Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 05:41 PM EST

PDB ID	:	7JLP
EMDB ID	:	EMD-22376
Title	:	cryo-EM structure of human ATG9A in nanodiscs
Authors	:	Maeda, S.; Otomo, T.
Deposited on	:	2020-07-30
Resolution	:	3.40 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:

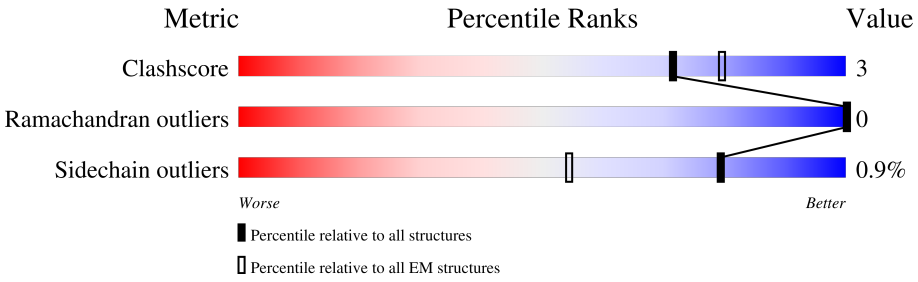
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	578	76% 8% 16%
1	B	578	76% 8% 16%
1	C	578	76% 7% 16%

2 Entry composition

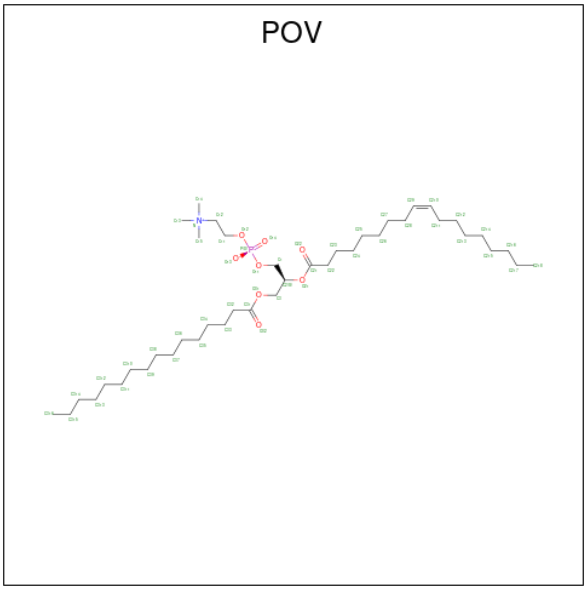
There are 2 unique types of molecules in this entry. The entry contains 12891 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Autophagy-related protein 9A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	485	Total	C	N	O	S	0	0
			3988	2627	674	664	23		
1	B	485	Total	C	N	O	S	0	0
			3988	2627	674	664	23		
1	C	485	Total	C	N	O	S	0	0
			3988	2627	674	664	23		

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			309	254	4	47	4	
2	A	1	Total	C	N	O	P	0
			309	254	4	47	4	
2	A	1	Total	C	N	O	P	0
			309	254	4	47	4	

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Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C N O P 309 254 4 47 4	0
2	A	1	Total C N O P 309 254 4 47 4	0
2	A	1	Total C N O P 309 254 4 47 4	0
2	A	1	Total C N O P 309 254 4 47 4	0
2	A	1	Total C N O P 309 254 4 47 4	0
2	A	1	Total C N O P 309 254 4 47 4	0
2	A	1	Total C N O P 309 254 4 47 4	0
2	A	1	Total C N O P 309 254 4 47 4	0
2	A	1	Total C N O P 309 254 4 47 4	0
2	A	1	Total C N O P 309 254 4 47 4	0
2	A	1	Total C N O P 309 254 4 47 4	0
2	A	1	Total C N O P 309 254 4 47 4	0
2	B	1	Total C N O P 309 254 4 47 4	0
2	B	1	Total C N O P 309 254 4 47 4	0
2	B	1	Total C N O P 309 254 4 47 4	0
2	B	1	Total C N O P 309 254 4 47 4	0
2	B	1	Total C N O P 309 254 4 47 4	0
2	B	1	Total C N O P 309 254 4 47 4	0
2	B	1	Total C N O P 309 254 4 47 4	0
2	B	1	Total C N O P 309 254 4 47 4	0
2	B	1	Total C N O P 309 254 4 47 4	0

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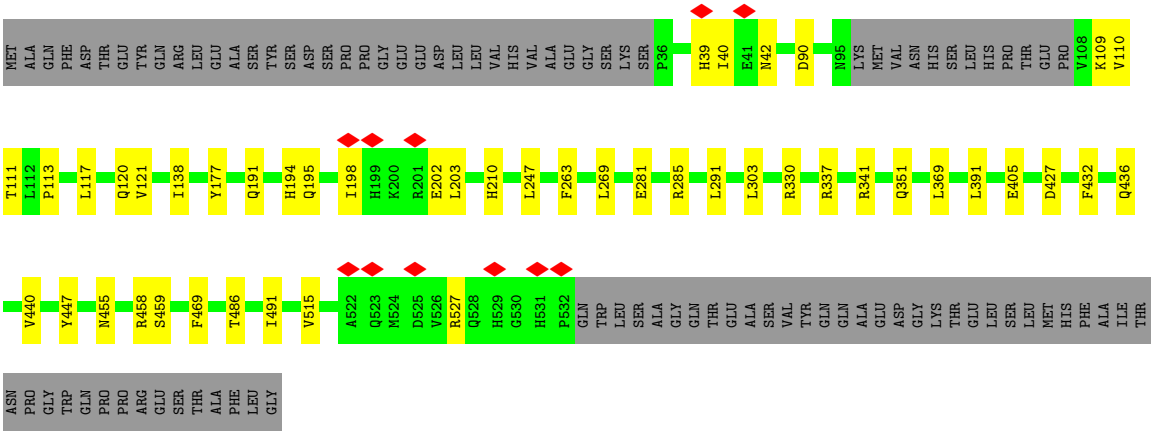
Mol	Chain	Residues	Atoms	AltConf
2	B	1	Total C N O P 309 254 4 47 4	0
2	B	1	Total C N O P 309 254 4 47 4	0
2	B	1	Total C N O P 309 254 4 47 4	0
2	B	1	Total C N O P 309 254 4 47 4	0
2	B	1	Total C N O P 309 254 4 47 4	0
2	B	1	Total C N O P 309 254 4 47 4	0
2	C	1	Total C N O P 309 254 4 47 4	0
2	C	1	Total C N O P 309 254 4 47 4	0
2	C	1	Total C N O P 309 254 4 47 4	0
2	C	1	Total C N O P 309 254 4 47 4	0
2	C	1	Total C N O P 309 254 4 47 4	0
2	C	1	Total C N O P 309 254 4 47 4	0
2	C	1	Total C N O P 309 254 4 47 4	0
2	C	1	Total C N O P 309 254 4 47 4	0
2	C	1	Total C N O P 309 254 4 47 4	0
2	C	1	Total C N O P 309 254 4 47 4	0
2	C	1	Total C N O P 309 254 4 47 4	0
2	C	1	Total C N O P 309 254 4 47 4	0
2	C	1	Total C N O P 309 254 4 47 4	0
2	C	1	Total C N O P 309 254 4 47 4	0
2	C	1	Total C N O P 309 254 4 47 4	0

3 Residue-property plots (i)

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.

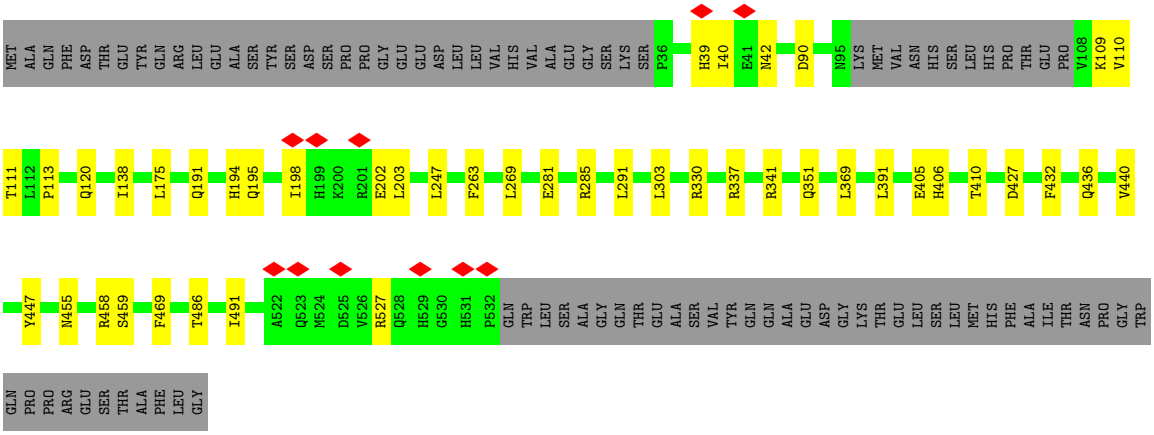
• Molecule 1: Autophagy-related protein 9A

Chain A:



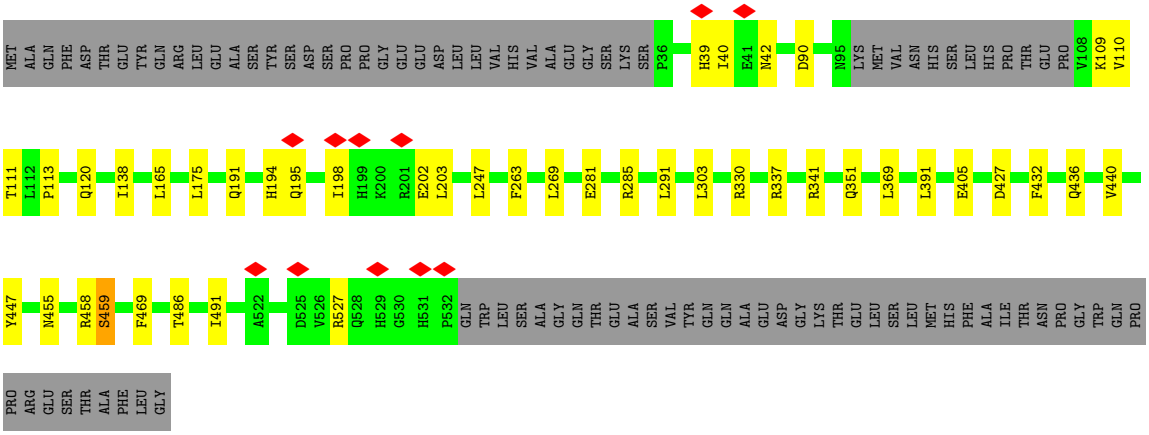
• Molecule 1: Autophagy-related protein 9A

Chain B:



• Molecule 1: Autophagy-related protein 9A

Chain C:


MET ALA GLN PHE ASP THR GLU TYR GLN ARG LEU GLU ALA SER TYR SER ASP SER PRO PRO GLY GLU GLU ASP LEU LEU VAL HIS VAL ALA GLU GLY SER LYS SER P36 H39 I40 E41 N42 D90 N95 LYS MET VAL ASN HIS SER LEU HIS PRO THR GLU PRO V108 K109 V110
T111 L112 P113 Q120 I138 L165 L175 Q191 H194 Q195 I198 H199 K200 R201 E202 L203 L247 F263 L269 E281 R285 L291 L303 R330 R337 R341 Q351 L369 L391 E405 D427 F432 Q436 V440
Y447 N455 R458 S459 F469 T486 I491 A522 D525 V526 R527 Q528 H529 G530 H531 P532 GLN TRP LEU SER ALA GLY GLN THR GLU ALA SER VAL TYR GLN GLN ALA GLU ASP GLY LYS THR GLU LEU SER LEU MET HIS PHE ALA ILE THR ASN PRO GLY TRP GLN PRO
PRO ARG GLU SER THR ALA PHE LEU GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	18276	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	66	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	73000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.276	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.029	Depositor
Map size (Å)	217.728, 217.728, 217.728	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.134, 1.134, 1.134	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/4100	0.39	0/5569
1	B	0.25	0/4100	0.39	0/5569
1	C	0.25	0/4100	0.39	0/5569
All	All	0.25	0/12300	0.39	0/16707

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

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	3988	0	4020	31	0
1	B	3988	0	4020	29	0
1	C	3988	0	4020	29	0
2	A	309	0	440	7	0
2	B	309	0	440	5	0
2	C	309	0	440	7	0
All	All	12891	0	13380	91	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 (91) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ARG:NH2	1:B:351:GLN:OE1	2.25	0.69
1:A:337:ARG:NH2	1:A:351:GLN:OE1	2.25	0.69
1:C:337:ARG:NH2	1:C:351:GLN:OE1	2.25	0.68
1:A:263:PHE:HA	1:A:269:LEU:HA	1.78	0.65
1:B:263:PHE:HA	1:B:269:LEU:HA	1.78	0.64
1:B:111:THR:HB	1:B:113:PRO:HD2	1.80	0.64
1:C:111:THR:HB	1:C:113:PRO:HD2	1.80	0.63
1:C:263:PHE:HA	1:C:269:LEU:HA	1.78	0.63
1:A:111:THR:HB	1:A:113:PRO:HD2	1.80	0.62
1:A:330:ARG:NH1	1:A:469:PHE:O	2.32	0.62
1:B:405:GLU:HG2	1:C:109:LYS:HD2	1.79	0.62
1:C:330:ARG:NH1	1:C:469:PHE:O	2.32	0.62
1:B:330:ARG:NH1	1:B:469:PHE:O	2.32	0.62
1:B:405:GLU:HG2	1:C:109:LYS:CD	2.29	0.62
1:A:109:LYS:HD2	1:C:405:GLU:HG2	1.87	0.55
1:B:369:LEU:HD23	1:B:432:PHE:HZ	1.72	0.54
1:C:369:LEU:HD23	1:C:432:PHE:HZ	1.72	0.54
1:A:191:GLN:HA	1:A:194:HIS:CE1	2.43	0.54
1:A:369:LEU:HD23	1:A:432:PHE:HZ	1.72	0.53
1:C:281:GLU:OE2	1:C:285:ARG:NH2	2.40	0.53
1:C:191:GLN:HA	1:C:194:HIS:CE1	2.43	0.53
1:B:191:GLN:HA	1:B:194:HIS:CE1	2.43	0.52
1:A:281:GLU:OE2	1:A:285:ARG:NH2	2.40	0.51
1:A:109:LYS:CD	1:C:405:GLU:HG2	2.41	0.50
1:B:341:ARG:O	1:B:527:ARG:NH2	2.32	0.50
1:A:341:ARG:O	1:A:527:ARG:NH2	2.32	0.50
1:B:281:GLU:OE2	1:B:285:ARG:NH2	2.40	0.50
1:C:40:ILE:HG22	1:C:42:ASN:H	1.78	0.49
1:A:40:ILE:HG22	1:A:42:ASN:H	1.78	0.48
1:C:341:ARG:O	1:C:527:ARG:NH2	2.32	0.48
1:B:40:ILE:HG22	1:B:42:ASN:H	1.78	0.48
1:B:303:LEU:HB3	2:B:602:POV:H37A	1.96	0.48
1:A:405:GLU:HG2	1:B:109:LYS:HD2	1.96	0.48
1:A:303:LEU:HB3	2:A:602:POV:H37A	1.96	0.47
1:B:436:GLN:O	1:B:440:VAL:HG23	2.15	0.47
1:A:455:ASN:HB2	1:A:458:ARG:HG2	1.97	0.47
1:C:202:GLU:HG2	1:C:203:LEU:H	1.79	0.47
1:A:291:LEU:HD12	1:A:491:ILE:HD12	1.97	0.47
1:B:202:GLU:HG2	1:B:203:LEU:H	1.79	0.47
1:B:455:ASN:HB2	1:B:458:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLU:HG2	1:A:203:LEU:H	1.79	0.46
1:C:303:LEU:HB3	2:C:604:POV:H37A	1.96	0.46
2:C:615:POV:H28A	2:C:615:POV:H211	1.74	0.46
1:C:291:LEU:HD12	1:C:491:ILE:HD12	1.97	0.46
1:C:436:GLN:O	1:C:440:VAL:HG23	2.14	0.46
1:C:455:ASN:HB2	1:C:458:ARG:HG2	1.97	0.46
1:A:436:GLN:O	1:A:440:VAL:HG23	2.14	0.46
1:A:39:HIS:O	1:A:39:HIS:ND1	2.47	0.46
2:B:615:POV:H29	2:C:613:POV:H26A	1.97	0.45
1:A:405:GLU:HG2	1:B:109:LYS:CD	2.46	0.45
1:A:405:GLU:CD	1:B:111:THR:HG22	2.37	0.45
2:A:611:POV:H26A	2:C:602:POV:H29	1.97	0.45
2:A:615:POV:H29	2:B:611:POV:H26A	1.97	0.45
1:B:291:LEU:HD12	1:B:491:ILE:HD12	1.97	0.45
1:C:138:ILE:HG23	2:C:603:POV:H31A	1.97	0.45
1:A:177:TYR:CE2	1:C:459:SER:HB2	2.52	0.45
1:B:138:ILE:HG23	2:B:601:POV:H31A	1.97	0.45
2:A:601:POV:H11A	2:A:601:POV:H14B	1.71	0.45
2:A:613:POV:H25	2:A:613:POV:H28A	1.82	0.45
1:A:138:ILE:HG23	2:A:601:POV:H31A	1.97	0.44
1:B:427:ASP:N	1:B:427:ASP:OD1	2.50	0.44
1:B:447:TYR:CE1	1:B:527:ARG:HB3	2.52	0.44
1:B:39:HIS:O	1:B:39:HIS:ND1	2.47	0.44
1:C:447:TYR:CE1	1:C:527:ARG:HB3	2.52	0.44
1:A:447:TYR:CE1	1:A:527:ARG:HB3	2.52	0.44
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.85	0.44
1:C:427:ASP:N	1:C:427:ASP:OD1	2.50	0.44
1:A:427:ASP:N	1:A:427:ASP:OD1	2.50	0.43
1:C:39:HIS:O	1:C:39:HIS:ND1	2.47	0.43
1:A:247:LEU:HD23	1:A:486:THR:HG23	2.01	0.43
2:C:615:POV:H28A	2:C:615:POV:H25	1.82	0.43
1:B:406:HIS:O	1:B:410:THR:OG1	2.27	0.43
1:C:247:LEU:HD23	1:C:486:THR:HG23	2.01	0.43
1:B:175:LEU:HA	1:B:175:LEU:HD23	1.86	0.42
1:B:195:GLN:HB2	1:B:198:ILE:HD11	2.01	0.42
1:B:247:LEU:HD23	1:B:486:THR:HG23	2.01	0.42
1:B:391:LEU:HD23	1:B:391:LEU:HA	1.85	0.42
1:C:195:GLN:HB2	1:C:198:ILE:HD11	2.01	0.42
2:C:615:POV:H11	2:C:615:POV:H13A	1.71	0.42
2:B:613:POV:H11	2:B:613:POV:H13A	1.71	0.42
1:C:175:LEU:HD23	1:C:175:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:GLU:HG2	1:C:203:LEU:N	2.35	0.42
1:A:202:GLU:HG2	1:A:203:LEU:N	2.35	0.42
1:A:195:GLN:HB2	1:A:198:ILE:HD11	2.01	0.42
1:C:165:LEU:HD23	1:C:165:LEU:HA	1.93	0.42
1:C:391:LEU:HD23	1:C:391:LEU:HA	1.85	0.42
1:B:202:GLU:HG2	1:B:203:LEU:N	2.35	0.41
1:A:458:ARG:HA	1:A:458:ARG:HD3	1.89	0.40
2:A:613:POV:H13A	2:A:613:POV:H11	1.71	0.40
1:A:117:LEU:HB3	1:A:121:VAL:HG13	2.03	0.40
1:A:210:HIS:HB3	1:A:515:VAL:HG11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	481/578 (83%)	459 (95%)	22 (5%)	0	100	100
1	B	481/578 (83%)	459 (95%)	22 (5%)	0	100	100
1	C	481/578 (83%)	459 (95%)	22 (5%)	0	100	100
All	All	1443/1734 (83%)	1377 (95%)	66 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/510 (84%)	427 (99%)	4 (1%)	78	90
1	B	431/510 (84%)	427 (99%)	4 (1%)	78	90
1	C	431/510 (84%)	427 (99%)	4 (1%)	78	90
All	All	1293/1530 (84%)	1281 (99%)	12 (1%)	79	90

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ASP
1	A	110	VAL
1	A	120	GLN
1	A	459	SER
1	B	90	ASP
1	B	110	VAL
1	B	120	GLN
1	B	459	SER
1	C	90	ASP
1	C	110	VAL
1	C	120	GLN
1	C	459	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	406	HIS
1	A	428	GLN
1	B	406	HIS
1	B	428	GLN
1	C	379	ASN
1	C	406	HIS
1	C	428	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

45 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	POV	B	605	-	17,17,51	0.97	1 (5%)	17,17,59	1.12	1 (5%)
2	POV	B	604	-	32,32,51	0.98	1 (3%)	37,39,59	1.05	1 (2%)
2	POV	B	609	-	17,17,51	0.96	1 (5%)	17,17,59	1.15	1 (5%)
2	POV	C	602	-	17,17,51	0.98	1 (5%)	17,17,59	1.11	1 (5%)
2	POV	C	613	-	16,16,51	1.00	1 (6%)	16,16,59	1.15	1 (6%)
2	POV	A	602	-	13,13,51	0.17	0	12,12,59	0.77	0
2	POV	B	602	-	13,13,51	0.17	0	12,12,59	0.77	0
2	POV	A	613	-	32,32,51	1.01	1 (3%)	37,38,59	1.01	1 (2%)
2	POV	B	607	-	13,13,51	0.47	0	13,13,59	1.09	1 (7%)
2	POV	B	603	-	34,34,51	1.03	1 (2%)	40,42,59	1.07	1 (2%)
2	POV	B	613	-	32,32,51	1.01	1 (3%)	37,38,59	1.01	1 (2%)
2	POV	B	614	-	7,7,51	0.20	0	6,6,59	0.63	0
2	POV	B	608	-	12,12,51	1.40	2 (16%)	12,12,59	1.59	3 (25%)
2	POV	B	606	-	17,17,51	0.97	1 (5%)	17,17,59	1.12	1 (5%)
2	POV	C	601	-	7,7,51	0.20	0	6,6,59	0.63	0
2	POV	A	603	-	34,34,51	1.03	1 (2%)	40,42,59	1.07	1 (2%)
2	POV	B	601	-	40,40,51	0.95	1 (2%)	46,48,59	1.05	2 (4%)
2	POV	B	610	-	17,17,51	0.97	1 (5%)	17,17,59	1.14	1 (5%)
2	POV	A	609	-	17,17,51	0.96	1 (5%)	17,17,59	1.15	1 (5%)
2	POV	A	612	-	10,10,51	0.49	0	10,10,59	1.13	1 (10%)
2	POV	A	607	-	13,13,51	0.47	0	13,13,59	1.09	1 (7%)
2	POV	C	614	-	10,10,51	0.50	0	10,10,59	1.13	1 (10%)
2	POV	A	606	-	17,17,51	0.97	1 (5%)	17,17,59	1.12	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	POV	A	614	-	7,7,51	0.20	0	6,6,59	0.63	0
2	POV	C	607	-	17,17,51	0.97	1 (5%)	17,17,59	1.13	1 (5%)
2	POV	A	615	-	17,17,51	0.98	1 (5%)	17,17,59	1.11	1 (5%)
2	POV	C	603	-	40,40,51	0.95	1 (2%)	46,48,59	1.05	1 (2%)
2	POV	A	608	-	12,12,51	1.39	2 (16%)	12,12,59	1.59	3 (25%)
2	POV	B	611	-	16,16,51	1.00	1 (6%)	16,16,59	1.15	1 (6%)
2	POV	C	605	-	34,34,51	1.03	1 (2%)	40,42,59	1.07	1 (2%)
2	POV	A	610	-	17,17,51	0.97	1 (5%)	17,17,59	1.14	1 (5%)
2	POV	C	608	-	17,17,51	0.97	1 (5%)	17,17,59	1.11	1 (5%)
2	POV	C	615	-	32,32,51	1.01	1 (3%)	37,38,59	1.01	1 (2%)
2	POV	A	604	-	32,32,51	0.98	1 (3%)	37,39,59	1.05	1 (2%)
2	POV	C	612	-	17,17,51	0.97	1 (5%)	17,17,59	1.13	1 (5%)
2	POV	C	606	-	32,32,51	0.98	1 (3%)	37,39,59	1.05	1 (2%)
2	POV	C	610	-	12,12,51	1.40	2 (16%)	12,12,59	1.60	3 (25%)
2	POV	B	615	-	17,17,51	0.98	1 (5%)	17,17,59	1.11	1 (5%)
2	POV	B	612	-	10,10,51	0.49	0	10,10,59	1.13	1 (10%)
2	POV	A	605	-	17,17,51	0.96	1 (5%)	17,17,59	1.12	1 (5%)
2	POV	C	611	-	17,17,51	0.96	1 (5%)	17,17,59	1.15	1 (5%)
2	POV	C	609	-	13,13,51	0.47	0	13,13,59	1.09	1 (7%)
2	POV	C	604	-	13,13,51	0.17	0	12,12,59	0.76	0
2	POV	A	601	-	40,40,51	0.95	1 (2%)	46,48,59	1.05	1 (2%)
2	POV	A	611	-	16,16,51	1.00	1 (6%)	16,16,59	1.15	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	B	605	-	-	5/15/15/55	-
2	POV	B	604	-	-	9/34/34/55	-
2	POV	B	609	-	-	8/15/15/55	-
2	POV	C	602	-	-	7/15/15/55	-
2	POV	C	613	-	-	8/14/14/55	-
2	POV	A	602	-	-	2/11/11/55	-
2	POV	B	602	-	-	2/11/11/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	A	613	-	-	14/33/33/55	-
2	POV	B	607	-	-	0/11/11/55	-
2	POV	B	603	-	-	17/38/38/55	-
2	POV	B	613	-	-	14/33/33/55	-
2	POV	B	614	-	-	0/5/5/55	-
2	POV	B	608	-	-	5/10/10/55	-
2	POV	B	606	-	-	7/15/15/55	-
2	POV	C	601	-	-	0/5/5/55	-
2	POV	A	603	-	-	17/38/38/55	-
2	POV	B	601	-	-	8/44/44/55	-
2	POV	B	610	-	-	4/15/15/55	-
2	POV	A	609	-	-	7/15/15/55	-
2	POV	A	612	-	-	3/8/8/55	-
2	POV	A	607	-	-	0/11/11/55	-
2	POV	C	614	-	-	3/8/8/55	-
2	POV	A	606	-	-	7/15/15/55	-
2	POV	A	614	-	-	0/5/5/55	-
2	POV	C	607	-	-	5/15/15/55	-
2	POV	A	615	-	-	7/15/15/55	-
2	POV	C	603	-	-	8/44/44/55	-
2	POV	A	608	-	-	5/10/10/55	-
2	POV	B	611	-	-	8/14/14/55	-
2	POV	C	605	-	-	17/38/38/55	-
2	POV	A	610	-	-	4/15/15/55	-
2	POV	C	608	-	-	7/15/15/55	-
2	POV	C	615	-	-	14/33/33/55	-
2	POV	A	604	-	-	9/34/34/55	-
2	POV	C	612	-	-	4/15/15/55	-
2	POV	C	606	-	-	9/34/34/55	-
2	POV	C	610	-	-	5/10/10/55	-
2	POV	B	615	-	-	7/15/15/55	-
2	POV	B	612	-	-	3/8/8/55	-
2	POV	A	605	-	-	5/15/15/55	-
2	POV	C	611	-	-	7/15/15/55	-
2	POV	C	609	-	-	0/11/11/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	C	604	-	-	2/11/11/55	-
2	POV	A	601	-	-	8/44/44/55	-
2	POV	A	611	-	-	8/14/14/55	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	608	POV	O32-C31	4.17	1.36	1.22
2	C	610	POV	O32-C31	4.17	1.36	1.22
2	A	608	POV	O32-C31	4.15	1.35	1.22
2	C	615	POV	P-O12	3.83	1.74	1.59
2	A	613	POV	P-O12	3.83	1.74	1.59
2	B	613	POV	P-O12	3.82	1.74	1.59
2	A	601	POV	P-O12	3.76	1.74	1.59
2	B	601	POV	P-O12	3.76	1.74	1.59
2	A	603	POV	P-O12	3.75	1.74	1.59
2	C	603	POV	P-O12	3.74	1.74	1.59
2	B	603	POV	P-O12	3.73	1.74	1.59
2	C	605	POV	P-O12	3.73	1.74	1.59
2	A	604	POV	P-O12	3.71	1.74	1.59
2	C	606	POV	P-O12	3.71	1.74	1.59
2	B	604	POV	P-O12	3.69	1.74	1.59
2	B	615	POV	C29-C210	3.61	1.52	1.31
2	C	602	POV	C29-C210	3.60	1.52	1.31
2	C	612	POV	C29-C210	3.60	1.52	1.31
2	B	610	POV	C29-C210	3.60	1.52	1.31
2	A	615	POV	C29-C210	3.60	1.52	1.31
2	A	610	POV	C29-C210	3.60	1.52	1.31
2	A	606	POV	C29-C210	3.60	1.52	1.31
2	C	608	POV	C29-C210	3.59	1.52	1.31
2	A	611	POV	C29-C210	3.59	1.52	1.31
2	B	606	POV	C29-C210	3.58	1.52	1.31
2	C	613	POV	C29-C210	3.58	1.52	1.31
2	B	611	POV	C29-C210	3.58	1.52	1.31
2	B	605	POV	C29-C210	3.57	1.52	1.31
2	C	607	POV	C29-C210	3.57	1.52	1.31
2	B	609	POV	C29-C210	3.56	1.52	1.31
2	A	609	POV	C29-C210	3.56	1.52	1.31
2	C	611	POV	C29-C210	3.55	1.52	1.31
2	A	605	POV	C29-C210	3.55	1.52	1.31
2	B	608	POV	O31-C31	-2.42	1.22	1.30
2	C	610	POV	O31-C31	-2.41	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	608	POV	O31-C31	-2.41	1.22	1.30

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	604	POV	O13-P-O14	3.76	130.81	112.24
2	C	606	POV	O13-P-O14	3.75	130.80	112.24
2	B	604	POV	O13-P-O14	3.75	130.79	112.24
2	C	615	POV	O13-P-O14	3.73	130.70	112.24
2	B	601	POV	O13-P-O14	3.73	130.69	112.24
2	A	613	POV	O13-P-O14	3.73	130.67	112.24
2	B	613	POV	O13-P-O14	3.73	130.67	112.24
2	A	601	POV	O13-P-O14	3.73	130.66	112.24
2	C	603	POV	O13-P-O14	3.72	130.61	112.24
2	B	603	POV	O13-P-O14	3.71	130.56	112.24
2	A	603	POV	O13-P-O14	3.70	130.55	112.24
2	C	605	POV	O13-P-O14	3.69	130.50	112.24
2	C	610	POV	O31-C31-C32	3.36	124.84	114.03
2	B	608	POV	O31-C31-C32	3.36	124.83	114.03
2	A	608	POV	O31-C31-C32	3.34	124.77	114.03
2	C	609	POV	C33-C32-C31	-2.75	107.54	114.47
2	A	607	POV	C33-C32-C31	-2.74	107.56	114.47
2	B	607	POV	C33-C32-C31	-2.74	107.56	114.47
2	B	612	POV	C33-C32-C31	-2.69	107.69	114.47
2	A	612	POV	C33-C32-C31	-2.68	107.73	114.47
2	C	614	POV	C33-C32-C31	-2.67	107.75	114.47
2	B	609	POV	C23-C22-C21	-2.66	107.77	114.47
2	A	609	POV	C23-C22-C21	-2.65	107.78	114.47
2	C	611	POV	C23-C22-C21	-2.65	107.80	114.47
2	C	610	POV	C33-C32-C31	-2.65	107.80	114.47
2	B	608	POV	C33-C32-C31	-2.63	107.84	114.47
2	B	610	POV	C23-C22-C21	-2.63	107.84	114.47
2	A	608	POV	C33-C32-C31	-2.62	107.86	114.47
2	B	611	POV	C23-C22-C21	-2.62	107.87	114.47
2	A	611	POV	C23-C22-C21	-2.62	107.88	114.47
2	C	613	POV	C23-C22-C21	-2.61	107.88	114.47
2	A	610	POV	C23-C22-C21	-2.61	107.89	114.47
2	C	612	POV	C23-C22-C21	-2.61	107.89	114.47
2	C	607	POV	C23-C22-C21	-2.57	108.00	114.47
2	B	605	POV	C23-C22-C21	-2.56	108.01	114.47
2	A	605	POV	C23-C22-C21	-2.56	108.02	114.47
2	B	606	POV	C23-C22-C21	-2.53	108.10	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	606	POV	C23-C22-C21	-2.51	108.14	114.47
2	C	608	POV	C23-C22-C21	-2.51	108.16	114.47
2	B	615	POV	C23-C22-C21	-2.50	108.18	114.47
2	C	602	POV	C23-C22-C21	-2.50	108.18	114.47
2	A	615	POV	C23-C22-C21	-2.49	108.19	114.47
2	B	608	POV	O32-C31-C32	-2.37	115.48	123.08
2	C	610	POV	O32-C31-C32	-2.36	115.50	123.08
2	A	608	POV	O32-C31-C32	-2.36	115.50	123.08
2	B	601	POV	C11-C12-N	-2.01	109.08	115.78

There are no chirality outliers.

All (289) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	POV	C11-O12-P-O13
2	A	601	POV	O21-C2-C3-O31
2	A	601	POV	O12-C11-C12-N
2	A	603	POV	O21-C2-C3-O31
2	A	603	POV	O12-C11-C12-N
2	A	604	POV	C11-O12-P-O11
2	A	604	POV	C11-O12-P-O13
2	A	604	POV	C11-O12-P-O14
2	A	604	POV	C1-C2-C3-O31
2	A	604	POV	O21-C2-C3-O31
2	A	605	POV	C211-C210-C29-C28
2	A	613	POV	C1-O11-P-O12
2	A	613	POV	C1-O11-P-O13
2	A	613	POV	C11-O12-P-O11
2	A	613	POV	C11-O12-P-O13
2	A	613	POV	C11-O12-P-O14
2	A	613	POV	O12-C11-C12-N
2	B	601	POV	C11-O12-P-O13
2	B	601	POV	O21-C2-C3-O31
2	B	601	POV	O12-C11-C12-N
2	B	603	POV	O21-C2-C3-O31
2	B	603	POV	O12-C11-C12-N
2	B	604	POV	C11-O12-P-O11
2	B	604	POV	C11-O12-P-O13
2	B	604	POV	C11-O12-P-O14
2	B	604	POV	C1-C2-C3-O31
2	B	604	POV	O21-C2-C3-O31
2	B	605	POV	C211-C210-C29-C28

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Mol	Chain	Res	Type	Atoms
2	B	613	POV	C1-O11-P-O12
2	B	613	POV	C1-O11-P-O13
2	B	613	POV	C11-O12-P-O11
2	B	613	POV	C11-O12-P-O13
2	B	613	POV	C11-O12-P-O14
2	B	613	POV	O12-C11-C12-N
2	C	603	POV	C11-O12-P-O13
2	C	603	POV	O21-C2-C3-O31
2	C	603	POV	O12-C11-C12-N
2	C	605	POV	O21-C2-C3-O31
2	C	605	POV	O12-C11-C12-N
2	C	606	POV	C11-O12-P-O11
2	C	606	POV	C11-O12-P-O13
2	C	606	POV	C11-O12-P-O14
2	C	606	POV	C1-C2-C3-O31
2	C	606	POV	O21-C2-C3-O31
2	C	607	POV	C211-C210-C29-C28
2	C	615	POV	C1-O11-P-O12
2	C	615	POV	C1-O11-P-O13
2	C	615	POV	C11-O12-P-O11
2	C	615	POV	C11-O12-P-O13
2	C	615	POV	C11-O12-P-O14
2	C	615	POV	O12-C11-C12-N
2	A	613	POV	O22-C21-O21-C2
2	B	613	POV	O22-C21-O21-C2
2	C	615	POV	O22-C21-O21-C2
2	A	613	POV	C22-C21-O21-C2
2	B	613	POV	C22-C21-O21-C2
2	C	615	POV	C22-C21-O21-C2
2	A	615	POV	C211-C210-C29-C28
2	B	615	POV	C211-C210-C29-C28
2	C	602	POV	C211-C210-C29-C28
2	A	609	POV	C21-C22-C23-C24
2	B	609	POV	C21-C22-C23-C24
2	C	611	POV	C21-C22-C23-C24
2	A	603	POV	C31-C32-C33-C34
2	B	603	POV	C31-C32-C33-C34
2	C	605	POV	C31-C32-C33-C34
2	A	601	POV	C11-O12-P-O11
2	A	603	POV	C11-O12-P-O11
2	B	601	POV	C11-O12-P-O11
2	B	603	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
2	C	603	POV	C11-O12-P-O11
2	C	605	POV	C11-O12-P-O11
2	A	608	POV	C33-C34-C35-C36
2	B	608	POV	C33-C34-C35-C36
2	C	610	POV	C33-C34-C35-C36
2	A	604	POV	C33-C34-C35-C36
2	B	604	POV	C33-C34-C35-C36
2	C	606	POV	C33-C34-C35-C36
2	A	603	POV	C33-C34-C35-C36
2	A	615	POV	C22-C23-C24-C25
2	B	603	POV	C33-C34-C35-C36
2	B	615	POV	C22-C23-C24-C25
2	C	602	POV	C22-C23-C24-C25
2	C	605	POV	C33-C34-C35-C36
2	A	605	POV	C23-C24-C25-C26
2	B	605	POV	C23-C24-C25-C26
2	C	607	POV	C23-C24-C25-C26
2	A	605	POV	C25-C26-C27-C28
2	B	605	POV	C25-C26-C27-C28
2	C	607	POV	C25-C26-C27-C28
2	A	608	POV	C32-C33-C34-C35
2	B	608	POV	C32-C33-C34-C35
2	C	610	POV	C32-C33-C34-C35
2	A	613	POV	C23-C24-C25-C26
2	B	613	POV	C23-C24-C25-C26
2	C	615	POV	C23-C24-C25-C26
2	C	607	POV	C24-C25-C26-C27
2	A	605	POV	C24-C25-C26-C27
2	A	606	POV	C211-C212-C213-C214
2	B	605	POV	C24-C25-C26-C27
2	B	606	POV	C211-C212-C213-C214
2	C	608	POV	C211-C212-C213-C214
2	A	601	POV	C26-C27-C28-C29
2	A	606	POV	C26-C27-C28-C29
2	B	601	POV	C26-C27-C28-C29
2	B	606	POV	C26-C27-C28-C29
2	C	603	POV	C26-C27-C28-C29
2	C	608	POV	C26-C27-C28-C29
2	A	601	POV	C34-C35-C36-C37
2	B	601	POV	C34-C35-C36-C37
2	C	603	POV	C34-C35-C36-C37
2	A	604	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
2	B	604	POV	C32-C33-C34-C35
2	C	606	POV	C32-C33-C34-C35
2	A	611	POV	C211-C212-C213-C214
2	B	611	POV	C211-C212-C213-C214
2	C	613	POV	C211-C212-C213-C214
2	B	606	POV	C25-C26-C27-C28
2	C	608	POV	C25-C26-C27-C28
2	A	606	POV	C25-C26-C27-C28
2	A	603	POV	C1-C2-C3-O31
2	B	603	POV	C1-C2-C3-O31
2	C	605	POV	C1-C2-C3-O31
2	A	609	POV	C211-C210-C29-C28
2	B	609	POV	C211-C210-C29-C28
2	C	611	POV	C211-C210-C29-C28
2	A	611	POV	C21-C22-C23-C24
2	B	611	POV	C21-C22-C23-C24
2	C	613	POV	C21-C22-C23-C24
2	C	615	POV	C21-C22-C23-C24
2	A	613	POV	C21-C22-C23-C24
2	B	613	POV	C21-C22-C23-C24
2	A	612	POV	C31-C32-C33-C34
2	B	612	POV	C31-C32-C33-C34
2	A	609	POV	C211-C212-C213-C214
2	B	609	POV	C211-C212-C213-C214
2	C	611	POV	C211-C212-C213-C214
2	C	614	POV	C31-C32-C33-C34
2	A	602	POV	C35-C36-C37-C38
2	B	602	POV	C35-C36-C37-C38
2	C	604	POV	C35-C36-C37-C38
2	A	603	POV	C35-C36-C37-C38
2	B	603	POV	C35-C36-C37-C38
2	C	605	POV	C35-C36-C37-C38
2	A	601	POV	C1-C2-C3-O31
2	B	601	POV	C1-C2-C3-O31
2	C	603	POV	C1-C2-C3-O31
2	C	606	POV	C39-C310-C311-C312
2	B	604	POV	C39-C310-C311-C312
2	A	604	POV	C39-C310-C311-C312
2	A	603	POV	C11-O12-P-O14
2	B	603	POV	C11-O12-P-O14
2	C	605	POV	C11-O12-P-O14
2	A	606	POV	C213-C214-C215-C216

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Mol	Chain	Res	Type	Atoms
2	B	606	POV	C213-C214-C215-C216
2	C	608	POV	C213-C214-C215-C216
2	A	603	POV	C12-C11-O12-P
2	B	603	POV	C12-C11-O12-P
2	C	605	POV	C12-C11-O12-P
2	A	603	POV	C21-C22-C23-C24
2	A	615	POV	C21-C22-C23-C24
2	B	603	POV	C21-C22-C23-C24
2	C	602	POV	C21-C22-C23-C24
2	C	605	POV	C21-C22-C23-C24
2	B	615	POV	C21-C22-C23-C24
2	A	604	POV	O12-C11-C12-N
2	B	604	POV	O12-C11-C12-N
2	C	606	POV	O12-C11-C12-N
2	C	605	POV	O31-C31-C32-C33
2	A	603	POV	O11-C1-C2-C3
2	B	603	POV	O11-C1-C2-C3
2	C	605	POV	O11-C1-C2-C3
2	A	603	POV	O31-C31-C32-C33
2	A	603	POV	O11-C1-C2-O21
2	B	603	POV	O11-C1-C2-O21
2	C	605	POV	O11-C1-C2-O21
2	B	603	POV	O31-C31-C32-C33
2	B	610	POV	C25-C26-C27-C28
2	C	612	POV	C25-C26-C27-C28
2	A	610	POV	C25-C26-C27-C28
2	C	604	POV	C36-C37-C38-C39
2	A	602	POV	C36-C37-C38-C39
2	B	602	POV	C36-C37-C38-C39
2	A	609	POV	O22-C21-C22-C23
2	B	609	POV	O22-C21-C22-C23
2	C	608	POV	O21-C21-C22-C23
2	C	611	POV	O22-C21-C22-C23
2	A	606	POV	O21-C21-C22-C23
2	B	606	POV	O21-C21-C22-C23
2	A	606	POV	O22-C21-C22-C23
2	A	615	POV	O21-C21-C22-C23
2	B	606	POV	O22-C21-C22-C23
2	B	615	POV	O21-C21-C22-C23
2	C	602	POV	O21-C21-C22-C23
2	C	608	POV	O22-C21-C22-C23
2	A	609	POV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
2	B	609	POV	C22-C23-C24-C25
2	C	611	POV	C22-C23-C24-C25
2	A	612	POV	O32-C31-C32-C33
2	B	612	POV	O32-C31-C32-C33
2	C	614	POV	O32-C31-C32-C33
2	A	612	POV	O31-C31-C32-C33
2	A	609	POV	O21-C21-C22-C23
2	B	612	POV	O31-C31-C32-C33
2	C	614	POV	O31-C31-C32-C33
2	A	615	POV	O22-C21-C22-C23
2	B	609	POV	O21-C21-C22-C23
2	B	615	POV	O22-C21-C22-C23
2	C	602	POV	O22-C21-C22-C23
2	C	611	POV	O21-C21-C22-C23
2	C	613	POV	C24-C25-C26-C27
2	A	611	POV	C23-C24-C25-C26
2	A	611	POV	C24-C25-C26-C27
2	B	611	POV	C24-C25-C26-C27
2	B	611	POV	C23-C24-C25-C26
2	A	608	POV	O31-C31-C32-C33
2	C	613	POV	C23-C24-C25-C26
2	B	608	POV	O31-C31-C32-C33
2	C	610	POV	O31-C31-C32-C33
2	B	606	POV	C24-C25-C26-C27
2	C	608	POV	C24-C25-C26-C27
2	A	615	POV	C29-C210-C211-C212
2	B	615	POV	C29-C210-C211-C212
2	C	602	POV	C29-C210-C211-C212
2	A	606	POV	C24-C25-C26-C27
2	C	613	POV	C25-C26-C27-C28
2	B	611	POV	C25-C26-C27-C28
2	A	611	POV	C25-C26-C27-C28
2	A	603	POV	C1-O11-P-O12
2	B	603	POV	C1-O11-P-O12
2	C	605	POV	C1-O11-P-O12
2	A	610	POV	C24-C25-C26-C27
2	B	610	POV	C24-C25-C26-C27
2	A	605	POV	C29-C210-C211-C212
2	B	605	POV	C29-C210-C211-C212
2	C	607	POV	C29-C210-C211-C212
2	C	612	POV	C24-C25-C26-C27
2	A	611	POV	C27-C28-C29-C210

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Mol	Chain	Res	Type	Atoms
2	B	611	POV	C27-C28-C29-C210
2	C	613	POV	C27-C28-C29-C210
2	A	611	POV	C210-C211-C212-C213
2	A	613	POV	C26-C27-C28-C29
2	B	611	POV	C210-C211-C212-C213
2	B	613	POV	C26-C27-C28-C29
2	C	613	POV	C210-C211-C212-C213
2	C	615	POV	C26-C27-C28-C29
2	C	610	POV	O32-C31-C32-C33
2	C	605	POV	C32-C33-C34-C35
2	A	603	POV	C32-C33-C34-C35
2	B	603	POV	C32-C33-C34-C35
2	A	608	POV	O32-C31-C32-C33
2	B	608	POV	O32-C31-C32-C33
2	A	601	POV	O31-C31-C32-C33
2	B	601	POV	O31-C31-C32-C33
2	C	603	POV	O31-C31-C32-C33
2	A	610	POV	C29-C210-C211-C212
2	A	611	POV	C29-C210-C211-C212
2	B	610	POV	C29-C210-C211-C212
2	B	611	POV	C29-C210-C211-C212
2	C	612	POV	C29-C210-C211-C212
2	C	613	POV	C29-C210-C211-C212
2	B	608	POV	C35-C36-C37-C38
2	A	608	POV	C35-C36-C37-C38
2	C	610	POV	C35-C36-C37-C38
2	A	609	POV	C27-C28-C29-C210
2	A	610	POV	C27-C28-C29-C210
2	A	615	POV	C27-C28-C29-C210
2	B	609	POV	C27-C28-C29-C210
2	B	615	POV	C27-C28-C29-C210
2	C	602	POV	C27-C28-C29-C210
2	C	611	POV	C27-C28-C29-C210
2	B	610	POV	C27-C28-C29-C210
2	C	612	POV	C27-C28-C29-C210
2	A	603	POV	C1-O11-P-O14
2	A	613	POV	O11-C1-C2-O21
2	B	603	POV	C1-O11-P-O14
2	B	613	POV	O11-C1-C2-O21
2	C	605	POV	C1-O11-P-O14
2	C	615	POV	C11-C12-N-C13
2	C	615	POV	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
2	A	613	POV	C11-C12-N-C13
2	B	613	POV	C11-C12-N-C13
2	C	605	POV	C36-C37-C38-C39
2	A	603	POV	C36-C37-C38-C39
2	B	603	POV	C36-C37-C38-C39
2	B	613	POV	O21-C21-C22-C23
2	B	609	POV	C29-C210-C211-C212
2	A	613	POV	O21-C21-C22-C23
2	C	615	POV	O21-C21-C22-C23

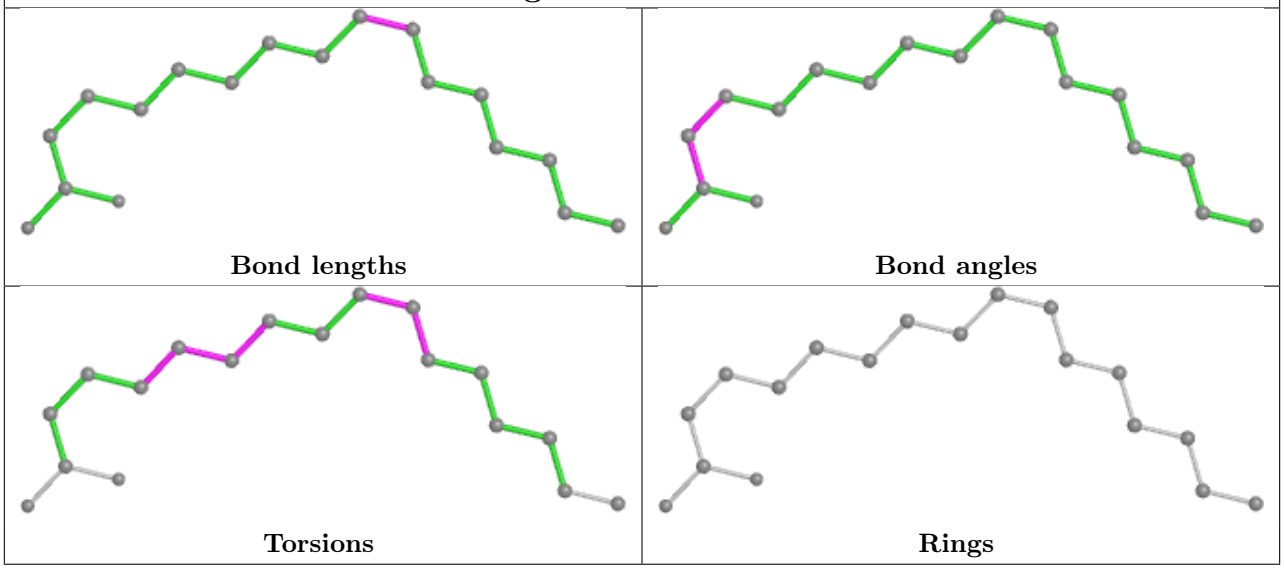
There are no ring outliers.

15 monomers are involved in 16 short contacts:

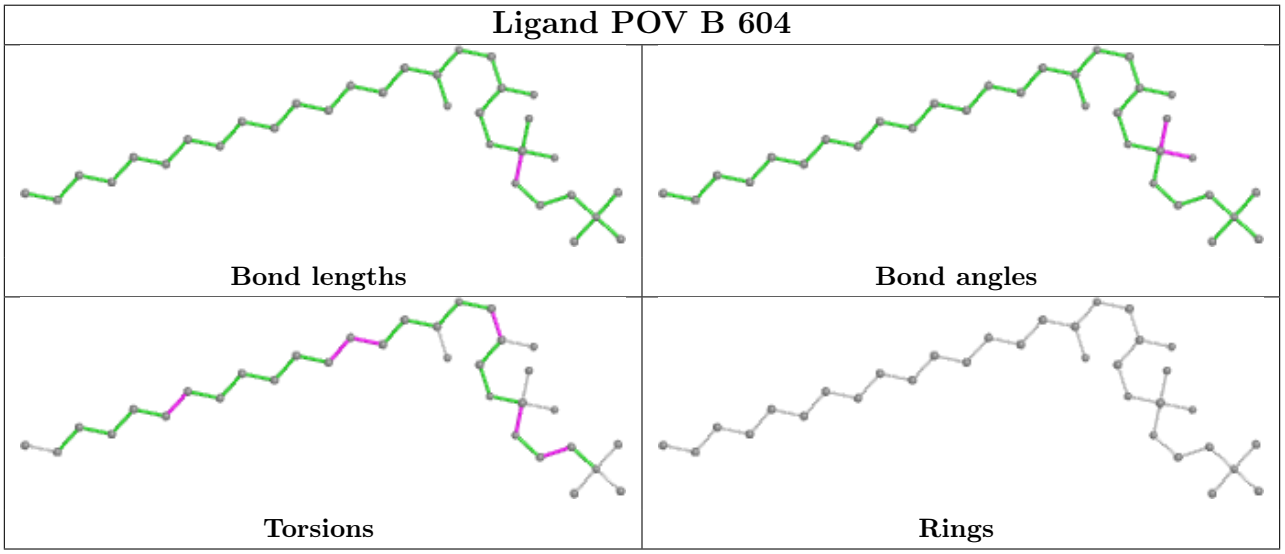
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	POV	1	0
2	C	613	POV	1	0
2	A	602	POV	1	0
2	B	602	POV	1	0
2	A	613	POV	2	0
2	B	613	POV	1	0
2	B	601	POV	1	0
2	A	615	POV	1	0
2	C	603	POV	1	0
2	B	611	POV	1	0
2	C	615	POV	3	0
2	B	615	POV	1	0
2	C	604	POV	1	0
2	A	601	POV	2	0
2	A	611	POV	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

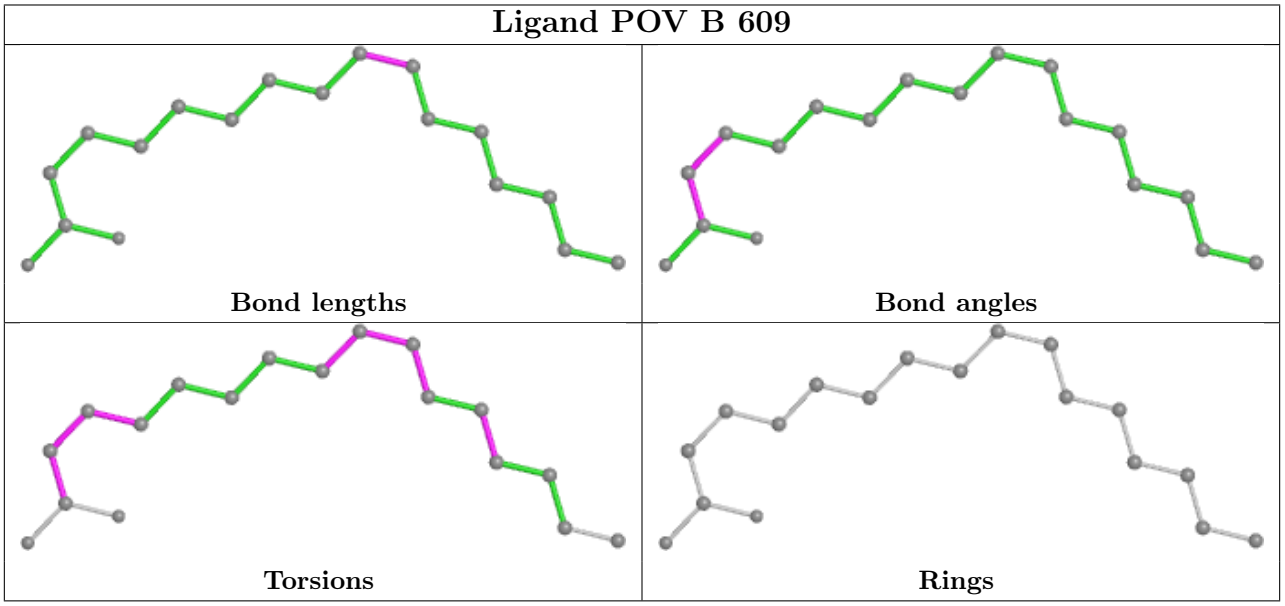
Ligand POV B 605



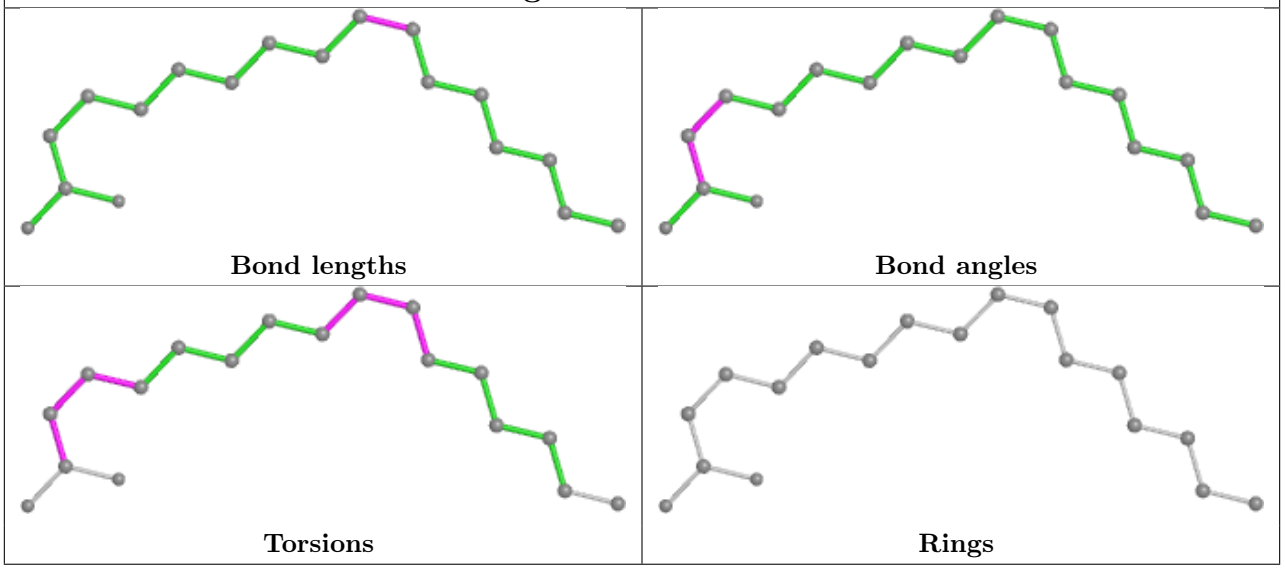
Ligand POV B 604



Ligand POV B 609



Ligand POV C 602



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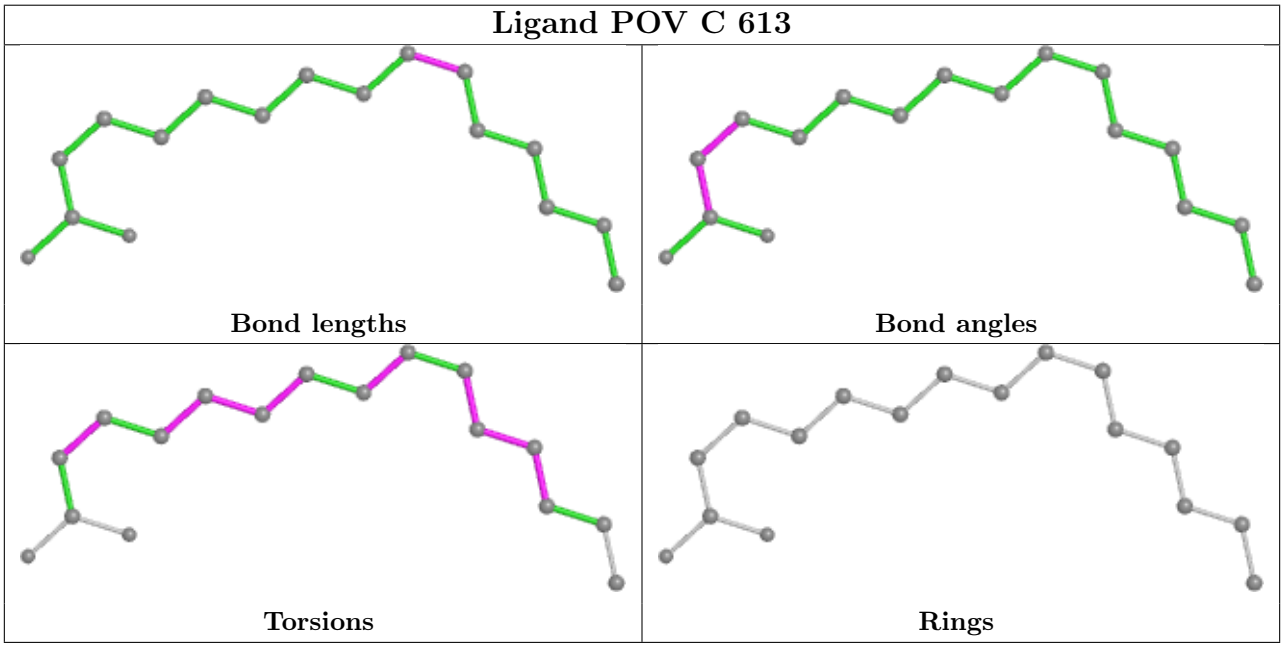
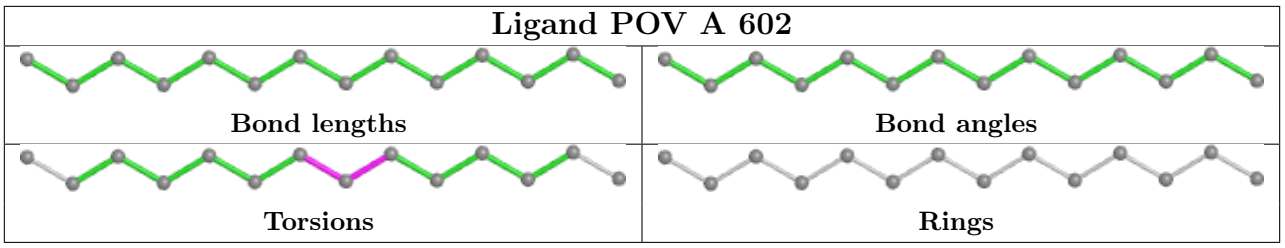


Ligand POV A 602



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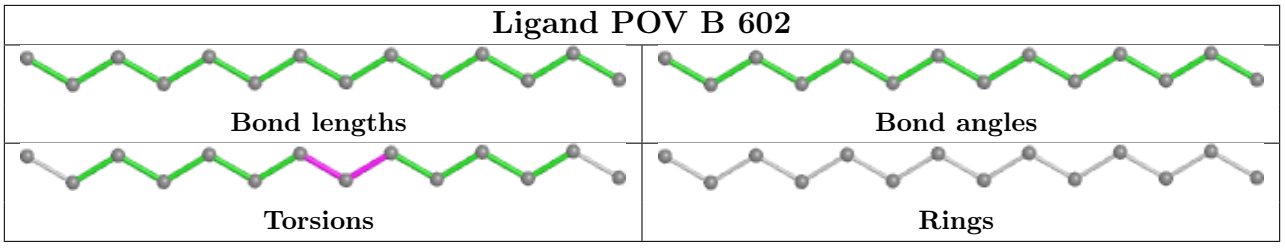

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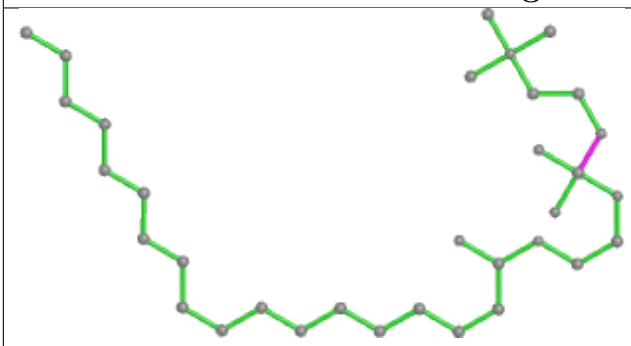
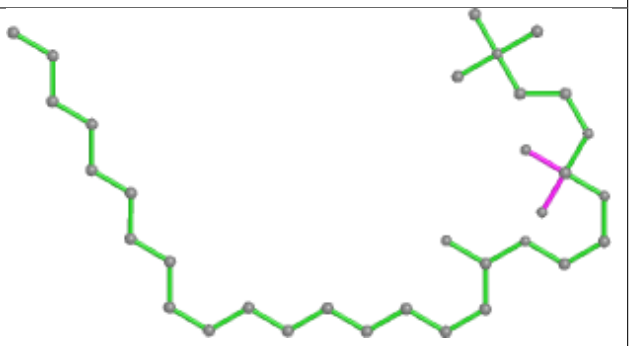
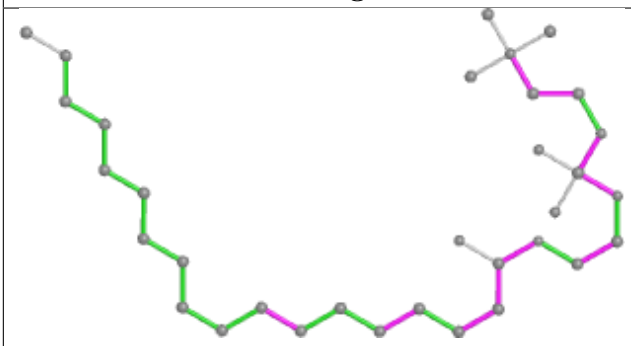


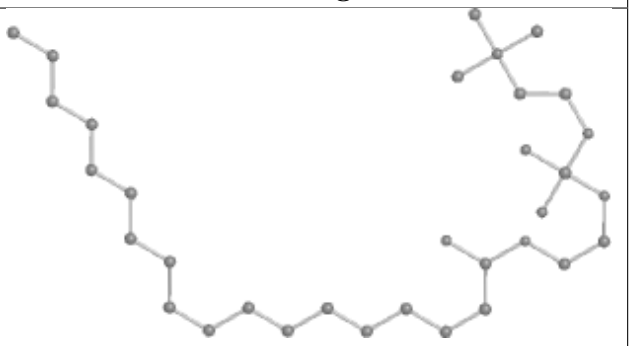
Bond lengths



Bond angles

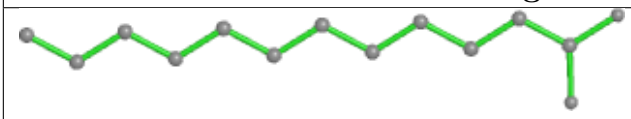


Torsions

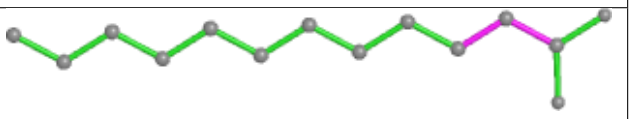


Rings

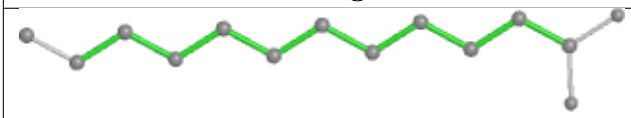
Ligand POV B 607



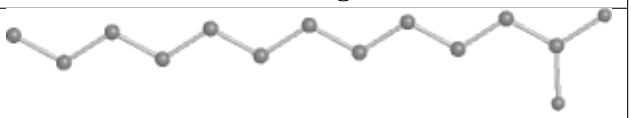
Bond lengths



Bond angles

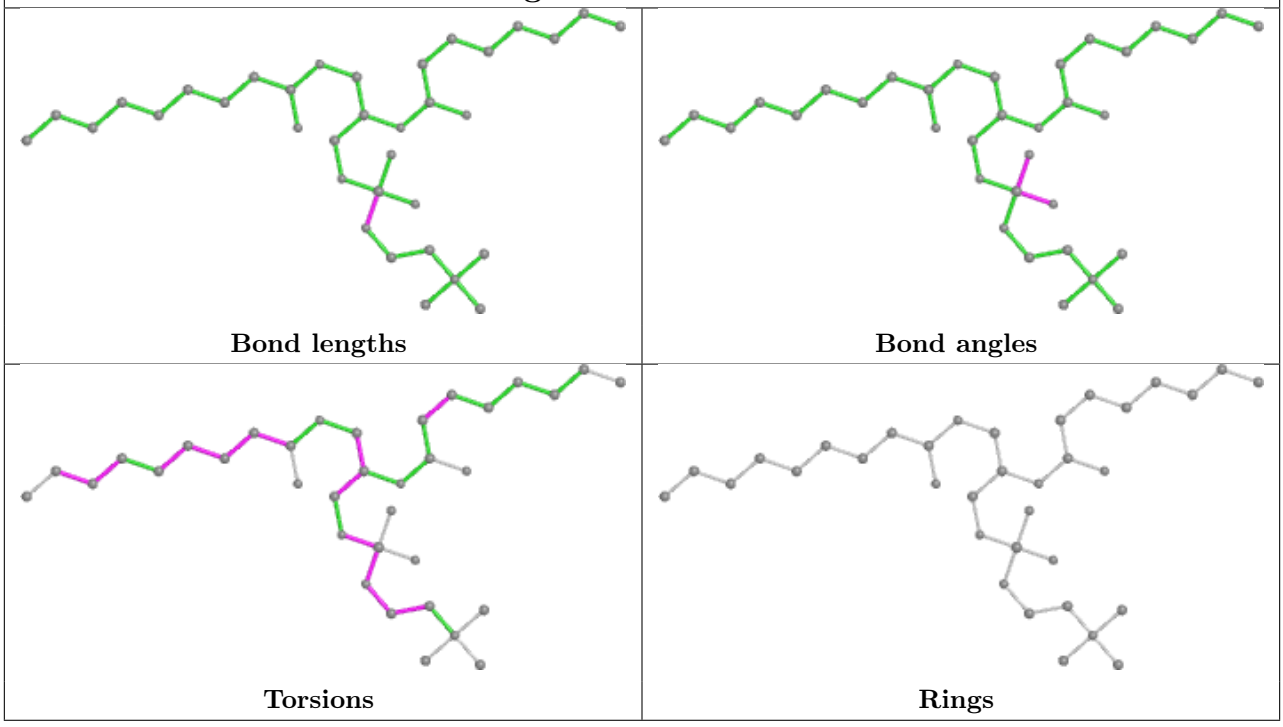


Torsions



Rings

Ligand POV B 603



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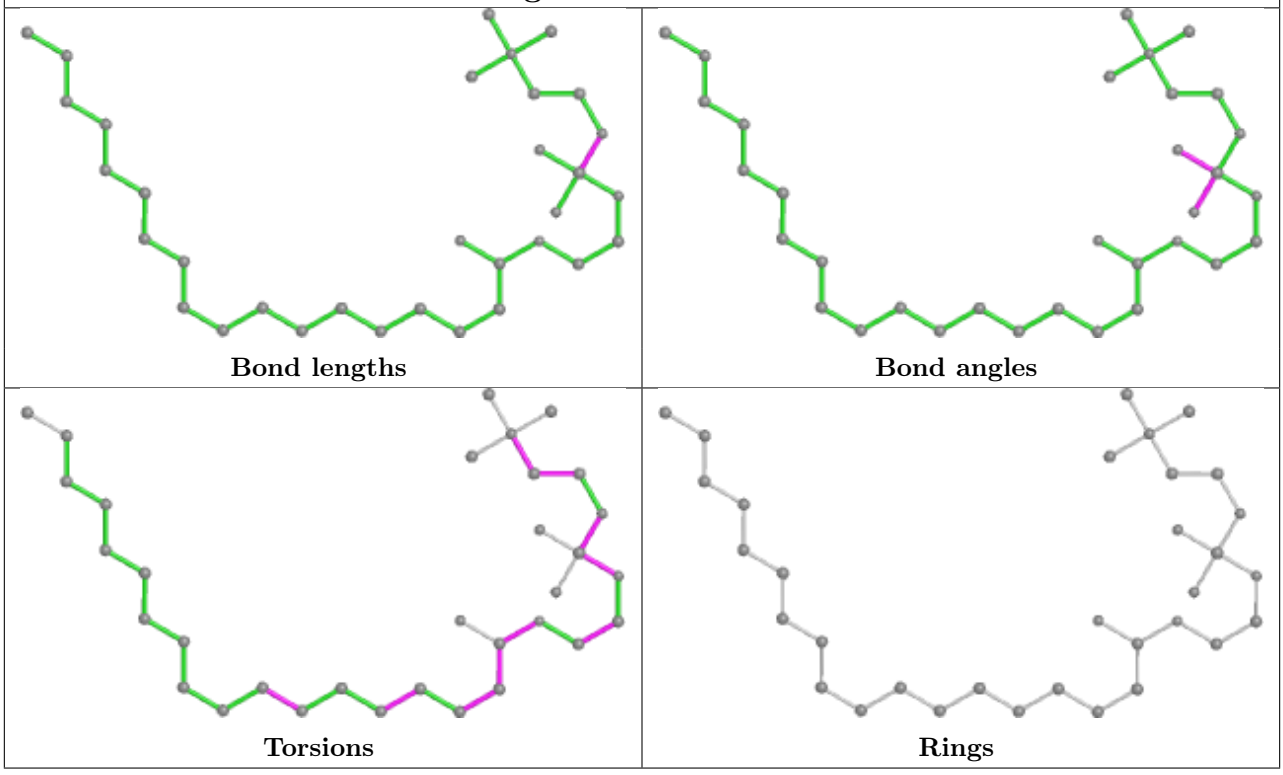
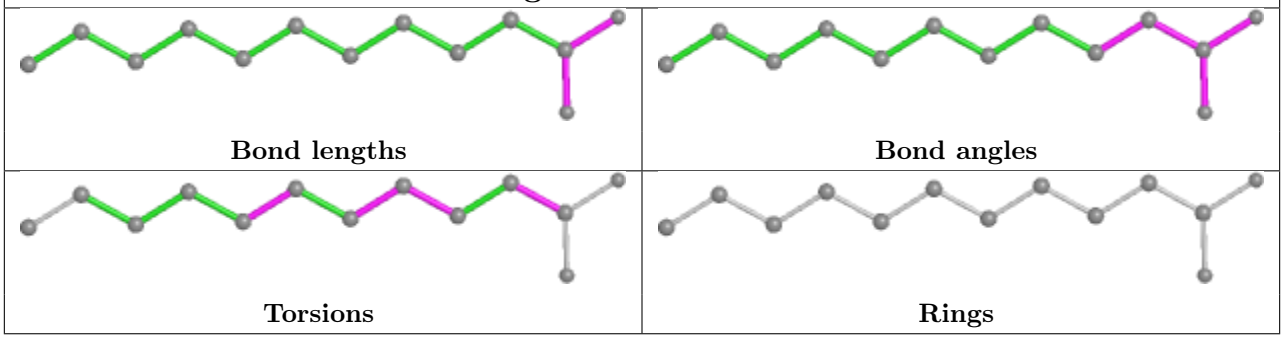


Ligand POV B 608



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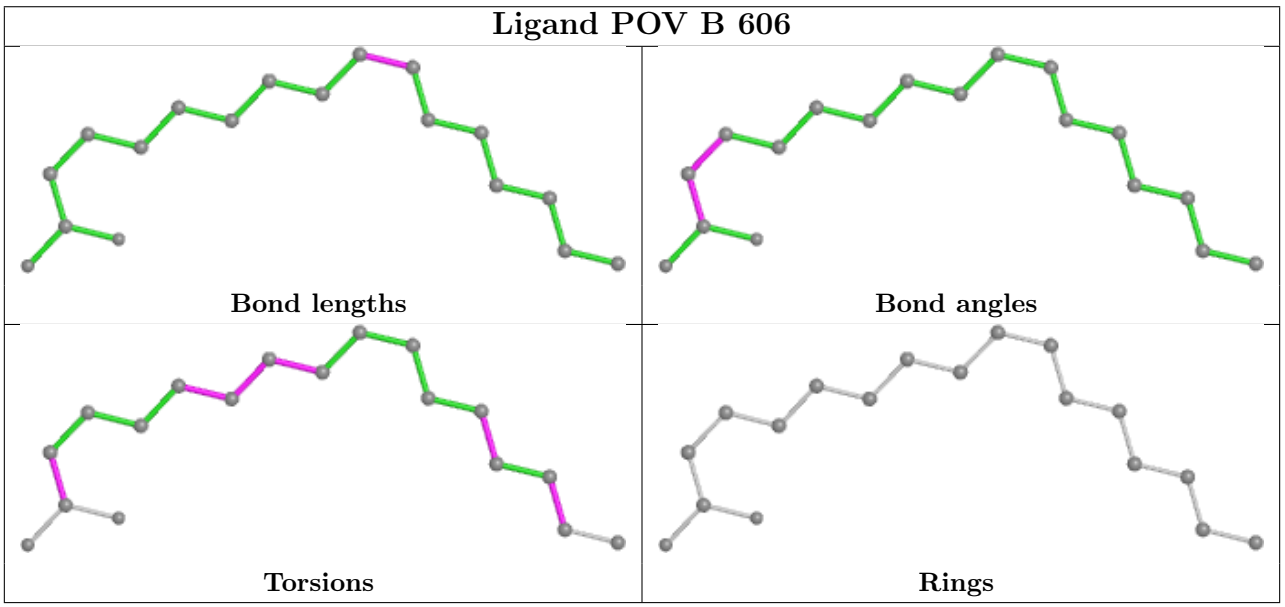
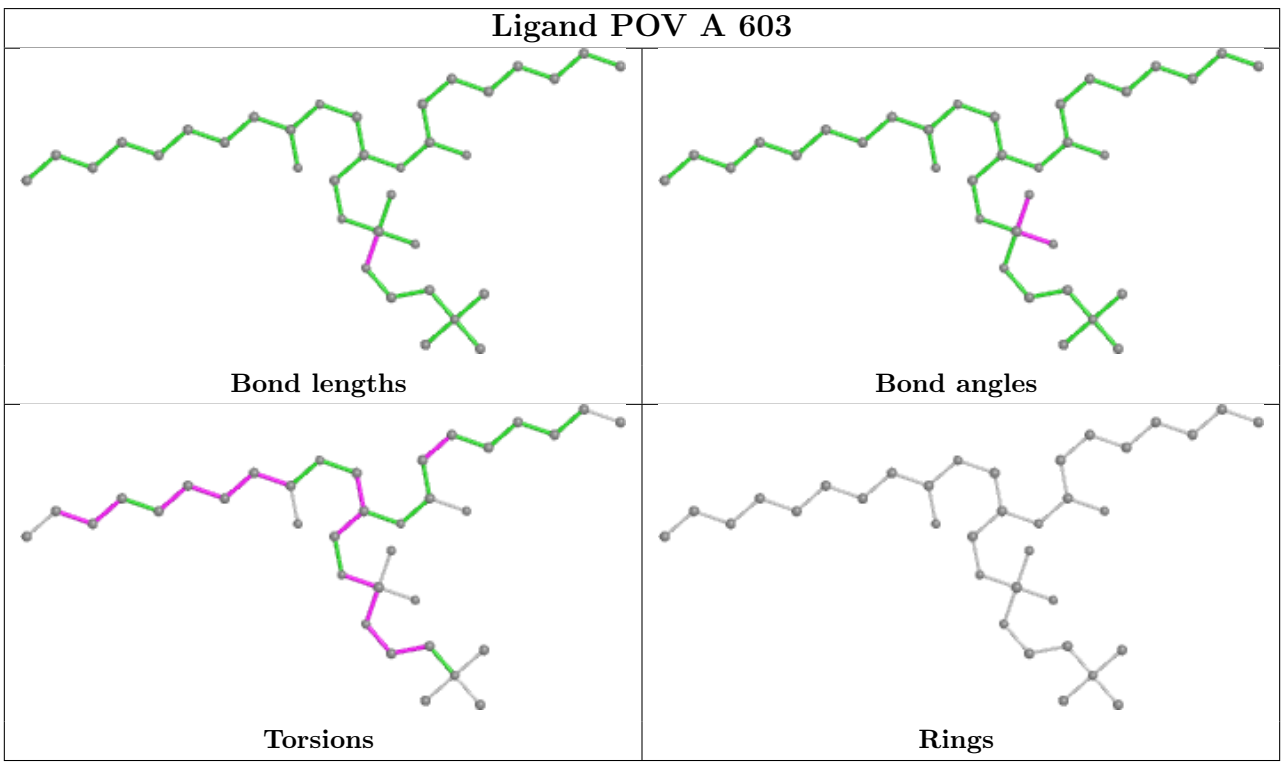
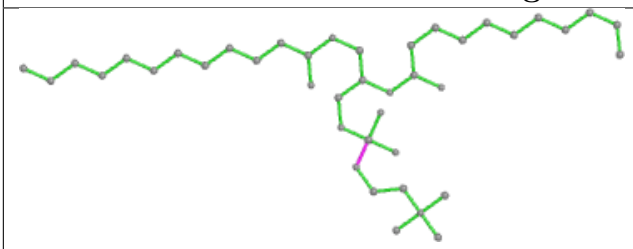


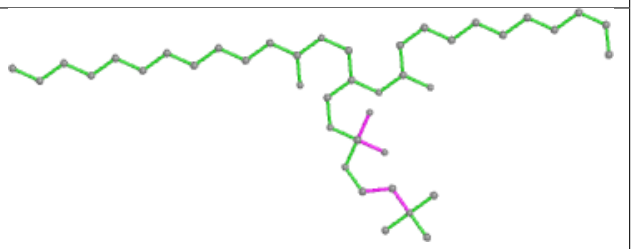
Ligand POV A 603



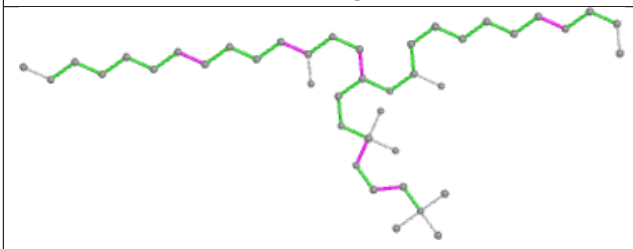
Ligand POV B 601



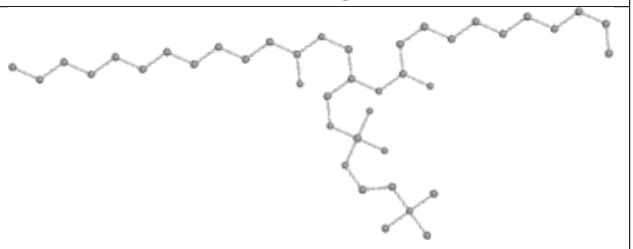
Bond lengths



Bond angles

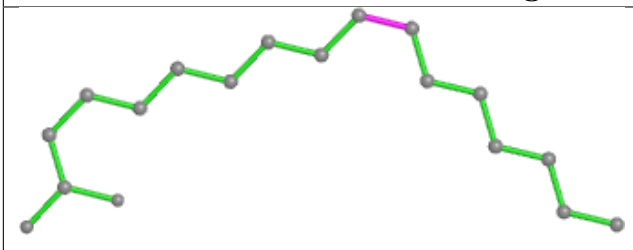


Torsions

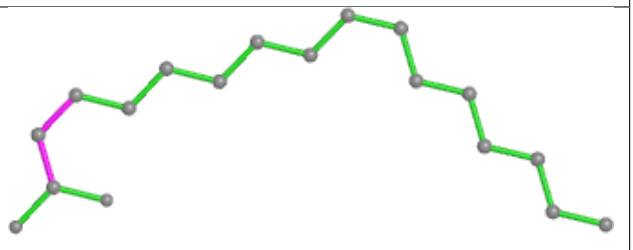


Rings

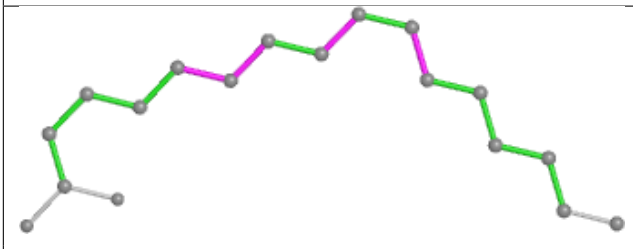
Ligand POV B 610



Bond lengths



Bond angles



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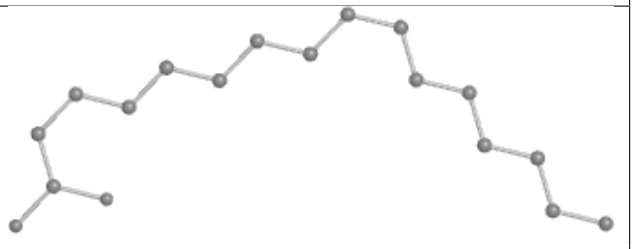

Rings

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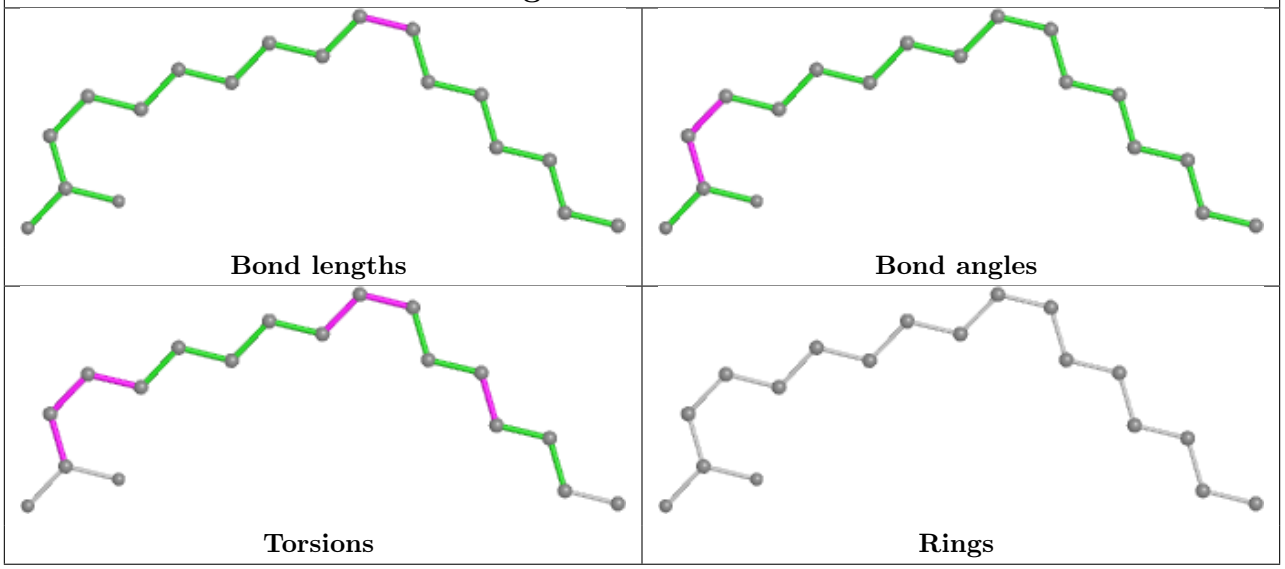

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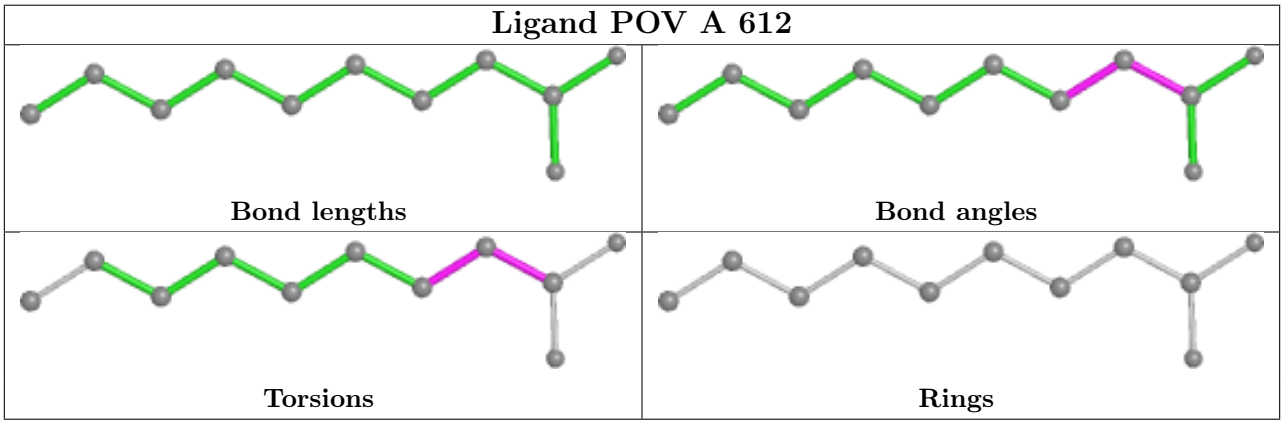

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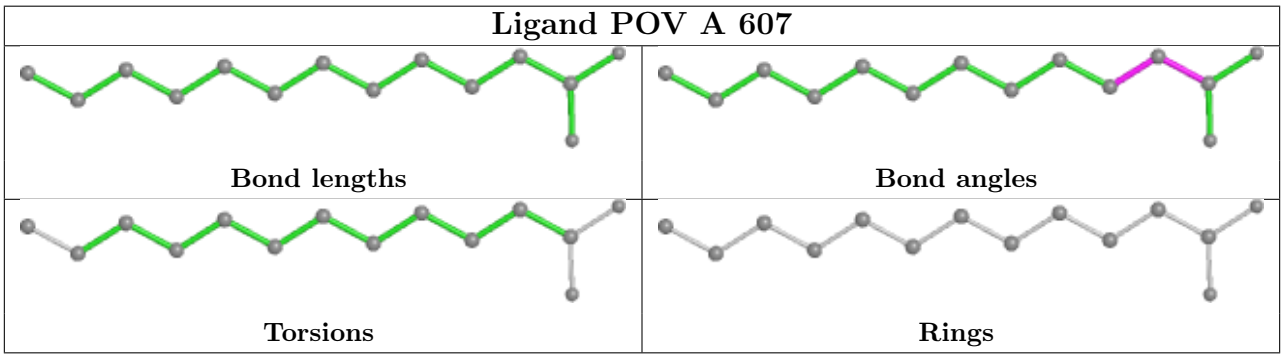
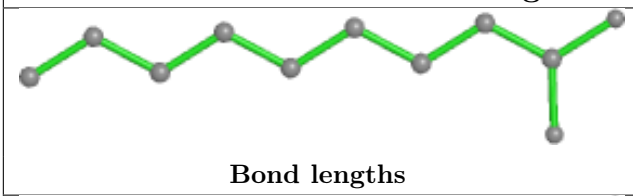
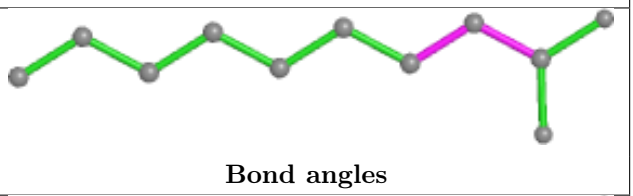
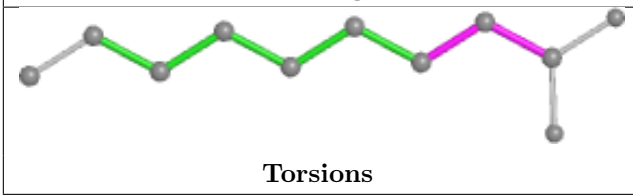
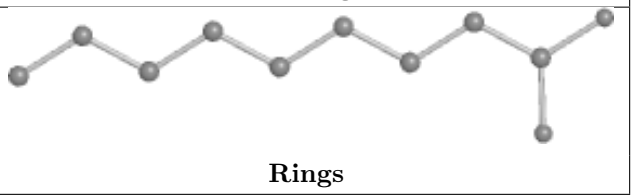


Ligand POV C 614

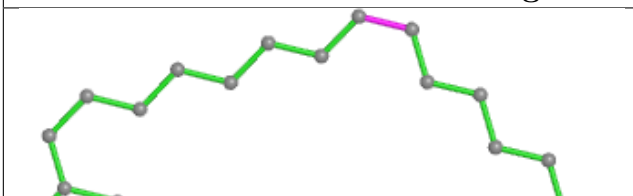

Bond lengths


Bond angles


Torsions


Rings

Ligand POV A 606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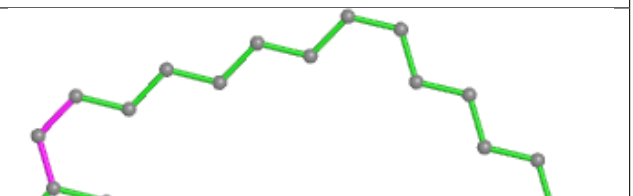
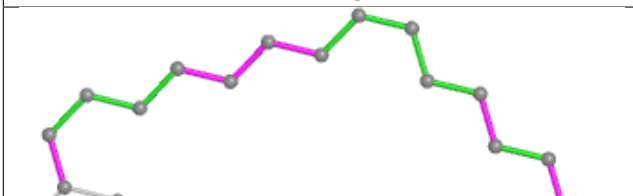

Bond angles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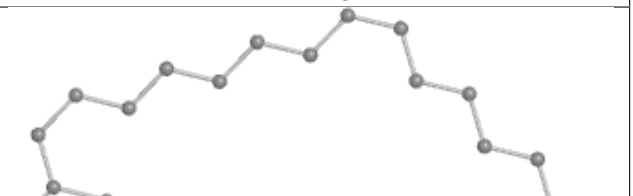
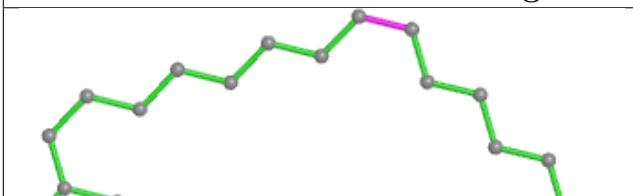
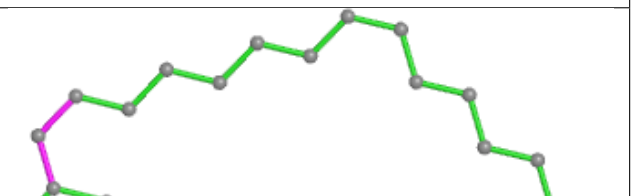
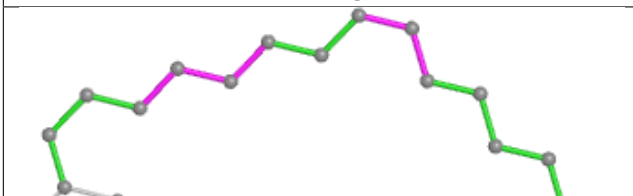
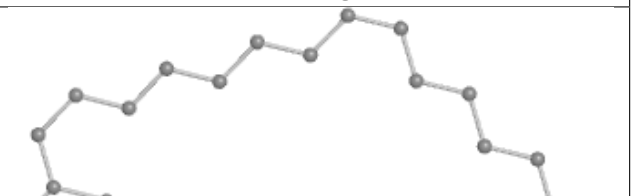

Rings

Ligand POV C 607

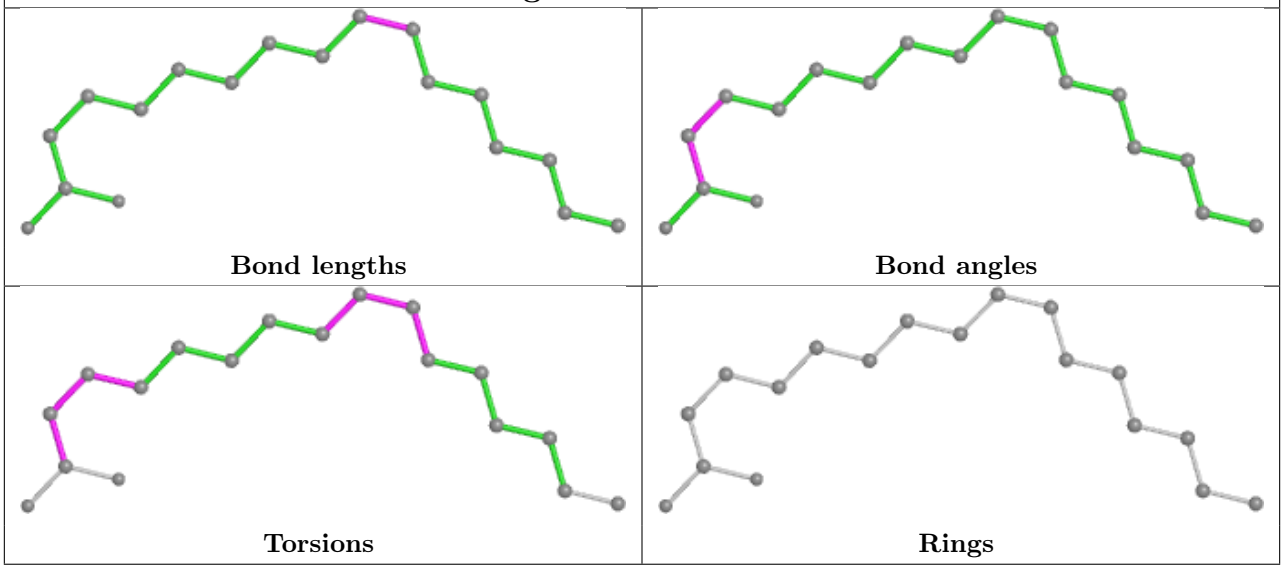

Bond lengths


Bond angles

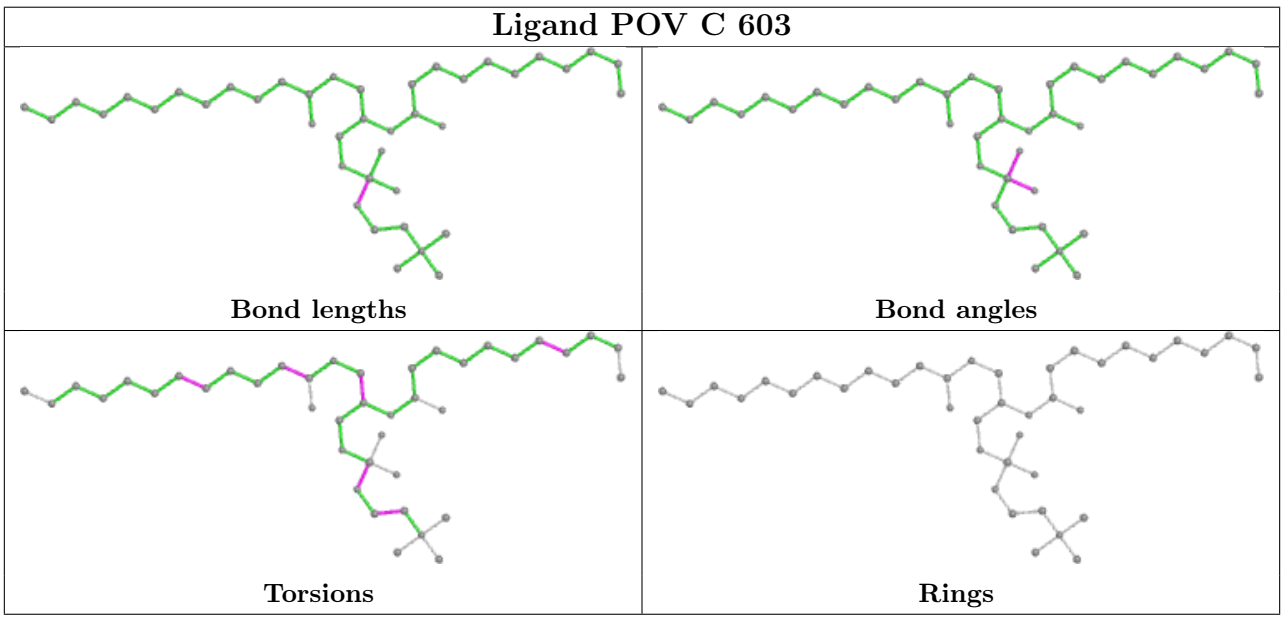

Torsions


Rings

Ligand POV A 615



Ligand POV C 603



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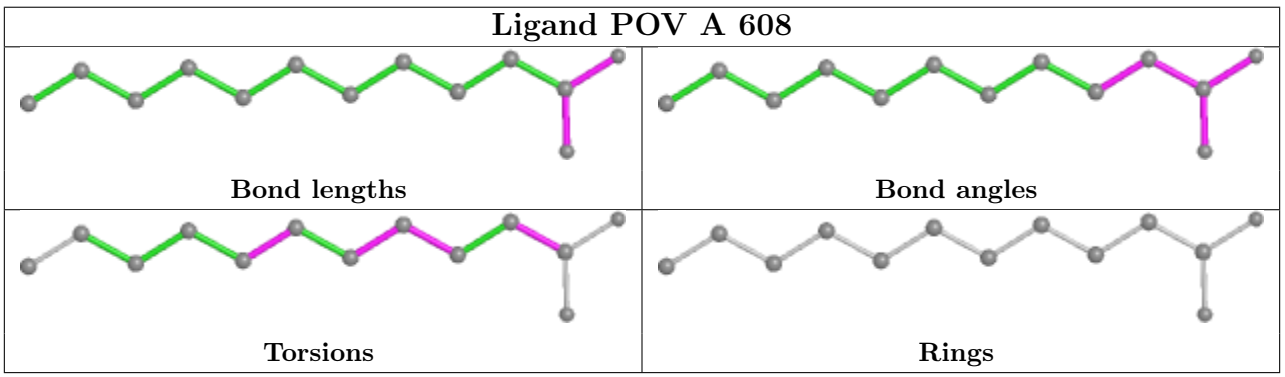
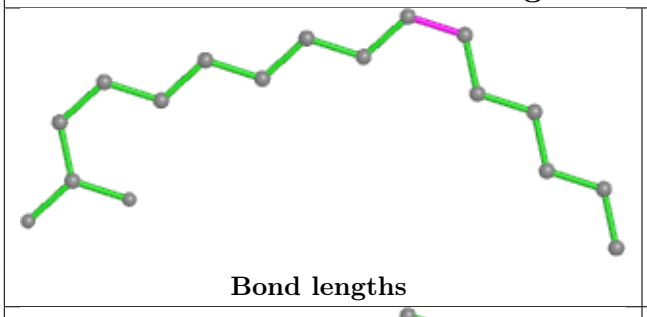
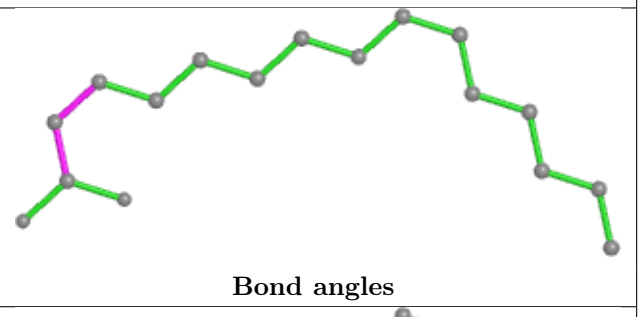


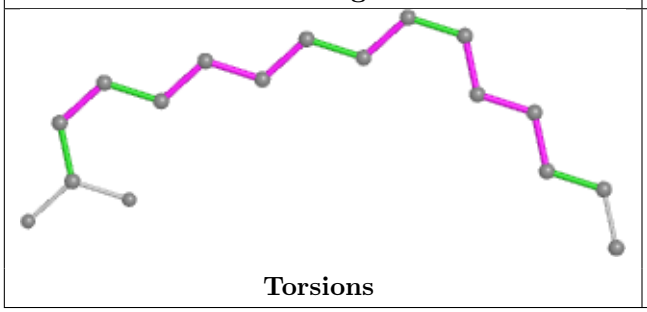
Ligand POV B 611



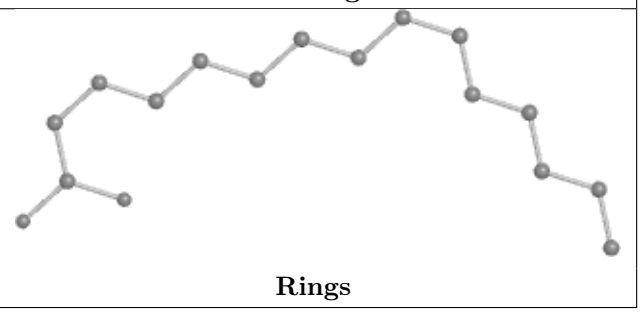
Bond lengths



Bond angles

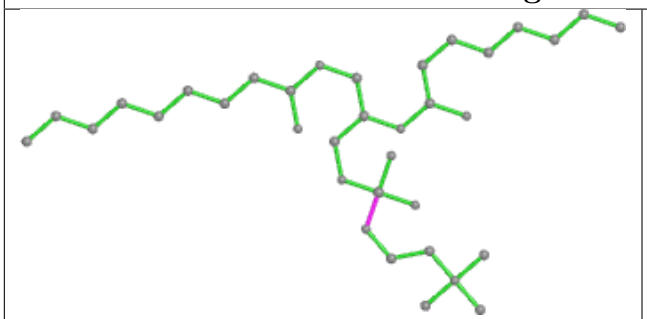


Torsions



Rings

Ligand POV C 605



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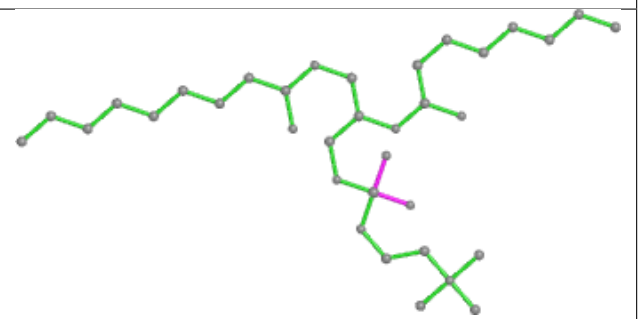
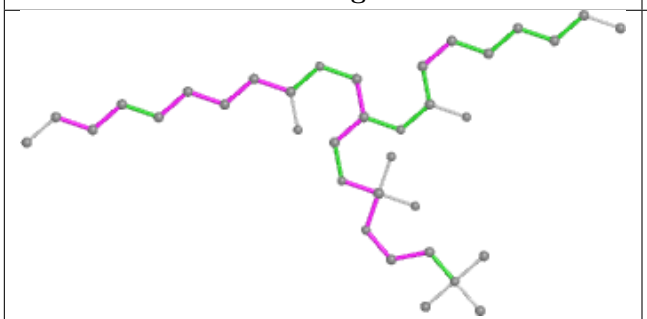


Bond angles



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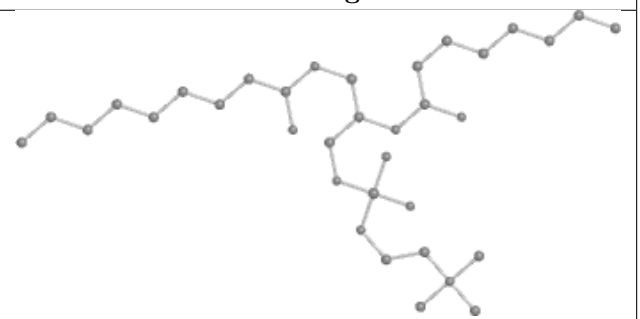
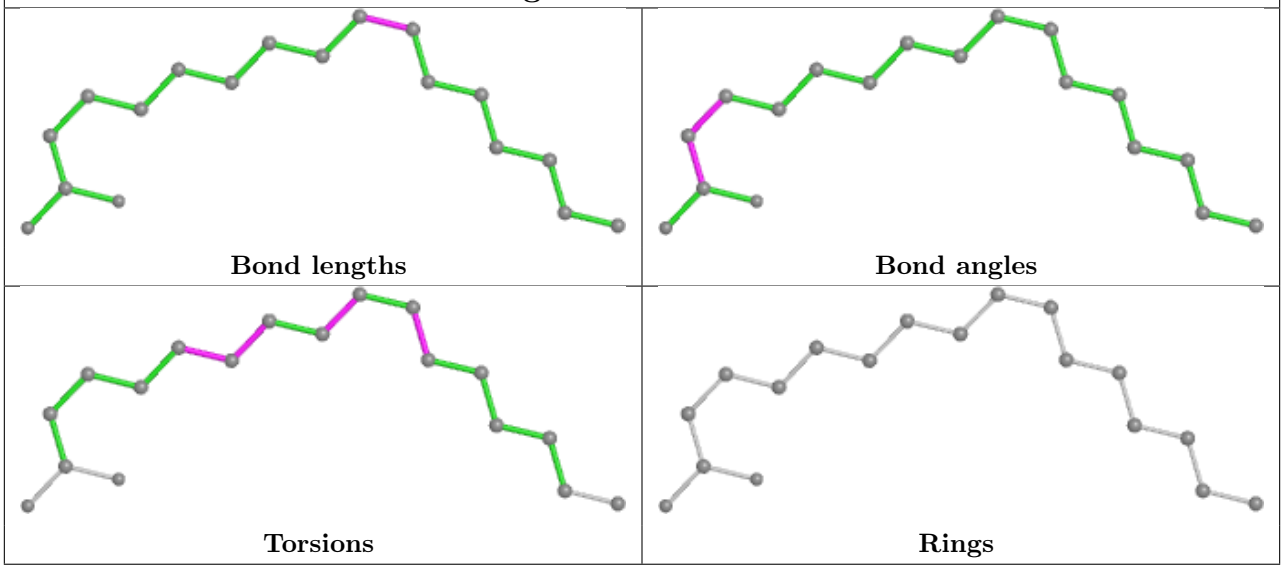


Rings

Ligand POV A 610



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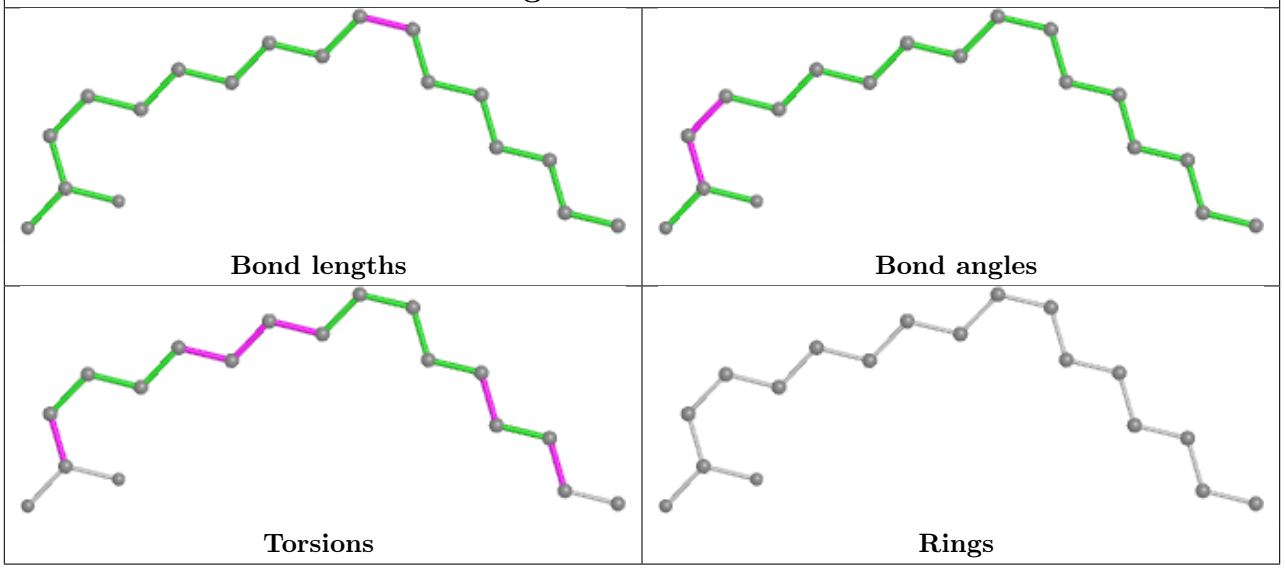

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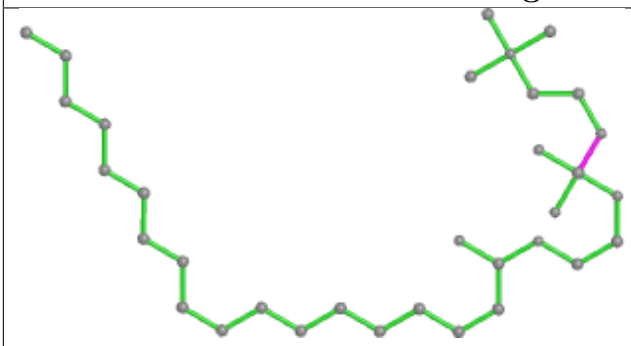
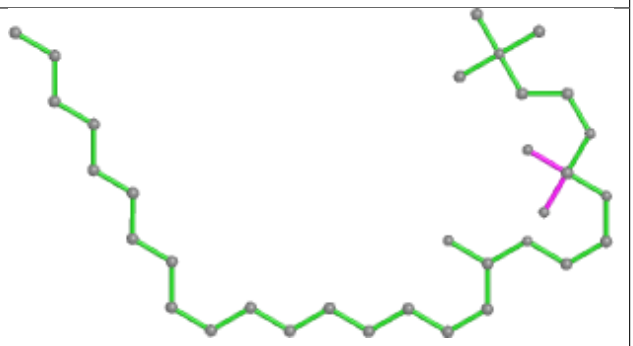
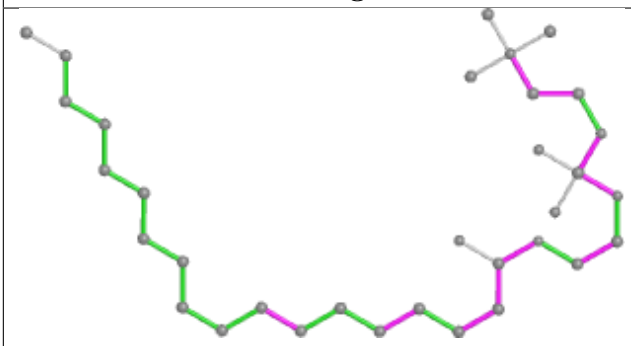


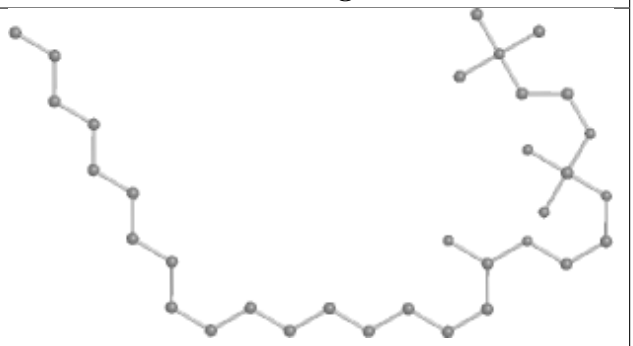
Bond lengths



Bond angles

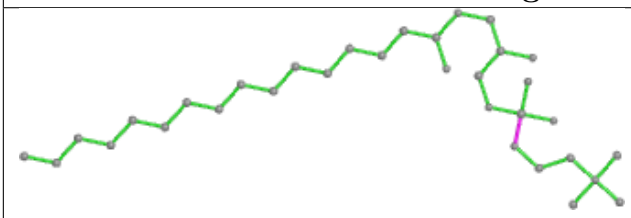


Torsions

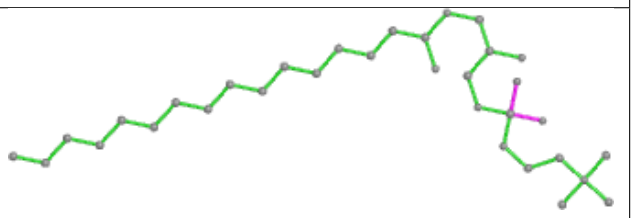


Rings

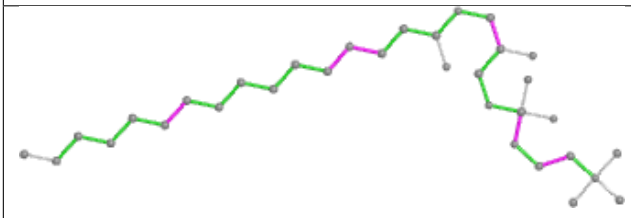
Ligand POV A 604



Bond lengths



Bond angles



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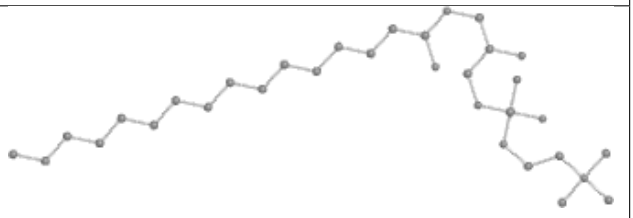
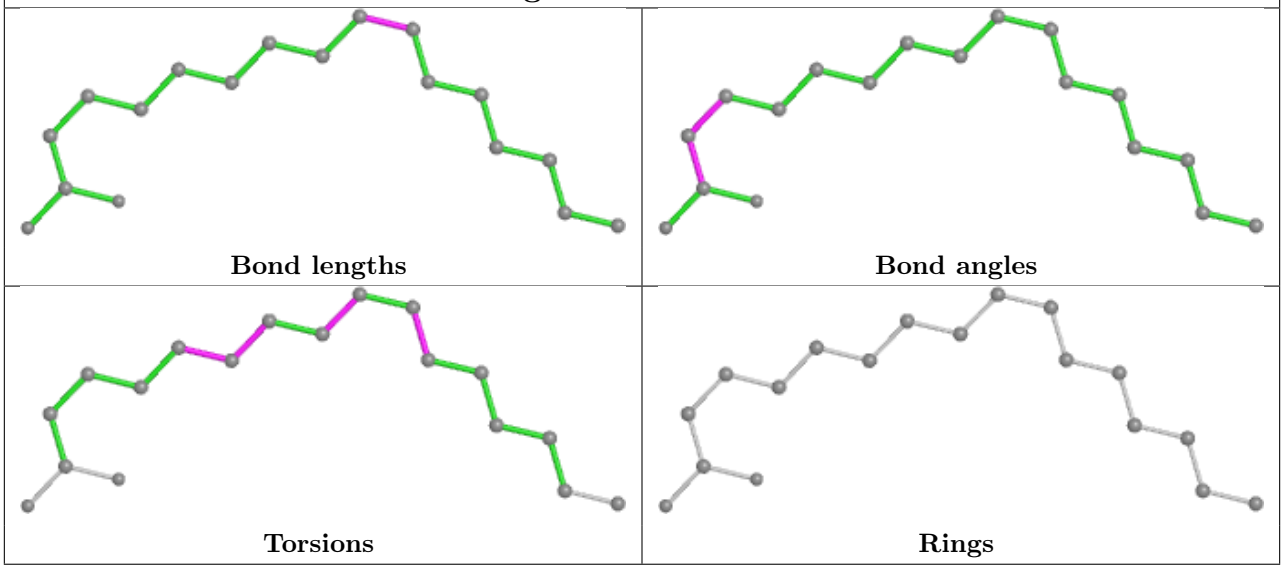


Rings

Ligand POV C 612



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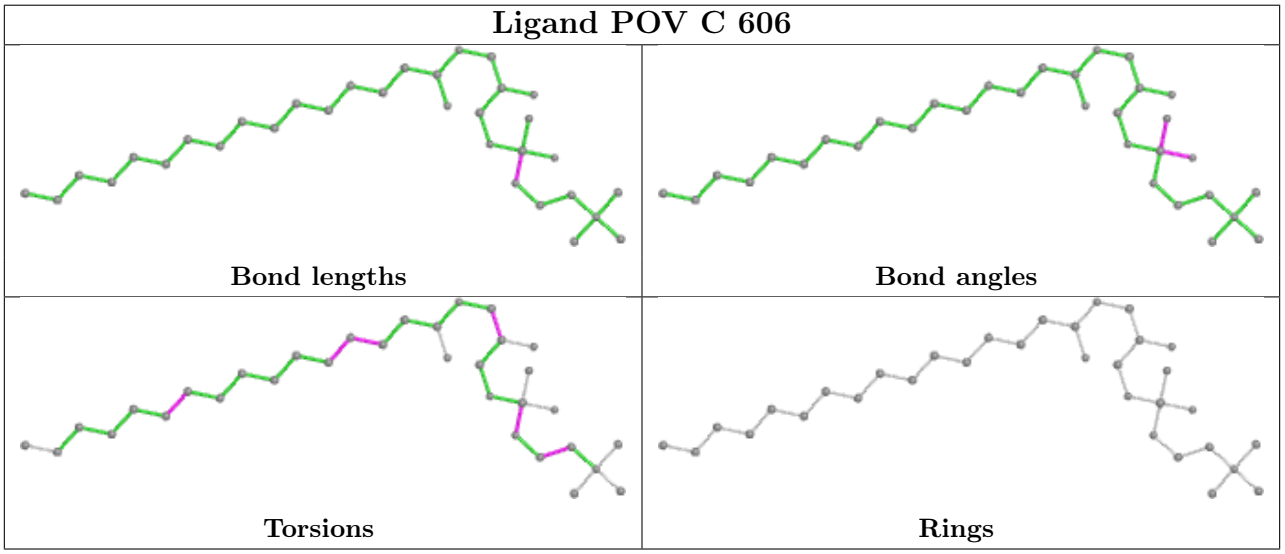

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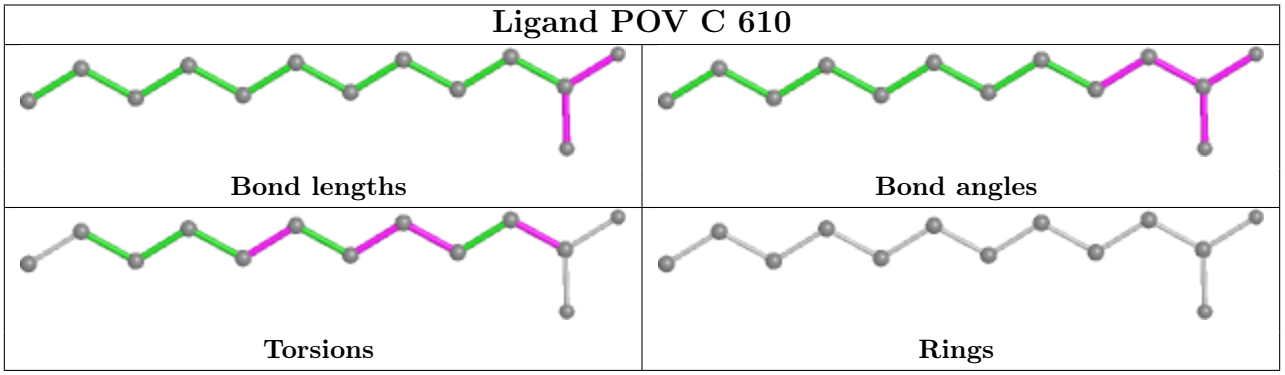

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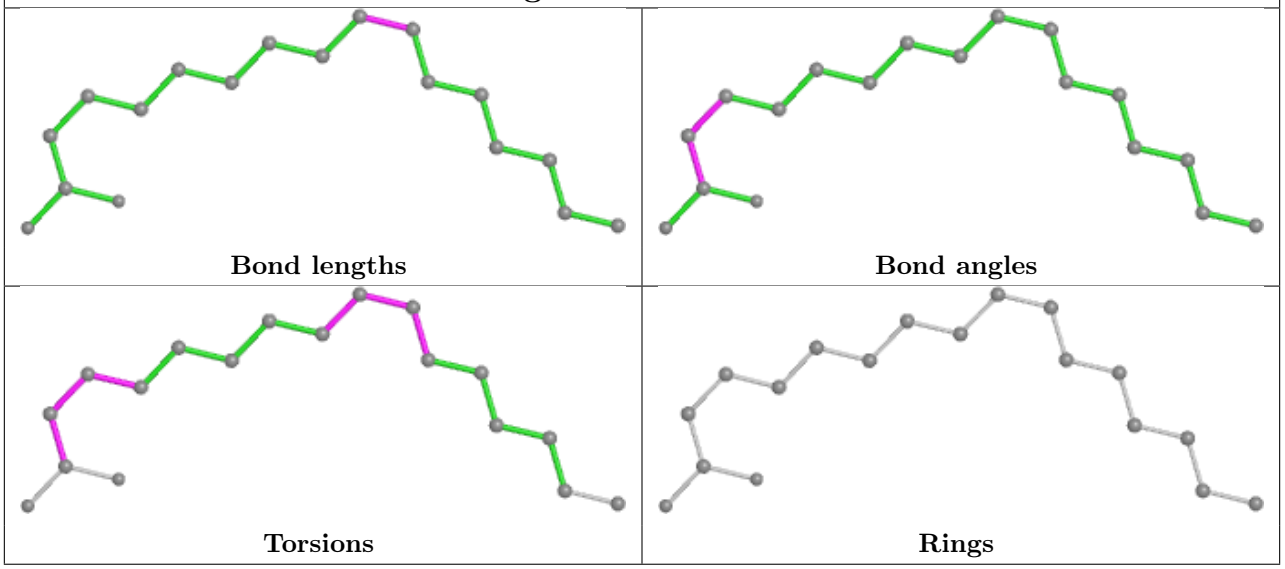

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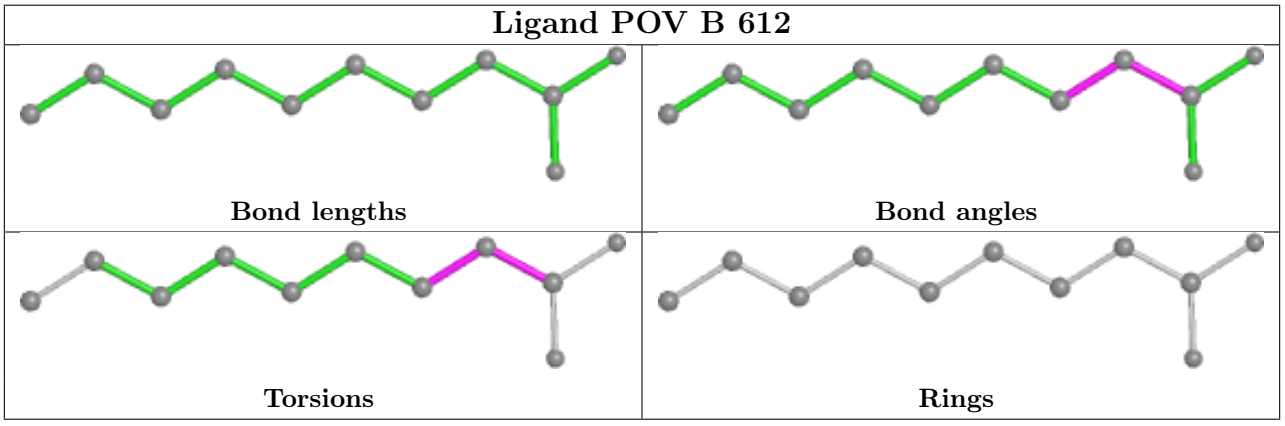

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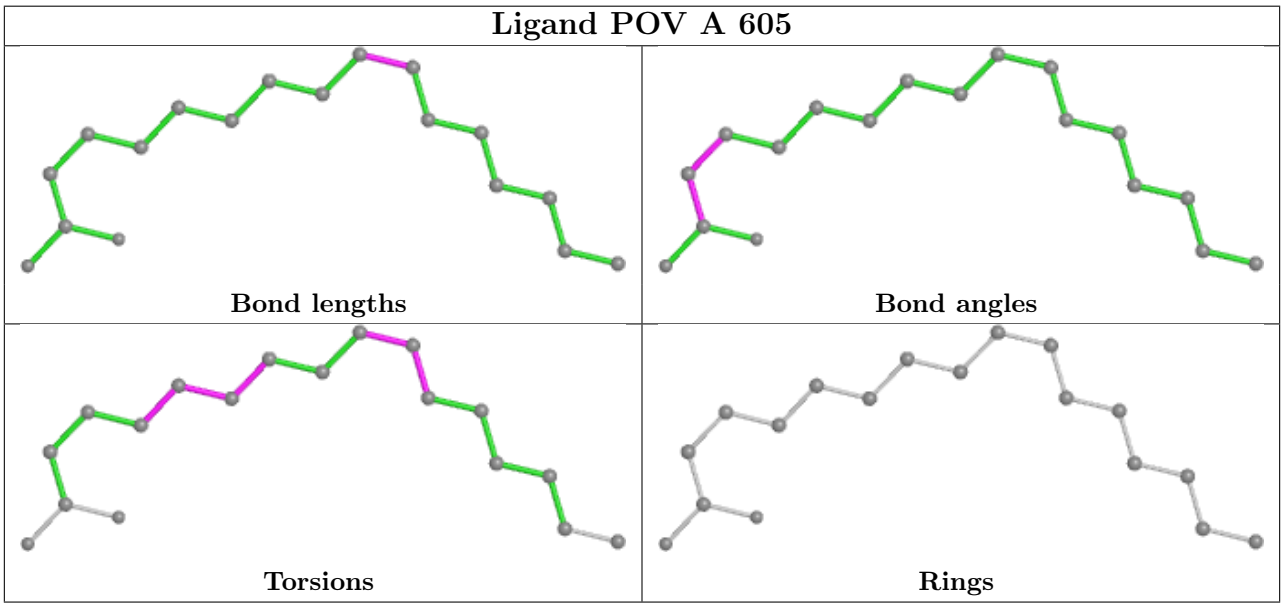

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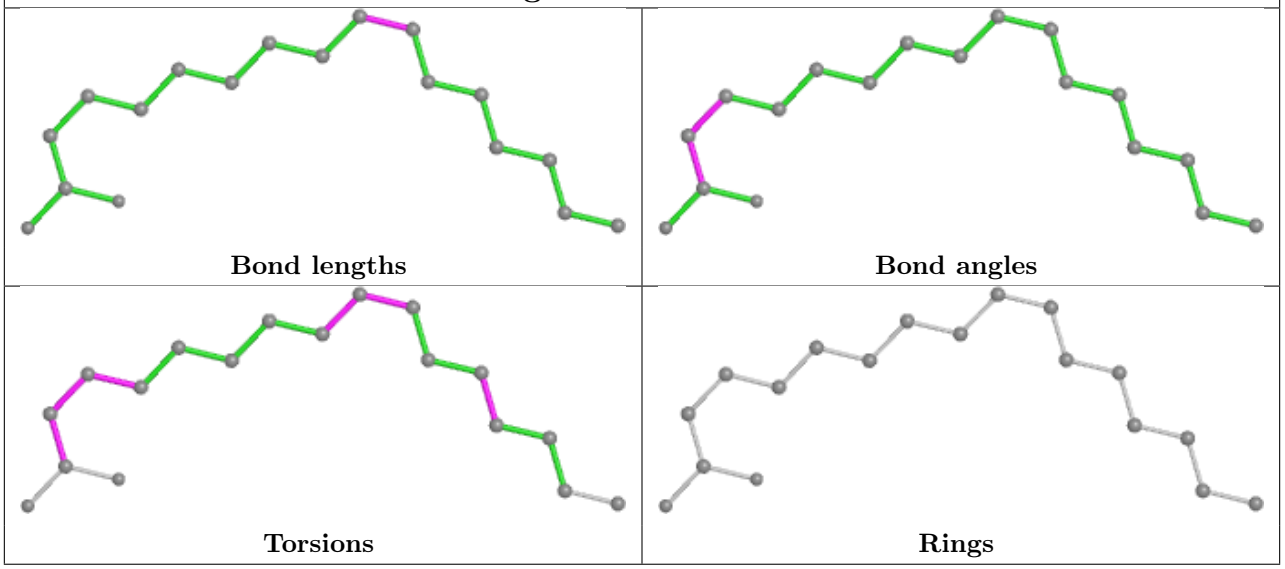

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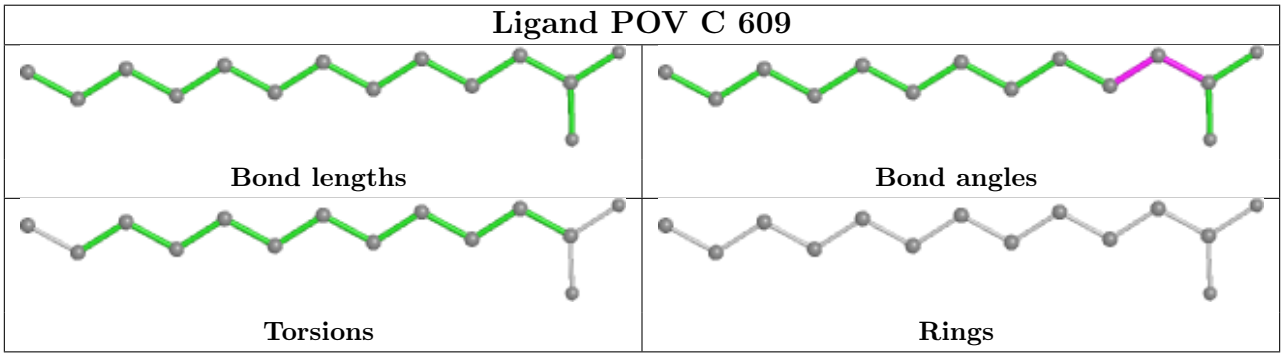

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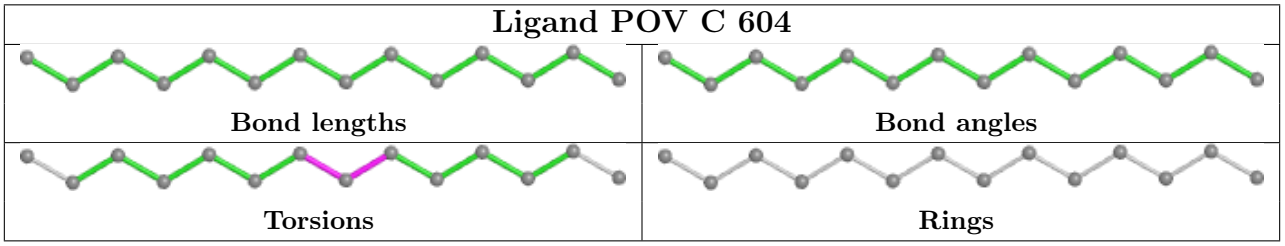

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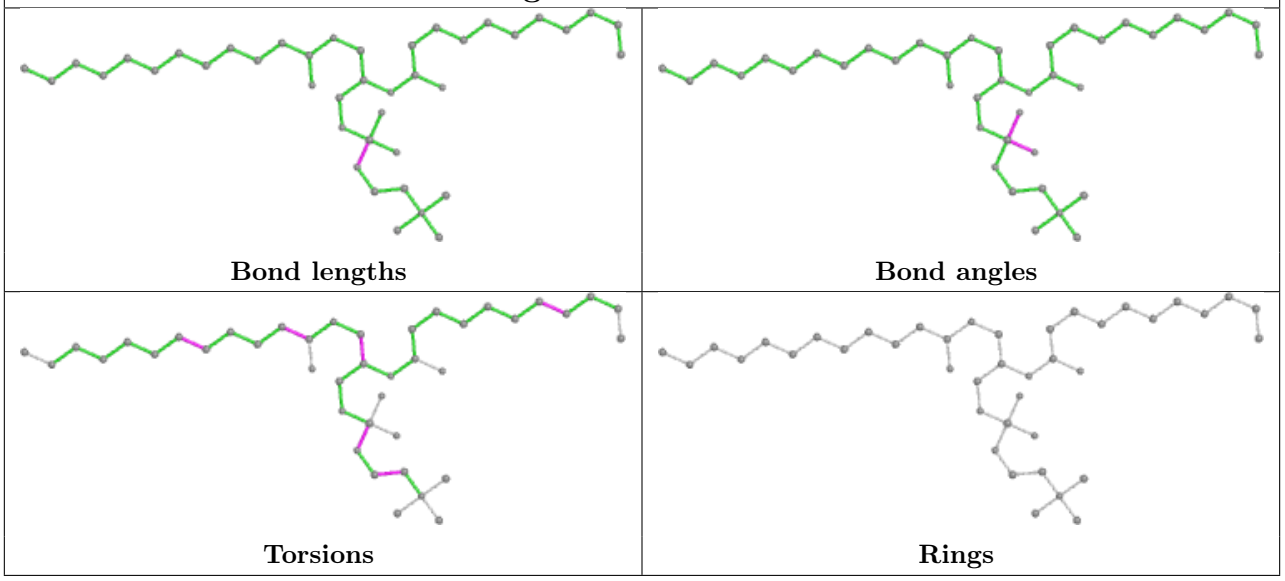

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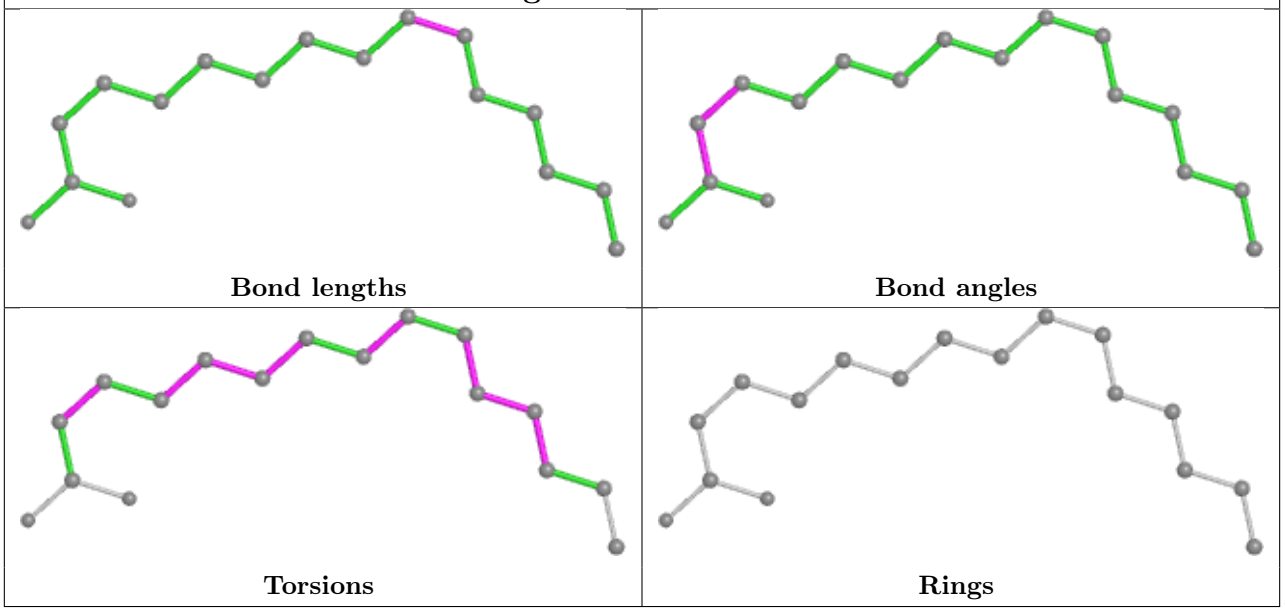


5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

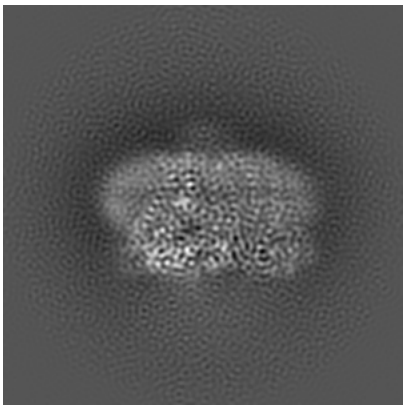
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22376. These allow visual inspection of the internal detail of the map and identification of artifacts.

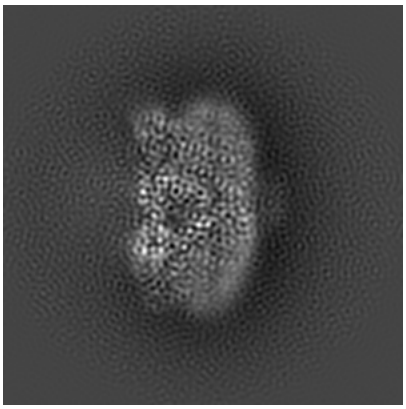
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

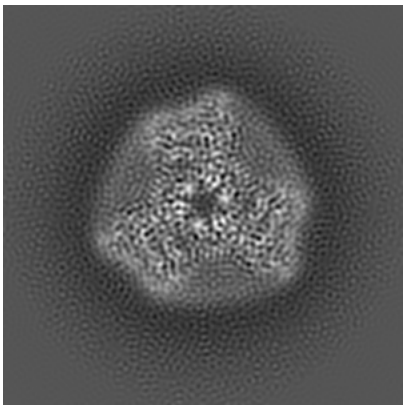
6.1.1 Primary map



X

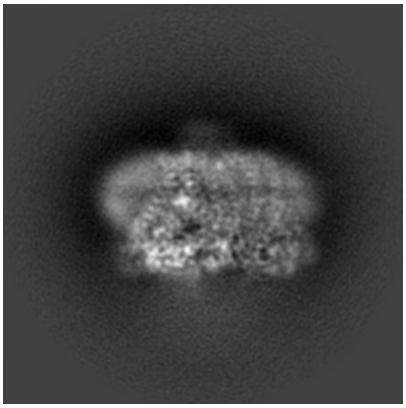


Y

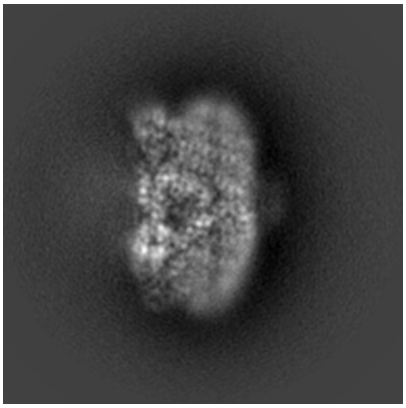


Z

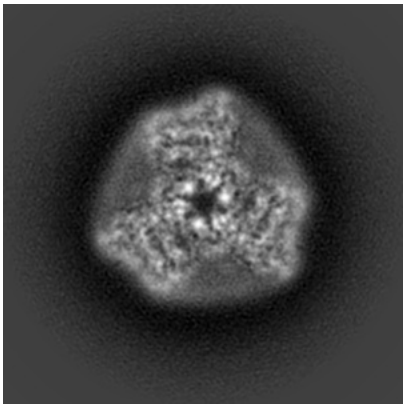
6.1.2 Raw map



X



Y

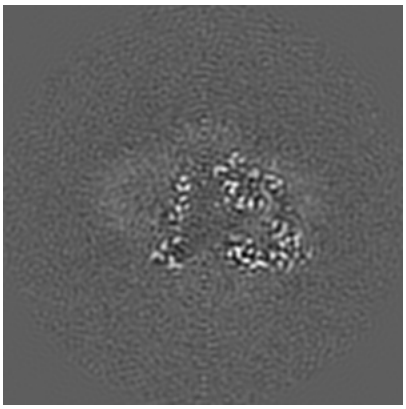


Z

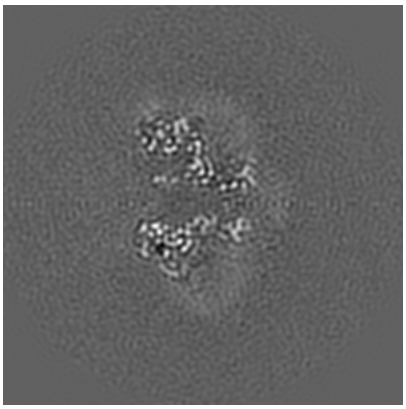
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

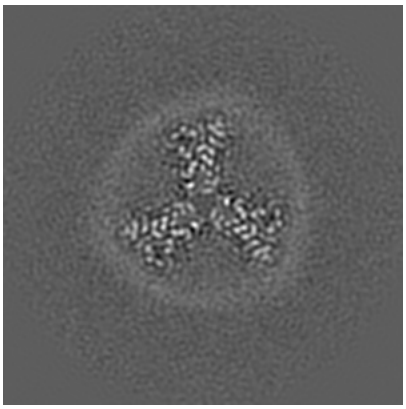
6.2.1 Primary map



X Index: 96

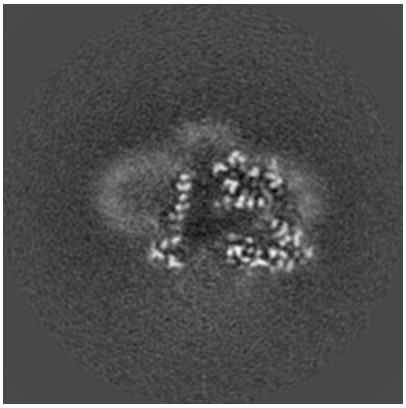


Y Index: 96

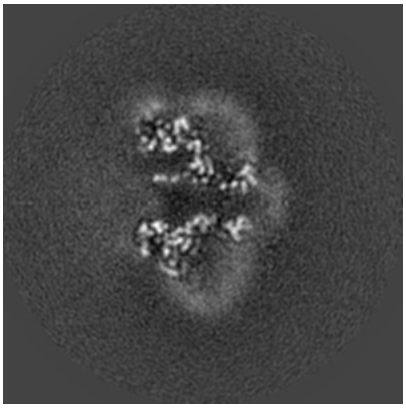


Z Index: 96

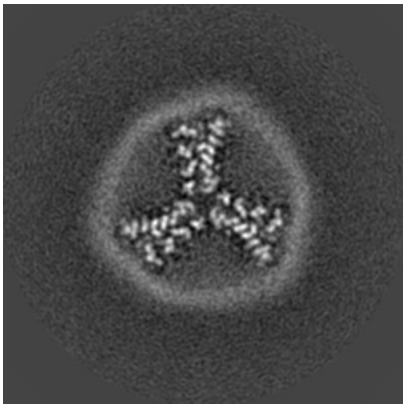
6.2.2 Raw map



X Index: 96



Y Index: 96

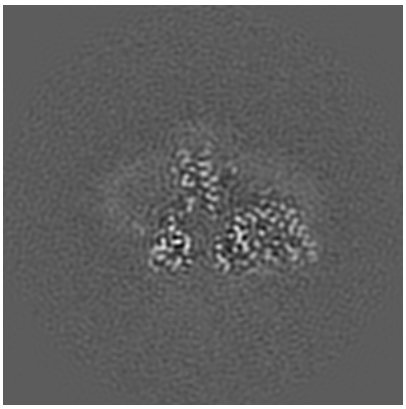


Z Index: 96

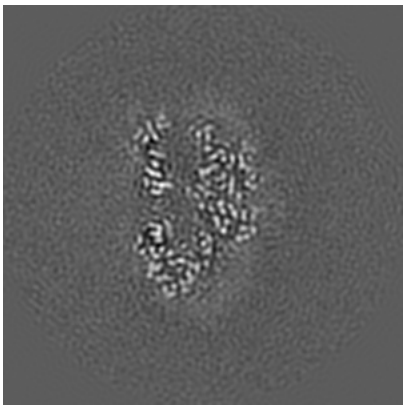
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

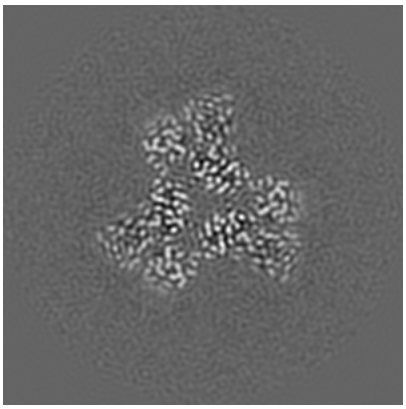
6.3.1 Primary map



X Index: 105

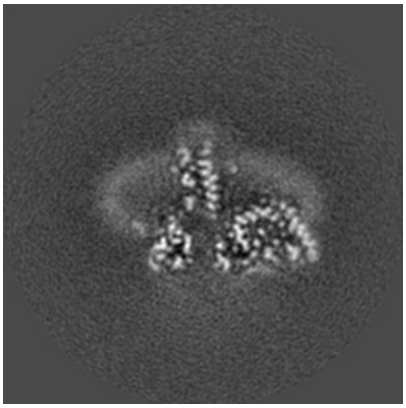


Y Index: 88

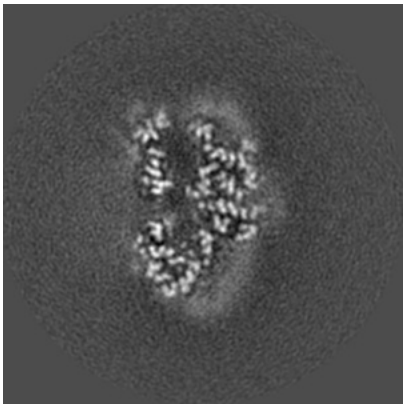


Z Index: 75

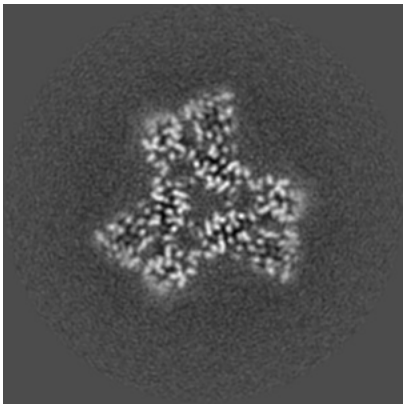
6.3.2 Raw map



X Index: 105



Y Index: 88



Z Index: 75

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

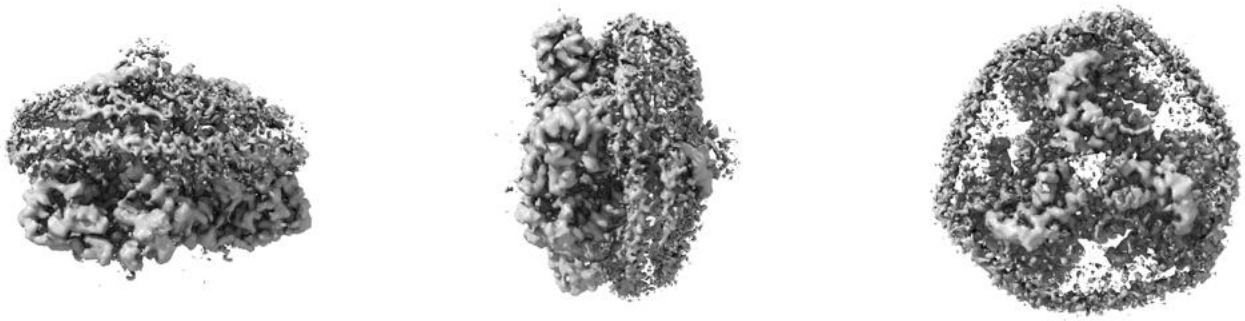
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.029. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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.

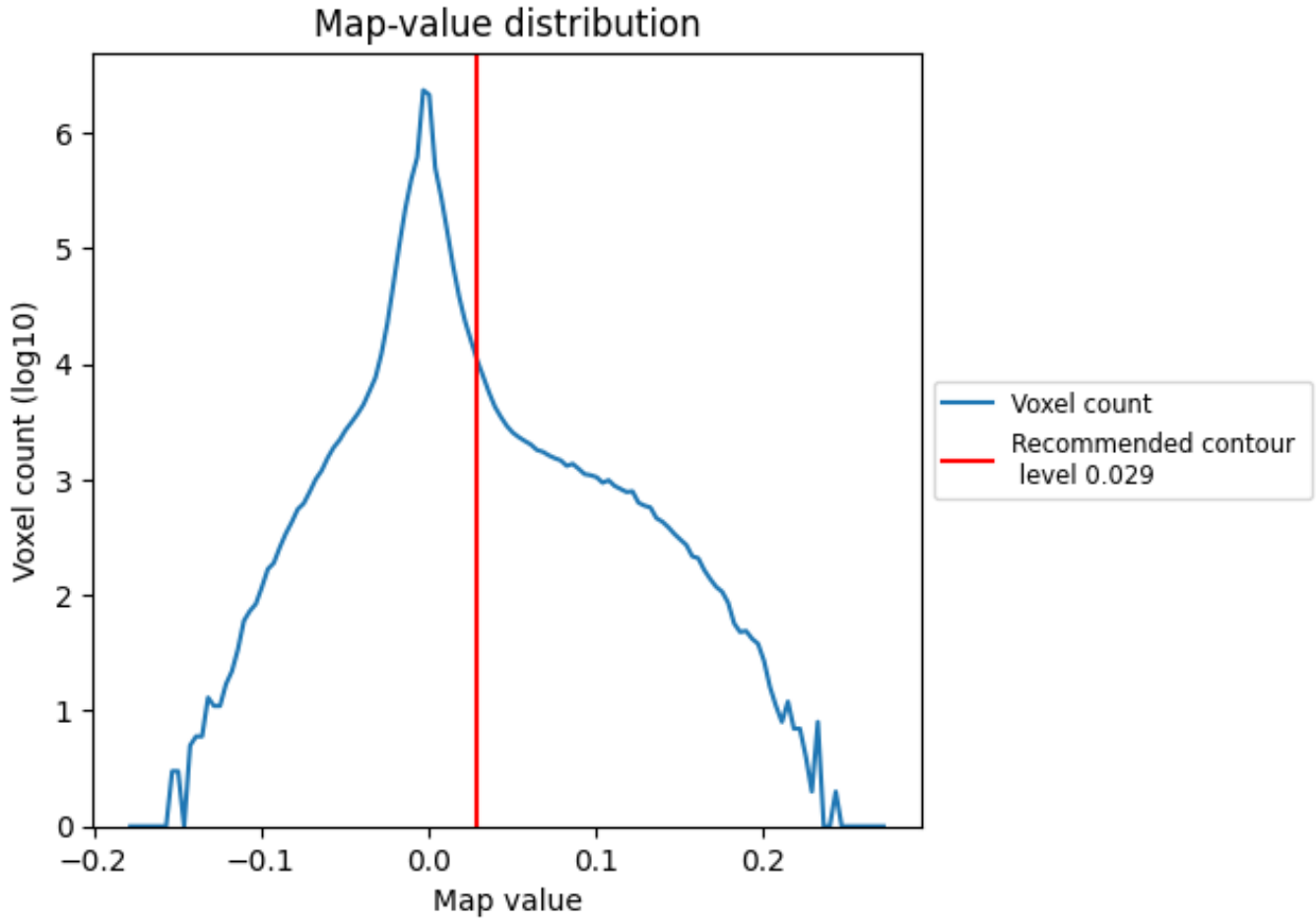
6.5 Mask visualisation (i)

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

7 Map analysis

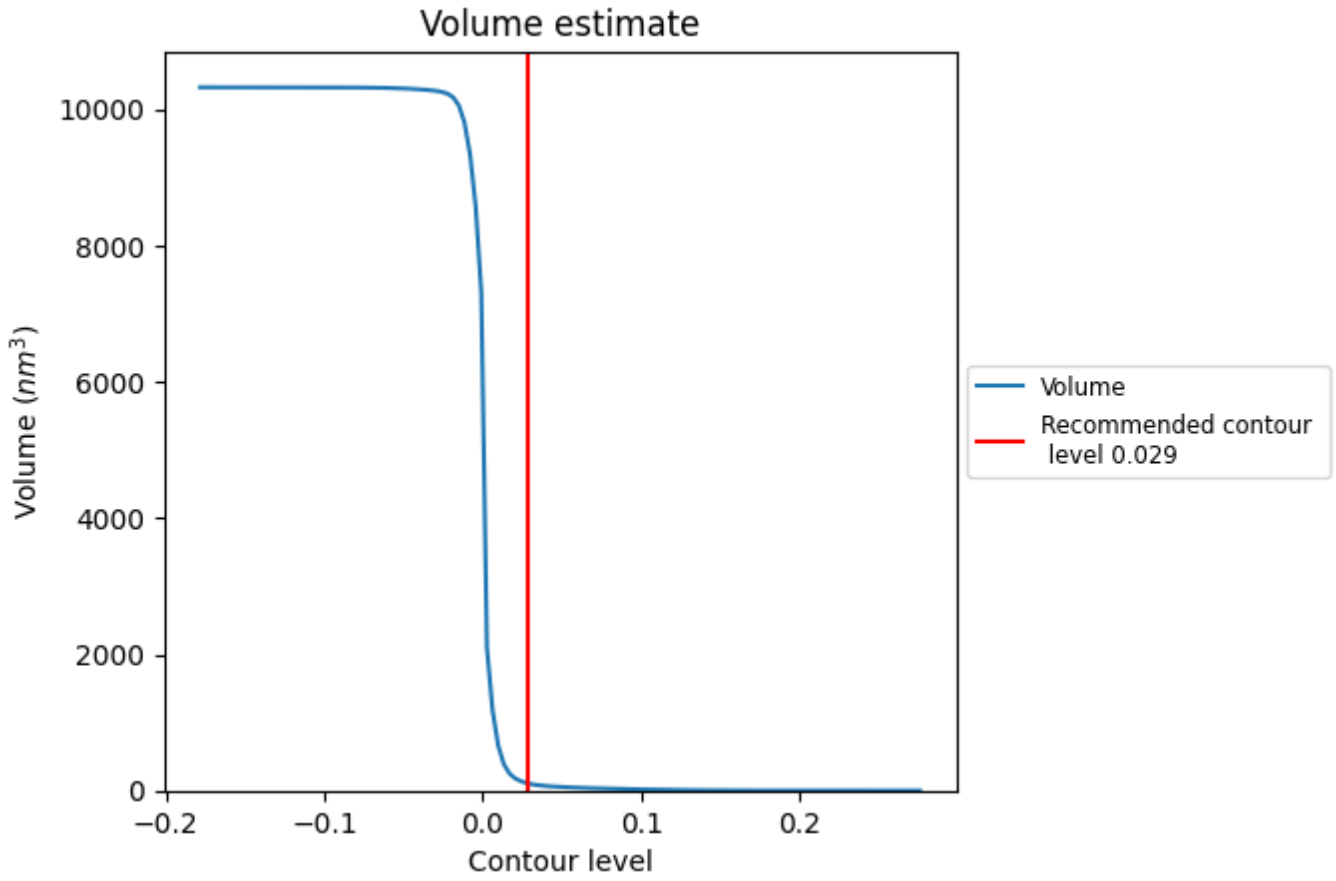
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

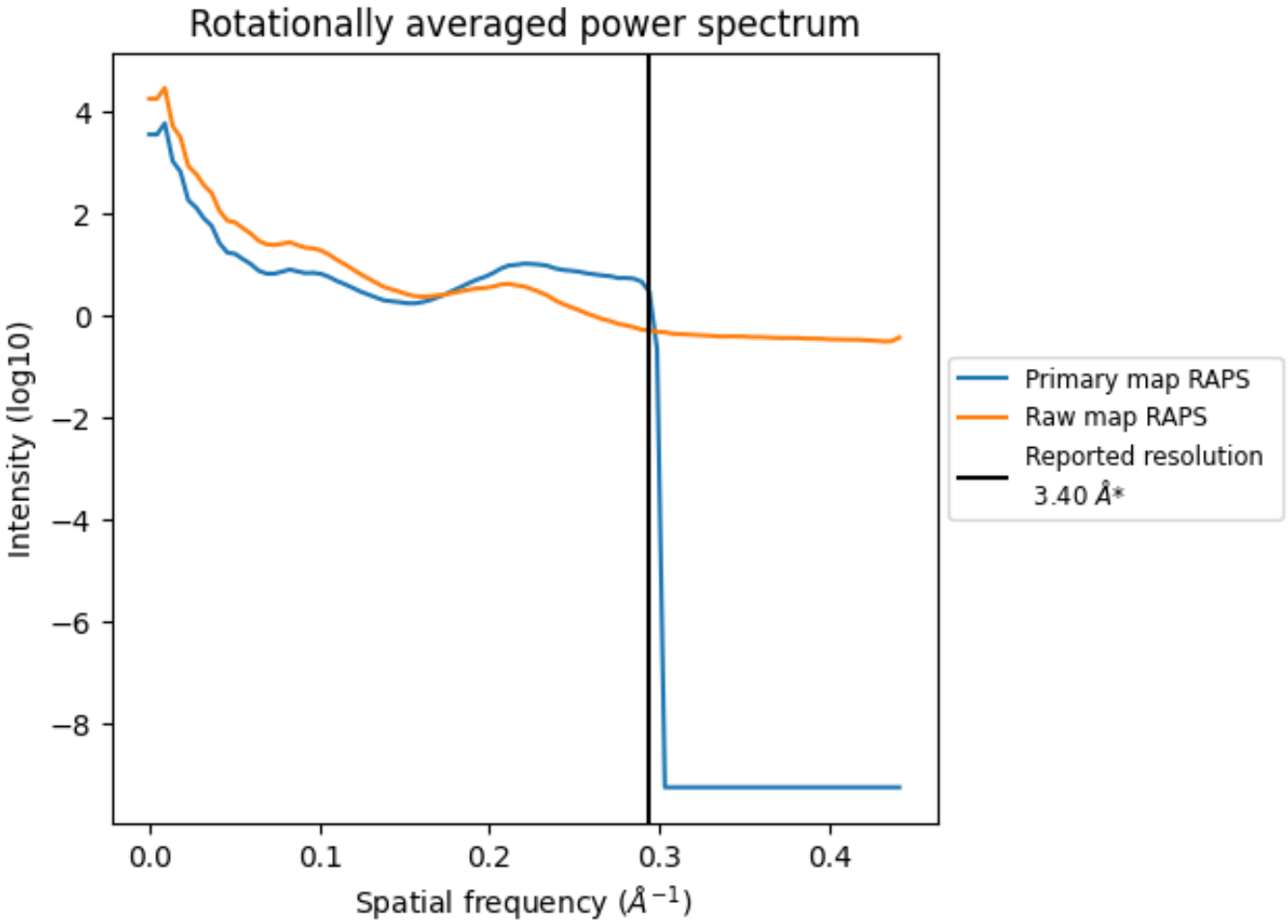
7.2 Volume estimate



The volume at the recommended contour level is 104 nm^3; this corresponds to an approximate mass of 94 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)

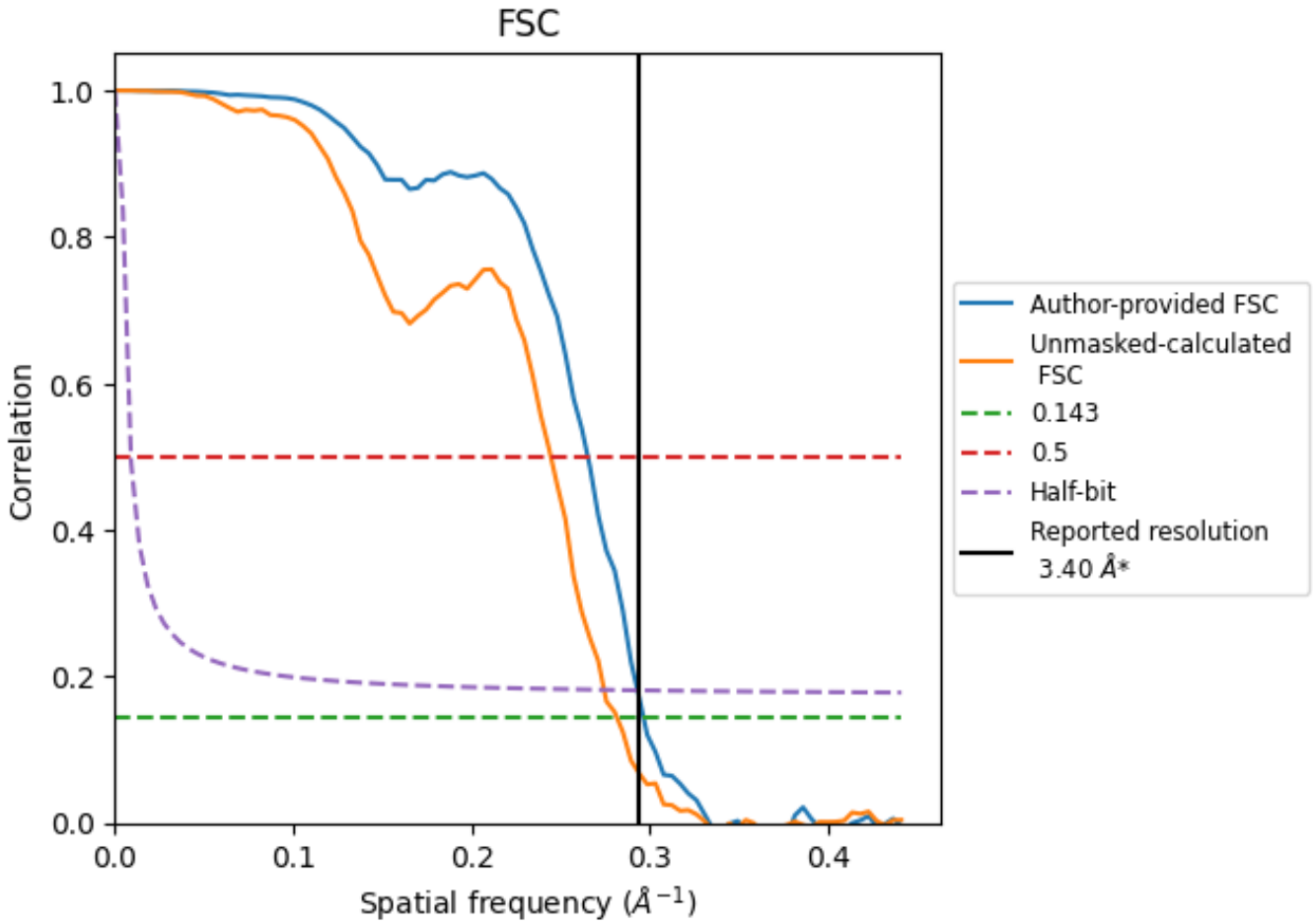


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

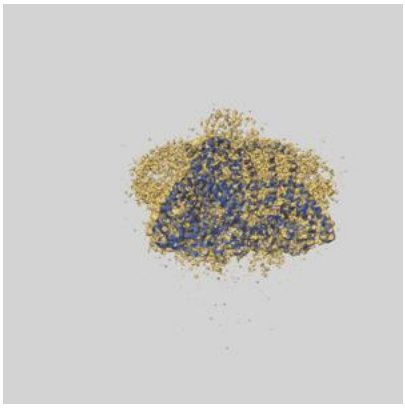
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.37	3.77	3.41
Unmasked-calculated*	3.55	4.09	3.65

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

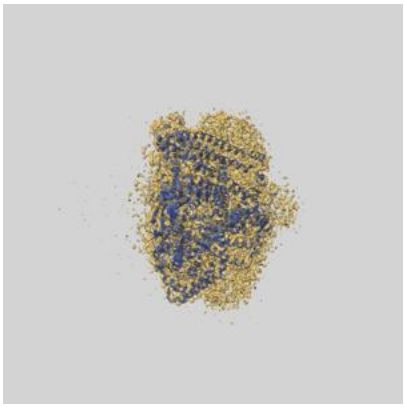
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22376 and PDB model 7JLP. Per-residue inclusion information can be found in section 3 on page 6.

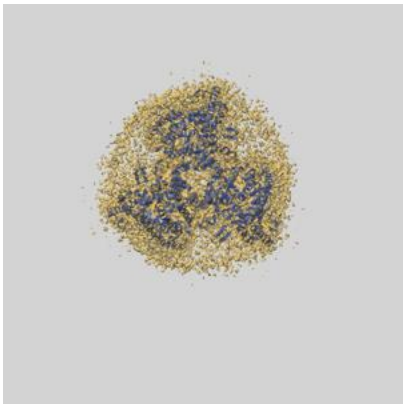
9.1 Map-model overlay



X



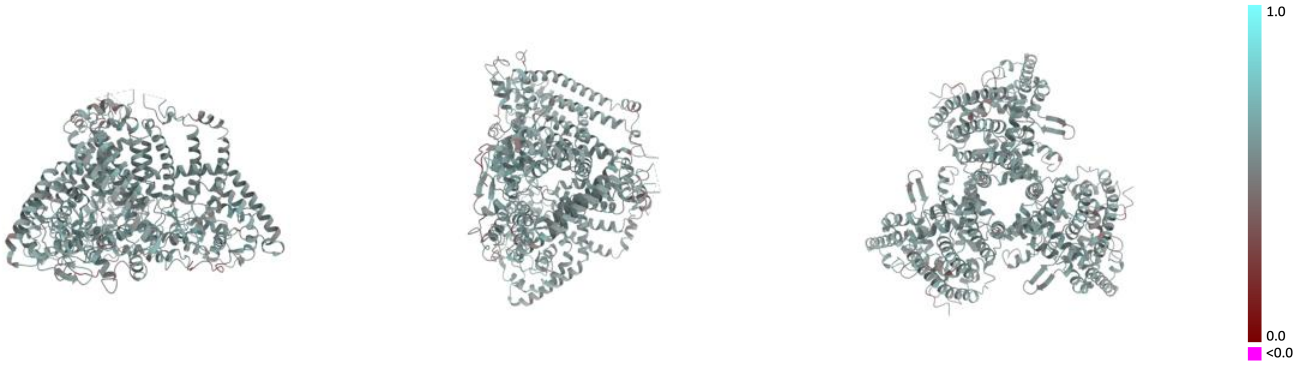
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.029 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.

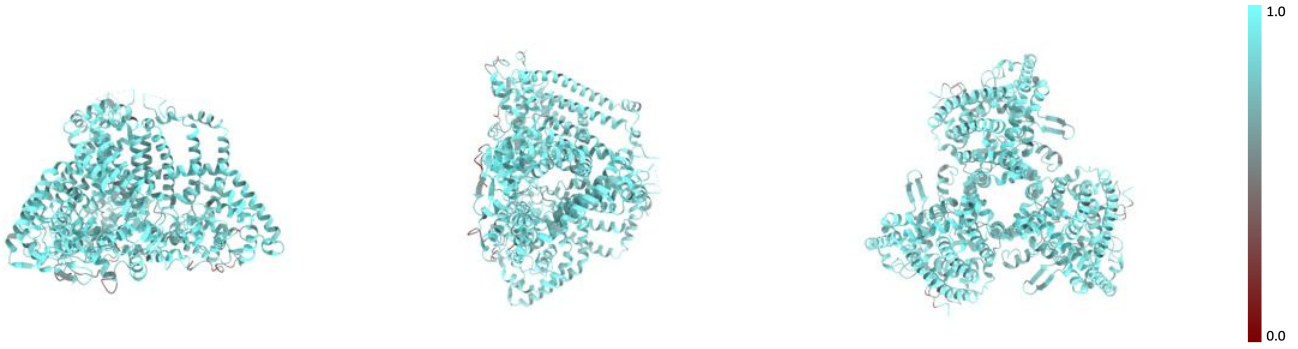
9.2 Q-score mapped to coordinate model



X Y Z

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

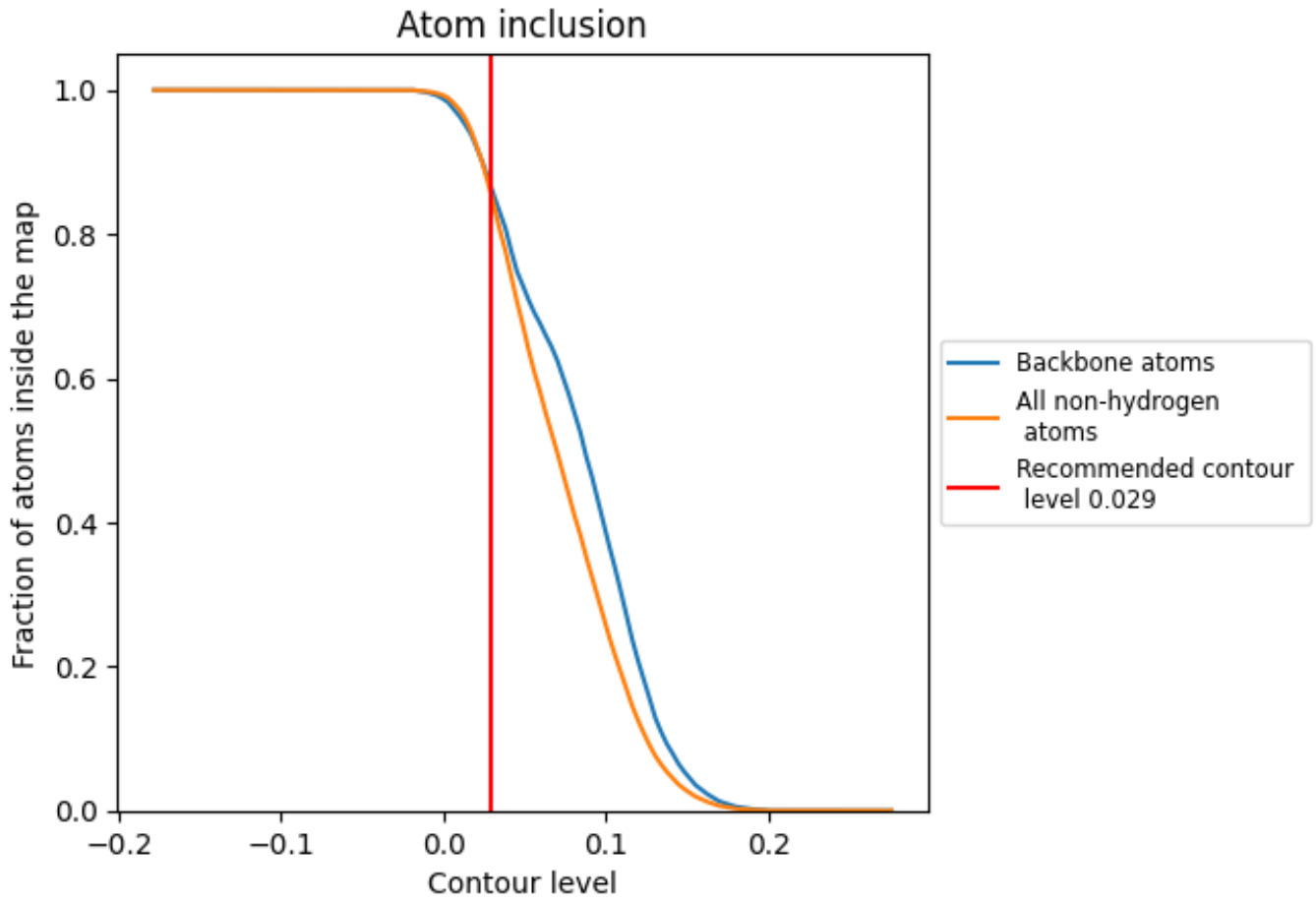
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.029).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.029) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8575	0.5520
A	0.8568	0.5510
B	0.8575	0.5530
C	0.8582	0.5530