Full wwPDB EM Validation Report (i)

Feb 24, 2024 – 12:47 PM EST

PDB ID	:	7K4B
EMDB ID	:	EMD-22663
Title	:	Cryo-EM structure of human TRPV6 in complex with (4- phenylcyclohexyl) piperazine inhibitor cis-22a
Authors	:	Neuberger, A.; Nadezhdin, K.D.; Singh, A.K.; Sobolevsky, A.I.
Deposited on	:	2020-09-15
Resolution	:	3.10 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 (i) 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 (1)) were used in the production of this report:

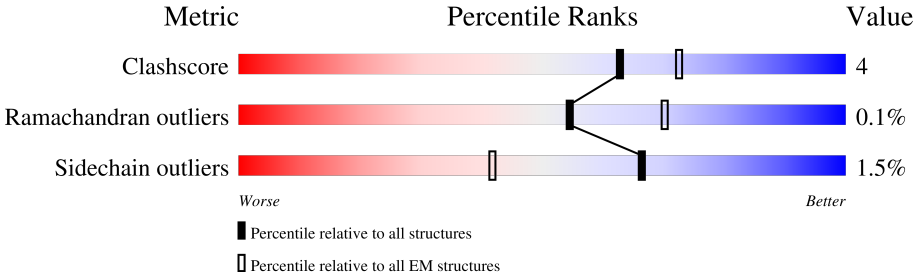
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 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	670	7% 78% 12% 9%
1	B	670	7% 78% 12% 9%
1	C	670	7% 79% 11% • 9%
1	D	670	7% 78% 12% • 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21118 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

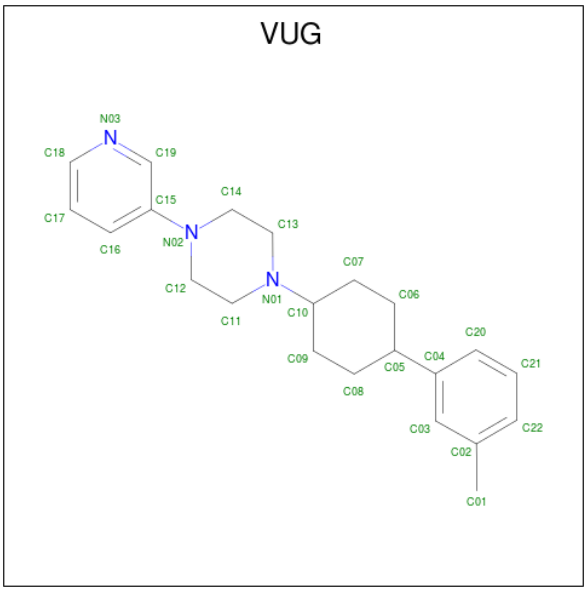
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	607	4891	3159	830	862	40	0	0
1	B	607	4891	3159	830	862	40	0	0
1	C	607	4891	3159	830	862	40	0	0
1	D	607	4891	3159	830	862	40	0	0

There are 12 discrepancies between the modelled and reference sequences:

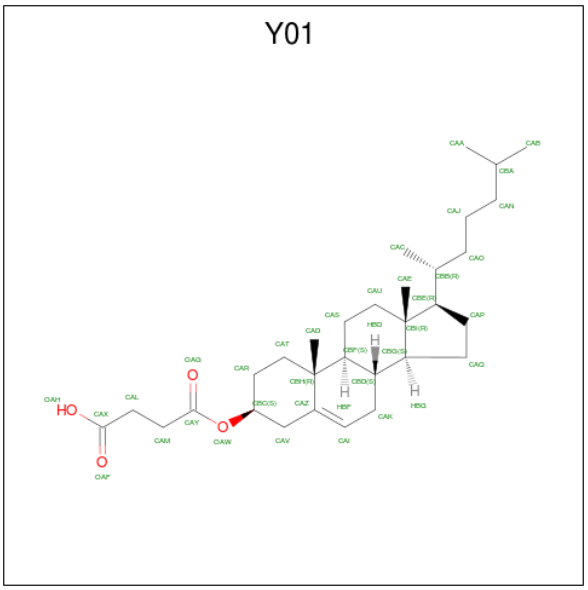
Chain	Residue	Modelled	Actual	Comment	Reference
A	668	VAL	-	expression tag	UNP Q9H1D0
A	669	PRO	-	expression tag	UNP Q9H1D0
A	670	ARG	-	expression tag	UNP Q9H1D0
B	668	VAL	-	expression tag	UNP Q9H1D0
B	669	PRO	-	expression tag	UNP Q9H1D0
B	670	ARG	-	expression tag	UNP Q9H1D0
C	668	VAL	-	expression tag	UNP Q9H1D0
C	669	PRO	-	expression tag	UNP Q9H1D0
C	670	ARG	-	expression tag	UNP Q9H1D0
D	668	VAL	-	expression tag	UNP Q9H1D0
D	669	PRO	-	expression tag	UNP Q9H1D0
D	670	ARG	-	expression tag	UNP Q9H1D0

- Molecule 2 is 1-[cis-4-(3-methylphenyl)cyclohexyl]-4-(pyridin-3-yl)piperazine (three-letter code: VUG) (formula: $C_{22}H_{29}N_3$) (labeled as "Ligand of Interest" by depositor).



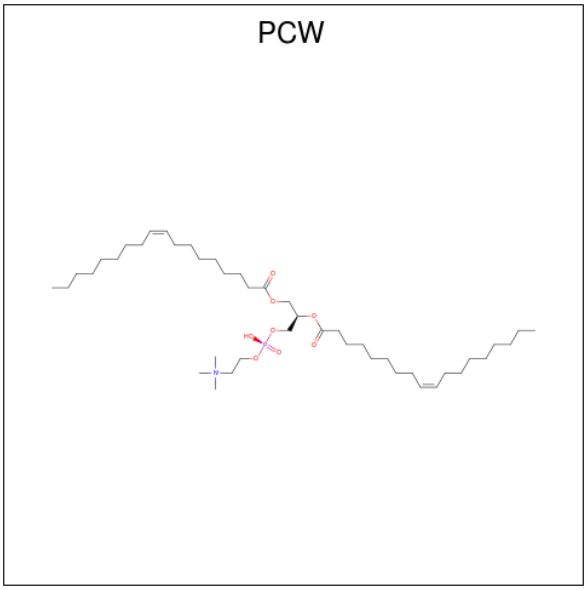
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
2	A	1	25	22	3	0
			Total	C	N	
2	A	1	25	22	3	0
			Total	C	N	
2	B	1	25	22	3	0
			Total	C	N	
2	B	1	25	22	3	0
			Total	C	N	
2	C	1	25	22	3	0

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
3	A	1	35	31	4		0
			Total	C	O		
3	A	1	35	31	4		0
			Total	C	O		
3	B	1	35	31	4		0
			Total	C	O		
3	B	1	35	31	4		0
			Total	C	O		
3	B	1	35	31	4		0
			Total	C	O		
3	C	1	35	31	4		0
			Total	C	O		
3	D	1	35	31	4		0
			Total	C	O		
3	D	1	35	31	4		0

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	51	41	1	8	1	0
			Total	C				
4	A	1	16	16				0
			Total	C				
4	A	1	11	11				0

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Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C 8 8	0
4	A	1	Total C 8 8	0
4	A	1	Total C N O P 39 29 1 8 1	0
4	A	1	Total C 16 16	0
4	A	1	Total C 13 13	0
4	A	1	Total C N O P 43 33 1 8 1	0
4	A	1	Total C N O P 51 41 1 8 1	0
4	A	1	Total C 15 15	0
4	A	1	Total C 16 16	0
4	B	1	Total C 15 15	0
4	B	1	Total C 16 16	0
4	B	1	Total C N O P 51 41 1 8 1	0
4	B	1	Total C 16 16	0
4	B	1	Total C 11 11	0
4	B	1	Total C 8 8	0
4	B	1	Total C 8 8	0
4	B	1	Total C N O P 39 29 1 8 1	0
4	B	1	Total C 16 16	0
4	B	1	Total C 13 13	0
4	B	1	Total C N O P 43 33 1 8 1	0
4	B	1	Total C N O P 51 41 1 8 1	0

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Mol	Chain	Residues	Atoms	AltConf
4	C	1	Total C 15 15	0
4	C	1	Total C 16 16	0
4	C	1	Total C N O P 51 41 1 8 1	0
4	C	1	Total C 16 16	0
4	C	1	Total C 11 11	0
4	C	1	Total C 8 8	0
4	C	1	Total C 8 8	0
4	C	1	Total C N O P 39 29 1 8 1	0
4	C	1	Total C 16 16	0
4	C	1	Total C 13 13	0
4	C	1	Total C N O P 43 33 1 8 1	0
4	C	1	Total C N O P 51 41 1 8 1	0
4	D	1	Total C 13 13	0
4	D	1	Total C N O P 43 33 1 8 1	0
4	D	1	Total C N O P 51 41 1 8 1	0
4	D	1	Total C 15 15	0
4	D	1	Total C 16 16	0
4	D	1	Total C N O P 51 41 1 8 1	0
4	D	1	Total C 16 16	0
4	D	1	Total C 11 11	0
4	D	1	Total C 8 8	0

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Mol	Chain	Residues	Atoms	AltConf
4	D	1	Total C 8 8	0
4	D	1	Total C N O P 39 29 1 8 1	0
4	D	1	Total C 16 16	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

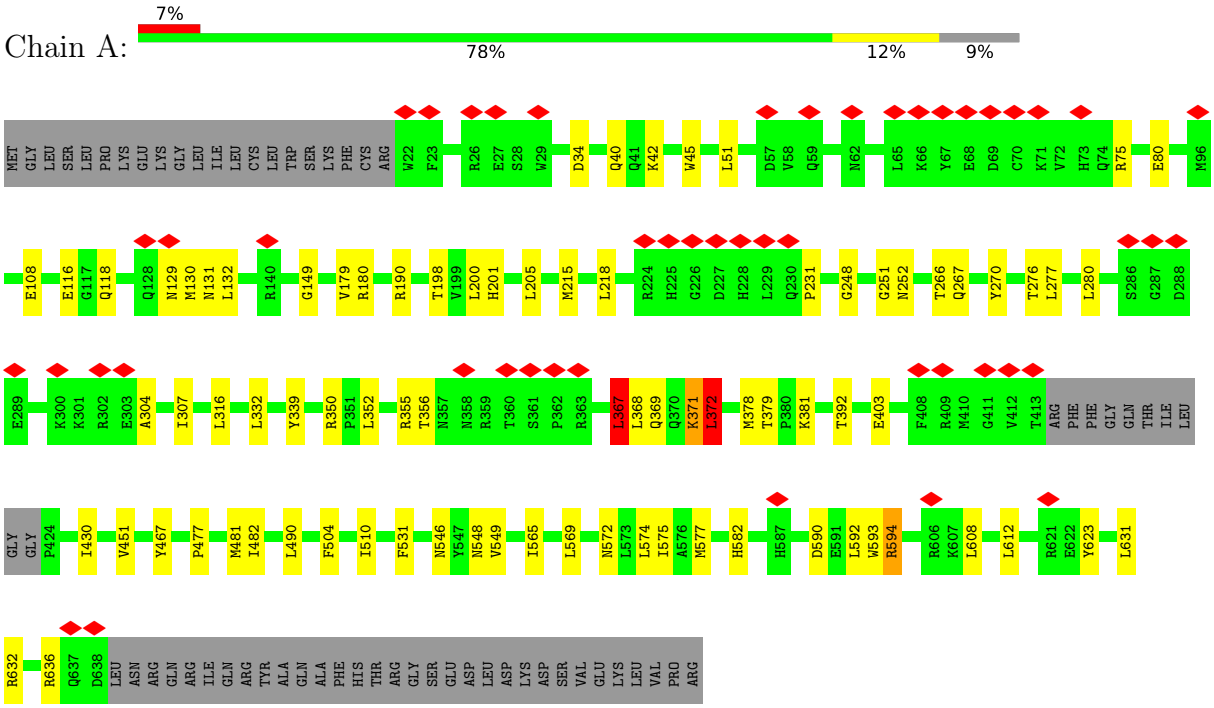
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Ca 1 1	0

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.

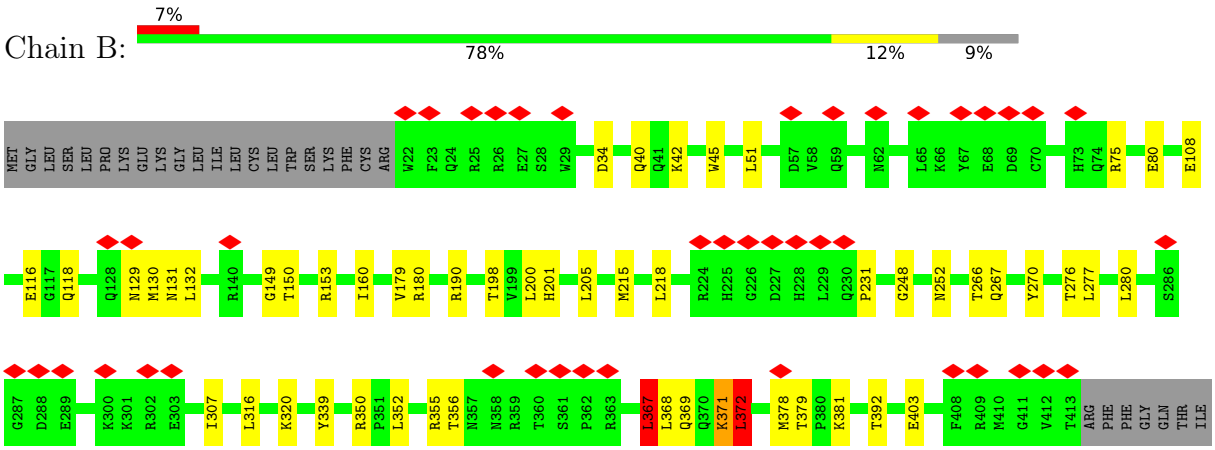
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

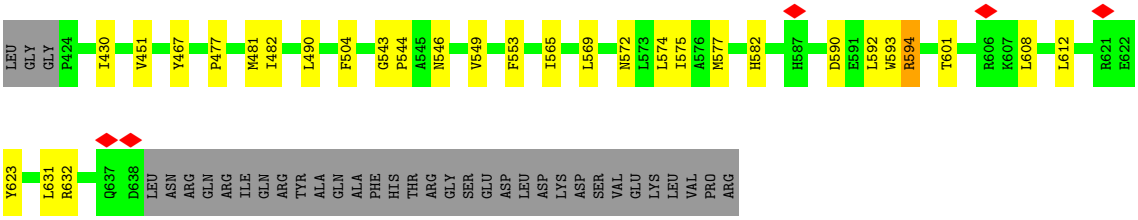
Chain A:



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

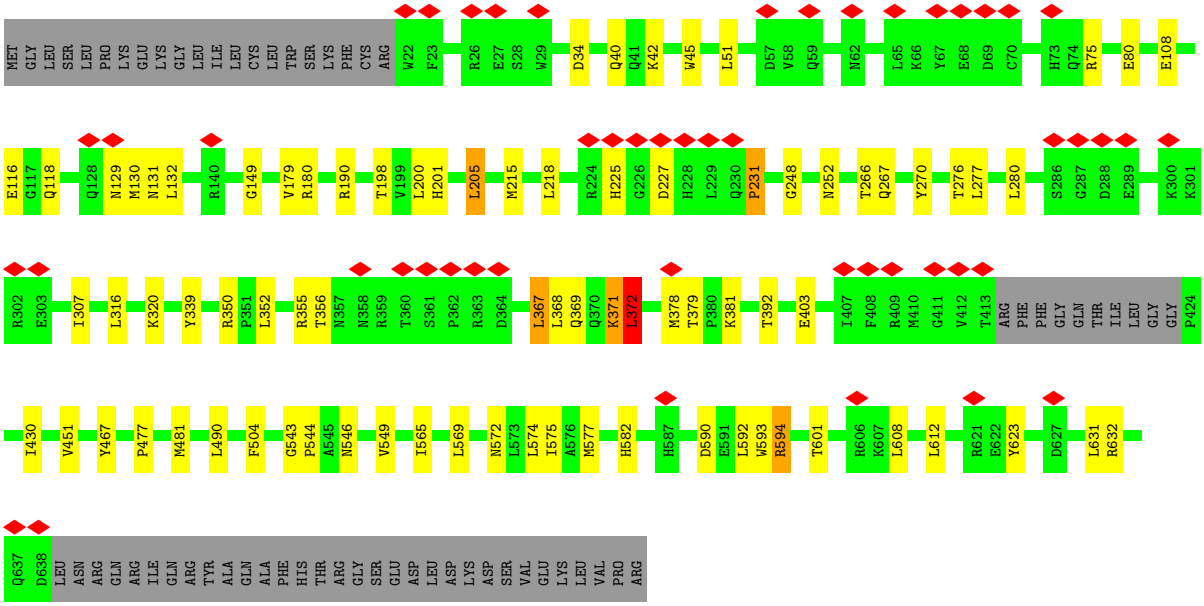
Chain B:





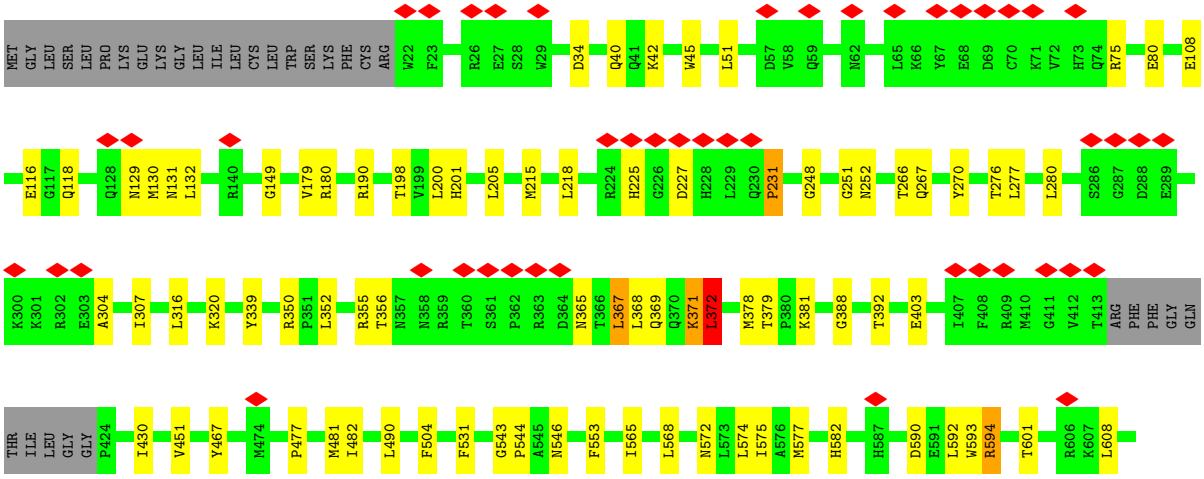
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

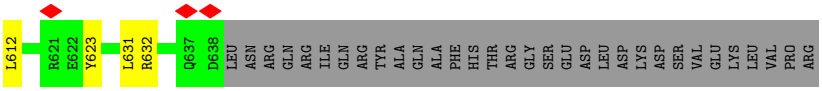
Chain C:



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

Chain D:




L612
R621
E622
Y623
L631
R632
Q637
D638
LEU
ASN
ARG
GLN
ARG
ILE
GLN
ARG
TYR
ALA
GLN
ALA
PHE
HIS
THR
ARG
GLY
SER
GLU
ASP
LEU
ASP
LYS
ASP
SER
VAL
GLU
LYS
LEU
VAL
PRO
ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	199015	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.768	Depositor
Minimum map value	-2.276	Depositor
Average map value	0.040	Depositor
Map value standard deviation	0.167	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	212.48, 212.48, 212.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: PCW, CA, VUG, Y01

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.41	0/5004	0.67	5/6788 (0.1%)
1	B	0.41	0/5004	0.67	5/6788 (0.1%)
1	C	0.41	0/5004	0.67	5/6788 (0.1%)
1	D	0.41	0/5004	0.67	5/6788 (0.1%)
All	All	0.41	0/20016	0.67	20/27152 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	372	LEU	CA-CB-CG	5.29	127.48	115.30
1	D	372	LEU	CA-CB-CG	5.29	127.48	115.30
1	B	367	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	372	LEU	CA-CB-CG	5.28	127.44	115.30
1	C	372	LEU	CA-CB-CG	5.28	127.44	115.30
1	D	367	LEU	CA-CB-CG	5.28	127.44	115.30
1	C	367	LEU	CA-CB-CG	5.27	127.43	115.30
1	A	367	LEU	CA-CB-CG	5.25	127.37	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	490	LEU	CA-CB-CG	5.20	127.25	115.30
1	D	490	LEU	CA-CB-CG	5.18	127.23	115.30
1	A	490	LEU	CA-CB-CG	5.18	127.22	115.30
1	B	490	LEU	CA-CB-CG	5.18	127.22	115.30
1	D	592	LEU	CA-CB-CG	5.09	127.00	115.30
1	C	592	LEU	CA-CB-CG	5.08	126.98	115.30
1	B	592	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	371	LYS	CA-CB-CG	5.06	124.54	113.40
1	A	592	LEU	CA-CB-CG	5.06	126.93	115.30
1	B	371	LYS	CA-CB-CG	5.04	124.49	113.40
1	C	371	LYS	CA-CB-CG	5.03	124.47	113.40
1	D	371	LYS	CA-CB-CG	5.03	124.47	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ASN	Peptide
1	B	129	ASN	Peptide
1	C	129	ASN	Peptide
1	D	129	ASN	Peptide

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	4891	0	4940	49	0
1	B	4891	0	4940	49	0
1	C	4891	0	4940	47	0
1	D	4891	0	4940	51	0
2	A	50	0	0	0	0
2	B	50	0	0	0	0
2	C	25	0	0	0	0
3	A	70	0	98	2	0
3	B	105	0	147	5	0
3	C	35	0	49	1	0
3	D	70	0	98	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	287	0	418	6	0
4	B	287	0	418	5	0
4	C	287	0	418	3	0
4	D	287	0	418	4	0
5	A	1	0	0	0	0
All	All	21118	0	21824	188	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (188) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:MET:HB3	1:C:132:LEU:H	1.61	0.66
1:A:198:THR:H	1:A:201:HIS:HD2	1.43	0.66
1:B:130:MET:HB3	1:B:132:LEU:H	1.61	0.65
1:B:198:THR:H	1:B:201:HIS:HD2	1.43	0.65
1:D:130:MET:HB3	1:D:132:LEU:H	1.61	0.65
1:D:198:THR:H	1:D:201:HIS:HD2	1.43	0.65
1:A:130:MET:HB3	1:A:132:LEU:H	1.61	0.65
1:B:379:THR:HG22	1:B:381:LYS:H	1.63	0.64
1:C:198:THR:H	1:C:201:HIS:HD2	1.43	0.64
1:A:379:THR:HG22	1:A:381:LYS:H	1.63	0.63
1:C:379:THR:HG22	1:C:381:LYS:H	1.63	0.63
1:D:379:THR:HG22	1:D:381:LYS:H	1.63	0.63
1:D:590:ASP:O	1:D:594:ARG:NH2	2.33	0.62
1:B:632:ARG:NH1	1:C:34:ASP:OD1	2.33	0.62
1:A:590:ASP:O	1:A:594:ARG:NH2	2.33	0.62
1:B:590:ASP:O	1:B:594:ARG:NH2	2.33	0.62
1:C:590:ASP:O	1:C:594:ARG:NH2	2.33	0.61
1:C:623:TYR:HA	1:D:42:LYS:HD2	1.81	0.61
1:C:267:GLN:HE21	1:C:277:LEU:HD22	1.66	0.60
1:A:267:GLN:HE21	1:A:277:LEU:HD22	1.66	0.60
1:D:267:GLN:HE21	1:D:277:LEU:HD22	1.66	0.60
1:B:267:GLN:HE21	1:B:277:LEU:HD22	1.66	0.59
1:A:632:ARG:NH1	1:B:34:ASP:OD1	2.35	0.57
1:A:350:ARG:HH22	1:A:451:VAL:HG12	1.71	0.56
1:D:350:ARG:HH22	1:D:451:VAL:HG12	1.71	0.56
1:A:623:TYR:HA	1:B:42:LYS:HD2	1.88	0.56
1:D:553:PHE:CE1	3:D:704:Y01:HAV2	2.41	0.56
1:C:350:ARG:HH22	1:C:451:VAL:HG12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ARG:HH22	1:B:451:VAL:HG12	1.71	0.54
1:B:198:THR:HG23	1:B:200:LEU:H	1.74	0.53
1:A:198:THR:HG23	1:A:200:LEU:H	1.74	0.53
1:C:198:THR:HG23	1:C:200:LEU:H	1.74	0.53
1:B:623:TYR:HA	1:C:42:LYS:HD2	1.91	0.53
1:C:40:GLN:NE2	1:C:80:GLU:OE2	2.42	0.52
1:B:40:GLN:NE2	1:B:80:GLU:OE2	2.42	0.52
1:C:477:PRO:HG3	1:C:593:TRP:HB2	1.92	0.52
1:A:40:GLN:NE2	1:A:80:GLU:OE2	2.42	0.52
1:A:477:PRO:HG3	1:A:593:TRP:HB2	1.92	0.52
1:D:40:GLN:NE2	1:D:80:GLU:OE2	2.42	0.52
1:D:477:PRO:HG3	1:D:593:TRP:HB2	1.92	0.52
1:B:477:PRO:HG3	1:B:593:TRP:HB2	1.92	0.52
1:D:198:THR:HG23	1:D:200:LEU:H	1.74	0.52
1:A:355:ARG:HD2	1:A:369:GLN:HA	1.92	0.51
1:B:355:ARG:HD2	1:B:369:GLN:HA	1.92	0.51
1:C:116:GLU:H	1:C:149:GLY:HA3	1.76	0.51
1:A:116:GLU:H	1:A:149:GLY:HA3	1.76	0.51
1:D:355:ARG:HD2	1:D:369:GLN:HA	1.92	0.51
1:C:355:ARG:HD2	1:C:369:GLN:HA	1.92	0.51
1:B:482:ILE:HG23	1:C:569:LEU:HD21	1.93	0.51
1:D:116:GLU:H	1:D:149:GLY:HA3	1.76	0.51
1:B:190:ARG:NH2	1:B:231:PRO:O	2.44	0.51
1:C:190:ARG:NH2	1:C:231:PRO:O	2.44	0.50
1:A:356:THR:H	1:A:371:LYS:HE3	1.76	0.50
1:D:356:THR:H	1:D:371:LYS:HE3	1.76	0.50
1:A:270:TYR:OH	1:B:118:GLN:NE2	2.45	0.50
1:D:280:LEU:HD11	1:D:316:LEU:HD22	1.94	0.50
1:B:356:THR:H	1:B:371:LYS:HE3	1.76	0.50
1:C:280:LEU:HD11	1:C:316:LEU:HD22	1.94	0.50
1:B:116:GLU:H	1:B:149:GLY:HA3	1.76	0.49
1:C:356:THR:H	1:C:371:LYS:HE3	1.76	0.49
1:D:190:ARG:NH2	1:D:231:PRO:O	2.44	0.49
1:A:42:LYS:HD2	1:D:623:TYR:HA	1.93	0.49
1:C:198:THR:HG22	1:C:201:HIS:CD2	2.47	0.49
1:A:34:ASP:OD1	1:D:632:ARG:NH1	2.43	0.49
1:A:198:THR:HG22	1:A:201:HIS:CD2	2.47	0.49
1:B:280:LEU:HD11	1:B:316:LEU:HD22	1.94	0.49
1:A:190:ARG:NH2	1:A:231:PRO:O	2.45	0.49
1:B:198:THR:HG22	1:B:201:HIS:CD2	2.47	0.49
1:A:280:LEU:HD11	1:A:316:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:VAL:HA	1:D:365:ASN:HA	1.94	0.49
1:A:569:LEU:HD21	1:D:482:ILE:HG23	1.95	0.49
1:C:75:ARG:NH1	1:C:108:GLU:OE2	2.46	0.49
1:D:75:ARG:NH1	1:D:108:GLU:OE2	2.46	0.48
1:D:198:THR:HG22	1:D:201:HIS:CD2	2.47	0.48
1:A:75:ARG:NH1	1:A:108:GLU:OE2	2.46	0.48
1:B:75:ARG:NH1	1:B:108:GLU:OE2	2.46	0.48
1:B:270:TYR:OH	1:C:118:GLN:NE2	2.47	0.48
1:D:45:TRP:HA	1:D:51:LEU:HD12	1.96	0.48
1:A:45:TRP:HA	1:A:51:LEU:HD12	1.96	0.48
1:C:266:THR:HG22	1:C:276:THR:HG22	1.96	0.48
1:C:632:ARG:NH1	1:D:34:ASP:OD1	2.42	0.48
4:D:702:PCW:H161	4:D:702:PCW:H132	1.63	0.48
1:B:45:TRP:HA	1:B:51:LEU:HD12	1.96	0.47
1:C:45:TRP:HA	1:C:51:LEU:HD12	1.96	0.47
1:A:482:ILE:HG23	1:B:569:LEU:HD21	1.97	0.47
1:B:266:THR:HG22	1:B:276:THR:HG22	1.95	0.47
4:B:707:PCW:H132	4:B:707:PCW:H162	1.68	0.47
1:D:266:THR:HG22	1:D:276:THR:HG22	1.96	0.47
1:B:352:LEU:HD12	1:B:372:LEU:HB3	1.97	0.47
1:C:608:LEU:HD12	1:C:612:LEU:HD22	1.97	0.47
1:C:352:LEU:HD12	1:C:372:LEU:HB3	1.97	0.46
1:D:608:LEU:HD12	1:D:612:LEU:HD22	1.97	0.46
1:A:352:LEU:HD12	1:A:372:LEU:HB3	1.97	0.46
4:C:713:PCW:H161	4:C:713:PCW:H132	1.57	0.46
1:A:266:THR:HG22	1:A:276:THR:HG22	1.96	0.46
1:A:574:LEU:HA	1:A:577:MET:HG2	1.98	0.46
1:B:632:ARG:HD3	1:C:34:ASP:HA	1.97	0.46
1:D:352:LEU:HD12	1:D:372:LEU:HB3	1.97	0.46
1:B:367:LEU:HG	1:C:549:VAL:HG11	1.97	0.46
1:B:403:GLU:HB3	1:B:430:ILE:HD11	1.98	0.46
1:C:403:GLU:HB3	1:C:430:ILE:HD11	1.98	0.46
1:A:608:LEU:HD12	1:A:612:LEU:HD22	1.97	0.46
4:A:703:PCW:H172	3:B:701:Y01:HAD3	1.98	0.46
1:A:632:ARG:HD3	1:B:34:ASP:HA	1.98	0.46
1:B:574:LEU:HA	1:B:577:MET:HG2	1.97	0.46
1:B:608:LEU:HD12	1:B:612:LEU:HD22	1.97	0.46
1:A:355:ARG:NH1	1:A:368:LEU:O	2.50	0.45
1:A:403:GLU:HB3	1:A:430:ILE:HD11	1.98	0.45
1:C:574:LEU:HA	1:C:577:MET:HG2	1.98	0.45
4:D:708:PCW:H132	4:D:708:PCW:H162	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ARG:NH1	1:C:368:LEU:O	2.50	0.45
1:C:572:ASN:HA	1:C:575:ILE:HG12	1.99	0.45
1:D:403:GLU:HB3	1:D:430:ILE:HD11	1.98	0.45
1:B:355:ARG:NH1	1:B:368:LEU:O	2.50	0.45
1:D:572:ASN:HA	1:D:575:ILE:HG12	1.99	0.45
1:D:355:ARG:NH1	1:D:368:LEU:O	2.50	0.45
4:A:703:PCW:H132	4:A:703:PCW:H162	1.68	0.45
1:C:180:ARG:HE	1:C:218:LEU:HD11	1.82	0.45
1:C:270:TYR:OH	1:D:118:GLN:NE2	2.50	0.45
1:B:180:ARG:HE	1:B:218:LEU:HD11	1.82	0.45
1:D:180:ARG:HE	1:D:218:LEU:HD11	1.82	0.45
1:A:180:ARG:HE	1:A:218:LEU:HD11	1.82	0.44
1:A:572:ASN:HA	1:A:575:ILE:HG12	1.99	0.44
1:B:572:ASN:HA	1:B:575:ILE:HG12	1.99	0.44
1:D:574:LEU:HA	1:D:577:MET:HG2	1.98	0.44
1:C:632:ARG:HD3	1:D:34:ASP:HA	1.99	0.44
1:B:481:MET:SD	1:B:582:HIS:NE2	2.91	0.44
1:A:339:TYR:HE1	1:A:392:THR:HA	1.83	0.44
4:A:711:PCW:H132	4:A:711:PCW:H161	1.60	0.44
3:B:706:Y01:HAD3	4:B:707:PCW:H172	1.99	0.44
1:C:280:LEU:HD22	1:C:631:LEU:HB2	2.00	0.44
1:C:339:TYR:HE1	1:C:392:THR:HA	1.83	0.44
1:B:543:GLY:HA2	1:B:544:PRO:HD3	1.85	0.44
1:C:481:MET:SD	1:C:582:HIS:NE2	2.91	0.44
1:B:339:TYR:HE1	1:B:392:THR:HA	1.83	0.43
1:D:179:VAL:HG21	1:D:215:MET:HE1	2.00	0.43
1:D:339:TYR:HE1	1:D:392:THR:HA	1.83	0.43
1:A:118:GLN:NE2	1:D:270:TYR:OH	2.51	0.43
1:A:481:MET:SD	1:A:582:HIS:NE2	2.91	0.43
4:A:712:PCW:H122	4:A:712:PCW:H31	1.88	0.43
4:B:715:PCW:H132	4:B:715:PCW:H161	1.59	0.43
1:C:248:GLY:HA2	1:C:307:ILE:HD13	2.01	0.43
4:C:705:PCW:H172	3:D:704:Y01:HAD3	1.98	0.43
1:D:504:PHE:HE2	1:D:565:ILE:HD11	1.84	0.43
1:B:248:GLY:HA2	1:B:307:ILE:HD13	2.01	0.43
1:D:481:MET:SD	1:D:582:HIS:NE2	2.91	0.43
1:A:548:ASN:O	1:D:365:ASN:ND2	2.52	0.43
1:B:280:LEU:HD22	1:B:631:LEU:HB2	2.00	0.43
1:B:504:PHE:HE2	1:B:565:ILE:HD11	1.84	0.43
1:D:248:GLY:HA2	1:D:307:ILE:HD13	2.01	0.43
1:D:467:TYR:CE2	3:D:707:Y01:HAR2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLY:HA2	1:A:307:ILE:HD13	2.01	0.43
1:A:467:TYR:CE2	3:A:702:Y01:HAR2	2.54	0.43
1:A:510:ILE:O	1:D:350:ARG:NH1	2.52	0.43
1:C:504:PHE:HE2	1:C:565:ILE:HD11	1.84	0.43
1:D:543:GLY:HA2	1:D:544:PRO:HD3	1.85	0.43
1:A:504:PHE:HE2	1:A:565:ILE:HD11	1.84	0.42
1:B:179:VAL:HG21	1:B:215:MET:HE1	2.00	0.42
1:A:636:ARG:HH11	1:B:160:ILE:HG22	1.85	0.42
1:D:225:HIS:ND1	1:D:227:ASP:O	2.49	0.42
1:A:280:LEU:HD22	1:A:631:LEU:HB2	2.00	0.42
1:B:467:TYR:CE2	3:B:705:Y01:HAR2	2.54	0.42
1:C:467:TYR:CE2	3:C:704:Y01:HAR2	2.54	0.42
1:C:574:LEU:HD12	1:D:568:LEU:HD11	2.02	0.42
1:D:280:LEU:HD22	1:D:631:LEU:HB2	2.00	0.42
1:C:225:HIS:ND1	1:C:227:ASP:O	2.49	0.42
4:D:702:PCW:H63	4:D:702:PCW:H42	1.88	0.42
1:A:367:LEU:HG	1:B:549:VAL:HG11	2.01	0.42
1:B:553:PHE:CE1	3:B:701:Y01:HAV2	2.55	0.42
1:D:388:GLY:HA3	4:D:703:PCW:H172	2.01	0.41
4:B:707:PCW:H42	4:B:707:PCW:H63	1.85	0.41
1:A:179:VAL:HG21	1:A:215:MET:HE1	2.02	0.41
4:A:703:PCW:H63	4:A:703:PCW:H42	1.85	0.41
1:A:251:GLY:HA2	1:A:304:ALA:HA	2.02	0.41
1:C:205:LEU:H	1:C:205:LEU:HG	1.73	0.41
4:A:711:PCW:H121	4:A:711:PCW:H31	1.87	0.41
1:D:320:LYS:HG3	1:D:601:THR:HG21	2.03	0.41
4:C:714:PCW:H63	4:C:714:PCW:H42	1.92	0.41
1:C:179:VAL:HG21	1:C:215:MET:HE1	2.01	0.41
1:A:332:LEU:HD13	1:A:332:LEU:HA	1.93	0.41
1:C:320:LYS:HG3	1:C:601:THR:HG21	2.03	0.41
1:C:543:GLY:HA2	1:C:544:PRO:HD3	1.85	0.41
1:D:251:GLY:HA2	1:D:304:ALA:HA	2.02	0.41
4:B:715:PCW:H63	4:B:715:PCW:H42	1.88	0.40
1:A:531:PHE:HB2	3:B:701:Y01:HAT2	2.04	0.40
1:B:320:LYS:HG3	1:B:601:THR:HG21	2.03	0.40
3:A:714:Y01:HAT2	1:D:531:PHE:HB2	2.04	0.40
1:B:150:THR:HA	1:B:153:ARG:HD3	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	603/670 (90%)	549 (91%)	54 (9%)	0	100	100
1	B	603/670 (90%)	548 (91%)	55 (9%)	0	100	100
1	C	603/670 (90%)	549 (91%)	53 (9%)	1 (0%)	47	79
1	D	603/670 (90%)	549 (91%)	53 (9%)	1 (0%)	47	79
All	All	2412/2680 (90%)	2195 (91%)	215 (9%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	231	PRO
1	D	231	PRO

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	529/584 (91%)	521 (98%)	8 (2%)	65	85
1	B	529/584 (91%)	521 (98%)	8 (2%)	65	85
1	C	529/584 (91%)	521 (98%)	8 (2%)	65	85
1	D	529/584 (91%)	521 (98%)	8 (2%)	65	85
All	All	2116/2336 (91%)	2084 (98%)	32 (2%)	66	85

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	205	LEU
1	A	252	ASN
1	A	367	LEU
1	A	372	LEU
1	A	378	MET
1	A	546	ASN
1	A	594	ARG
1	B	131	ASN
1	B	205	LEU
1	B	252	ASN
1	B	367	LEU
1	B	372	LEU
1	B	378	MET
1	B	546	ASN
1	B	594	ARG
1	C	131	ASN
1	C	205	LEU
1	C	252	ASN
1	C	367	LEU
1	C	372	LEU
1	C	378	MET
1	C	546	ASN
1	C	594	ARG
1	D	131	ASN
1	D	205	LEU
1	D	252	ASN
1	D	367	LEU
1	D	372	LEU
1	D	378	MET
1	D	546	ASN
1	D	594	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	131	ASN
1	A	201	HIS
1	A	206	GLN
1	A	252	ASN
1	A	267	GLN
1	A	522	HIS

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Mol	Chain	Res	Type
1	B	118	GLN
1	B	131	ASN
1	B	201	HIS
1	B	206	GLN
1	B	252	ASN
1	B	267	GLN
1	B	365	ASN
1	B	522	HIS
1	C	118	GLN
1	C	131	ASN
1	C	201	HIS
1	C	206	GLN
1	C	252	ASN
1	C	267	GLN
1	C	522	HIS
1	D	118	GLN
1	D	131	ASN
1	D	201	HIS
1	D	206	GLN
1	D	252	ASN
1	D	267	GLN
1	D	365	ASN
1	D	522	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 62 ligands modelled in this entry, 1 is monoatomic - leaving 61 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PCW	C	701	-	14,14,53	0.74	0	13,13,61	0.44	0
4	PCW	B	713	-	15,15,53	1.41	2 (13%)	14,14,61	0.72	0
4	PCW	C	710	-	38,38,53	1.22	3 (7%)	44,46,61	1.09	3 (6%)
3	Y01	B	706	-	38,38,38	0.46	0	57,57,57	0.69	0
2	VUG	B	717	-	28,28,28	1.92	5 (17%)	37,38,38	1.24	3 (8%)
4	PCW	B	715	-	42,42,53	1.20	3 (7%)	47,50,61	1.15	3 (6%)
4	PCW	A	704	-	15,15,53	1.44	2 (13%)	14,14,61	0.68	0
3	Y01	D	704	-	38,38,38	0.46	0	57,57,57	0.69	0
4	PCW	B	708	-	15,15,53	1.44	2 (13%)	14,14,61	0.68	0
2	VUG	C	703	-	28,28,28	1.89	4 (14%)	37,38,38	1.66	9 (24%)
3	Y01	A	702	-	38,38,38	0.49	0	57,57,57	0.75	1 (1%)
4	PCW	A	712	-	50,50,53	1.12	3 (6%)	56,58,61	1.04	3 (5%)
4	PCW	D	712	-	7,7,53	0.73	0	6,6,61	0.31	0
4	PCW	D	713	-	38,38,53	1.22	3 (7%)	44,46,61	1.09	3 (6%)
4	PCW	D	701	-	12,12,53	0.76	0	11,11,61	0.40	0
4	PCW	D	705	-	14,14,53	0.75	0	13,13,61	0.43	0
4	PCW	D	708	-	50,50,53	1.10	3 (6%)	56,58,61	0.99	4 (7%)
4	PCW	B	707	-	50,50,53	1.10	3 (6%)	56,58,61	1.00	4 (7%)
4	PCW	C	709	-	7,7,53	0.73	0	6,6,61	0.30	0
4	PCW	A	708	-	38,38,53	1.22	3 (7%)	44,46,61	1.09	3 (6%)
4	PCW	C	705	-	50,50,53	1.10	3 (6%)	56,58,61	1.00	4 (7%)
4	PCW	B	716	-	50,50,53	1.12	3 (6%)	56,58,61	1.04	3 (5%)
4	PCW	C	706	-	15,15,53	1.43	2 (13%)	14,14,61	0.68	0
2	VUG	B	704	-	28,28,28	1.87	4 (14%)	37,38,38	1.68	9 (24%)
4	PCW	C	711	-	15,15,53	1.41	2 (13%)	14,14,61	0.71	0
4	PCW	A	706	-	7,7,53	0.72	0	6,6,61	0.33	0
4	PCW	C	714	-	50,50,53	1.12	3 (6%)	56,58,61	1.04	3 (5%)
4	PCW	D	714	-	15,15,53	1.41	2 (13%)	14,14,61	0.74	0
4	PCW	D	706	-	15,15,53	1.44	2 (13%)	14,14,61	0.69	0
4	PCW	D	711	-	7,7,53	0.72	0	6,6,61	0.33	0
4	PCW	B	710	-	7,7,53	0.72	0	6,6,61	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PCW	A	707	-	7,7,53	0.73	0	6,6,61	0.31	0
4	PCW	B	703	-	15,15,53	1.44	2 (13%)	14,14,61	0.67	0
4	PCW	A	716	-	15,15,53	1.44	2 (13%)	14,14,61	0.68	0
4	PCW	B	711	-	7,7,53	0.73	0	6,6,61	0.31	0
4	PCW	D	709	-	15,15,53	1.43	2 (13%)	14,14,61	0.67	0
4	PCW	C	712	-	12,12,53	0.76	0	11,11,61	0.39	0
4	PCW	C	702	-	15,15,53	1.43	2 (13%)	14,14,61	0.67	0
2	VUG	A	701	-	28,28,28	1.87	5 (17%)	37,38,38	1.70	9 (24%)
3	Y01	A	714	-	38,38,38	0.46	0	57,57,57	0.69	0
4	PCW	B	709	-	10,10,53	0.80	0	8,9,61	0.36	0
4	PCW	D	710	-	10,10,53	0.80	0	8,9,61	0.34	0
4	PCW	A	710	-	12,12,53	0.76	0	11,11,61	0.39	0
4	PCW	C	713	-	42,42,53	1.20	3 (7%)	47,50,61	1.16	3 (6%)
4	PCW	A	711	-	42,42,53	1.20	3 (7%)	47,50,61	1.15	3 (6%)
3	Y01	D	707	-	38,38,38	0.49	0	57,57,57	0.75	1 (1%)
4	PCW	C	707	-	10,10,53	0.80	0	8,9,61	0.36	0
4	PCW	B	702	-	14,14,53	0.75	0	13,13,61	0.44	0
4	PCW	A	715	-	14,14,53	0.74	0	13,13,61	0.43	0
4	PCW	B	714	-	12,12,53	0.75	0	11,11,61	0.40	0
4	PCW	D	702	-	42,42,53	1.20	3 (7%)	47,50,61	1.16	3 (6%)
3	Y01	B	701	-	38,38,38	0.46	0	57,57,57	0.69	0
3	Y01	B	705	-	38,38,38	0.49	0	57,57,57	0.75	1 (1%)
4	PCW	A	703	-	50,50,53	1.09	3 (6%)	56,58,61	1.03	4 (7%)
4	PCW	D	703	-	50,50,53	1.12	3 (6%)	56,58,61	1.03	3 (5%)
3	Y01	C	704	-	38,38,38	0.49	0	57,57,57	0.75	1 (1%)
4	PCW	C	708	-	7,7,53	0.72	0	6,6,61	0.32	0
4	PCW	A	709	-	15,15,53	1.41	2 (13%)	14,14,61	0.76	0
2	VUG	A	713	-	28,28,28	1.88	4 (14%)	37,38,38	1.68	9 (24%)
4	PCW	A	705	-	10,10,53	0.80	0	8,9,61	0.35	0
4	PCW	B	712	-	38,38,53	1.22	3 (7%)	44,46,61	1.09	3 (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
4	PCW	C	701	-	-	6/12/12/57	-
4	PCW	B	713	-	-	7/13/13/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	C	710	-	-	22/42/42/57	-
3	Y01	B	706	-	-	8/19/77/77	0/4/4/4
2	VUG	B	717	-	-	0/12/32/32	0/4/4/4
4	PCW	B	715	-	-	28/46/46/57	-
4	PCW	A	704	-	-	11/13/13/57	-
3	Y01	D	704	-	-	8/19/77/77	0/4/4/4
4	PCW	B	708	-	-	11/13/13/57	-
2	VUG	C	703	-	-	2/12/32/32	0/4/4/4
3	Y01	A	702	-	-	14/19/77/77	0/4/4/4
4	PCW	A	712	-	-	25/54/54/57	-
4	PCW	D	712	-	-	2/5/5/57	-
4	PCW	D	713	-	-	21/42/42/57	-
4	PCW	D	701	-	-	4/10/10/57	-
4	PCW	D	705	-	-	6/12/12/57	-
4	PCW	D	708	-	-	21/54/54/57	-
4	PCW	B	707	-	-	24/54/54/57	-
4	PCW	C	709	-	-	2/5/5/57	-
4	PCW	A	708	-	-	22/42/42/57	-
4	PCW	C	705	-	-	23/54/54/57	-
4	PCW	B	716	-	-	26/54/54/57	-
4	PCW	C	706	-	-	11/13/13/57	-
2	VUG	B	704	-	-	2/12/32/32	0/4/4/4
4	PCW	C	711	-	-	7/13/13/57	-
4	PCW	A	706	-	-	2/5/5/57	-
4	PCW	C	714	-	-	26/54/54/57	-
4	PCW	D	714	-	-	7/13/13/57	-
4	PCW	D	706	-	-	6/13/13/57	-
4	PCW	D	711	-	-	2/5/5/57	-
4	PCW	B	710	-	-	2/5/5/57	-
4	PCW	A	707	-	-	2/5/5/57	-
4	PCW	B	703	-	-	7/13/13/57	-
4	PCW	A	716	-	-	6/13/13/57	-
4	PCW	B	711	-	-	2/5/5/57	-
4	PCW	D	709	-	-	11/13/13/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	C	712	-	-	4/10/10/57	-
4	PCW	C	702	-	-	7/13/13/57	-
2	VUG	A	701	-	-	2/12/32/32	0/4/4/4
3	Y01	A	714	-	-	8/19/77/77	0/4/4/4
4	PCW	B	709	-	-	4/8/8/57	-
4	PCW	D	710	-	-	4/8/8/57	-
4	PCW	A	710	-	-	4/10/10/57	-
4	PCW	C	713	-	-	28/46/46/57	-
4	PCW	A	711	-	-	27/46/46/57	-
3	Y01	D	707	-	-	14/19/77/77	0/4/4/4
4	PCW	C	707	-	-	2/8/8/57	-
4	PCW	B	702	-	-	6/12/12/57	-
4	PCW	A	715	-	-	6/12/12/57	-
4	PCW	B	714	-	-	4/10/10/57	-
4	PCW	D	702	-	-	28/46/46/57	-
3	Y01	B	701	-	-	8/19/77/77	0/4/4/4
3	Y01	B	705	-	-	14/19/77/77	0/4/4/4
4	PCW	A	703	-	-	24/54/54/57	-
4	PCW	D	703	-	-	24/54/54/57	-
3	Y01	C	704	-	-	14/19/77/77	0/4/4/4
4	PCW	C	708	-	-	2/5/5/57	-
4	PCW	A	709	-	-	7/13/13/57	-
2	VUG	A	713	-	-	2/12/32/32	0/4/4/4
4	PCW	A	705	-	-	4/8/8/57	-
4	PCW	B	712	-	-	22/42/42/57	-

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	713	VUG	C13-N01	-5.08	1.37	1.47
2	B	704	VUG	C13-N01	-4.99	1.37	1.47
2	C	703	VUG	C13-N01	-4.98	1.37	1.47
2	A	701	VUG	C13-N01	-4.97	1.37	1.47
2	B	717	VUG	C13-N01	-4.94	1.37	1.47
2	A	713	VUG	C11-N01	-4.82	1.37	1.47
2	C	703	VUG	C11-N01	-4.81	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	717	VUG	C11-N01	-4.80	1.37	1.47
2	A	701	VUG	C11-N01	-4.75	1.37	1.47
2	B	704	VUG	C11-N01	-4.69	1.38	1.47
2	C	703	VUG	C10-N01	-4.10	1.37	1.48
2	A	713	VUG	C10-N01	-4.10	1.37	1.48
2	B	704	VUG	C10-N01	-4.06	1.37	1.48
2	A	701	VUG	C10-N01	-4.06	1.37	1.48
4	B	708	PCW	C20-C19	4.05	1.55	1.31
4	D	709	PCW	C20-C19	4.04	1.55	1.31
4	A	704	PCW	C20-C19	4.04	1.55	1.31
4	C	706	PCW	C20-C19	4.03	1.55	1.31
4	D	706	PCW	C20-C19	4.00	1.54	1.31
4	B	703	PCW	C20-C19	3.99	1.54	1.31
4	A	716	PCW	C20-C19	3.98	1.54	1.31
4	C	702	PCW	C20-C19	3.98	1.54	1.31
4	B	713	PCW	C20-C19	3.96	1.54	1.31
4	C	711	PCW	C20-C19	3.95	1.54	1.31
4	A	709	PCW	C20-C19	3.95	1.54	1.31
4	D	714	PCW	C20-C19	3.94	1.54	1.31
2	B	717	VUG	C10-N01	-3.90	1.38	1.48
2	C	703	VUG	C15-N02	3.71	1.48	1.38
2	B	704	VUG	C15-N02	3.65	1.48	1.38
2	A	713	VUG	C15-N02	3.59	1.48	1.38
2	A	701	VUG	C15-N02	3.58	1.48	1.38
2	B	717	VUG	C15-N02	3.49	1.48	1.38
4	D	703	PCW	O3-C11	3.14	1.42	1.33
4	C	714	PCW	O3-C11	3.13	1.42	1.33
4	A	712	PCW	O3-C11	3.12	1.42	1.33
4	B	716	PCW	O3-C11	3.12	1.42	1.33
4	A	708	PCW	O3-C11	3.05	1.42	1.33
4	C	710	PCW	O3-C11	3.04	1.42	1.33
4	D	713	PCW	O3-C11	3.04	1.42	1.33
4	C	713	PCW	O3-C11	3.02	1.42	1.33
4	B	715	PCW	O3-C11	3.02	1.42	1.33
4	D	702	PCW	O3-C11	3.01	1.42	1.33
4	B	712	PCW	O3-C11	3.00	1.42	1.33
4	A	711	PCW	O3-C11	2.99	1.42	1.33
4	D	703	PCW	O2-C31	2.90	1.42	1.34
4	C	713	PCW	O2-C31	2.90	1.42	1.34
4	D	702	PCW	O2-C31	2.89	1.42	1.34
4	B	716	PCW	O2-C31	2.89	1.42	1.34
4	B	715	PCW	O2-C31	2.89	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	711	PCW	O2-C31	2.88	1.42	1.34
4	C	714	PCW	O2-C31	2.88	1.42	1.34
4	A	712	PCW	O2-C31	2.87	1.42	1.34
4	C	705	PCW	O3-C11	2.86	1.41	1.33
4	A	703	PCW	O2-C31	2.86	1.42	1.34
4	D	708	PCW	O3-C11	2.84	1.41	1.33
4	B	707	PCW	O3-C11	2.84	1.41	1.33
4	C	705	PCW	O2-C31	2.82	1.42	1.34
4	A	703	PCW	O3-C11	2.82	1.41	1.33
4	B	712	PCW	O2-C31	2.82	1.42	1.34
4	D	713	PCW	O2-C31	2.82	1.42	1.34
4	A	708	PCW	O2-C31	2.81	1.42	1.34
4	C	710	PCW	O2-C31	2.81	1.42	1.34
4	B	707	PCW	O2-C31	2.80	1.42	1.34
4	D	708	PCW	O2-C31	2.76	1.42	1.34
4	B	713	PCW	C18-C19	-2.71	1.34	1.50
4	A	709	PCW	C18-C19	-2.70	1.34	1.50
4	D	714	PCW	C18-C19	-2.69	1.34	1.50
4	D	706	PCW	C18-C19	-2.68	1.35	1.50
4	B	703	PCW	C18-C19	-2.68	1.35	1.50
4	C	711	PCW	C18-C19	-2.68	1.35	1.50
4	A	716	PCW	C18-C19	-2.67	1.35	1.50
4	C	702	PCW	C18-C19	-2.67	1.35	1.50
4	A	704	PCW	C18-C19	-2.64	1.35	1.50
4	B	708	PCW	C18-C19	-2.63	1.35	1.50
4	D	708	PCW	O2-C2	-2.63	1.40	1.46
4	C	706	PCW	C18-C19	-2.63	1.35	1.50
4	D	709	PCW	C18-C19	-2.62	1.35	1.50
4	B	707	PCW	O2-C2	-2.60	1.40	1.46
4	C	705	PCW	O2-C2	-2.59	1.40	1.46
4	B	712	PCW	O2-C2	-2.54	1.40	1.46
4	A	703	PCW	O2-C2	-2.54	1.40	1.46
4	A	708	PCW	O2-C2	-2.53	1.40	1.46
2	B	717	VUG	C12-N02	-2.53	1.42	1.46
4	D	713	PCW	O2-C2	-2.52	1.40	1.46
4	C	710	PCW	O2-C2	-2.51	1.40	1.46
4	C	714	PCW	O2-C2	-2.48	1.40	1.46
4	B	716	PCW	O2-C2	-2.47	1.40	1.46
4	D	703	PCW	O2-C2	-2.46	1.40	1.46
4	A	712	PCW	O2-C2	-2.44	1.40	1.46
4	D	702	PCW	O2-C2	-2.41	1.40	1.46
4	B	715	PCW	O2-C2	-2.40	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	713	PCW	O2-C2	-2.40	1.40	1.46
4	A	711	PCW	O2-C2	-2.38	1.40	1.46
2	A	701	VUG	C12-N02	-2.02	1.43	1.46

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	VUG	C11-N01-C13	4.29	116.92	109.08
4	C	713	PCW	O2-C31-C32	4.22	120.59	111.50
4	D	702	PCW	O2-C31-C32	4.22	120.59	111.50
4	A	711	PCW	O2-C31-C32	4.21	120.57	111.50
4	B	715	PCW	O2-C31-C32	4.19	120.53	111.50
2	B	704	VUG	C11-N01-C13	4.11	116.59	109.08
4	C	713	PCW	C7-N-C6	4.04	119.37	108.97
4	A	711	PCW	C7-N-C6	4.04	119.35	108.97
4	B	716	PCW	O2-C31-C32	4.04	120.20	111.50
4	D	703	PCW	O2-C31-C32	4.03	120.18	111.50
4	D	702	PCW	C7-N-C6	4.02	119.32	108.97
4	A	712	PCW	O2-C31-C32	4.02	120.17	111.50
4	B	715	PCW	C7-N-C6	4.02	119.32	108.97
4	C	714	PCW	O2-C31-C32	4.02	120.16	111.50
4	A	703	PCW	O2-C31-C32	4.00	120.12	111.50
4	B	707	PCW	O2-C31-C32	3.97	120.05	111.50
2	A	713	VUG	C11-N01-C13	3.94	116.27	109.08
2	C	703	VUG	C11-N01-C13	3.93	116.26	109.08
4	C	705	PCW	O2-C31-C32	3.90	119.92	111.50
4	D	708	PCW	O2-C31-C32	3.90	119.92	111.50
4	D	713	PCW	O2-C31-C32	3.73	119.53	111.50
4	A	708	PCW	O2-C31-C32	3.72	119.52	111.50
4	C	710	PCW	O2-C31-C32	3.71	119.49	111.50
4	B	712	PCW	O2-C31-C32	3.70	119.48	111.50
4	A	712	PCW	C7-N-C6	3.70	118.49	108.97
4	B	716	PCW	C7-N-C6	3.69	118.45	108.97
4	C	714	PCW	C7-N-C6	3.68	118.44	108.97
4	D	703	PCW	C7-N-C6	3.68	118.44	108.97
4	A	708	PCW	C7-N-C6	3.68	118.43	108.97
4	D	713	PCW	C7-N-C6	3.67	118.42	108.97
4	B	712	PCW	C7-N-C6	3.67	118.41	108.97
4	C	710	PCW	C7-N-C6	3.67	118.40	108.97
4	A	703	PCW	C7-N-C6	3.59	118.19	108.97
4	B	707	PCW	C7-N-C6	3.58	118.18	108.97
4	C	705	PCW	C7-N-C6	3.57	118.15	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	708	PCW	C7-N-C6	3.57	118.14	108.97
2	B	717	VUG	C11-N01-C13	3.44	115.36	109.08
2	A	713	VUG	C18-N03-C19	3.29	122.54	116.85
2	B	704	VUG	C18-N03-C19	3.17	122.34	116.85
2	C	703	VUG	C18-N03-C19	3.16	122.31	116.85
2	A	701	VUG	C18-N03-C19	3.14	122.29	116.85
2	A	713	VUG	C15-C19-N03	-3.09	119.50	122.92
4	B	716	PCW	O3-C11-C12	3.07	121.55	111.91
4	C	714	PCW	O3-C11-C12	3.07	121.53	111.91
4	D	702	PCW	O3-C11-C12	3.06	121.53	111.91
4	A	712	PCW	O3-C11-C12	3.04	121.44	111.91
4	B	715	PCW	O3-C11-C12	3.03	121.42	111.91
4	C	713	PCW	O3-C11-C12	3.03	121.42	111.91
4	A	711	PCW	O3-C11-C12	3.02	121.37	111.91
2	A	701	VUG	C15-C19-N03	-3.01	119.59	122.92
2	A	701	VUG	C12-C11-N01	2.99	116.31	110.59
4	D	703	PCW	O3-C11-C12	2.96	121.19	111.91
2	B	717	VUG	C18-N03-C19	2.94	121.93	116.85
2	B	704	VUG	C15-C19-N03	-2.92	119.69	122.92
2	B	704	VUG	C12-C11-N01	2.90	116.14	110.59
2	C	703	VUG	C12-C11-N01	2.84	116.02	110.59
2	A	713	VUG	C12-C11-N01	2.81	115.97	110.59
2	C	703	VUG	C15-C19-N03	-2.76	119.87	122.92
2	B	704	VUG	C08-C05-C04	-2.75	106.35	112.79
2	A	713	VUG	C13-C14-N02	2.72	115.99	110.70
2	C	703	VUG	C13-C14-N02	2.71	115.96	110.70
2	A	701	VUG	C08-C05-C04	-2.70	106.47	112.79
2	C	703	VUG	C08-C05-C04	-2.68	106.51	112.79
4	A	703	PCW	C3-C2-C1	-2.62	105.59	111.79
4	A	708	PCW	O3-C11-C12	2.58	120.00	111.91
4	D	713	PCW	O3-C11-C12	2.58	120.00	111.91
2	B	704	VUG	C13-C14-N02	2.58	115.70	110.70
2	A	713	VUG	C08-C05-C04	-2.57	106.76	112.79
2	B	717	VUG	C12-N02-C14	-2.57	105.84	111.52
4	B	712	PCW	O3-C11-C12	2.57	119.97	111.91
4	C	710	PCW	O3-C11-C12	2.55	119.91	111.91
2	A	701	VUG	C13-C14-N02	2.43	115.42	110.70
2	A	701	VUG	C14-C13-N01	2.42	115.22	110.59
2	C	703	VUG	C08-C05-C06	2.30	114.35	109.56
4	B	707	PCW	C3-C2-C1	-2.29	106.38	111.79
4	C	705	PCW	C3-C2-C1	-2.28	106.38	111.79
2	A	713	VUG	C08-C05-C06	2.27	114.28	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	708	PCW	C3-C2-C1	-2.26	106.44	111.79
2	A	701	VUG	C08-C05-C06	2.25	114.24	109.56
2	A	713	VUG	C14-C13-N01	2.24	114.87	110.59
2	B	704	VUG	C14-C13-N01	2.22	114.85	110.59
2	B	704	VUG	C08-C05-C06	2.20	114.15	109.56
3	D	707	Y01	CAT-CAR-CBC	2.19	114.07	110.33
3	C	704	Y01	CAT-CAR-CBC	2.19	114.06	110.33
3	A	702	Y01	CAT-CAR-CBC	2.18	114.05	110.33
3	B	705	Y01	CAT-CAR-CBC	2.18	114.04	110.33
2	B	704	VUG	C04-C03-C02	-2.17	118.94	121.39
4	D	708	PCW	O3-C11-C12	2.15	118.66	111.91
4	C	705	PCW	O3-C11-C12	2.15	118.64	111.91
2	A	701	VUG	C04-C03-C02	-2.15	118.97	121.39
4	B	707	PCW	O3-C11-C12	2.13	118.58	111.91
2	C	703	VUG	C14-C13-N01	2.10	114.62	110.59
2	C	703	VUG	C04-C03-C02	-2.10	119.02	121.39
4	A	703	PCW	O3-C11-C12	2.08	118.43	111.91
2	A	713	VUG	C04-C03-C02	-2.05	119.08	121.39

There are no chirality outliers.

All (655) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	PCW	O4P-C4-C5-N
4	A	703	PCW	C32-C31-O2-C2
4	A	703	PCW	C4-O4P-P-O1P
4	A	703	PCW	C4-O4P-P-O2P
4	A	708	PCW	O4P-C4-C5-N
4	A	708	PCW	C32-C31-O2-C2
4	A	711	PCW	O4P-C4-C5-N
4	A	711	PCW	C12-C11-O3-C3
4	A	711	PCW	O11-C11-O3-C3
4	A	711	PCW	C32-C31-O2-C2
4	A	711	PCW	C39-C40-C41-C42
4	A	711	PCW	C1-O3P-P-O1P
4	A	711	PCW	C1-O3P-P-O2P
4	A	711	PCW	C4-O4P-P-O2P
4	A	711	PCW	C4-O4P-P-O3P
4	A	712	PCW	O4P-C4-C5-N
4	A	712	PCW	C12-C11-O3-C3
4	A	712	PCW	O11-C11-O3-C3
4	B	707	PCW	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
4	B	707	PCW	C32-C31-O2-C2
4	B	707	PCW	C4-O4P-P-O1P
4	B	707	PCW	C4-O4P-P-O2P
4	B	712	PCW	O4P-C4-C5-N
4	B	712	PCW	C32-C31-O2-C2
4	B	715	PCW	O4P-C4-C5-N
4	B	715	PCW	C12-C11-O3-C3
4	B	715	PCW	O11-C11-O3-C3
4	B	715	PCW	C32-C31-O2-C2
4	B	715	PCW	C39-C40-C41-C42
4	B	715	PCW	C1-O3P-P-O1P
4	B	715	PCW	C1-O3P-P-O2P
4	B	715	PCW	C4-O4P-P-O2P
4	B	715	PCW	C4-O4P-P-O3P
4	B	716	PCW	O4P-C4-C5-N
4	B	716	PCW	C12-C11-O3-C3
4	B	716	PCW	O11-C11-O3-C3
4	C	705	PCW	O4P-C4-C5-N
4	C	705	PCW	C32-C31-O2-C2
4	C	705	PCW	C4-O4P-P-O1P
4	C	705	PCW	C4-O4P-P-O2P
4	C	710	PCW	O4P-C4-C5-N
4	C	710	PCW	C32-C31-O2-C2
4	C	710	PCW	C4-O4P-P-O2P
4	C	713	PCW	O4P-C4-C5-N
4	C	713	PCW	C12-C11-O3-C3
4	C	713	PCW	O11-C11-O3-C3
4	C	713	PCW	C32-C31-O2-C2
4	C	713	PCW	C39-C40-C41-C42
4	C	713	PCW	C1-O3P-P-O1P
4	C	713	PCW	C1-O3P-P-O2P
4	C	713	PCW	C4-O4P-P-O2P
4	C	713	PCW	C4-O4P-P-O3P
4	C	714	PCW	O4P-C4-C5-N
4	C	714	PCW	C12-C11-O3-C3
4	C	714	PCW	O11-C11-O3-C3
4	D	702	PCW	O4P-C4-C5-N
4	D	702	PCW	C12-C11-O3-C3
4	D	702	PCW	O11-C11-O3-C3
4	D	702	PCW	C32-C31-O2-C2
4	D	702	PCW	C39-C40-C41-C42
4	D	702	PCW	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
4	D	702	PCW	C1-O3P-P-O2P
4	D	702	PCW	C4-O4P-P-O2P
4	D	702	PCW	C4-O4P-P-O3P
4	D	703	PCW	O4P-C4-C5-N
4	D	703	PCW	C12-C11-O3-C3
4	D	703	PCW	O11-C11-O3-C3
4	D	708	PCW	O4P-C4-C5-N
4	D	708	PCW	C32-C31-O2-C2
4	D	708	PCW	C4-O4P-P-O1P
4	D	708	PCW	C4-O4P-P-O2P
4	D	713	PCW	O4P-C4-C5-N
4	D	713	PCW	C32-C31-O2-C2
4	B	707	PCW	O11-C11-O3-C3
4	C	705	PCW	O11-C11-O3-C3
4	D	708	PCW	C12-C11-O3-C3
4	A	703	PCW	O11-C11-O3-C3
4	D	708	PCW	O11-C11-O3-C3
4	A	703	PCW	O31-C31-O2-C2
4	A	708	PCW	O31-C31-O2-C2
4	A	711	PCW	O31-C31-O2-C2
4	B	707	PCW	O31-C31-O2-C2
4	B	712	PCW	O31-C31-O2-C2
4	B	715	PCW	O31-C31-O2-C2
4	C	705	PCW	O31-C31-O2-C2
4	C	710	PCW	O31-C31-O2-C2
4	C	713	PCW	O31-C31-O2-C2
4	D	702	PCW	O31-C31-O2-C2
4	D	708	PCW	O31-C31-O2-C2
4	D	713	PCW	O31-C31-O2-C2
4	A	703	PCW	C12-C11-O3-C3
4	B	707	PCW	C12-C11-O3-C3
4	C	705	PCW	C12-C11-O3-C3
3	A	714	Y01	CAX-CAL-CAM-CAY
3	B	701	Y01	CAX-CAL-CAM-CAY
3	B	706	Y01	CAX-CAL-CAM-CAY
3	D	704	Y01	CAX-CAL-CAM-CAY
3	A	714	Y01	CAO-CBB-CBE-CBI
3	B	701	Y01	CAO-CBB-CBE-CBI
3	B	706	Y01	CAO-CBB-CBE-CBI
3	D	704	Y01	CAO-CBB-CBE-CBI
4	C	713	PCW	C13-C14-C15-C16
4	A	711	PCW	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
4	B	715	PCW	C13-C14-C15-C16
4	D	702	PCW	C13-C14-C15-C16
3	A	714	Y01	CAC-CBB-CBE-CBI
3	B	701	Y01	CAC-CBB-CBE-CBI
3	B	706	Y01	CAC-CBB-CBE-CBI
3	D	704	Y01	CAC-CBB-CBE-CBI
4	C	714	PCW	C24-C25-C26-C27
4	B	716	PCW	C24-C25-C26-C27
4	D	708	PCW	C11-C12-C13-C14
4	A	703	PCW	C11-C12-C13-C14
4	B	716	PCW	C31-C32-C33-C34
4	C	714	PCW	C31-C32-C33-C34
4	D	702	PCW	C11-C12-C13-C14
4	D	703	PCW	C31-C32-C33-C34
4	C	713	PCW	C15-C16-C17-C18
4	A	712	PCW	C31-C32-C33-C34
4	B	707	PCW	C11-C12-C13-C14
4	B	715	PCW	C11-C12-C13-C14
4	C	705	PCW	C11-C12-C13-C14
4	C	713	PCW	C11-C12-C13-C14
4	A	712	PCW	C24-C25-C26-C27
4	A	711	PCW	C11-C12-C13-C14
4	C	702	PCW	C13-C14-C15-C16
4	A	703	PCW	C4-O4P-P-O3P
4	A	711	PCW	C1-O3P-P-O4P
4	B	707	PCW	C4-O4P-P-O3P
4	B	715	PCW	C1-O3P-P-O4P
4	C	705	PCW	C4-O4P-P-O3P
4	C	713	PCW	C1-O3P-P-O4P
4	D	702	PCW	C1-O3P-P-O4P
4	D	708	PCW	C4-O4P-P-O3P
4	B	715	PCW	C15-C16-C17-C18
3	A	714	Y01	CAJ-CAN-CBA-CAA
3	B	701	Y01	CAJ-CAN-CBA-CAA
4	D	706	PCW	C11-C12-C13-C14
4	B	703	PCW	C13-C14-C15-C16
4	D	708	PCW	C20-C21-C22-C23
4	C	706	PCW	C22-C23-C24-C25
3	A	702	Y01	CAM-CAY-OAW-CBC
3	B	705	Y01	CAM-CAY-OAW-CBC
3	C	704	Y01	CAM-CAY-OAW-CBC
3	D	707	Y01	CAM-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
4	A	704	PCW	C22-C23-C24-C25
4	A	707	PCW	C13-C14-C15-C16
4	B	708	PCW	C22-C23-C24-C25
4	B	711	PCW	C13-C14-C15-C16
4	C	709	PCW	C13-C14-C15-C16
4	D	709	PCW	C15-C16-C17-C18
3	B	706	Y01	CAJ-CAN-CBA-CAA
3	D	704	Y01	CAJ-CAN-CBA-CAA
4	B	708	PCW	C15-C16-C17-C18
4	C	706	PCW	C15-C16-C17-C18
4	D	709	PCW	C22-C23-C24-C25
4	D	712	PCW	C13-C14-C15-C16
3	A	702	Y01	OAG-CAY-OAW-CBC
3	B	705	Y01	OAG-CAY-OAW-CBC
3	C	704	Y01	OAG-CAY-OAW-CBC
3	D	707	Y01	OAG-CAY-OAW-CBC
4	A	703	PCW	C31-C32-C33-C34
4	A	704	PCW	C15-C16-C17-C18
4	A	704	PCW	C13-C14-C15-C16
4	B	708	PCW	C13-C14-C15-C16
3	A	714	Y01	CAJ-CAO-CBB-CAC
3	B	701	Y01	CAJ-CAO-CBB-CAC
3	B	706	Y01	CAJ-CAO-CBB-CAC
3	D	704	Y01	CAJ-CAO-CBB-CAC
4	A	711	PCW	C32-C33-C34-C35
4	B	715	PCW	C32-C33-C34-C35
4	A	712	PCW	C34-C35-C36-C37
4	C	706	PCW	C13-C14-C15-C16
4	C	713	PCW	C32-C33-C34-C35
4	A	704	PCW	C12-C13-C14-C15
4	D	702	PCW	C32-C33-C34-C35
4	D	709	PCW	C13-C14-C15-C16
4	A	711	PCW	C15-C16-C17-C18
4	D	703	PCW	C13-C14-C15-C16
3	A	714	Y01	CAC-CBB-CBE-CAP
3	B	701	Y01	CAC-CBB-CBE-CAP
3	B	706	Y01	CAC-CBB-CBE-CAP
3	D	704	Y01	CAC-CBB-CBE-CAP
4	B	708	PCW	C12-C13-C14-C15
4	A	703	PCW	C20-C21-C22-C23
4	A	703	PCW	C36-C37-C38-C39
4	A	705	PCW	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
4	B	707	PCW	C20-C21-C22-C23
4	B	707	PCW	C36-C37-C38-C39
4	C	705	PCW	C20-C21-C22-C23
4	C	705	PCW	C36-C37-C38-C39
4	D	710	PCW	C16-C17-C18-C19
4	C	706	PCW	C12-C13-C14-C15
4	D	709	PCW	C12-C13-C14-C15
3	A	714	Y01	CAJ-CAN-CBA-CAB
3	B	701	Y01	CAJ-CAN-CBA-CAB
3	B	706	Y01	CAJ-CAN-CBA-CAB
3	D	704	Y01	CAJ-CAN-CBA-CAB
4	A	712	PCW	C35-C36-C37-C38
4	C	713	PCW	C14-C15-C16-C17
4	A	711	PCW	C14-C15-C16-C17
4	B	716	PCW	C34-C35-C36-C37
4	C	714	PCW	C34-C35-C36-C37
4	A	708	PCW	C12-C13-C14-C15
4	B	712	PCW	C12-C13-C14-C15
4	B	715	PCW	C14-C15-C16-C17
4	C	710	PCW	C12-C13-C14-C15
4	D	713	PCW	C12-C13-C14-C15
4	A	712	PCW	C13-C14-C15-C16
4	B	703	PCW	C11-C12-C13-C14
3	A	702	Y01	CAJ-CAN-CBA-CAB
3	B	705	Y01	CAJ-CAN-CBA-CAB
3	C	704	Y01	CAJ-CAN-CBA-CAB
3	D	707	Y01	CAJ-CAN-CBA-CAB
4	A	716	PCW	C11-C12-C13-C14
4	D	702	PCW	C14-C15-C16-C17
4	B	702	PCW	C16-C17-C18-C19
4	C	701	PCW	C16-C17-C18-C19
4	C	707	PCW	C16-C17-C18-C19
4	C	712	PCW	C20-C21-C22-C23
4	C	713	PCW	C16-C17-C18-C19
4	D	701	PCW	C20-C21-C22-C23
4	D	702	PCW	C16-C17-C18-C19
4	D	703	PCW	C36-C37-C38-C39
4	D	708	PCW	C36-C37-C38-C39
4	C	702	PCW	C11-C12-C13-C14
4	D	703	PCW	C34-C35-C36-C37
4	A	708	PCW	C2-C1-O3P-P
4	B	712	PCW	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
4	C	710	PCW	C2-C1-O3P-P
4	D	713	PCW	C2-C1-O3P-P
4	C	705	PCW	C31-C32-C33-C34
4	A	708	PCW	C12-C11-O3-C3
4	B	712	PCW	C12-C11-O3-C3
4	C	710	PCW	C12-C11-O3-C3
4	D	713	PCW	C12-C11-O3-C3
3	C	704	Y01	CAN-CAJ-CAO-CBB
4	A	712	PCW	C32-C31-O2-C2
4	D	703	PCW	C32-C31-O2-C2
4	B	716	PCW	C13-C14-C15-C16
4	D	708	PCW	C13-C14-C15-C16
3	A	702	Y01	CAN-CAJ-CAO-CBB
3	B	705	Y01	CAN-CAJ-CAO-CBB
3	D	707	Y01	CAN-CAJ-CAO-CBB
4	B	716	PCW	C35-C36-C37-C38
4	C	714	PCW	C35-C36-C37-C38
3	A	714	Y01	CAO-CBB-CBE-CAP
3	B	701	Y01	CAO-CBB-CBE-CAP
3	B	706	Y01	CAO-CBB-CBE-CAP
3	D	704	Y01	CAO-CBB-CBE-CAP
4	A	712	PCW	C36-C37-C38-C39
4	A	715	PCW	C16-C17-C18-C19
4	B	709	PCW	C16-C17-C18-C19
4	B	716	PCW	C36-C37-C38-C39
4	C	713	PCW	C36-C37-C38-C39
4	C	714	PCW	C36-C37-C38-C39
4	D	702	PCW	C36-C37-C38-C39
4	C	714	PCW	C13-C14-C15-C16
4	A	711	PCW	C33-C34-C35-C36
4	B	715	PCW	C33-C34-C35-C36
4	C	713	PCW	C33-C34-C35-C36
4	B	716	PCW	C11-C12-C13-C14
4	C	714	PCW	C11-C12-C13-C14
4	D	702	PCW	C33-C34-C35-C36
4	A	716	PCW	C13-C14-C15-C16
4	C	705	PCW	C13-C14-C15-C16
4	B	707	PCW	C31-C32-C33-C34
4	B	716	PCW	C32-C31-O2-C2
4	C	714	PCW	C32-C31-O2-C2
4	C	713	PCW	C19-C20-C21-C22
4	B	716	PCW	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
4	C	714	PCW	O31-C31-O2-C2
4	D	703	PCW	O31-C31-O2-C2
4	C	705	PCW	C14-C15-C16-C17
4	D	708	PCW	C14-C15-C16-C17
4	B	707	PCW	C13-C14-C15-C16
4	B	707	PCW	C14-C15-C16-C17
4	A	711	PCW	C16-C17-C18-C19
4	A	711	PCW	C36-C37-C38-C39
4	B	715	PCW	C16-C17-C18-C19
4	B	715	PCW	C36-C37-C38-C39
4	C	710	PCW	C16-C17-C18-C19
4	D	705	PCW	C16-C17-C18-C19
4	D	713	PCW	C16-C17-C18-C19
4	A	708	PCW	O11-C11-O3-C3
4	B	712	PCW	O11-C11-O3-C3
4	C	710	PCW	O11-C11-O3-C3
4	D	713	PCW	O11-C11-O3-C3
4	A	712	PCW	O31-C31-O2-C2
4	D	703	PCW	C35-C36-C37-C38
4	D	711	PCW	C14-C15-C16-C17
4	A	708	PCW	C19-C20-C21-C22
4	A	711	PCW	C19-C20-C21-C22
4	B	712	PCW	C19-C20-C21-C22
4	B	715	PCW	C19-C20-C21-C22
4	C	710	PCW	C19-C20-C21-C22
4	D	702	PCW	C19-C20-C21-C22
4	D	713	PCW	C19-C20-C21-C22
4	B	707	PCW	C1-O3P-P-O4P
4	C	705	PCW	C1-O3P-P-O4P
4	A	703	PCW	C14-C15-C16-C17
4	B	712	PCW	C16-C17-C18-C19
4	B	714	PCW	C20-C21-C22-C23
4	A	715	PCW	C14-C15-C16-C17
4	B	710	PCW	C14-C15-C16-C17
4	C	708	PCW	C14-C15-C16-C17
4	A	706	PCW	C14-C15-C16-C17
4	C	713	PCW	C12-C13-C14-C15
4	A	704	PCW	C11-C12-C13-C14
4	D	709	PCW	C11-C12-C13-C14
4	D	714	PCW	C21-C22-C23-C24
4	B	708	PCW	C11-C12-C13-C14
4	C	706	PCW	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
4	D	714	PCW	C11-C12-C13-C14
4	A	712	PCW	C11-C12-C13-C14
4	A	709	PCW	C11-C12-C13-C14
4	B	713	PCW	C11-C12-C13-C14
4	C	711	PCW	C11-C12-C13-C14
4	D	705	PCW	C14-C15-C16-C17
4	A	708	PCW	C16-C17-C18-C19
4	A	710	PCW	C20-C21-C22-C23
4	A	715	PCW	C20-C21-C22-C23
4	A	716	PCW	C20-C21-C22-C23
4	B	702	PCW	C20-C21-C22-C23
4	B	703	PCW	C20-C21-C22-C23
4	C	701	PCW	C20-C21-C22-C23
4	C	702	PCW	C20-C21-C22-C23
4	D	705	PCW	C20-C21-C22-C23
4	D	706	PCW	C20-C21-C22-C23
4	A	703	PCW	C13-C14-C15-C16
4	B	715	PCW	C12-C13-C14-C15
4	B	702	PCW	C14-C15-C16-C17
4	D	703	PCW	C22-C23-C24-C25
4	A	711	PCW	C12-C13-C14-C15
4	D	703	PCW	C25-C26-C27-C28
4	C	705	PCW	C12-C13-C14-C15
4	D	702	PCW	C12-C13-C14-C15
4	D	703	PCW	C24-C25-C26-C27
4	A	708	PCW	C17-C18-C19-C20
4	D	713	PCW	C17-C18-C19-C20
4	D	706	PCW	C13-C14-C15-C16
4	A	708	PCW	O3P-C1-C2-C3
4	B	712	PCW	O3P-C1-C2-C3
4	C	710	PCW	O3P-C1-C2-C3
4	D	713	PCW	O3P-C1-C2-C3
4	D	703	PCW	C14-C15-C16-C17
4	A	704	PCW	C21-C22-C23-C24
4	B	707	PCW	C12-C13-C14-C15
4	B	708	PCW	C21-C22-C23-C24
4	D	703	PCW	C11-C12-C13-C14
4	D	708	PCW	C31-C32-C33-C34
4	C	706	PCW	C21-C22-C23-C24
4	D	709	PCW	C21-C22-C23-C24
4	B	712	PCW	C17-C18-C19-C20
4	C	710	PCW	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
4	A	712	PCW	C25-C26-C27-C28
4	C	701	PCW	C14-C15-C16-C17
4	D	709	PCW	C23-C24-C25-C26
4	A	703	PCW	C12-C13-C14-C15
4	C	706	PCW	C23-C24-C25-C26
4	A	704	PCW	C23-C24-C25-C26
4	A	703	PCW	C1-O3P-P-O4P
4	A	708	PCW	C1-O3P-P-O4P
4	B	712	PCW	C1-O3P-P-O4P
4	C	710	PCW	C1-O3P-P-O4P
4	D	708	PCW	C1-O3P-P-O4P
4	D	713	PCW	C1-O3P-P-O4P
4	B	716	PCW	C25-C26-C27-C28
4	B	708	PCW	C23-C24-C25-C26
3	A	702	Y01	CAJ-CAN-CBA-CAA
3	B	705	Y01	CAJ-CAN-CBA-CAA
3	C	704	Y01	CAJ-CAN-CBA-CAA
3	D	707	Y01	CAJ-CAN-CBA-CAA
4	A	712	PCW	C15-C16-C17-C18
4	C	714	PCW	C25-C26-C27-C28
4	D	703	PCW	C42-C43-C44-C45
4	A	712	PCW	C19-C20-C21-C22
4	C	714	PCW	C41-C42-C43-C44
4	D	702	PCW	C15-C16-C17-C18
4	A	710	PCW	C22-C23-C24-C25
3	D	707	Y01	CAC-CBB-CBE-CBI
4	B	714	PCW	C22-C23-C24-C25
4	B	716	PCW	C19-C20-C21-C22
3	A	702	Y01	CAO-CBB-CBE-CBI
3	B	705	Y01	CAO-CBB-CBE-CBI
3	C	704	Y01	CAO-CBB-CBE-CBI
3	D	707	Y01	CAO-CBB-CBE-CBI
4	B	716	PCW	C41-C42-C43-C44
4	A	712	PCW	C41-C42-C43-C44
4	C	714	PCW	C19-C20-C21-C22
3	A	702	Y01	CAC-CBB-CBE-CBI
3	B	705	Y01	CAC-CBB-CBE-CBI
3	C	704	Y01	CAC-CBB-CBE-CBI
4	A	708	PCW	O3P-C1-C2-O2
4	B	712	PCW	O3P-C1-C2-O2
4	C	710	PCW	O3P-C1-C2-O2
4	D	713	PCW	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	712	PCW	C22-C23-C24-C25
4	D	701	PCW	C22-C23-C24-C25
4	A	708	PCW	C33-C34-C35-C36
4	D	708	PCW	C12-C13-C14-C15
4	B	711	PCW	C14-C15-C16-C17
4	C	710	PCW	C33-C34-C35-C36
4	D	712	PCW	C14-C15-C16-C17
4	A	707	PCW	C14-C15-C16-C17
4	C	709	PCW	C14-C15-C16-C17
4	A	709	PCW	C21-C22-C23-C24
4	B	716	PCW	C15-C16-C17-C18
4	A	708	PCW	C4-O4P-P-O3P
4	B	712	PCW	C4-O4P-P-O3P
4	C	710	PCW	C4-O4P-P-O3P
4	D	708	PCW	C15-C16-C17-C18
4	D	714	PCW	C15-C16-C17-C18
4	A	708	PCW	C1-O3P-P-O1P
4	A	708	PCW	C4-O4P-P-O1P
4	A	708	PCW	C4-O4P-P-O2P
4	B	707	PCW	C1-O3P-P-O1P
4	B	712	PCW	C1-O3P-P-O1P
4	B	712	PCW	C4-O4P-P-O1P
4	B	712	PCW	C4-O4P-P-O2P
4	C	705	PCW	C1-O3P-P-O1P
4	C	710	PCW	C1-O3P-P-O1P
4	C	710	PCW	C4-O4P-P-O1P
4	D	713	PCW	C1-O3P-P-O1P
4	D	713	PCW	C4-O4P-P-O1P
4	B	712	PCW	C33-C34-C35-C36
4	B	713	PCW	C21-C22-C23-C24
4	C	711	PCW	C21-C22-C23-C24
4	C	706	PCW	C20-C21-C22-C23
4	D	709	PCW	C20-C21-C22-C23
4	A	712	PCW	C42-C43-C44-C45
4	A	712	PCW	C22-C23-C24-C25
4	D	703	PCW	C19-C20-C21-C22
3	A	702	Y01	CAO-CBB-CBE-CAP
3	B	705	Y01	CAO-CBB-CBE-CAP
3	C	704	Y01	CAO-CBB-CBE-CAP
4	A	711	PCW	O2-C2-C3-O3
4	B	715	PCW	O2-C2-C3-O3
4	C	713	PCW	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	D	702	PCW	O2-C2-C3-O3
4	A	704	PCW	C19-C20-C21-C22
4	B	708	PCW	C19-C20-C21-C22
4	C	706	PCW	C19-C20-C21-C22
4	D	709	PCW	C19-C20-C21-C22
4	C	708	PCW	C12-C13-C14-C15
4	B	710	PCW	C12-C13-C14-C15
4	A	706	PCW	C12-C13-C14-C15
4	D	711	PCW	C12-C13-C14-C15
3	D	707	Y01	CAO-CBB-CBE-CAP
4	C	714	PCW	C15-C16-C17-C18
4	D	713	PCW	C33-C34-C35-C36
4	B	713	PCW	C22-C23-C24-C25
4	C	711	PCW	C22-C23-C24-C25
4	A	715	PCW	C23-C24-C25-C26
4	D	703	PCW	C23-C24-C25-C26
4	A	704	PCW	C14-C15-C16-C17
4	C	705	PCW	C15-C16-C17-C18
4	B	708	PCW	C14-C15-C16-C17
4	B	716	PCW	C22-C23-C24-C25
4	A	715	PCW	C19-C20-C21-C22
3	A	702	Y01	CAC-CBB-CBE-CAP
3	B	705	Y01	CAC-CBB-CBE-CAP
3	C	704	Y01	CAC-CBB-CBE-CAP
3	D	707	Y01	CAC-CBB-CBE-CAP
4	A	703	PCW	O2-C2-C3-O3
4	B	702	PCW	C23-C24-C25-C26
4	B	716	PCW	C12-C13-C14-C15
4	C	706	PCW	C14-C15-C16-C17
4	D	703	PCW	C12-C13-C14-C15
4	D	713	PCW	C4-O4P-P-O3P
4	B	716	PCW	C42-C43-C44-C45
4	A	709	PCW	C12-C13-C14-C15
4	B	707	PCW	C15-C16-C17-C18
4	B	713	PCW	C15-C16-C17-C18
4	A	703	PCW	C1-C2-C3-O3
4	D	708	PCW	C25-C26-C27-C28
4	C	714	PCW	C12-C13-C14-C15
4	C	714	PCW	C22-C23-C24-C25
4	A	709	PCW	C15-C16-C17-C18
4	C	711	PCW	C12-C13-C14-C15
4	C	701	PCW	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
4	C	714	PCW	C42-C43-C44-C45
4	B	715	PCW	C37-C38-C39-C40
4	D	702	PCW	C37-C38-C39-C40
4	D	705	PCW	C19-C20-C21-C22
4	D	706	PCW	C19-C20-C21-C22
4	B	708	PCW	C20-C21-C22-C23
4	D	709	PCW	C14-C15-C16-C17
4	A	712	PCW	C12-C13-C14-C15
4	B	702	PCW	C19-C20-C21-C22
4	C	702	PCW	C19-C20-C21-C22
4	A	709	PCW	C22-C23-C24-C25
3	A	702	Y01	CAJ-CAO-CBB-CAC
3	B	705	Y01	CAJ-CAO-CBB-CAC
3	C	704	Y01	CAJ-CAO-CBB-CAC
3	D	707	Y01	CAJ-CAO-CBB-CAC
4	D	703	PCW	C41-C42-C43-C44
4	D	705	PCW	C23-C24-C25-C26
4	A	704	PCW	C20-C21-C22-C23
4	A	716	PCW	C19-C20-C21-C22
4	B	703	PCW	C19-C20-C21-C22
4	C	702	PCW	C15-C16-C17-C18
4	A	711	PCW	C20-C21-C22-C23
4	B	715	PCW	C20-C21-C22-C23
4	C	705	PCW	C25-C26-C27-C28
4	C	713	PCW	C20-C21-C22-C23
4	D	702	PCW	C20-C21-C22-C23
3	A	702	Y01	CAM-CAL-CAX-OAH
3	B	705	Y01	CAM-CAL-CAX-OAH
3	C	704	Y01	CAM-CAL-CAX-OAH
3	D	707	Y01	CAM-CAL-CAX-OAH
4	A	711	PCW	C37-C38-C39-C40
4	C	713	PCW	C37-C38-C39-C40
4	B	707	PCW	C25-C26-C27-C28
4	A	703	PCW	C25-C26-C27-C28
3	A	702	Y01	CAM-CAL-CAX-OAF
3	B	705	Y01	CAM-CAL-CAX-OAF
3	C	704	Y01	CAM-CAL-CAX-OAF
3	D	707	Y01	CAM-CAL-CAX-OAF
4	A	705	PCW	C14-C15-C16-C17
4	A	703	PCW	C15-C16-C17-C18
4	B	707	PCW	C1-C2-C3-O3
4	C	705	PCW	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	D	714	PCW	C12-C13-C14-C15
4	C	701	PCW	C19-C20-C21-C22
4	B	713	PCW	C12-C13-C14-C15
4	D	710	PCW	C12-C13-C14-C15
4	D	714	PCW	C23-C24-C25-C26
4	D	703	PCW	C39-C40-C41-C42
4	B	707	PCW	O2-C2-C3-O3
4	C	705	PCW	O2-C2-C3-O3
4	A	716	PCW	C18-C19-C20-C21
4	C	702	PCW	C18-C19-C20-C21
4	A	705	PCW	C12-C13-C14-C15
4	B	703	PCW	C18-C19-C20-C21
4	A	709	PCW	C23-C24-C25-C26
4	A	703	PCW	C39-C40-C41-C42
4	A	703	PCW	C19-C20-C21-C22
4	C	705	PCW	C39-C40-C41-C42
4	D	710	PCW	C14-C15-C16-C17
4	B	713	PCW	C23-C24-C25-C26
4	B	707	PCW	C39-C40-C41-C42
4	D	710	PCW	C17-C18-C19-C20
2	A	701	VUG	C20-C04-C05-C08
4	A	712	PCW	C39-C40-C41-C42
4	B	716	PCW	C39-C40-C41-C42
4	C	707	PCW	C17-C18-C19-C20
4	C	714	PCW	C39-C40-C41-C42
2	A	713	VUG	C20-C04-C05-C08
2	B	704	VUG	C20-C04-C05-C08
2	C	703	VUG	C20-C04-C05-C08
4	A	712	PCW	C23-C24-C25-C26
4	A	712	PCW	O2-C31-C32-C33
4	B	716	PCW	O2-C31-C32-C33
4	D	703	PCW	O2-C31-C32-C33
4	B	714	PCW	C19-C20-C21-C22
4	D	708	PCW	C39-C40-C41-C42
4	C	714	PCW	C40-C41-C42-C43
4	A	711	PCW	C1-C2-C3-O3
4	B	715	PCW	C1-C2-C3-O3
4	C	713	PCW	C1-C2-C3-O3
4	D	702	PCW	C1-C2-C3-O3
4	A	710	PCW	C15-C16-C17-C18
4	D	706	PCW	C18-C19-C20-C21
3	A	702	Y01	CAL-CAM-CAY-OAW

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Mol	Chain	Res	Type	Atoms
3	B	705	Y01	CAL-CAM-CAY-OAW
3	C	704	Y01	CAL-CAM-CAY-OAW
3	D	707	Y01	CAL-CAM-CAY-OAW
4	B	709	PCW	C14-C15-C16-C17
4	C	714	PCW	O2-C31-C32-C33
4	A	710	PCW	C19-C20-C21-C22
4	B	709	PCW	C17-C18-C19-C20
4	C	701	PCW	C17-C18-C19-C20
4	B	707	PCW	C21-C22-C23-C24
4	C	711	PCW	C23-C24-C25-C26
4	A	705	PCW	C17-C18-C19-C20
4	B	702	PCW	C17-C18-C19-C20
4	D	701	PCW	C19-C20-C21-C22
4	A	703	PCW	C21-C22-C23-C24
4	A	708	PCW	O2-C31-C32-C33
4	C	710	PCW	O2-C31-C32-C33
4	C	711	PCW	C15-C16-C17-C18
4	B	712	PCW	O2-C31-C32-C33
4	D	713	PCW	O2-C31-C32-C33
4	B	709	PCW	C12-C13-C14-C15
4	B	703	PCW	C15-C16-C17-C18
4	A	712	PCW	C17-C18-C19-C20
4	C	712	PCW	C19-C20-C21-C22
4	A	708	PCW	O3-C11-C12-C13
4	B	712	PCW	O3-C11-C12-C13
4	C	710	PCW	O3-C11-C12-C13
4	D	713	PCW	O3-C11-C12-C13
4	A	704	PCW	C17-C18-C19-C20
4	A	715	PCW	C17-C18-C19-C20
4	A	716	PCW	C17-C18-C19-C20
4	B	703	PCW	C17-C18-C19-C20
4	B	707	PCW	C19-C20-C21-C22
4	B	708	PCW	C17-C18-C19-C20
4	B	713	PCW	C17-C18-C19-C20
4	B	716	PCW	C17-C18-C19-C20
4	C	702	PCW	C17-C18-C19-C20
4	C	706	PCW	C17-C18-C19-C20
4	C	711	PCW	C17-C18-C19-C20
4	C	714	PCW	C17-C18-C19-C20
4	D	706	PCW	C17-C18-C19-C20
4	D	709	PCW	C17-C18-C19-C20
4	B	714	PCW	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
4	A	709	PCW	C17-C18-C19-C20
4	D	714	PCW	C17-C18-C19-C20
4	B	716	PCW	C40-C41-C42-C43
4	C	710	PCW	O11-C11-C12-C13
4	C	705	PCW	C21-C22-C23-C24
4	A	703	PCW	C1-O3P-P-O1P
4	A	712	PCW	C1-O3P-P-O1P
4	B	716	PCW	C1-O3P-P-O1P
4	C	714	PCW	C1-O3P-P-O1P
4	D	703	PCW	C1-O3P-P-O1P
4	D	708	PCW	C1-O3P-P-O1P
4	A	708	PCW	O11-C11-C12-C13
4	A	712	PCW	O31-C31-C32-C33
4	B	712	PCW	O11-C11-C12-C13
4	D	703	PCW	O31-C31-C32-C33
4	D	713	PCW	O11-C11-C12-C13
4	D	714	PCW	C22-C23-C24-C25
4	B	716	PCW	O31-C31-C32-C33
4	C	714	PCW	O31-C31-C32-C33
3	A	702	Y01	CAL-CAM-CAY-OAG
3	B	705	Y01	CAL-CAM-CAY-OAG
3	C	704	Y01	CAL-CAM-CAY-OAG
3	D	707	Y01	CAL-CAM-CAY-OAG
4	A	711	PCW	C5-C4-O4P-P
4	B	715	PCW	C5-C4-O4P-P
4	C	713	PCW	C5-C4-O4P-P
4	D	702	PCW	C5-C4-O4P-P
4	A	708	PCW	O31-C31-C32-C33
4	C	710	PCW	O31-C31-C32-C33
2	C	703	VUG	C03-C04-C05-C08
4	B	712	PCW	O31-C31-C32-C33
4	D	705	PCW	C17-C18-C19-C20
4	B	715	PCW	O2-C31-C32-C33
2	A	713	VUG	C03-C04-C05-C08
2	B	704	VUG	C03-C04-C05-C08
4	D	713	PCW	O31-C31-C32-C33
4	A	711	PCW	O2-C31-C32-C33
4	B	716	PCW	C23-C24-C25-C26
4	C	714	PCW	C23-C24-C25-C26
2	A	701	VUG	C03-C04-C05-C08
4	C	713	PCW	O2-C31-C32-C33
4	D	702	PCW	O2-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
4	D	701	PCW	C15-C16-C17-C18
4	C	713	PCW	O31-C31-C32-C33
4	D	702	PCW	O31-C31-C32-C33
4	D	708	PCW	O3-C11-C12-C13
4	B	715	PCW	O31-C31-C32-C33
4	C	712	PCW	C15-C16-C17-C18

There are no ring outliers.

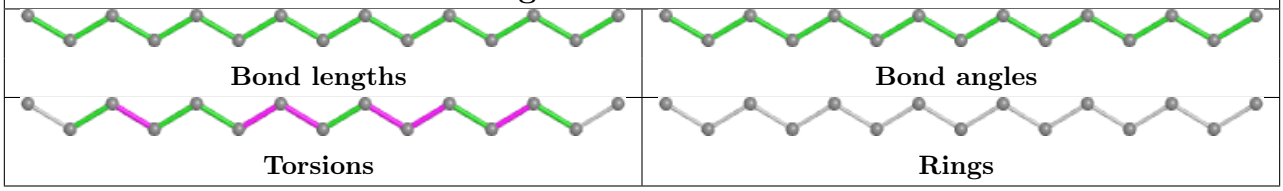
19 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	706	Y01	1	0
4	B	715	PCW	2	0
3	D	704	Y01	2	0
3	A	702	Y01	1	0
4	A	712	PCW	1	0
4	D	708	PCW	1	0
4	B	707	PCW	3	0
4	C	705	PCW	1	0
4	C	714	PCW	1	0
3	A	714	Y01	1	0
4	C	713	PCW	1	0
4	A	711	PCW	2	0
3	D	707	Y01	1	0
4	D	702	PCW	2	0
3	B	701	Y01	3	0
3	B	705	Y01	1	0
4	A	703	PCW	3	0
4	D	703	PCW	1	0
3	C	704	Y01	1	0

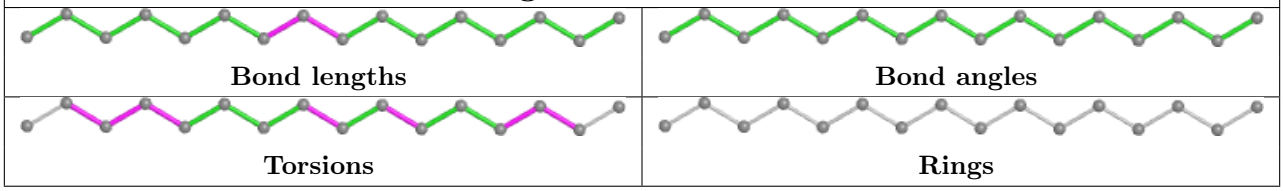
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 PCW C 701



Ligand PCW B 713



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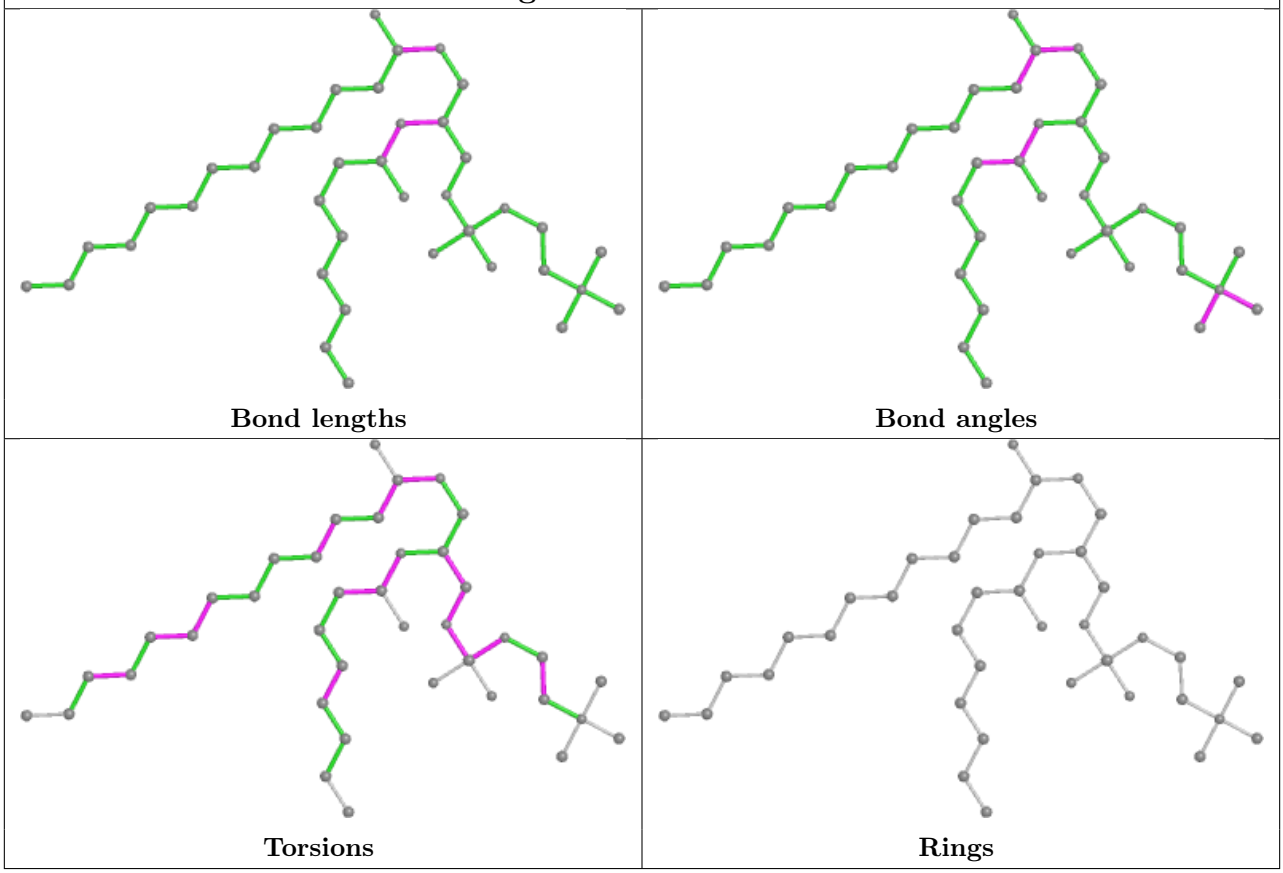
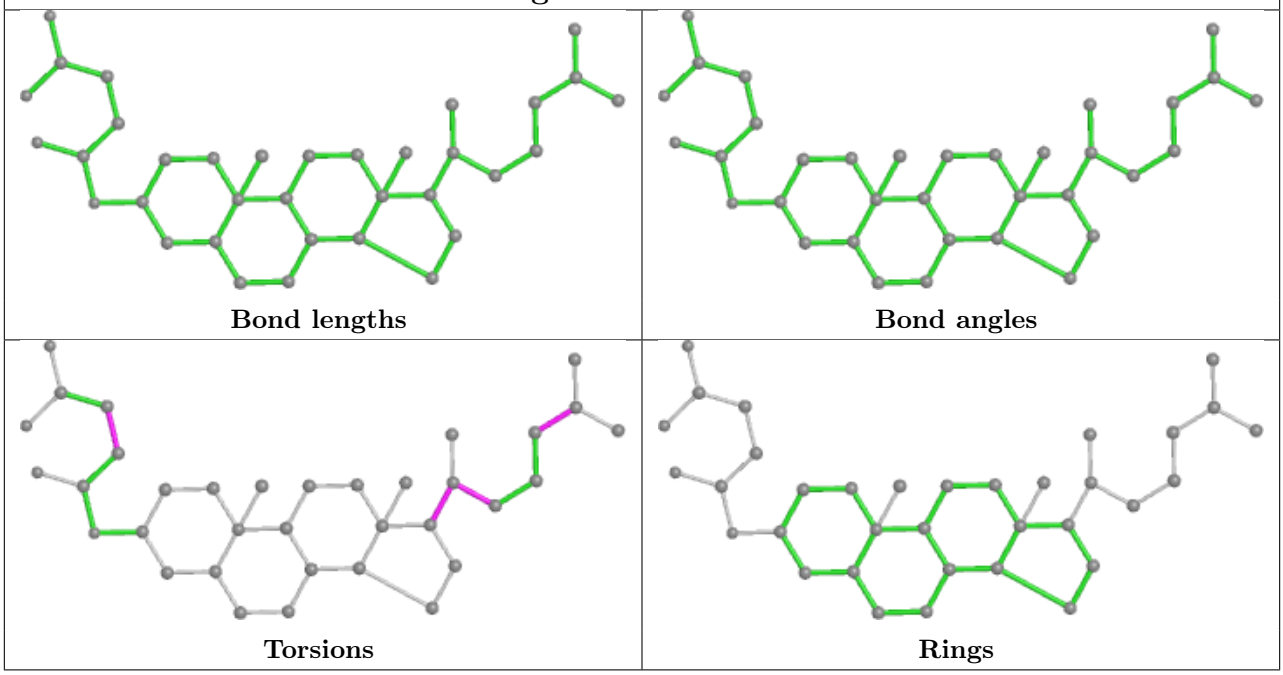
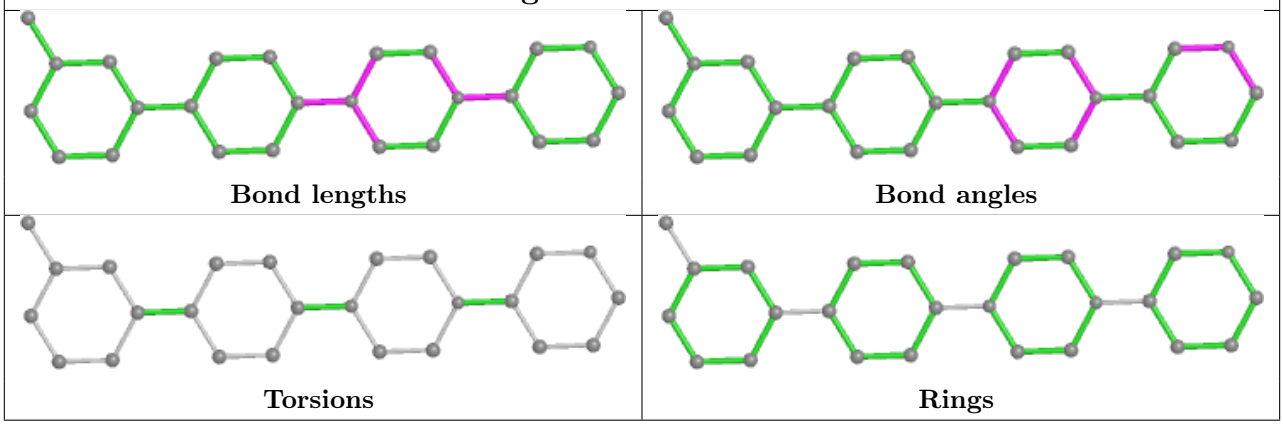


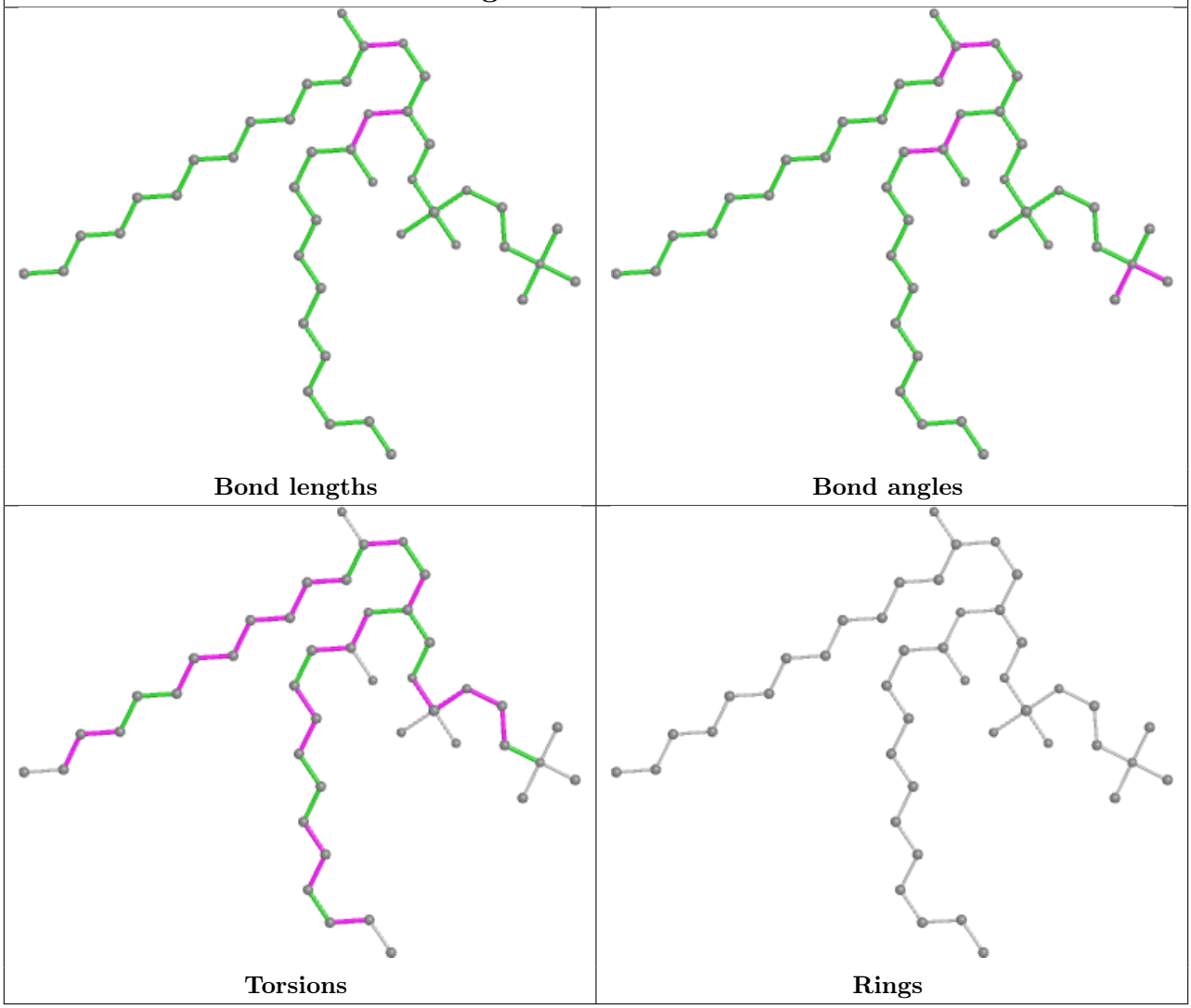
Ligand Y01 B 706



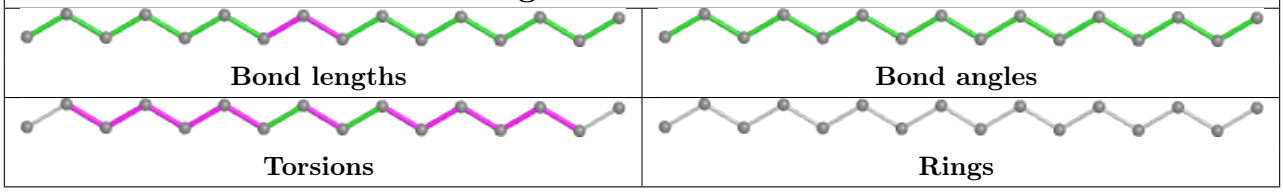
Ligand VUG B 717



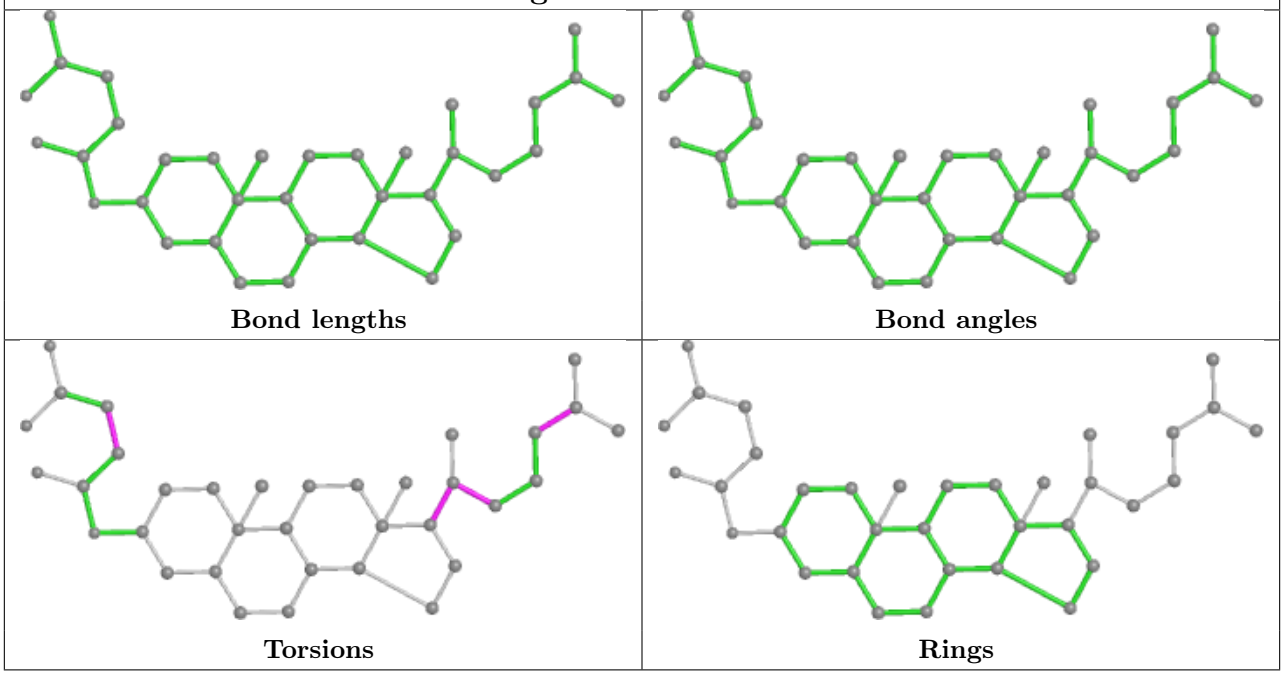
Ligand PCW B 715



Ligand PCW A 704



Ligand Y01 D 704



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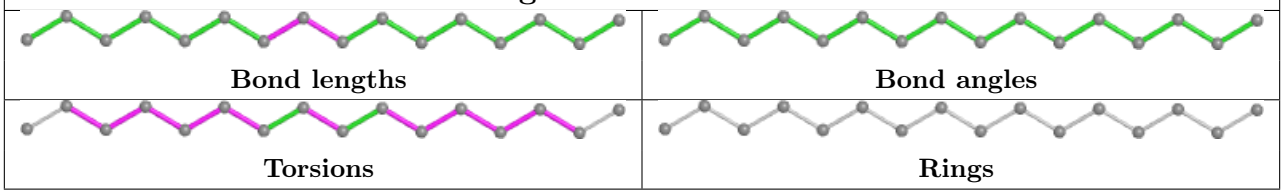
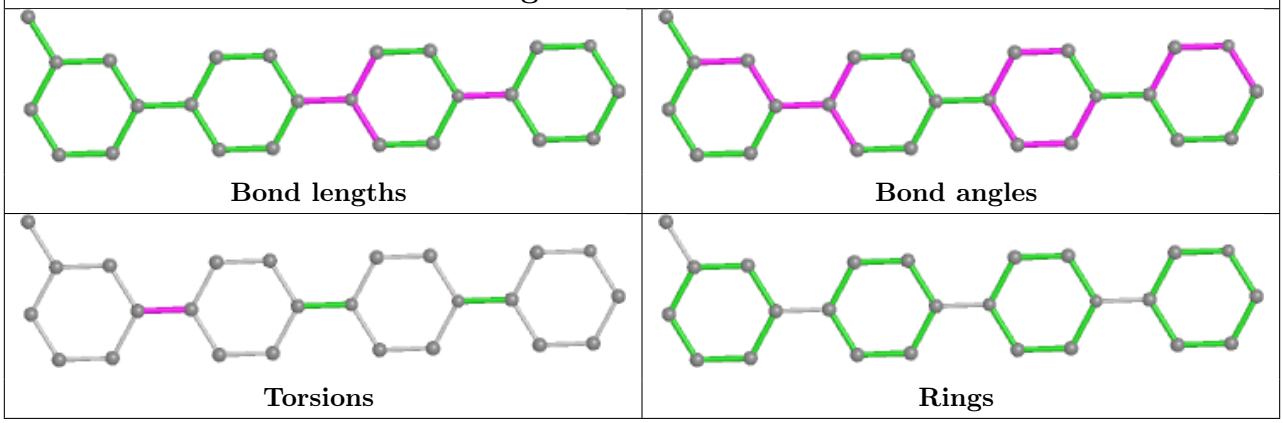


Ligand VUG C 703



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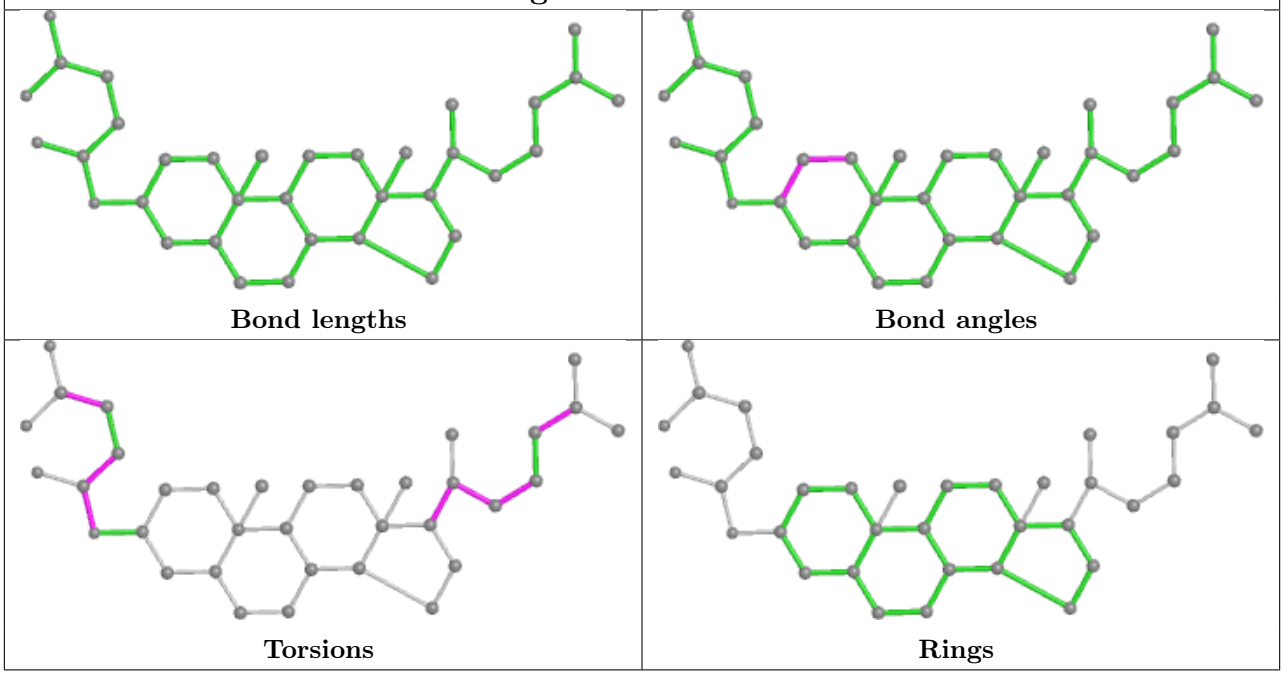

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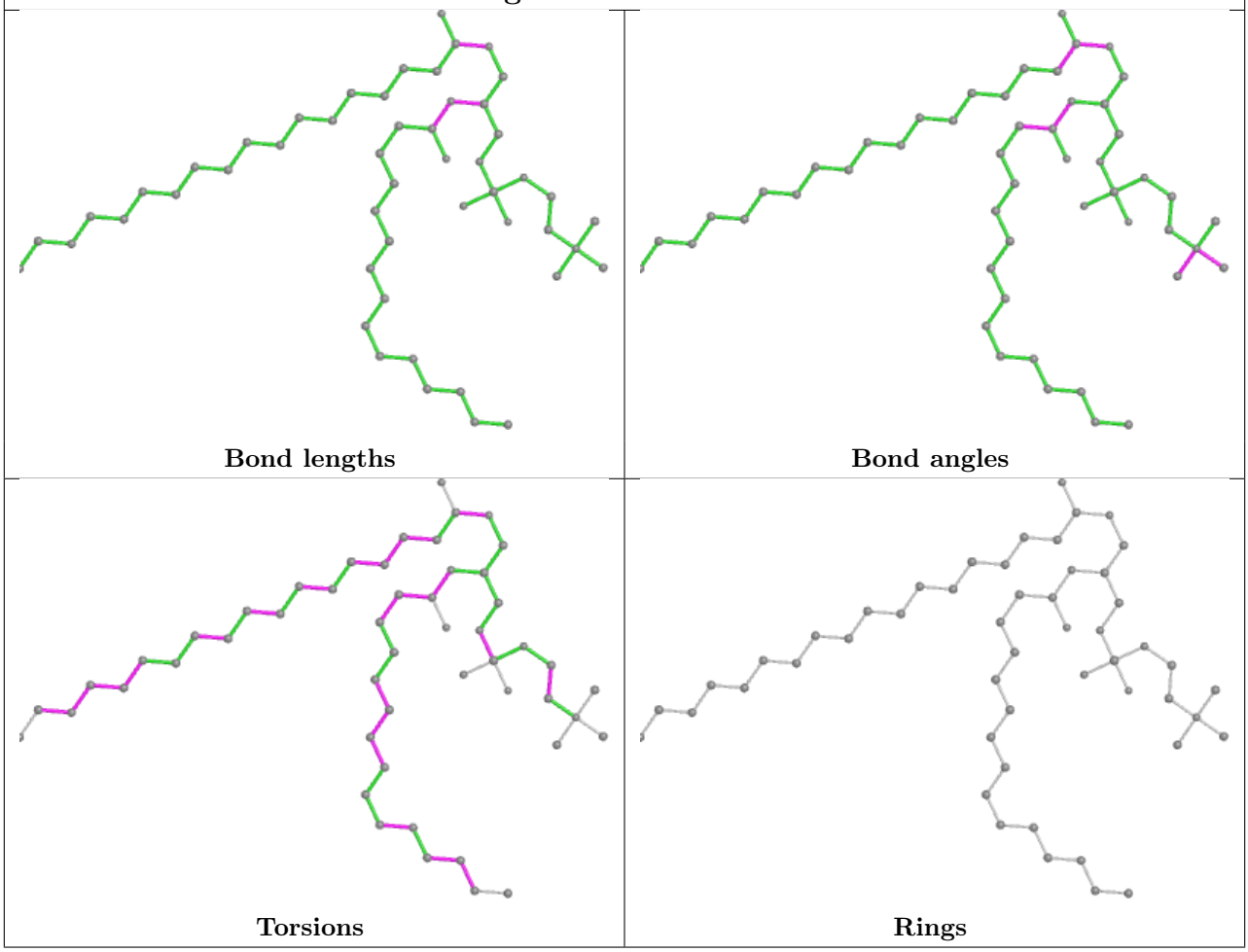

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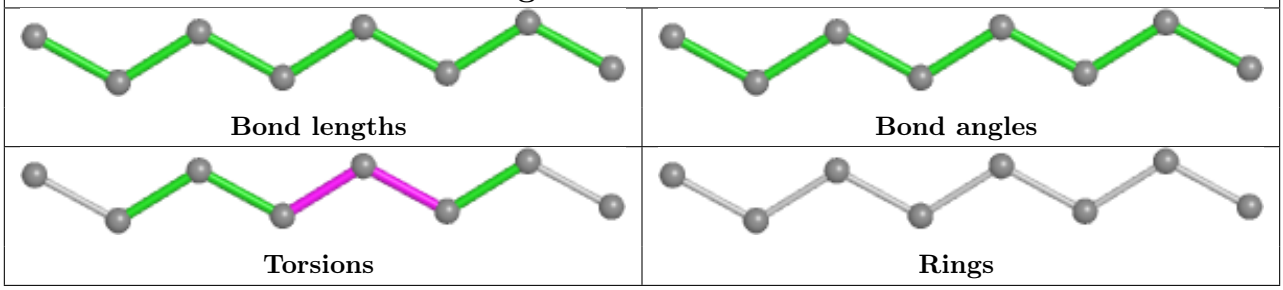

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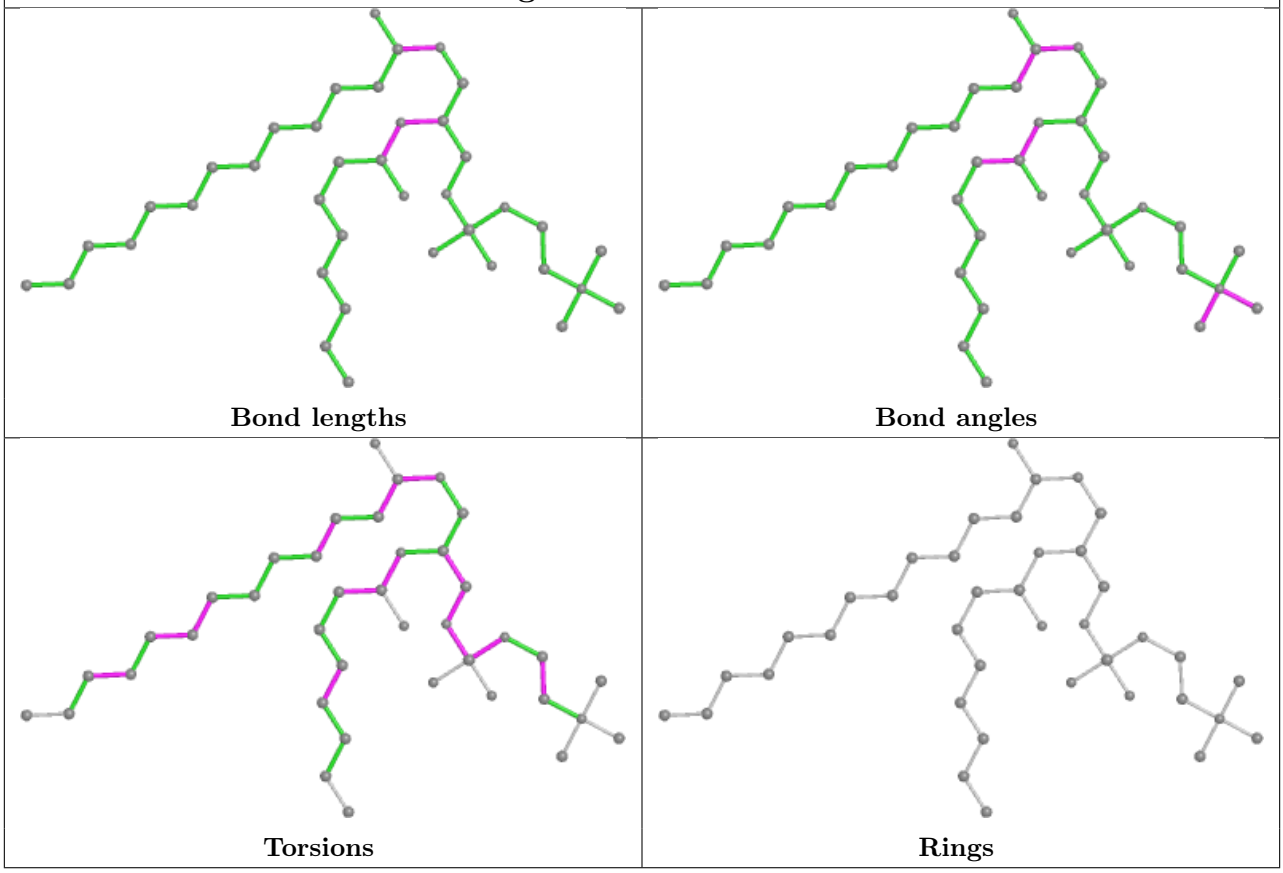

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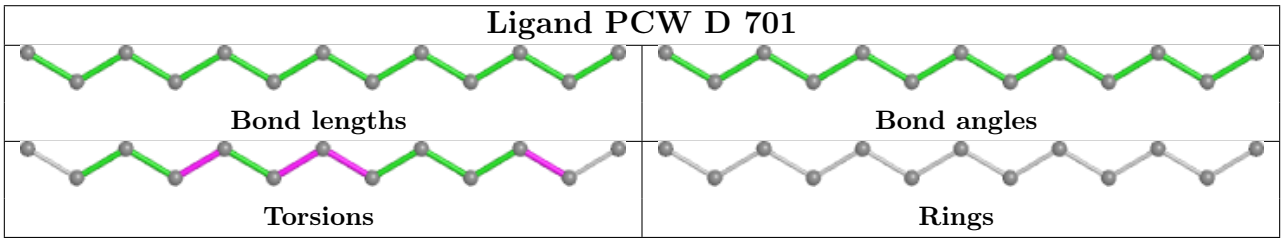

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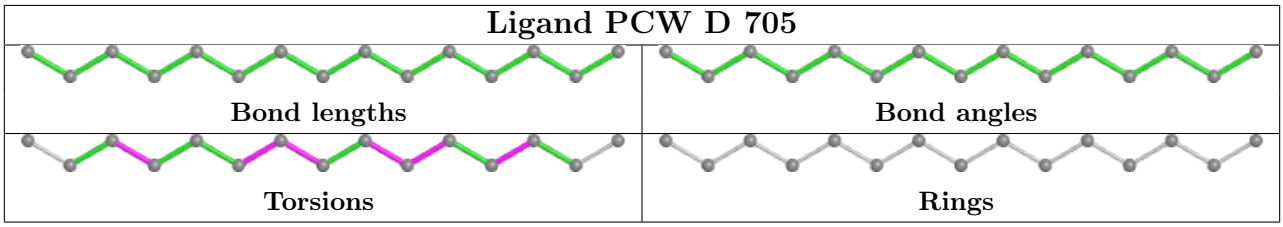

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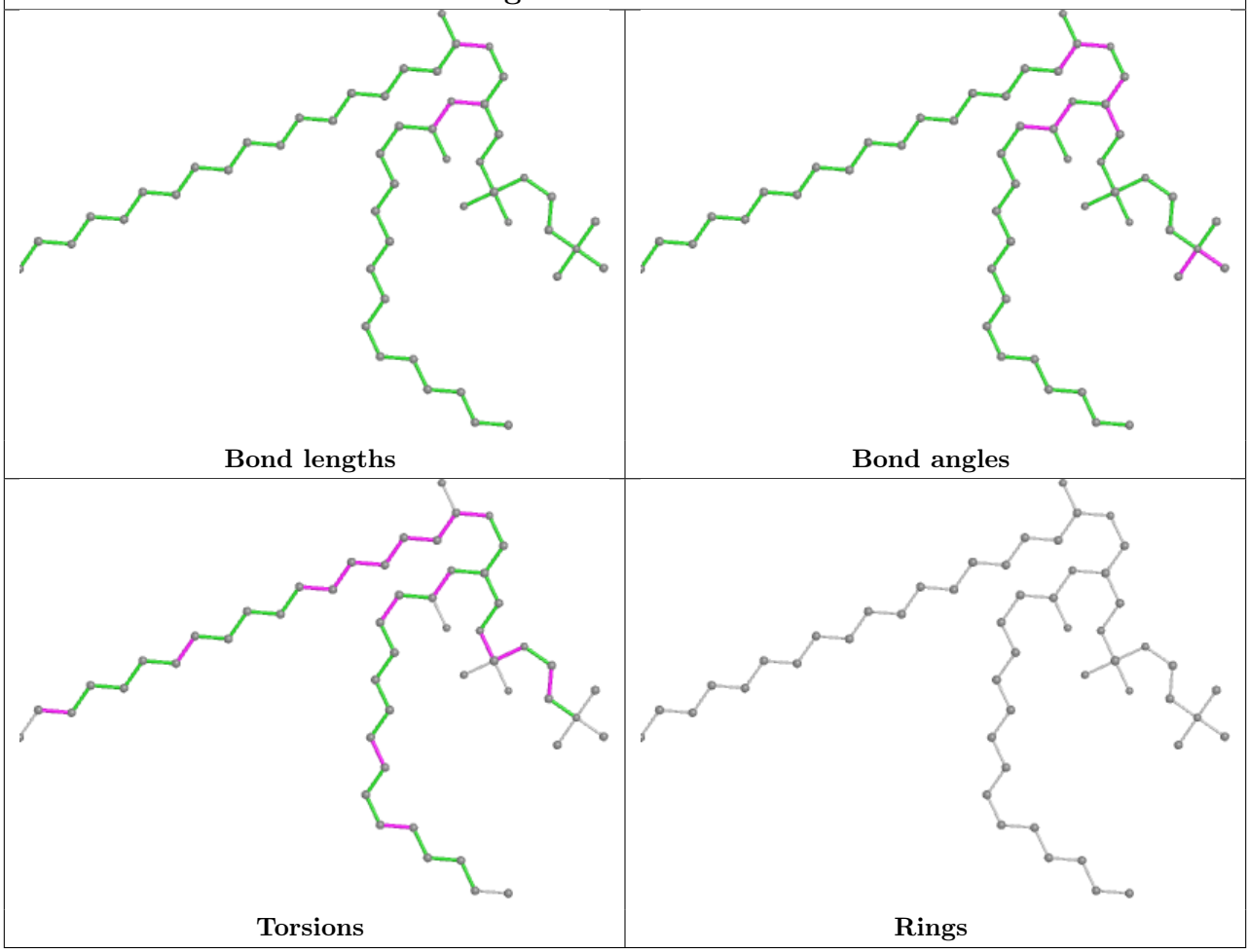
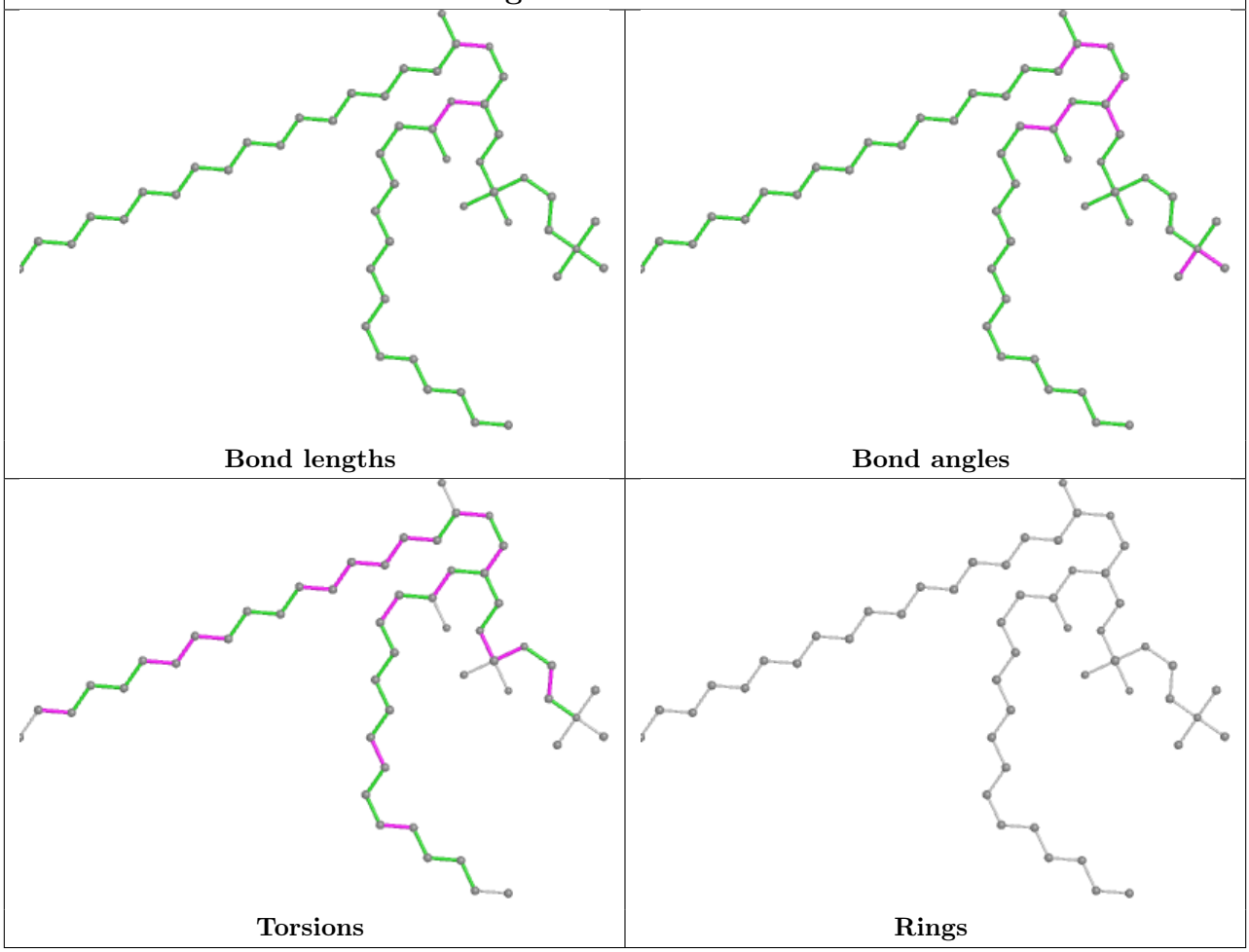


Ligand PCW B 707



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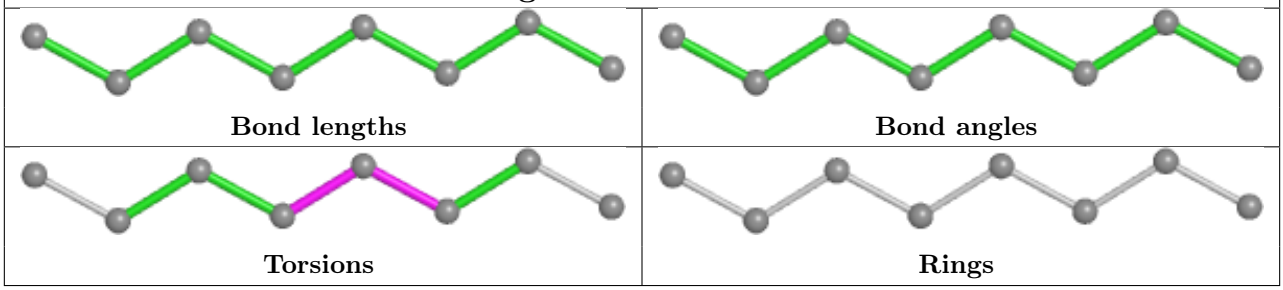

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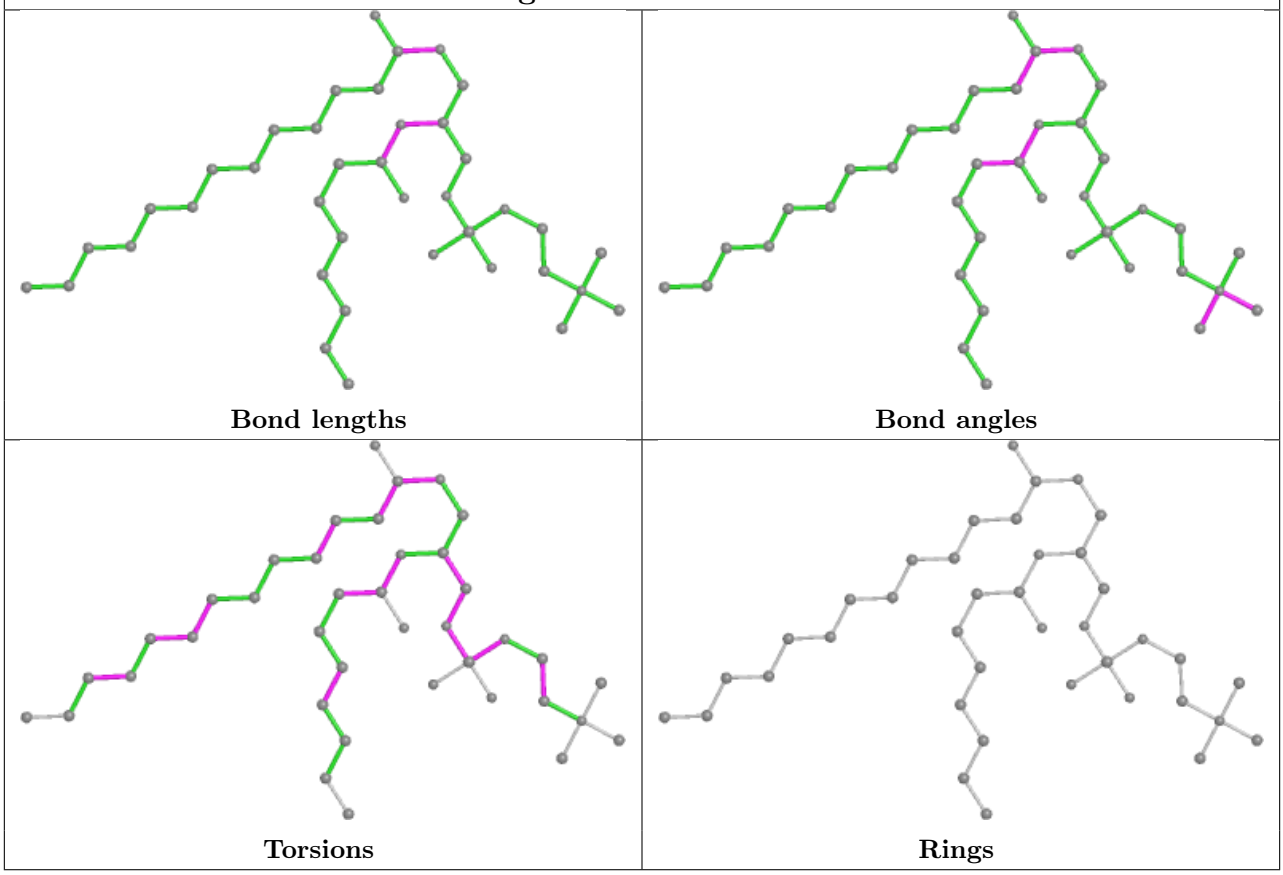

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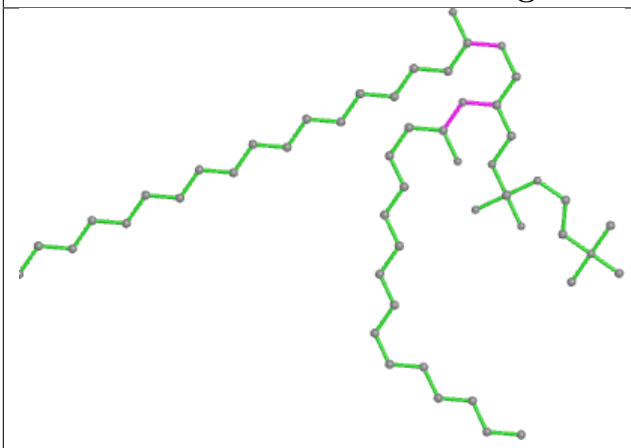
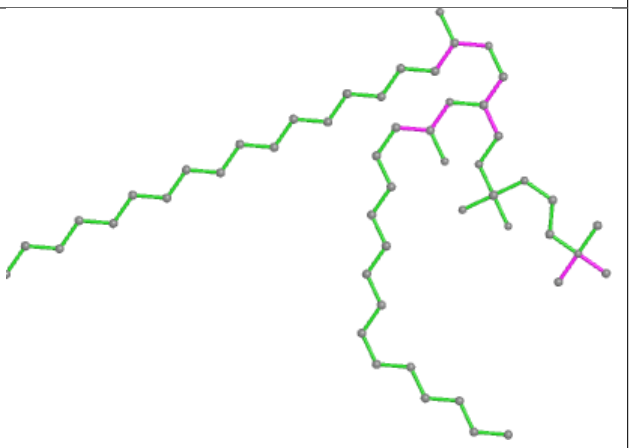
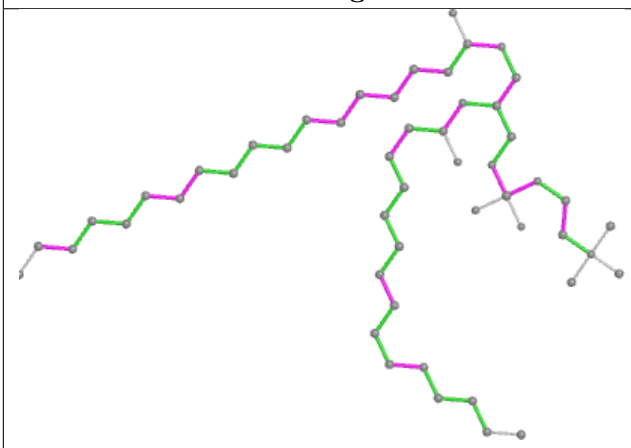
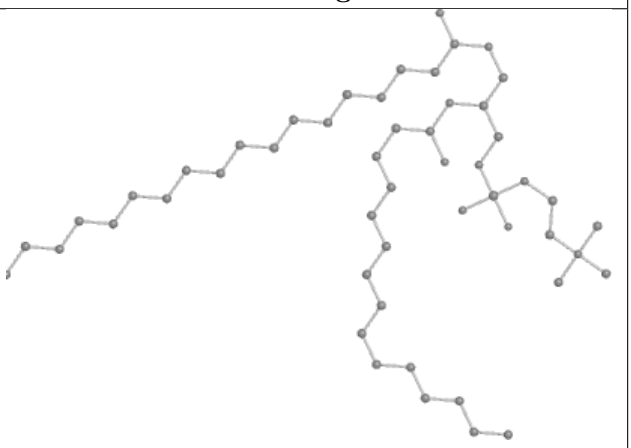
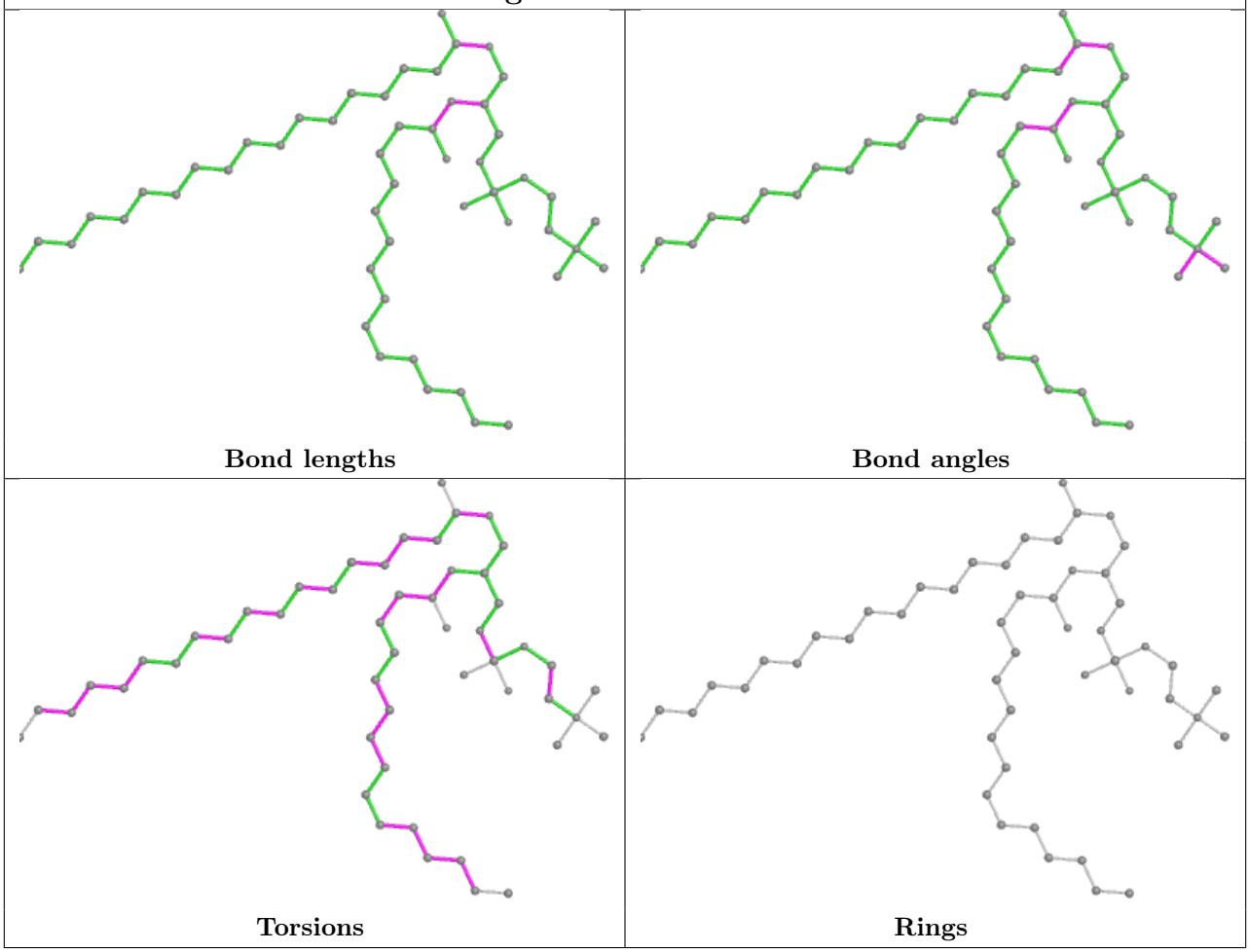
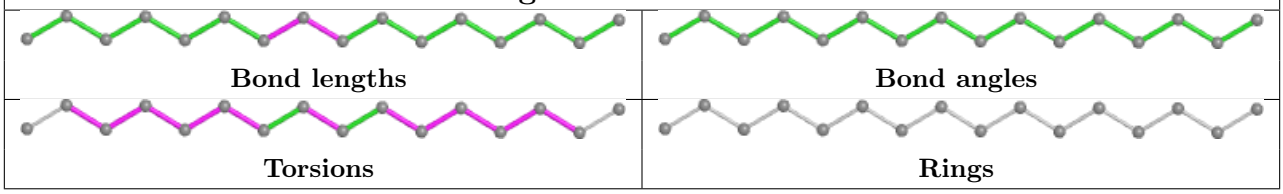
 Bond lengths	 Bond angles
 Torsions	 Rings

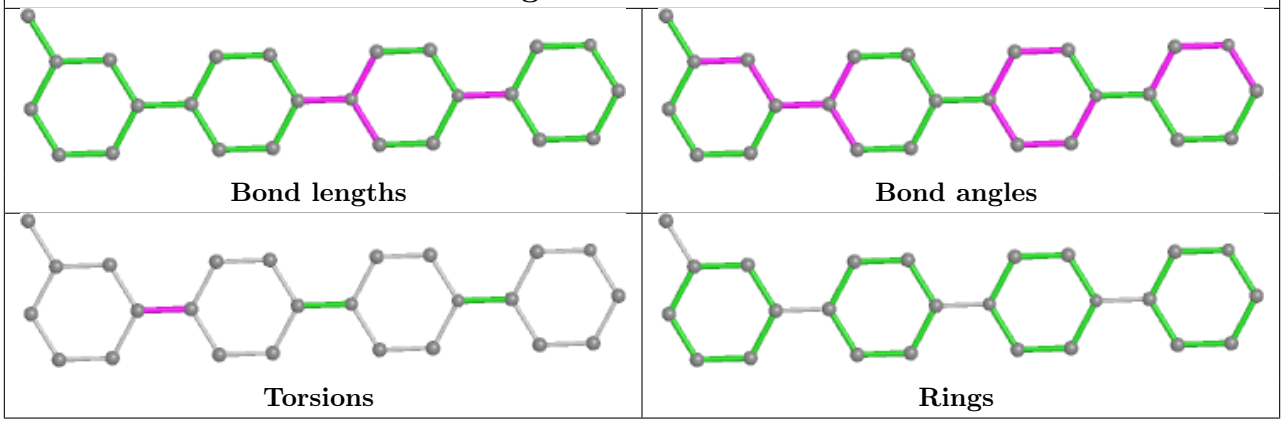
Ligand PCW B 716



Ligand PCW C 706



Ligand VUG B 704



Ligand PCW C 711

Bond lengths

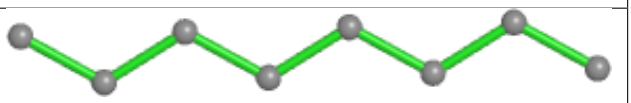
Bond angles

Torsions

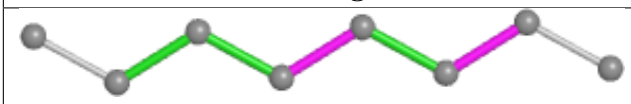
Rings

Ligand PCW A 706

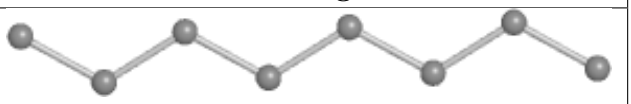
Bond lengths



Bond angles

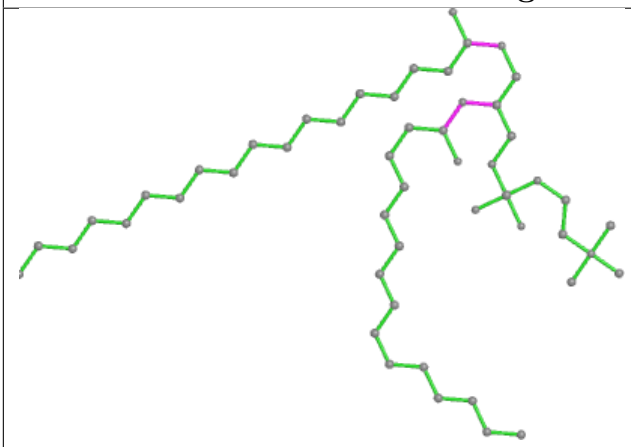


Torsions

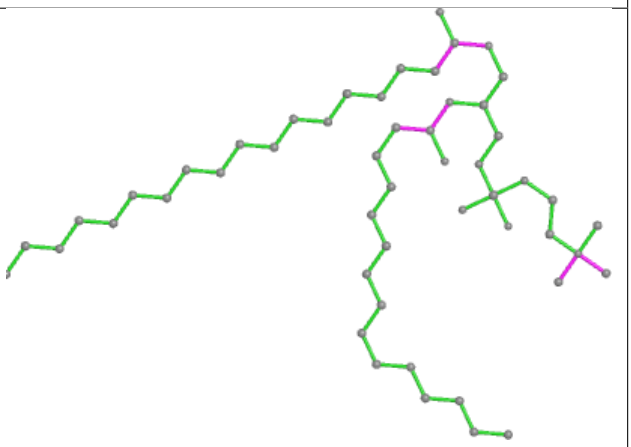


Rings

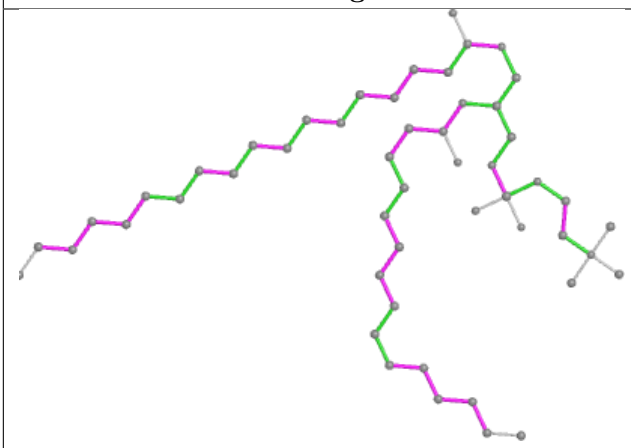
Ligand PCW C 714



Bond lengths



Bond angles



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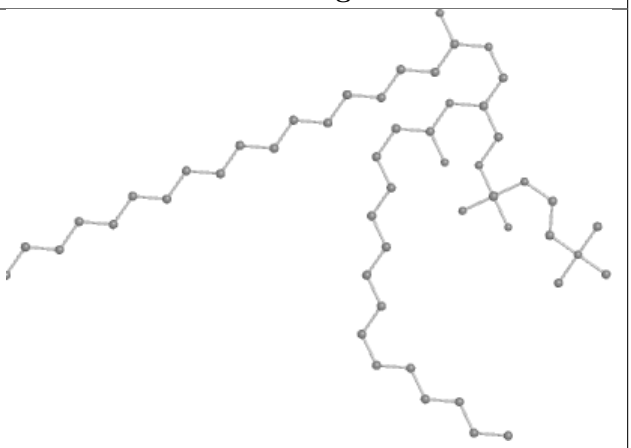
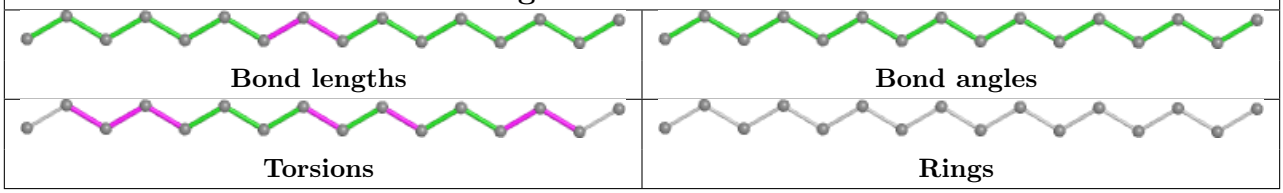
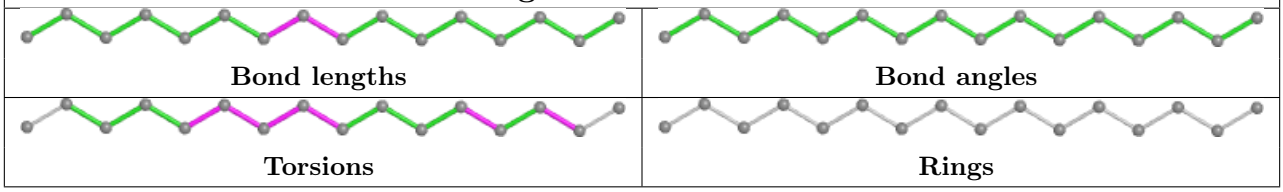


Rings

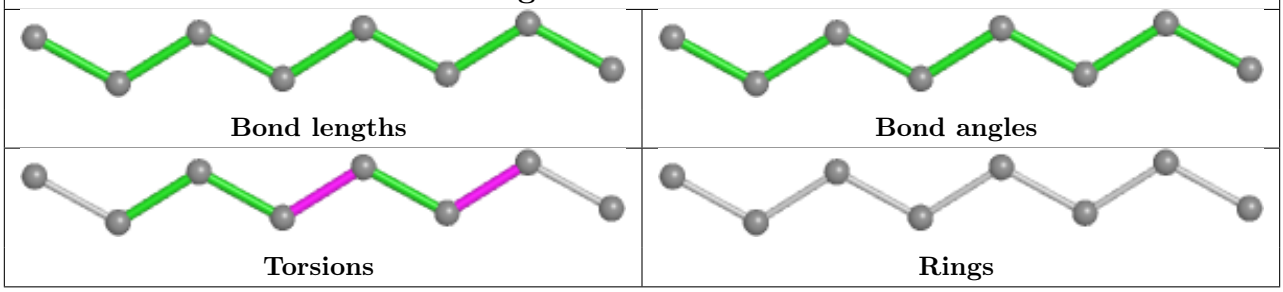
Ligand PCW D 714



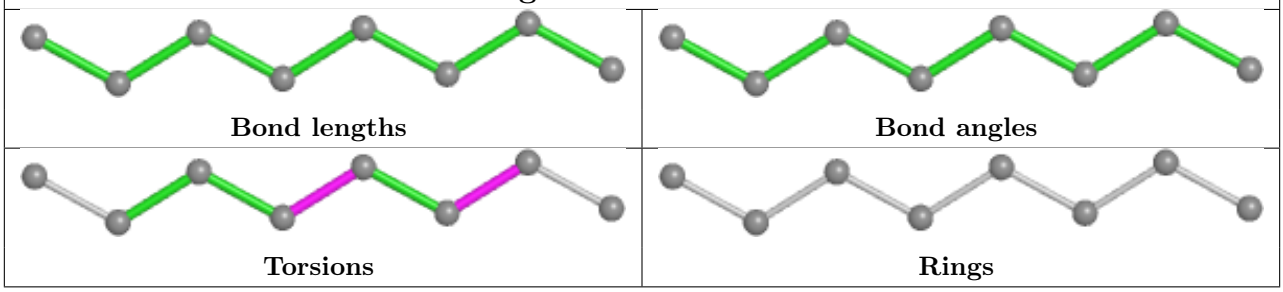
Ligand PCW D 706



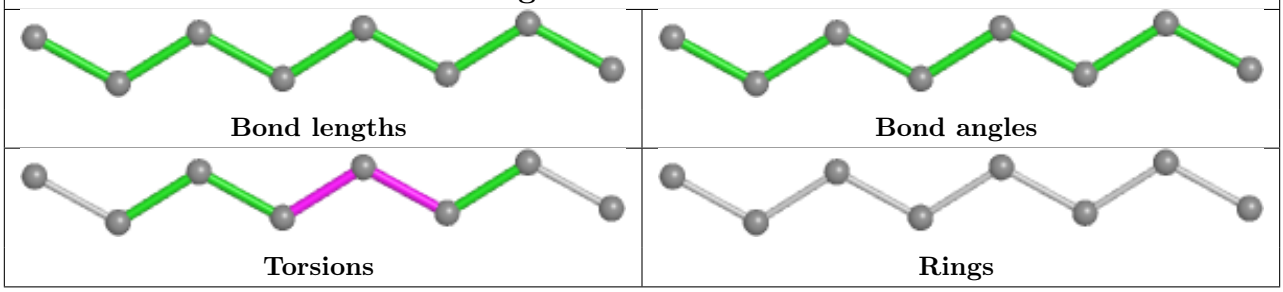
Ligand PCW D 711



Ligand PCW B 710



Ligand PCW A 707



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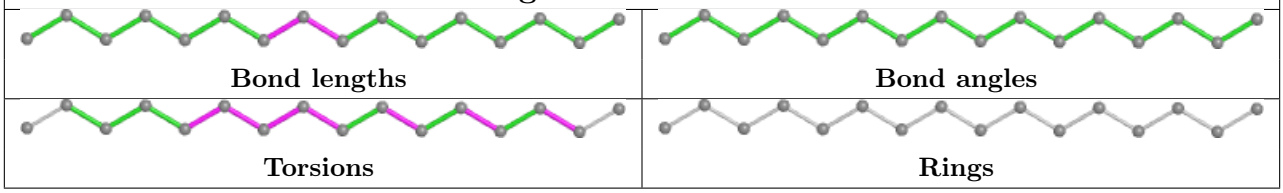

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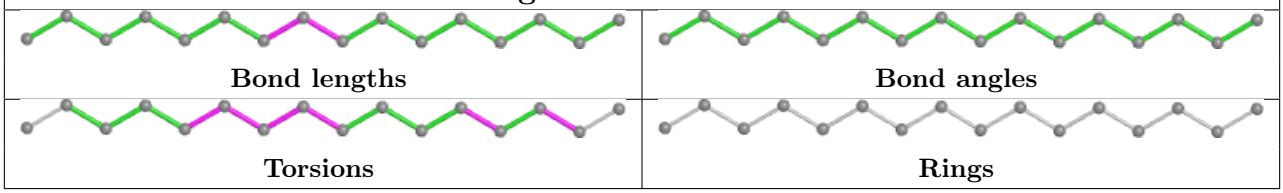
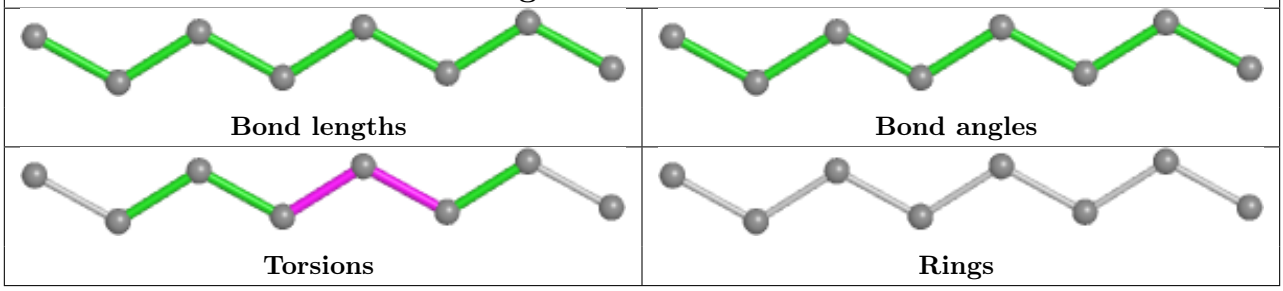


Ligand PCW B 711



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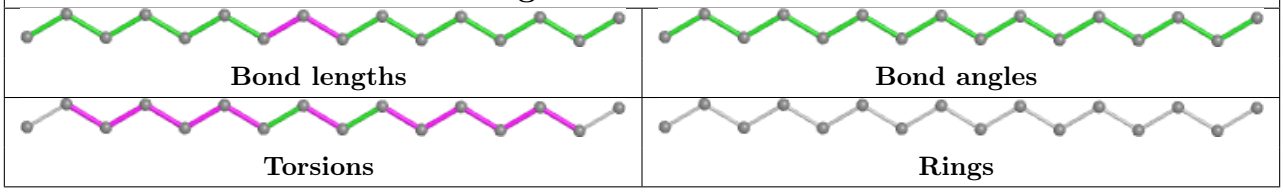
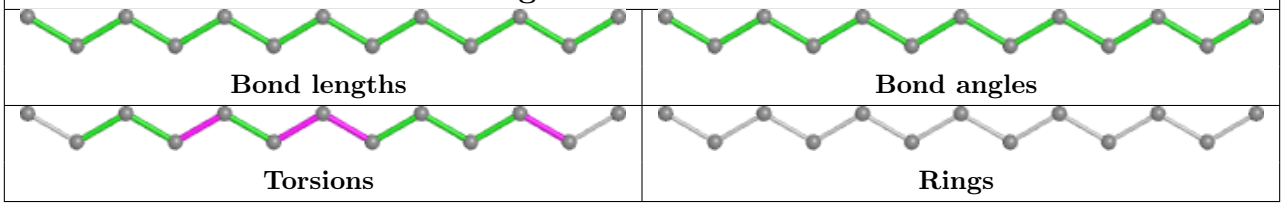
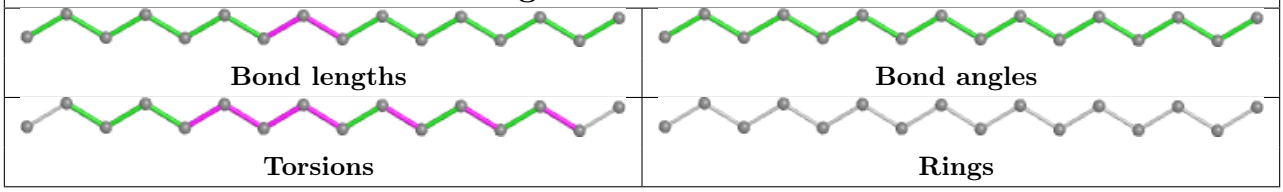


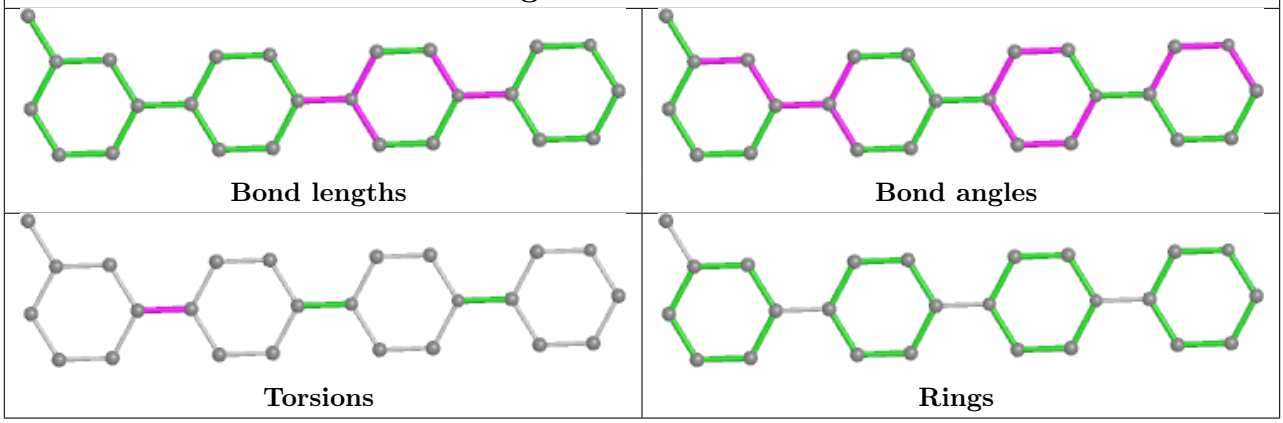
Ligand PCW C 712



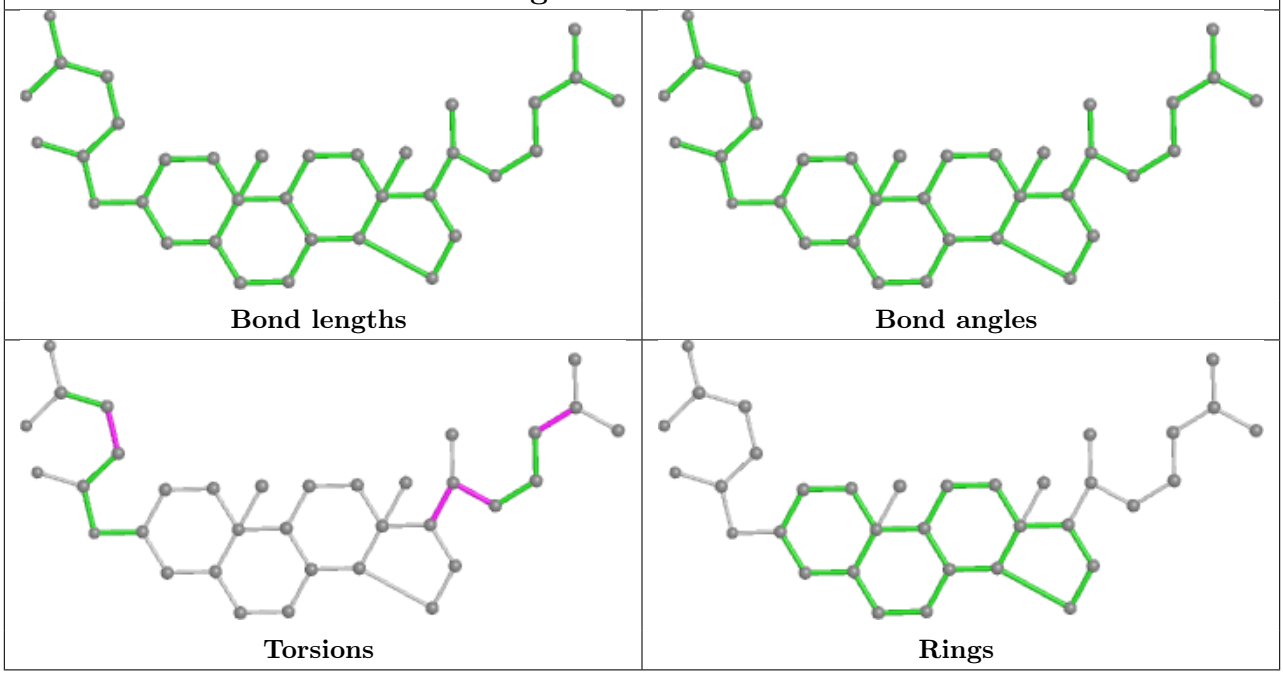
Ligand PCW C 702



Ligand VUG A 701



Ligand Y01 A 714



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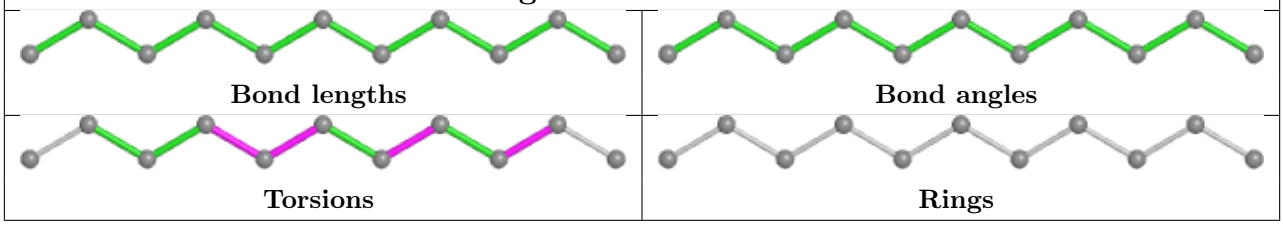

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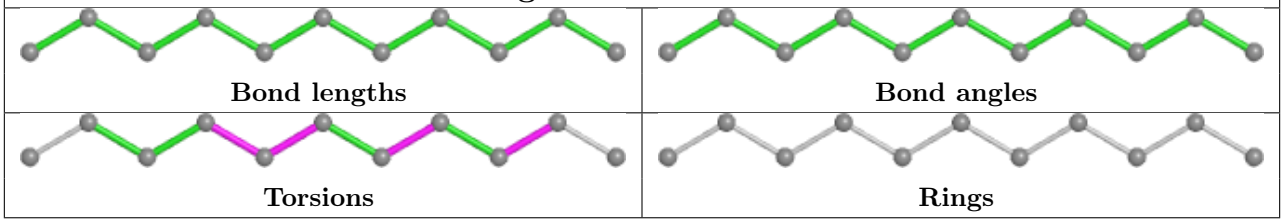

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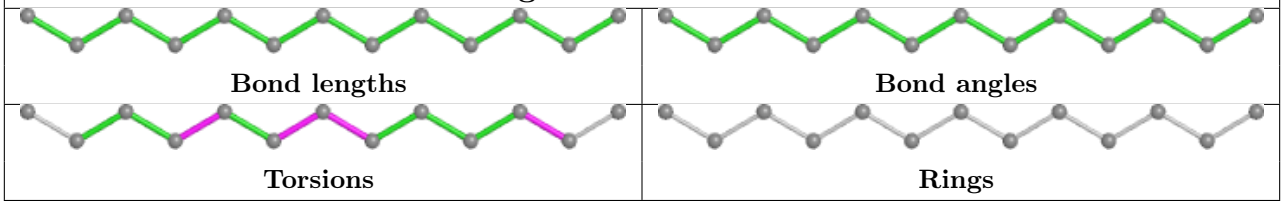

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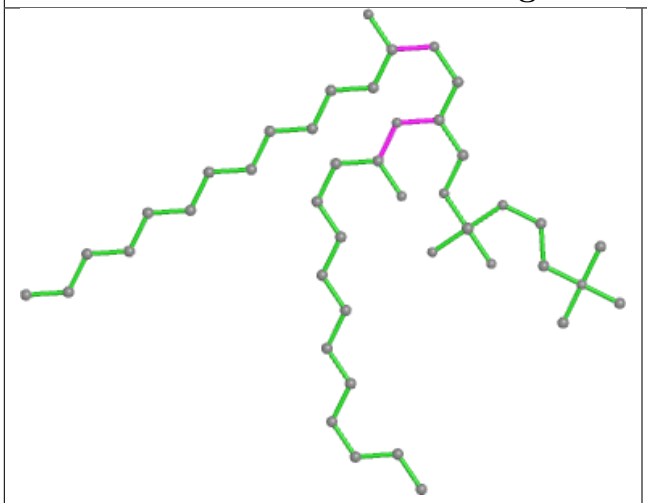
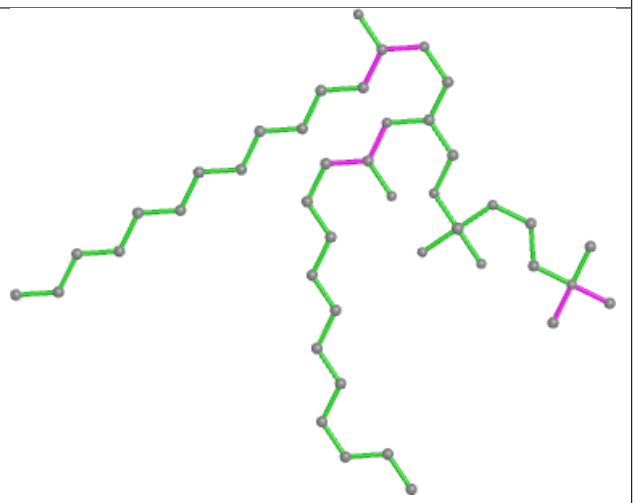
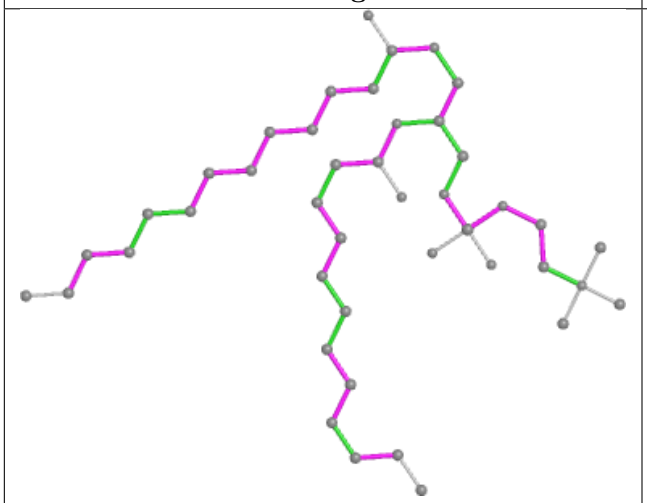


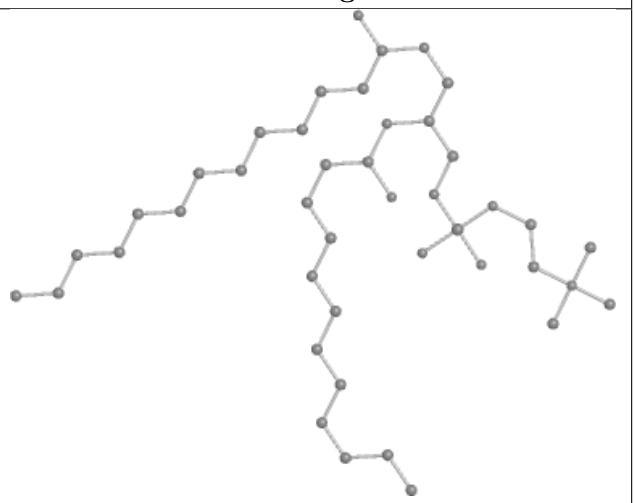
Bond lengths



Bond angles

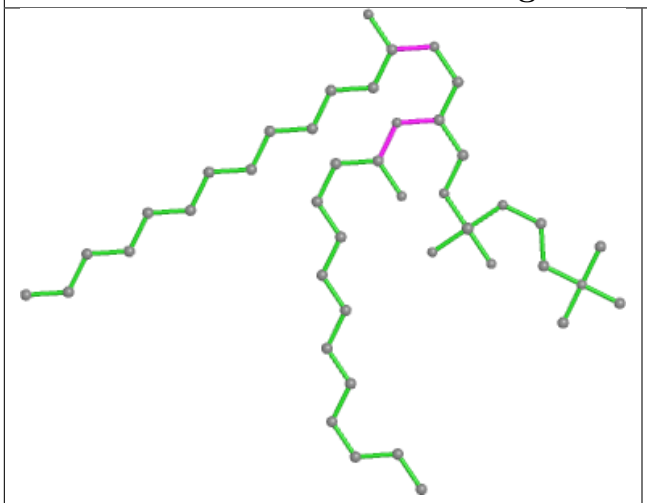


Torsions

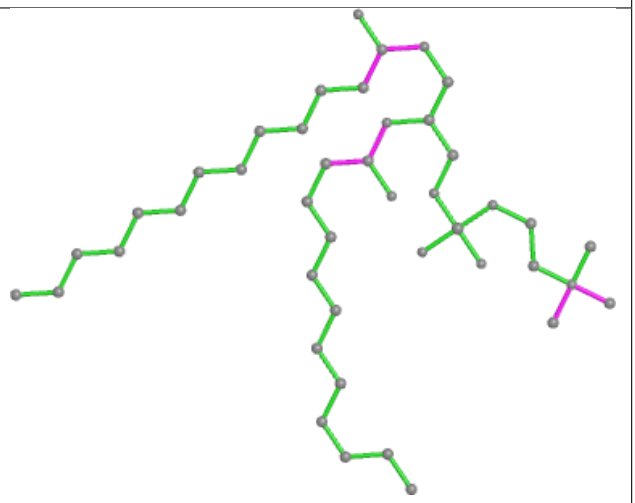


Rings

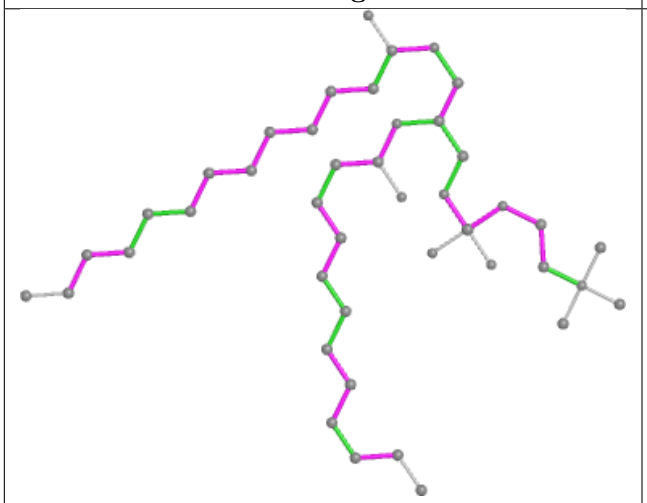
Ligand PCW A 711



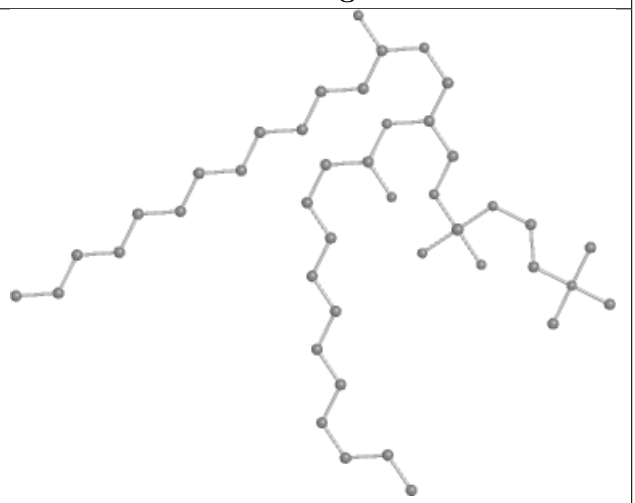
Bond lengths



Bond angles

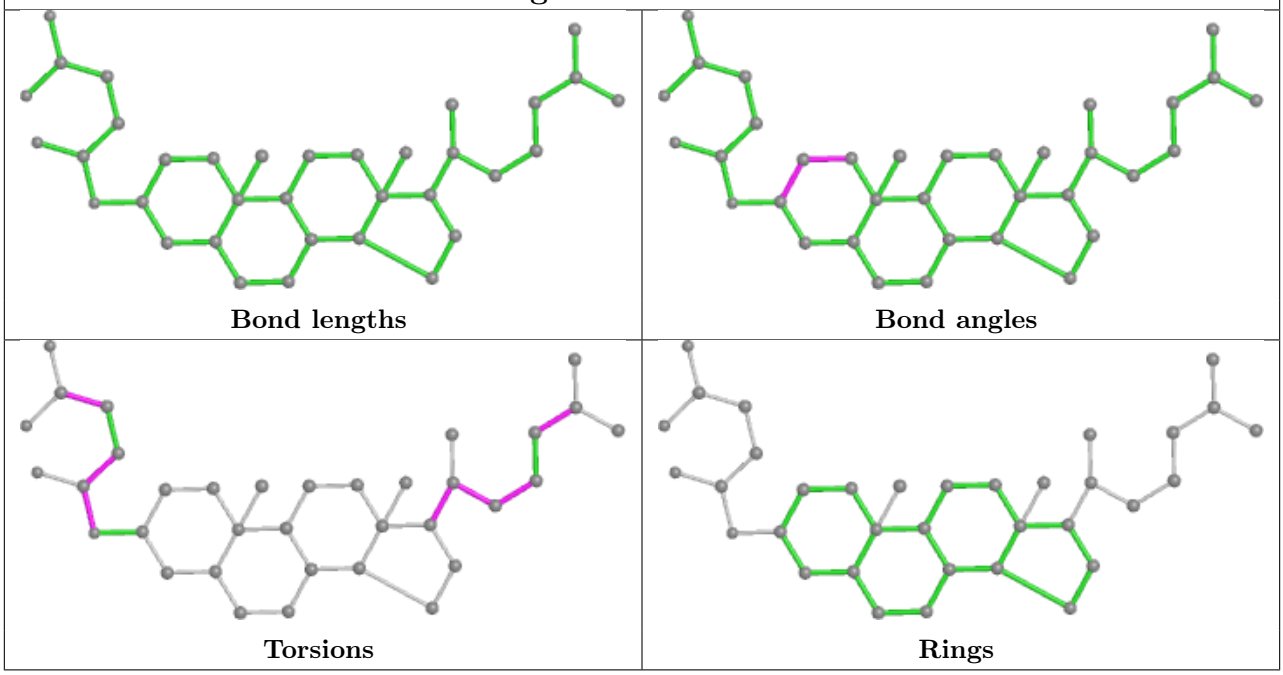


Torsions

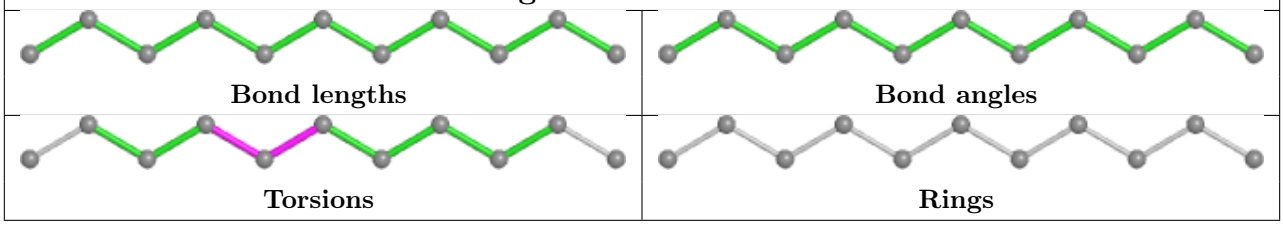


Rings

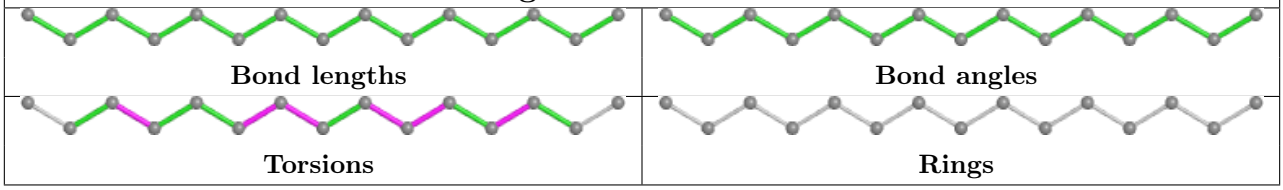
Ligand Y01 D 707



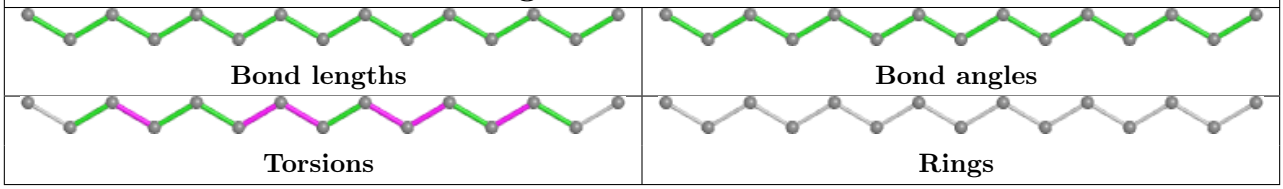
Ligand PCW C 707



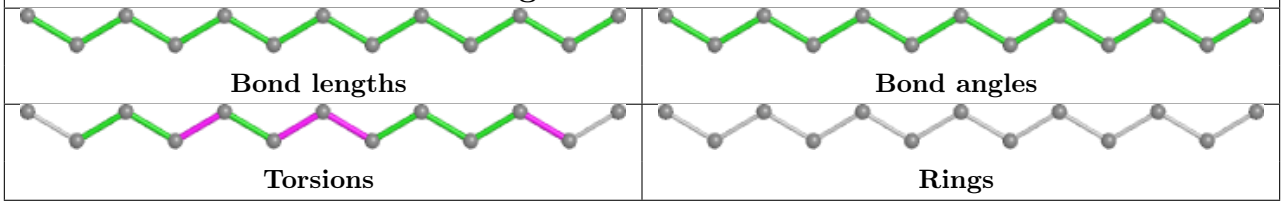
Ligand PCW B 702



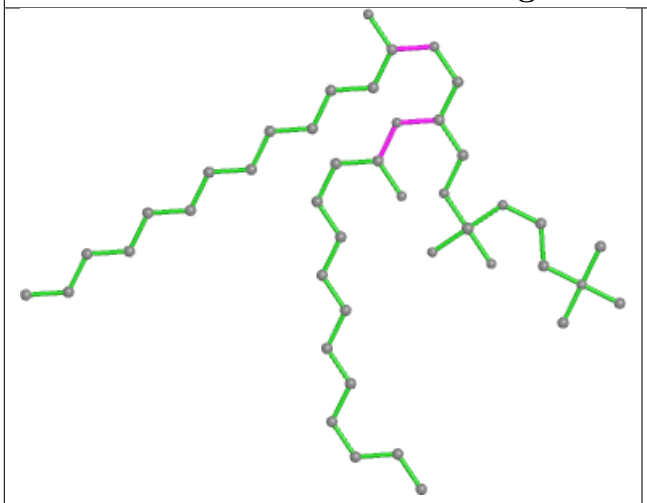
Ligand PCW A 715



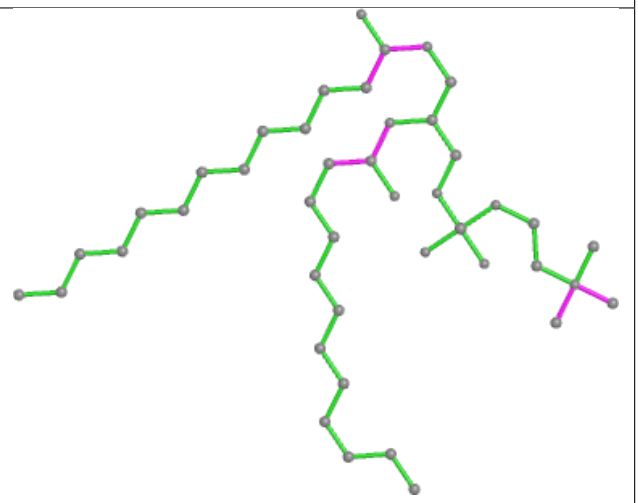
Ligand PCW B 714



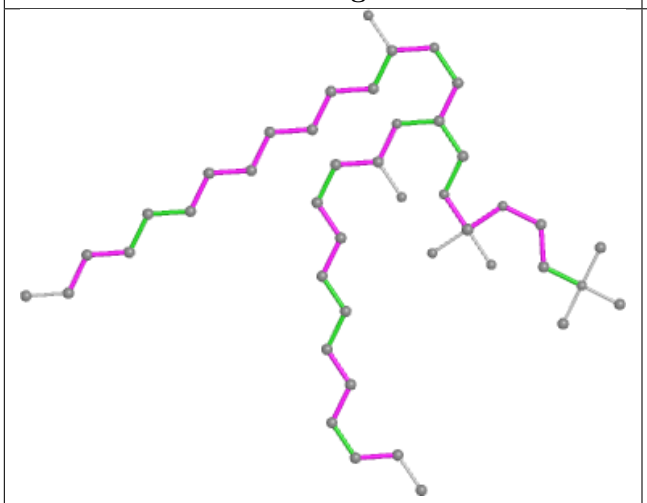
Ligand PCW D 702



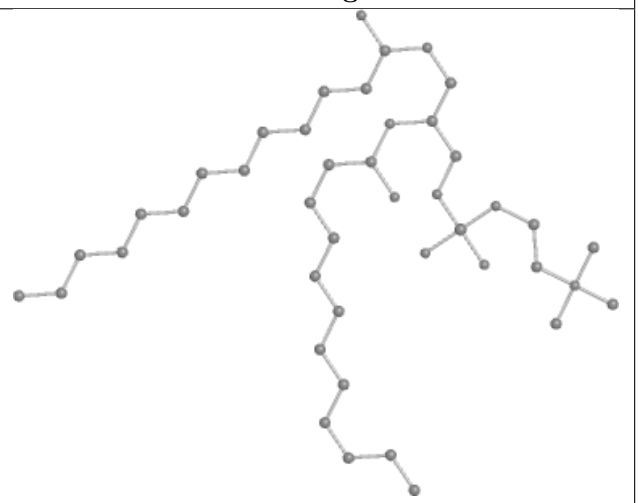
Bond lengths



Bond angles

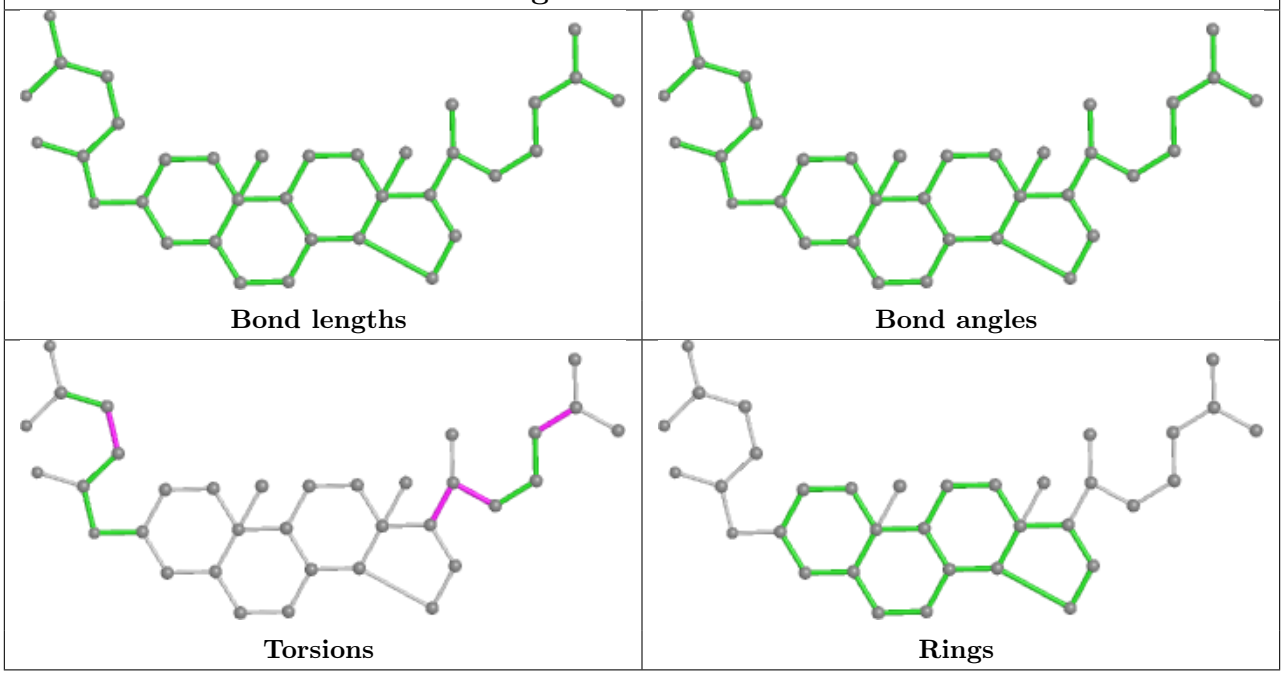


Torsions

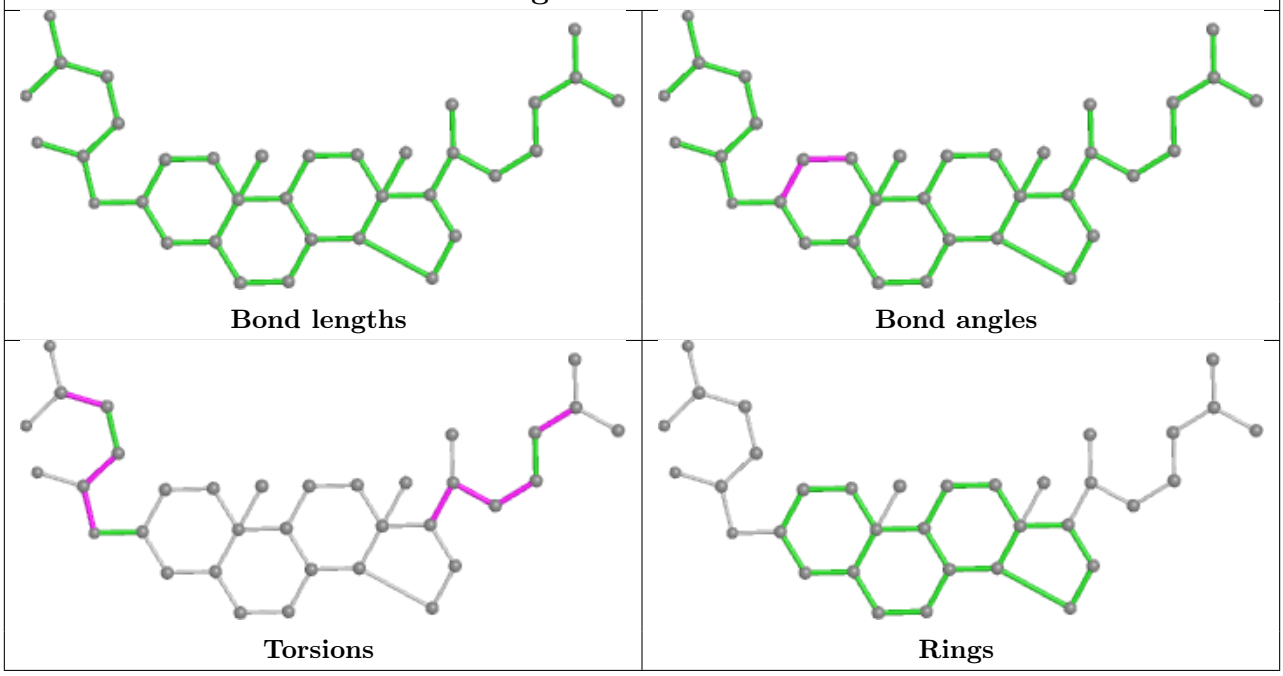


Rings

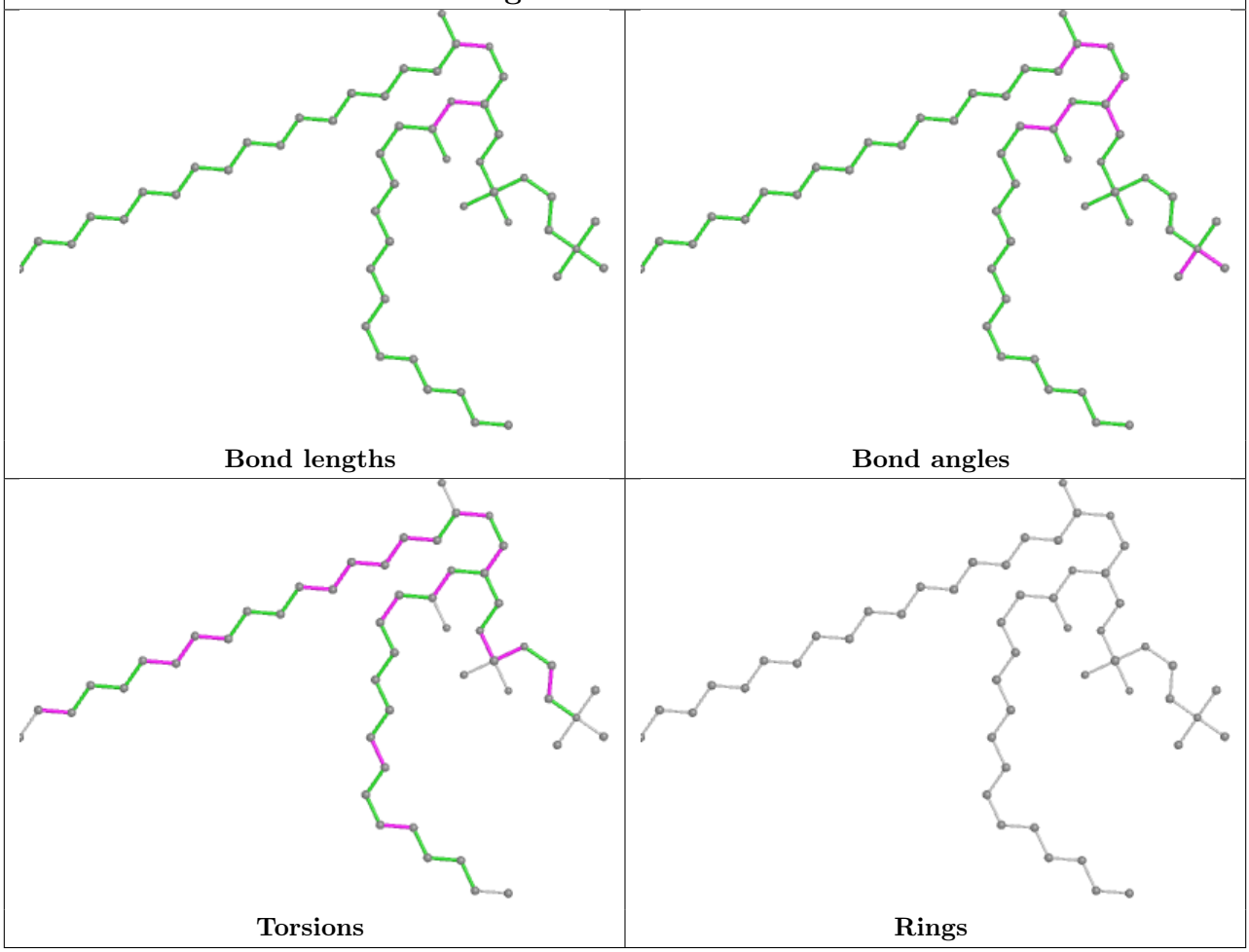
Ligand Y01 B 701



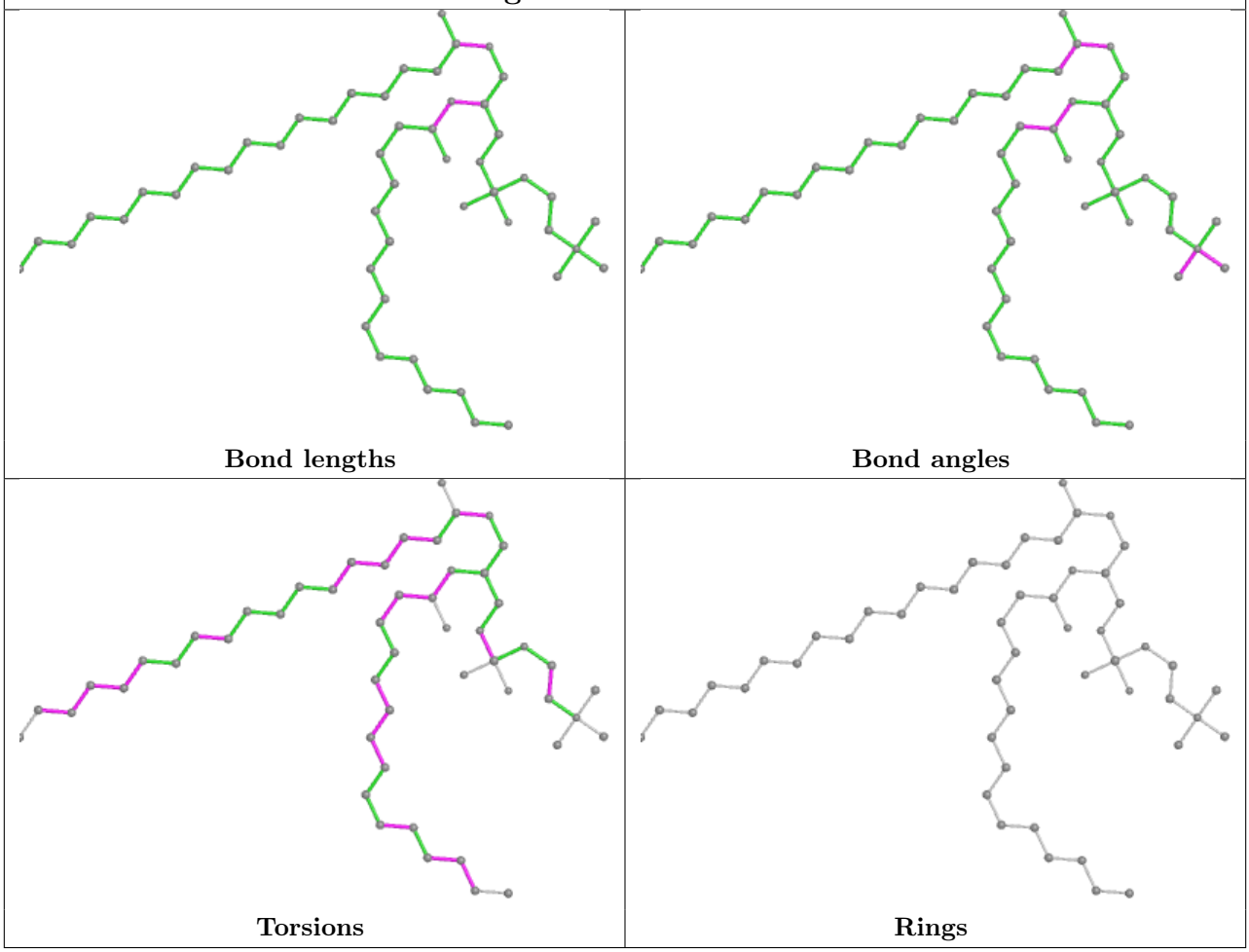
Ligand Y01 B 705



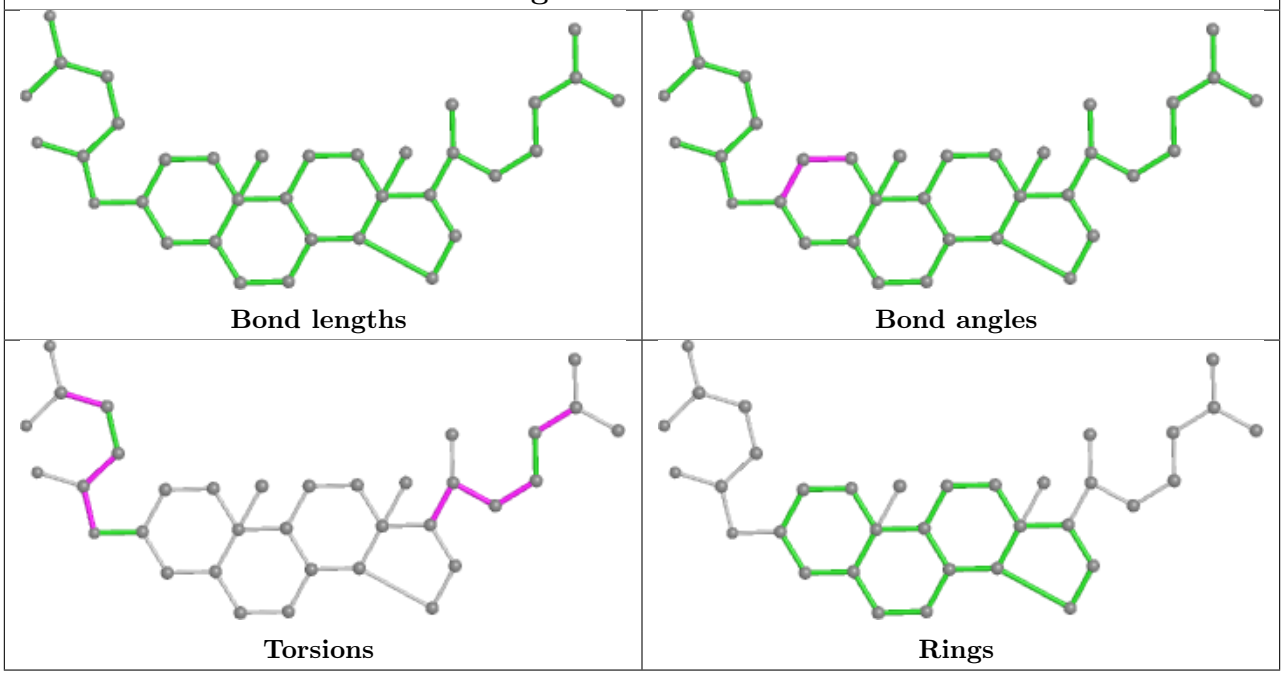
Ligand PCW A 703

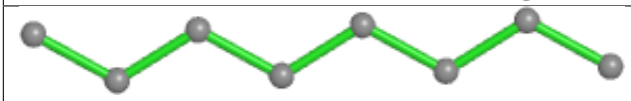
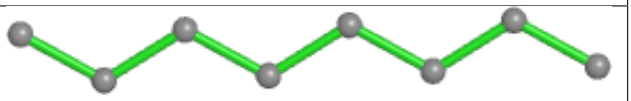
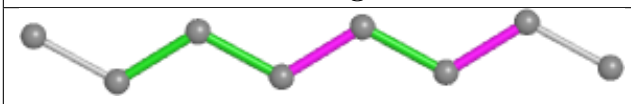
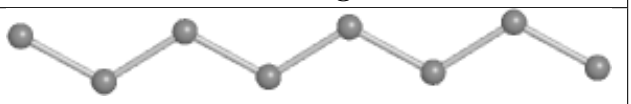


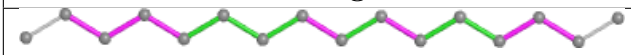
Ligand PCW D 703

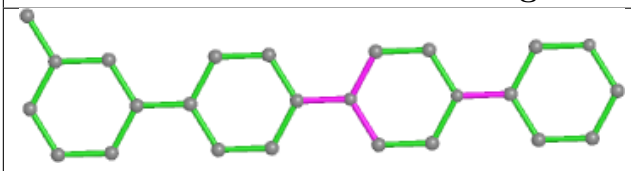
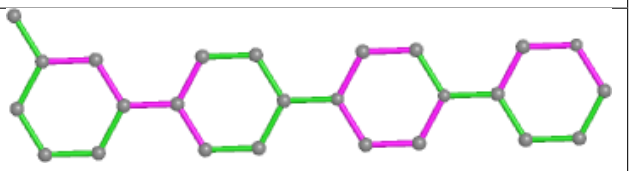
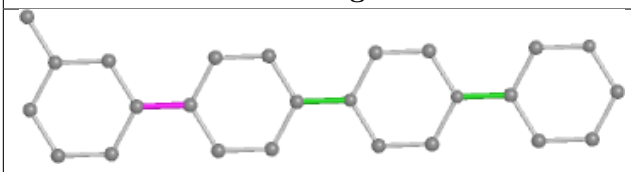
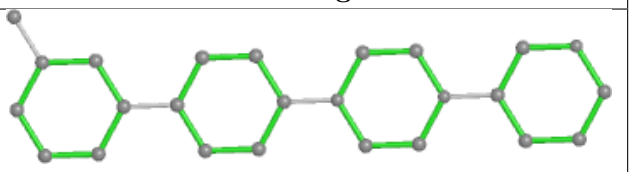


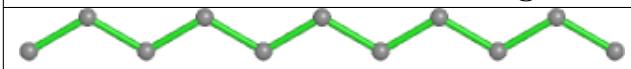
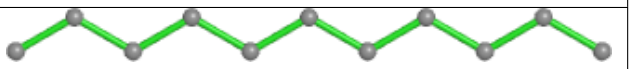
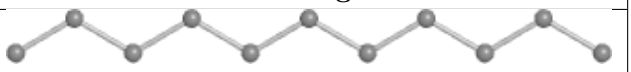
Ligand Y01 C 704

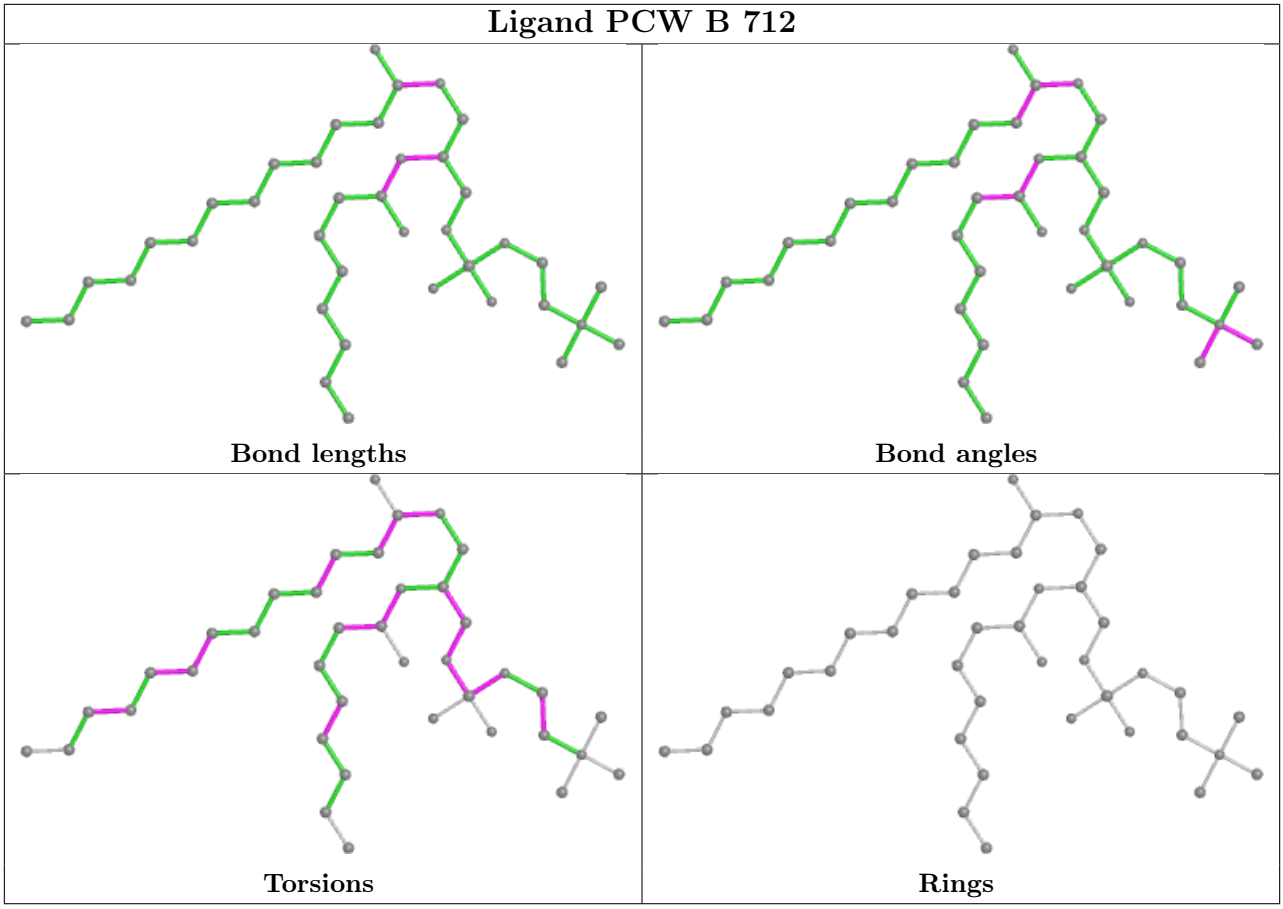


Ligand PCW C 708	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCW A 709	
Bond lengths	Bond angles
 Torsions	Rings

Ligand VUG A 713	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCW A 705	
 Bond lengths	 Bond angles
Torsions	 Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

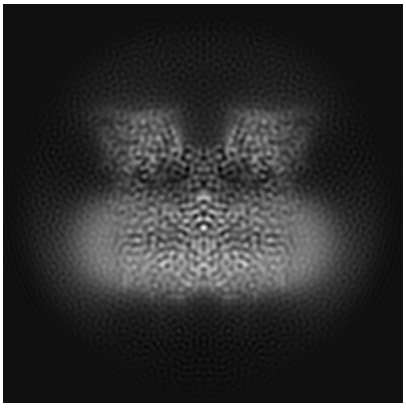
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22663. These allow visual inspection of the internal detail of the map and identification of artifacts.

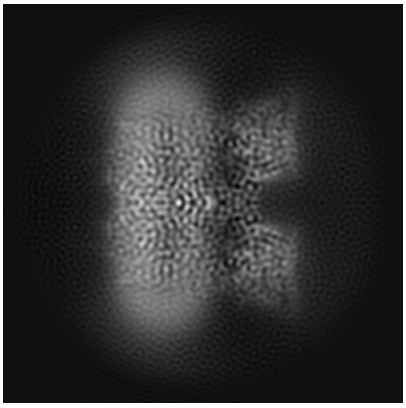
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

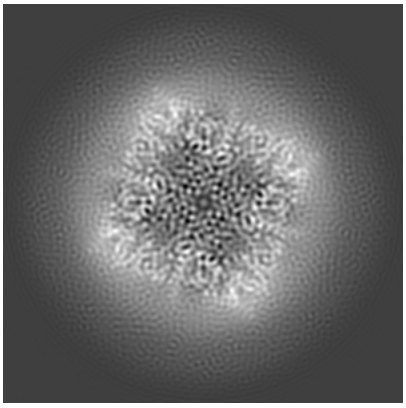
6.1.1 Primary map



X



Y

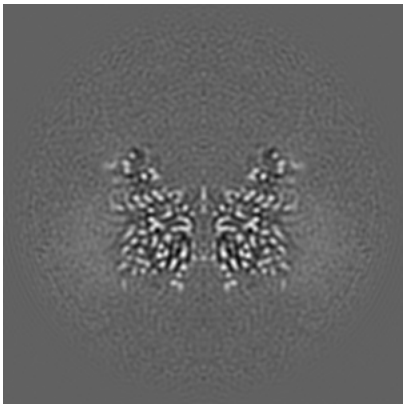


Z

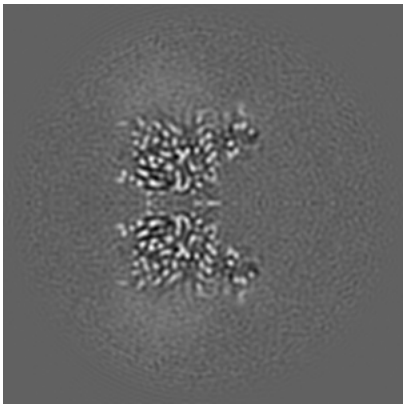
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

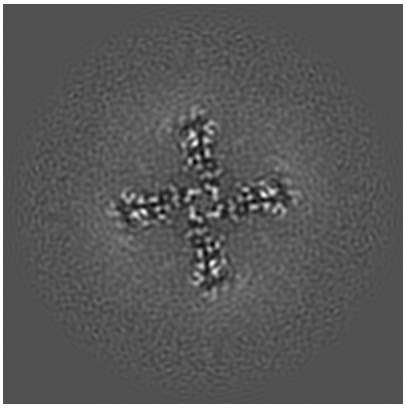
6.2.1 Primary map



X Index: 128



Y Index: 128

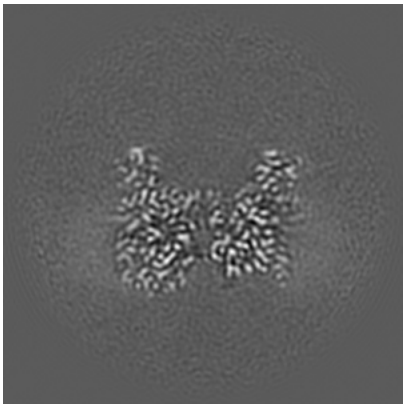


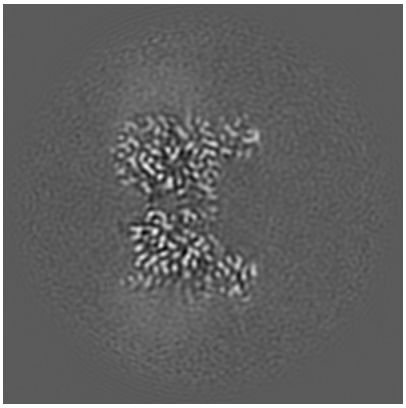
Z Index: 128

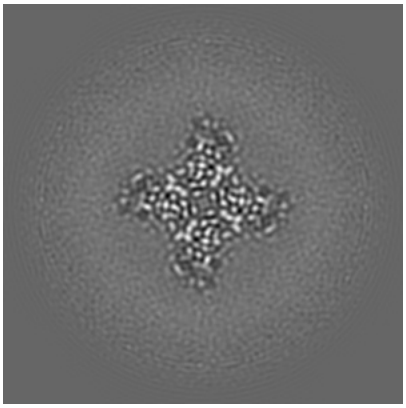
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 125

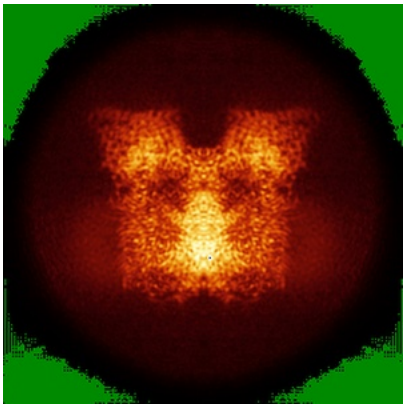

Y Index: 125

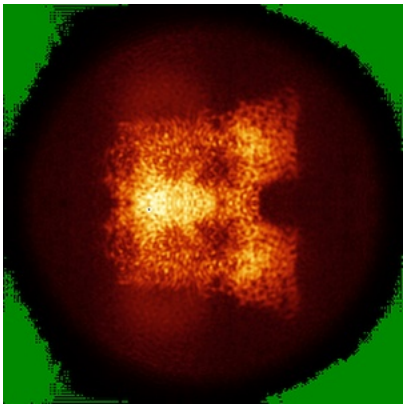

Z Index: 96

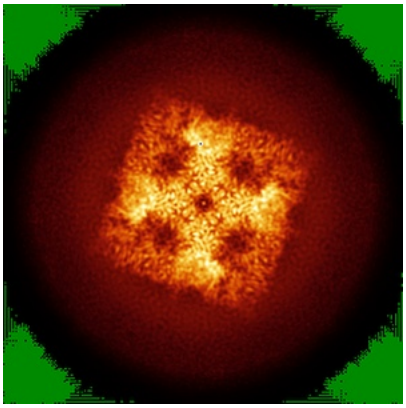
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

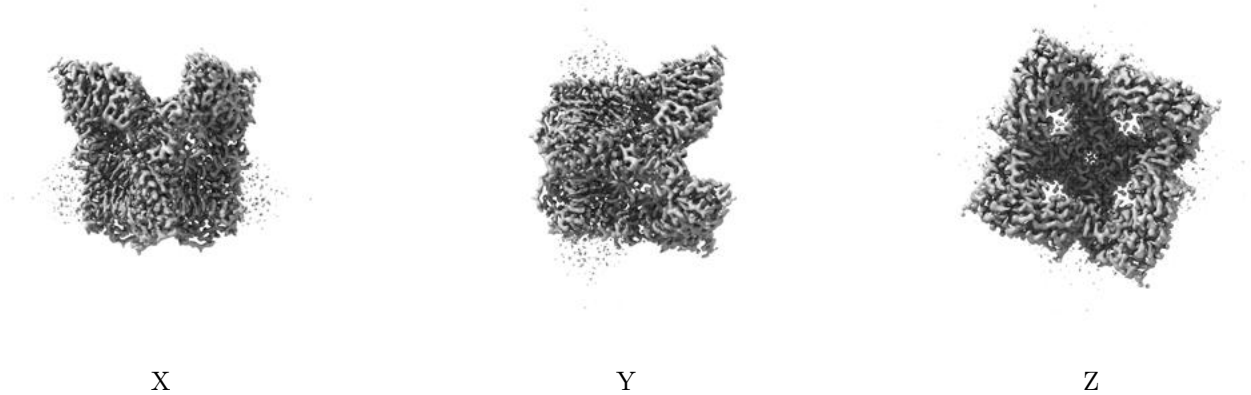

Y


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

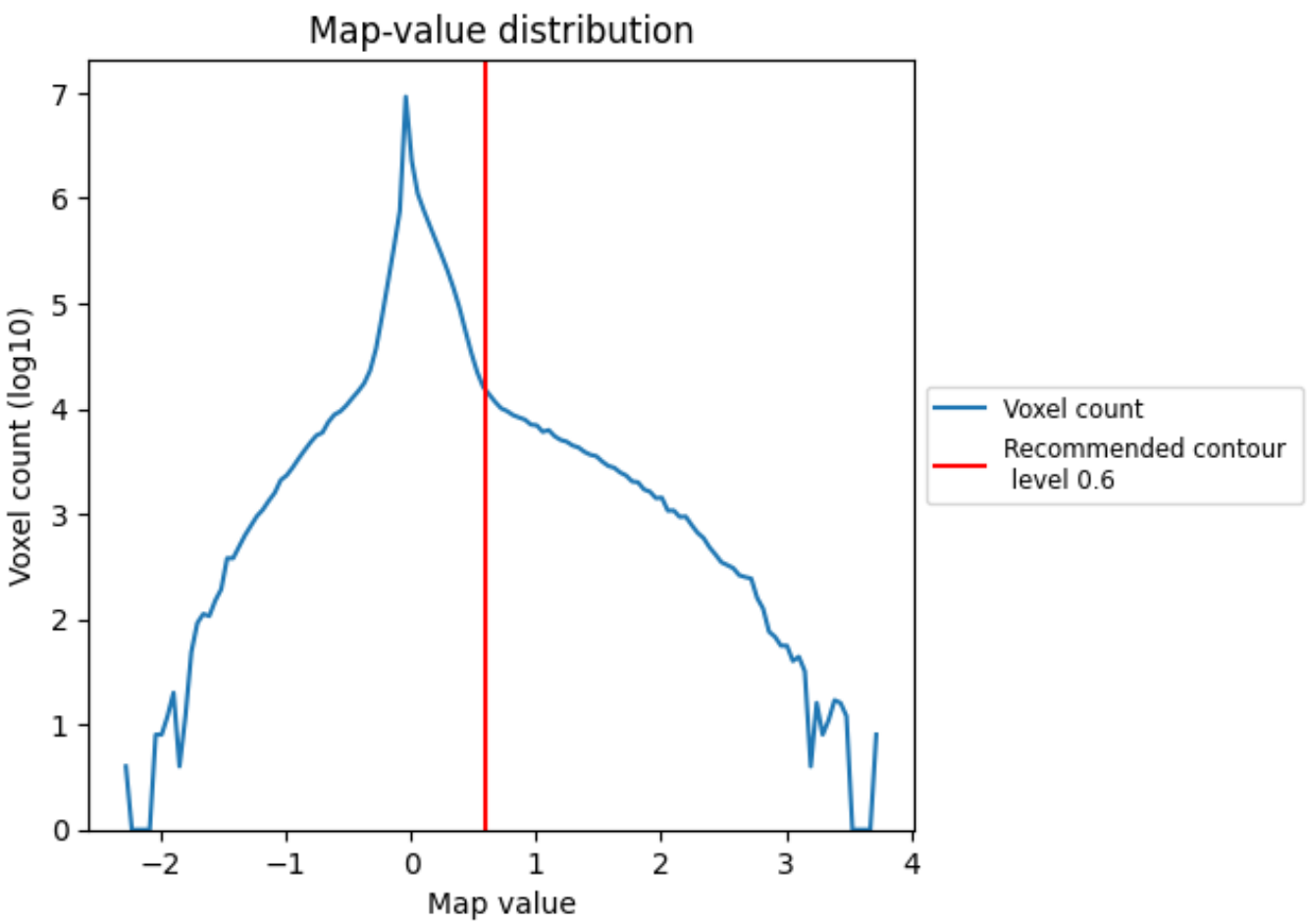
6.6 Mask visualisation (i)

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

7 Map analysis (i)

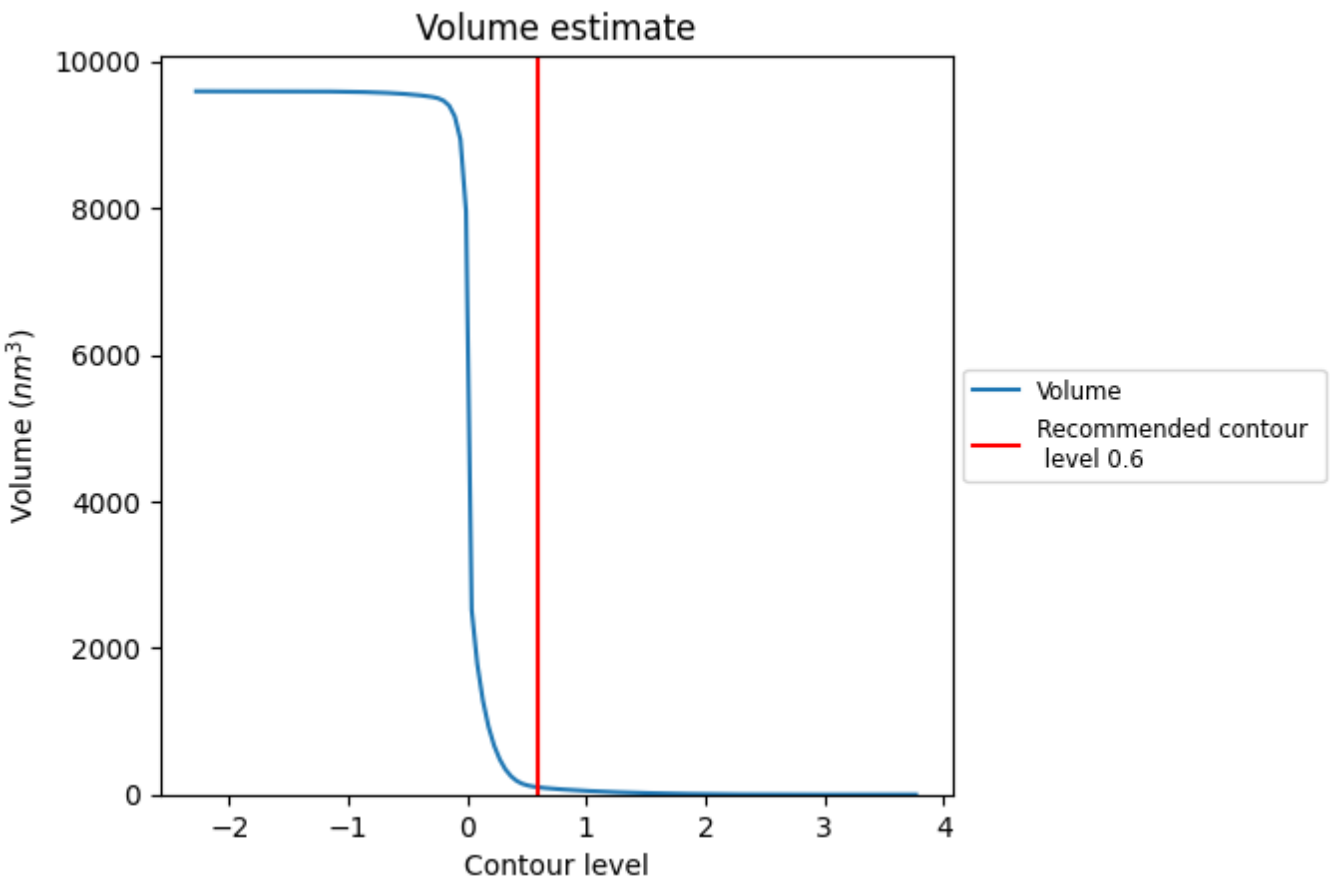
This section contains the results of statistical analysis of the map.

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.

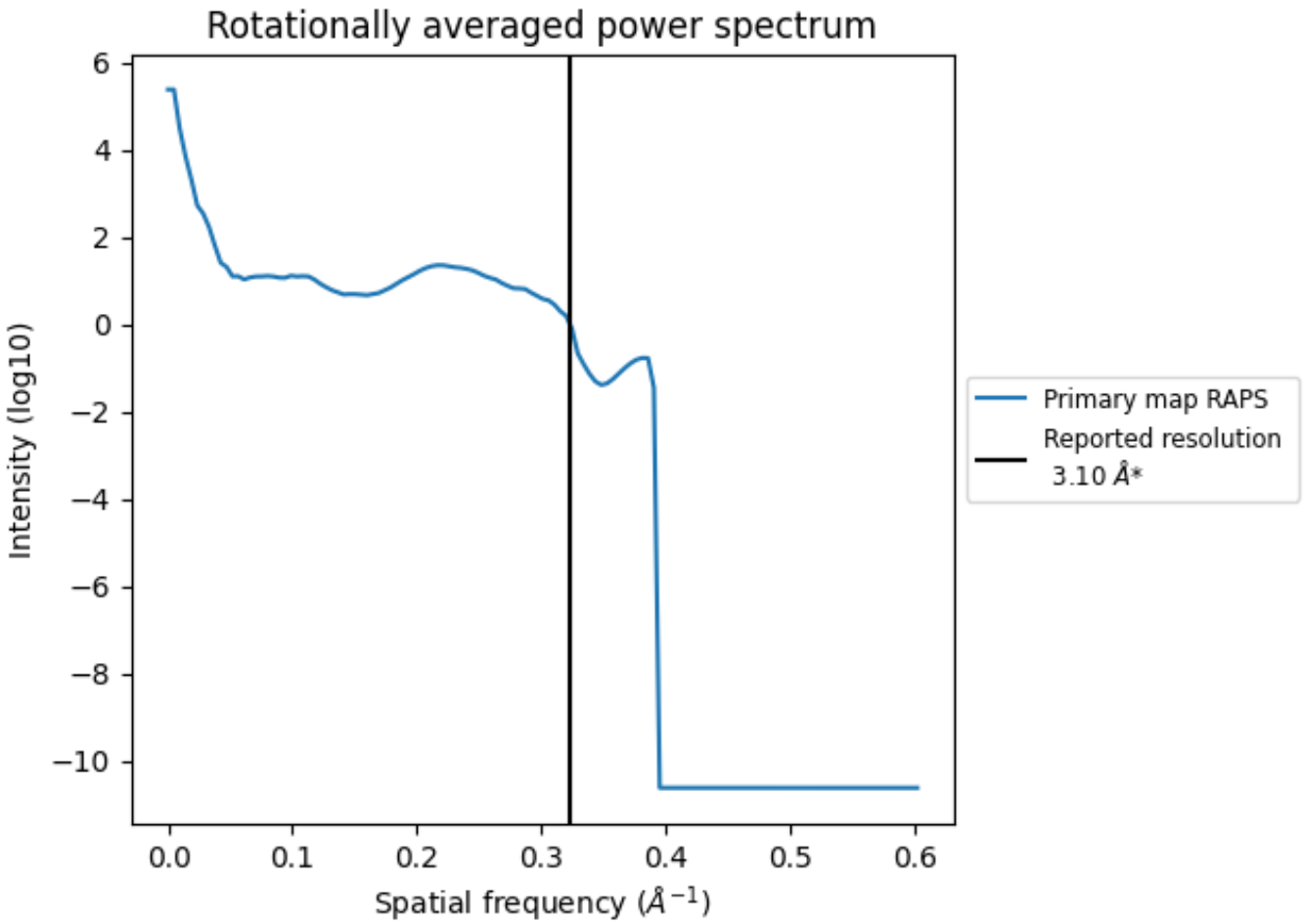
7.2 Volume estimate (i)



The volume at the recommended contour level is 99 nm^3; this corresponds to an approximate mass of 89 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 0.323 Å^{-1}

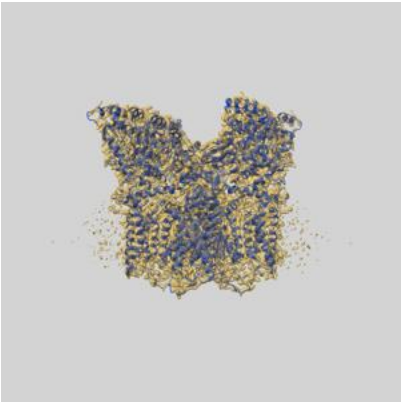
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

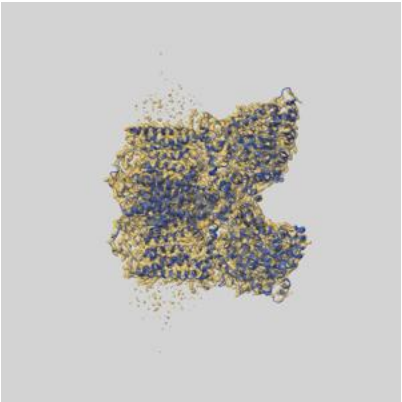
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22663 and PDB model 7K4B. Per-residue inclusion information can be found in section 3 on page 9.

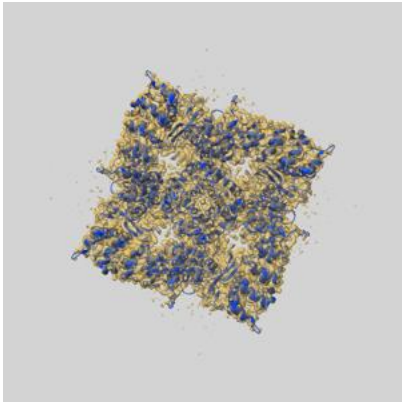
9.1 Map-model overlay (i)



X



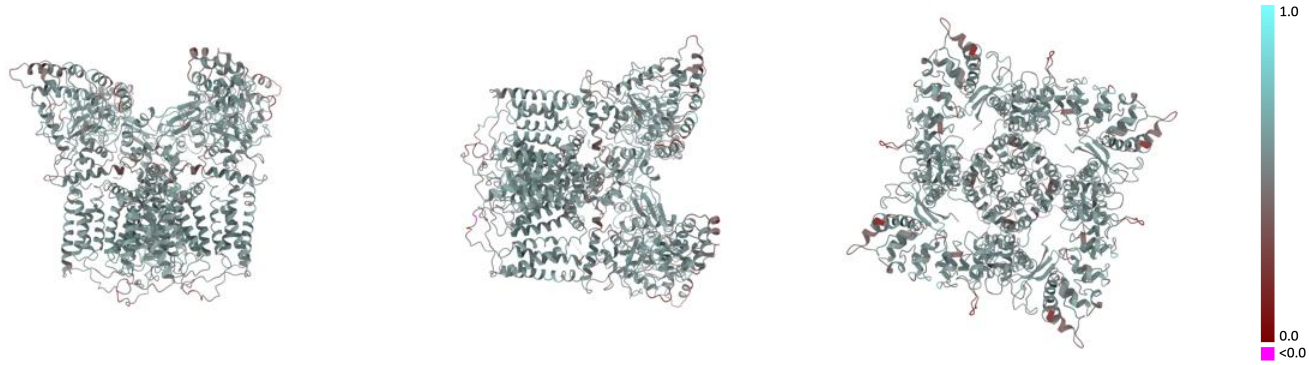
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

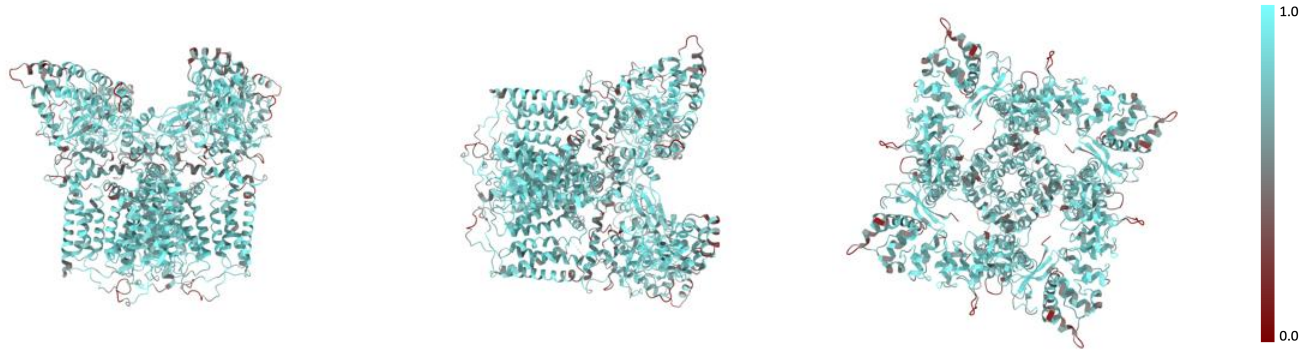
9.2 Q-score mapped to coordinate model (i)



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.

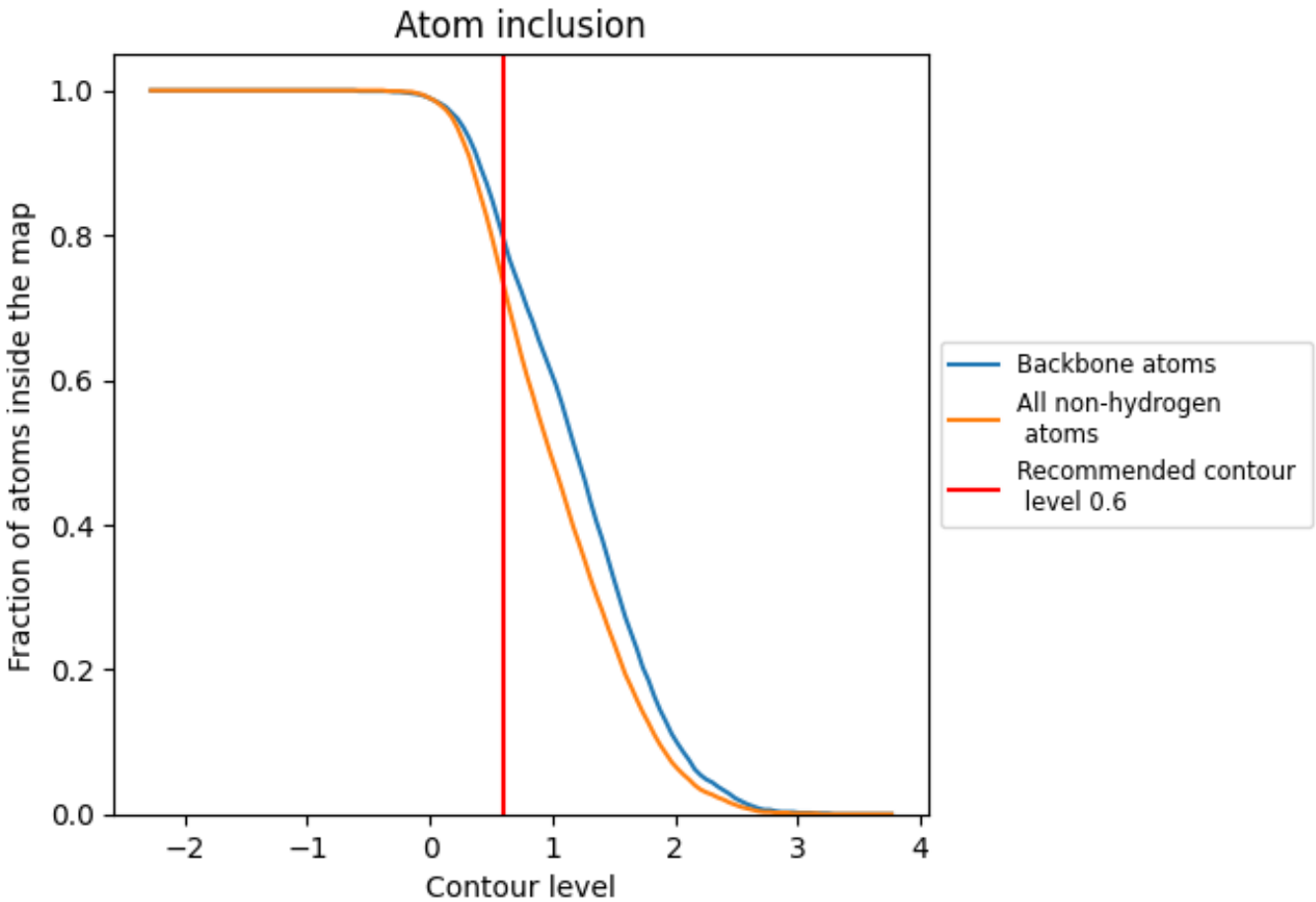
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7320	0.5330
A	0.7300	0.5320
B	0.7310	0.5330
C	0.7320	0.5350
D	0.7330	0.5340