Full wwPDB EM Validation Report ⓘ

Jan 5, 2025 – 10:41 PM EST

PDB ID	:	9CUJ
EMDB ID	:	EMD-45935
Title	:	Structure of human full-length derived TRPV6 channel in apo open state
Authors	:	Neuberger, A.; Nadezhdin, K.D.; Sobolevsky, A.I.
Deposited on	:	2024-07-26
Resolution	:	2.78 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

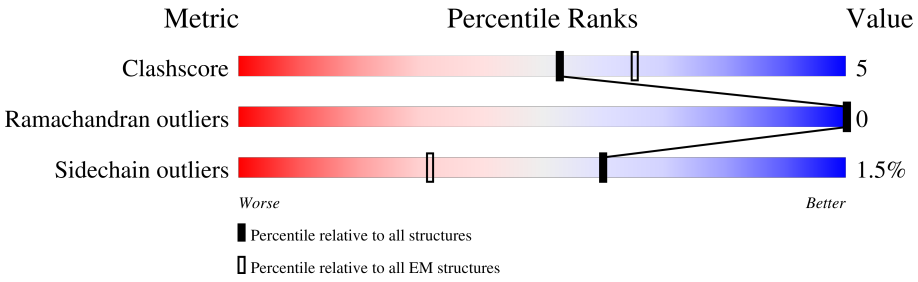
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.78 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	765	71% 8% • 20%
1	B	765	71% 9% 20%
1	C	765	71% 8% • 20%
1	D	765	71% 8% • 20%

2 Entry composition

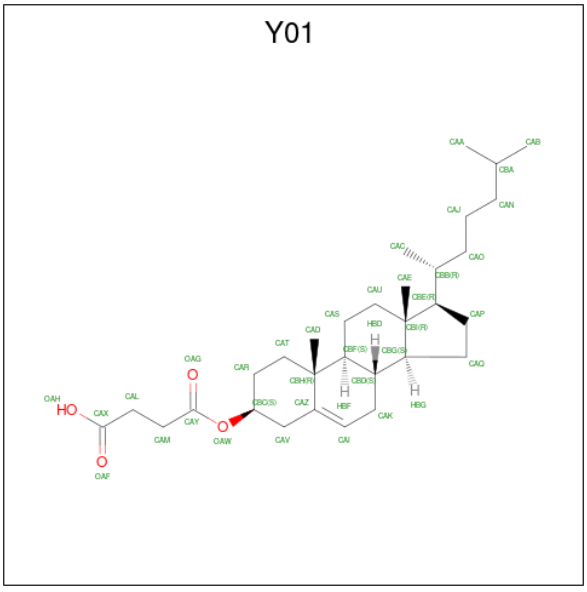
There are 6 unique types of molecules in this entry. The entry contains 21557 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	610	Total	C	N	O	S	0	0
			4895	3164	829	862	40		
1	B	610	Total	C	N	O	S	0	0
			4895	3164	829	862	40		
1	C	610	Total	C	N	O	S	0	0
			4895	3164	829	862	40		
1	D	610	Total	C	N	O	S	0	0
			4895	3164	829	862	40		

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	

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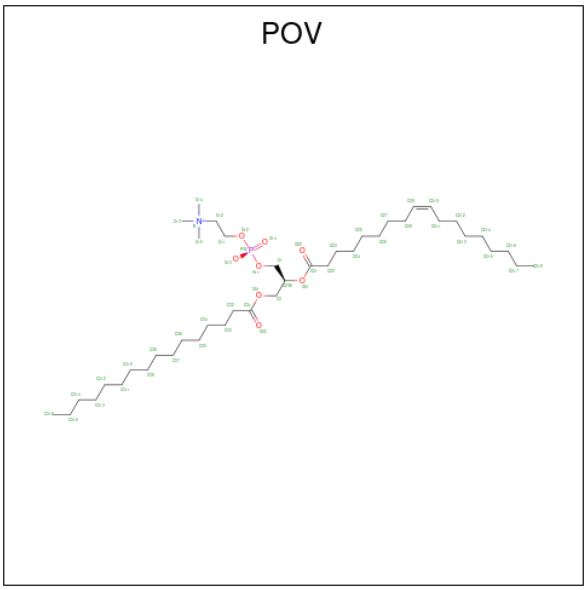
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C O 35 31 4	0
2	B	1	Total C O 35 31 4	0
2	B	1	Total C O 35 31 4	0
2	B	1	Total C O 35 31 4	0
2	C	1	Total C O 35 31 4	0
2	C	1	Total C O 35 31 4	0
2	C	1	Total C O 35 31 4	0
2	D	1	Total C O 35 31 4	0
2	D	1	Total C O 35 31 4	0
2	D	1	Total C O 35 31 4	0

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



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C O 20 18 2	0

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

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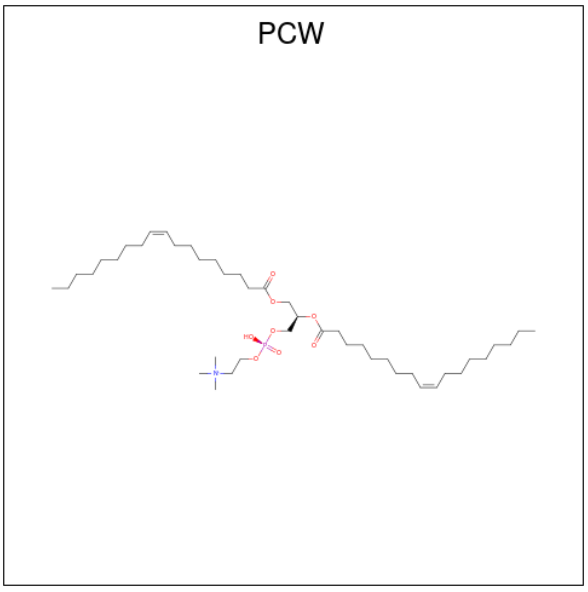
Mol	Chain	Residues	Atoms	AltConf
3	C	1	Total C N O P 52 42 1 8 1	0
3	C	1	Total C N O P 52 42 1 8 1	0
3	D	1	Total C N O P 52 42 1 8 1	0
3	D	1	Total C N O P 52 42 1 8 1	0
3	D	1	Total C N O P 52 42 1 8 1	0
3	D	1	Total C O 20 18 2	0
3	D	1	Total C N O P 52 42 1 8 1	0
3	D	1	Total C N O P 52 42 1 8 1	0
3	D	1	Total C O 19 17 2	0
3	D	1	Total C O 14 12 2	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
4	A	1	Total C 14 14	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 13 13	0
4	A	1	Total C 15 15	0
4	B	1	Total C 14 14	0
4	B	1	Total C 8 8	0
4	B	1	Total C 8 8	0
4	B	1	Total C 13 13	0
4	B	1	Total C 15 15	0
4	C	1	Total C 14 14	0
4	C	1	Total C 8 8	0
4	C	1	Total C 8 8	0
4	C	1	Total C 13 13	0
4	C	1	Total C 15 15	0
4	D	1	Total C 13 13	0
4	D	1	Total C 15 15	0
4	D	1	Total C 14 14	0
4	D	1	Total C 8 8	0
4	D	1	Total C 8 8	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

- Molecule 6 is water.

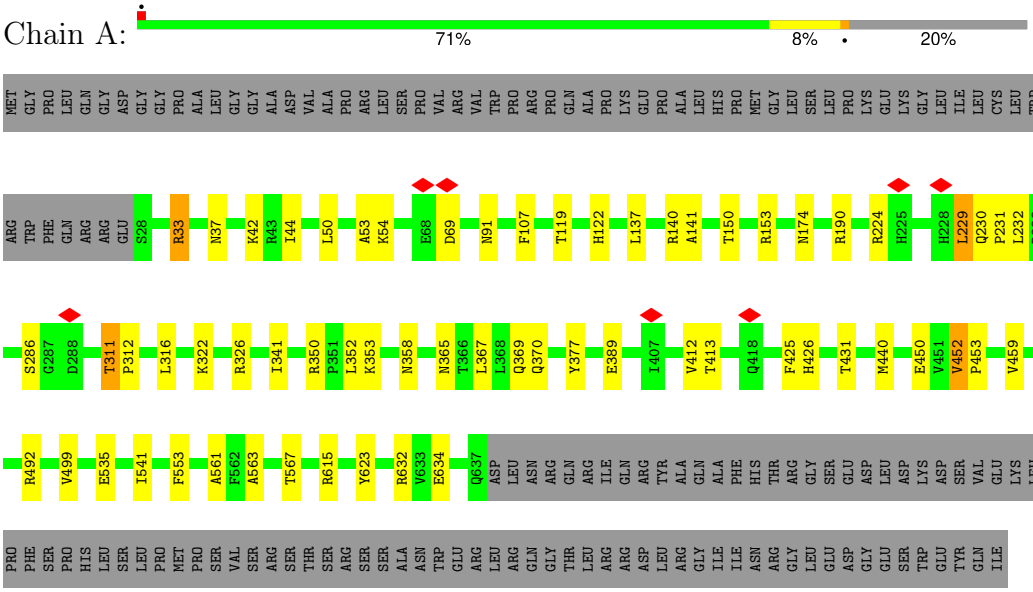
Mol	Chain	Residues	Atoms	AltConf
6	A	18	Total O 18 18	0
6	B	18	Total O 18 18	0
6	C	18	Total O 18 18	0
6	D	18	Total O 18 18	0

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.

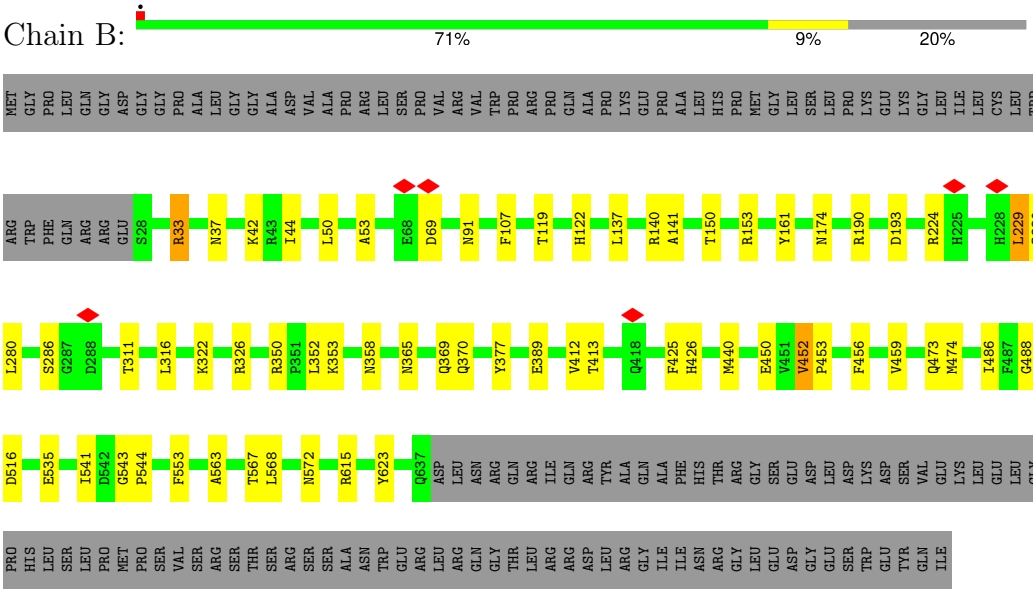
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

Chain A:



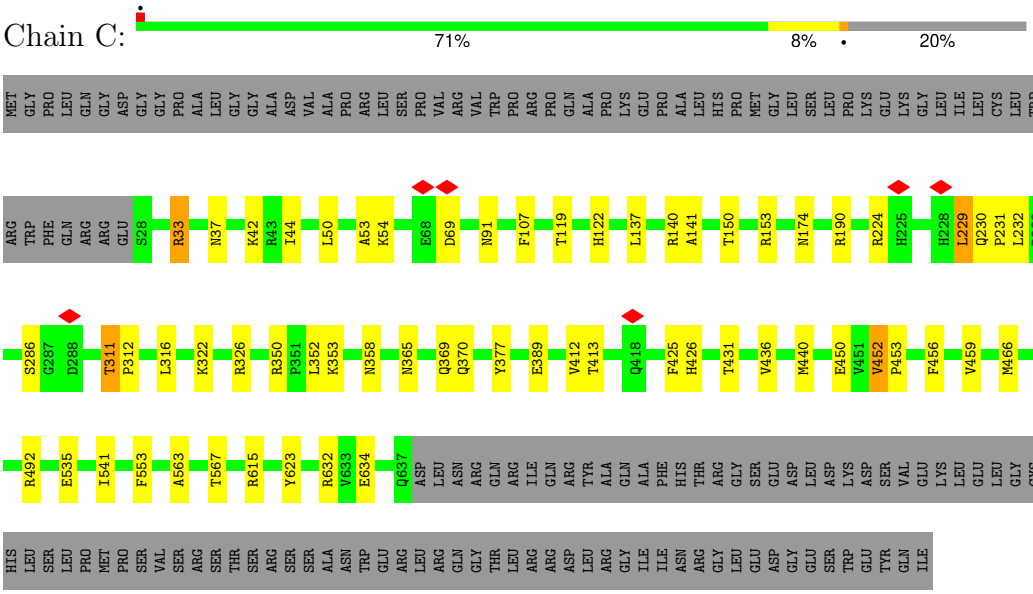
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

Chain B:



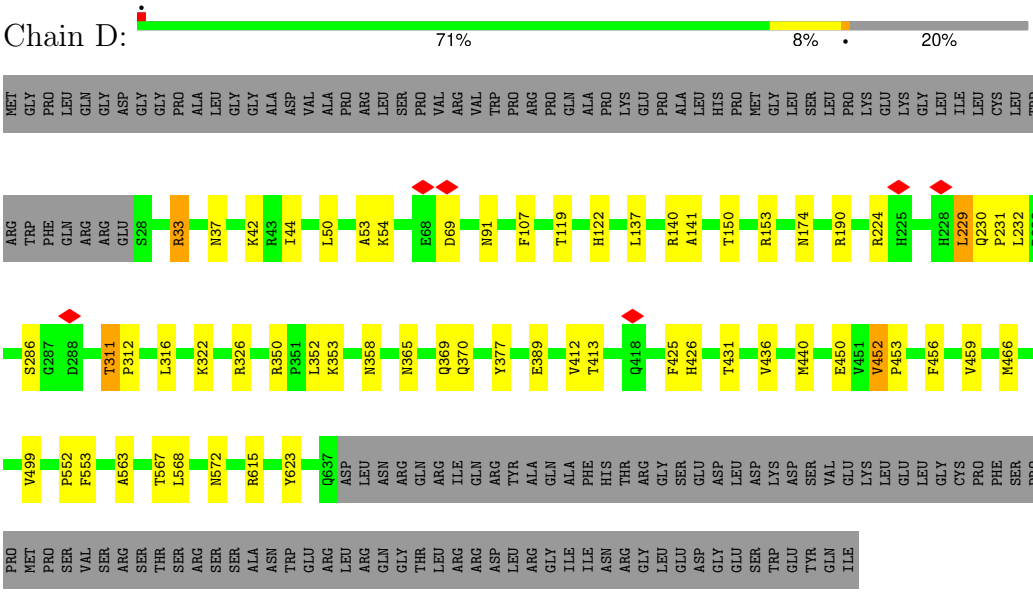
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

Chain C:



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

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	554157	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)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.509	Depositor
Minimum map value	-1.794	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.0959	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

5.1 Standard geometry

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

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	0.33	0/5008	0.58	1/6795 (0.0%)
1	B	0.33	0/5008	0.58	1/6795 (0.0%)
1	C	0.33	0/5008	0.58	1/6795 (0.0%)
1	D	0.33	0/5008	0.58	1/6795 (0.0%)
All	All	0.33	0/20032	0.58	4/27180 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	69	ASP	CB-CG-OD1	8.66	126.10	118.30
1	B	69	ASP	CB-CG-OD1	8.62	126.06	118.30
1	D	69	ASP	CB-CG-OD1	8.60	126.04	118.30
1	C	69	ASP	CB-CG-OD1	8.59	126.03	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4895	0	4954	43	0
1	B	4895	0	4954	40	0
1	C	4895	0	4954	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4895	0	4954	41	0
2	A	105	0	147	6	0
2	B	105	0	147	6	0
2	C	105	0	147	9	0
2	D	105	0	147	7	0
3	A	313	0	480	20	0
3	B	313	0	480	16	0
3	C	313	0	480	21	0
3	D	313	0	480	20	0
4	A	58	0	90	4	0
4	B	58	0	90	4	0
4	C	58	0	90	5	0
4	D	58	0	90	5	0
5	A	1	0	0	0	0
6	A	18	0	0	1	0
6	B	18	0	0	0	0
6	C	18	0	0	1	0
6	D	18	0	0	1	0
All	All	21557	0	22684	224	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 5.

All (224) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:GLN:HE22	1:D:450:GLU:H	1.40	0.70
1:A:370:GLN:HE22	1:A:450:GLU:H	1.40	0.70
1:B:370:GLN:HE22	1:B:450:GLU:H	1.40	0.69
1:C:370:GLN:HE22	1:C:450:GLU:H	1.40	0.68
1:C:459:VAL:HG21	2:C:804:Y01:HAN1	1.78	0.66
1:B:459:VAL:HG21	2:B:804:Y01:HAN1	1.78	0.65
1:D:459:VAL:HG21	2:D:808:Y01:HAN1	1.79	0.64
1:A:459:VAL:HG21	2:A:802:Y01:HAN1	1.80	0.62
1:D:452:VAL:HG13	1:D:453:PRO:HD3	1.84	0.60
1:C:452:VAL:HG13	1:C:453:PRO:HD3	1.84	0.60
1:A:452:VAL:HG13	1:A:453:PRO:HD3	1.84	0.58
1:B:231:PRO:HD2	1:B:234:LEU:HD12	1.85	0.58
1:B:452:VAL:HG13	1:B:453:PRO:HD3	1.84	0.58
1:C:231:PRO:HD2	1:C:234:LEU:HD12	1.85	0.58
1:A:474:MET:HB3	1:B:492:ARG:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:PRO:HD2	1:D:234:LEU:HD12	1.85	0.57
1:A:231:PRO:HD2	1:A:234:LEU:HD12	1.85	0.56
3:B:806:POV:H22A	4:B:810:PCW:H172	1.87	0.56
3:C:806:POV:H22A	4:C:810:PCW:H172	1.87	0.56
1:C:425:PHE:HB2	2:C:803:Y01:HAL2	1.88	0.56
1:B:425:PHE:HB2	2:B:803:Y01:HAL2	1.87	0.55
1:A:42:LYS:HD3	1:D:623:TYR:HA	1.89	0.55
1:B:44:ILE:HG13	1:B:50:LEU:HB3	1.89	0.55
1:D:119:THR:H	1:D:122:HIS:HD2	1.55	0.55
1:D:425:PHE:HB2	2:D:807:Y01:HAL2	1.88	0.55
1:A:425:PHE:HB2	2:A:801:Y01:HAL2	1.89	0.55
1:B:119:THR:H	1:B:122:HIS:HD2	1.55	0.55
3:B:815:POV:H27	3:C:806:POV:H32A	1.89	0.55
1:C:44:ILE:HG13	1:C:50:LEU:HB3	1.89	0.55
1:C:119:THR:H	1:C:122:HIS:HD2	1.55	0.55
3:A:804:POV:H22A	4:A:808:PCW:H172	1.88	0.54
3:A:813:POV:H27	3:B:806:POV:H32A	1.89	0.54
3:C:815:POV:H27	3:D:810:POV:H32A	1.89	0.54
3:D:810:POV:H22A	4:D:814:PCW:H172	1.87	0.54
1:A:44:ILE:HG13	1:A:50:LEU:HB3	1.89	0.54
1:A:119:THR:H	1:A:122:HIS:HD2	1.55	0.54
1:D:44:ILE:HG13	1:D:50:LEU:HB3	1.89	0.54
1:A:623:TYR:HA	1:B:42:LYS:HD3	1.90	0.54
1:B:623:TYR:HA	1:C:42:LYS:HD3	1.91	0.53
1:B:229:LEU:HD23	1:B:230:GLN:H	1.75	0.52
1:D:229:LEU:HD23	1:D:230:GLN:H	1.75	0.52
1:A:492:ARG:HD2	1:D:474:MET:HB3	1.93	0.51
1:C:229:LEU:HD23	1:C:230:GLN:H	1.75	0.51
1:C:353:LYS:HE3	1:C:369:GLN:HE21	1.76	0.51
1:D:353:LYS:HE3	1:D:369:GLN:HE21	1.76	0.51
1:C:623:TYR:HA	1:D:42:LYS:HD3	1.93	0.51
1:A:229:LEU:HD23	1:A:230:GLN:H	1.75	0.51
1:B:563:ALA:O	1:B:567:THR:OG1	2.29	0.51
1:C:474:MET:HB3	1:D:492:ARG:HD2	1.93	0.50
3:A:804:POV:H32A	3:D:803:POV:H27	1.93	0.50
1:A:353:LYS:HE3	1:A:369:GLN:HE21	1.76	0.50
1:B:353:LYS:HE3	1:B:369:GLN:HE21	1.76	0.50
1:B:322:LYS:HG2	1:B:326:ARG:HH12	1.77	0.50
3:D:806:POV:H21F	3:D:806:POV:H31H	1.94	0.49
3:C:802:POV:H21F	3:C:802:POV:H31H	1.94	0.49
1:C:563:ALA:O	1:C:567:THR:OG1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:ALA:O	1:D:567:THR:OG1	2.29	0.49
1:C:322:LYS:HG2	1:C:326:ARG:HH12	1.77	0.49
1:D:322:LYS:HG2	1:D:326:ARG:HH12	1.77	0.49
3:A:816:POV:H31H	3:A:816:POV:H21F	1.94	0.49
1:A:563:ALA:O	1:A:567:THR:OG1	2.29	0.48
1:A:190:ARG:HG2	1:A:232:LEU:HD13	1.96	0.48
1:A:322:LYS:HG2	1:A:326:ARG:HH12	1.77	0.48
1:D:190:ARG:HG2	1:D:232:LEU:HD13	1.96	0.48
1:C:377:TYR:OH	1:C:389:GLU:OE1	2.32	0.48
1:C:486:ILE:HD12	2:C:804:Y01:HAD3	1.96	0.47
1:D:53:ALA:O	1:D:91:ASN:ND2	2.47	0.47
1:C:190:ARG:HG2	1:C:232:LEU:HD13	1.96	0.47
3:B:802:POV:H31H	3:B:802:POV:H21F	1.94	0.47
1:C:440:MET:HG3	3:C:808:POV:H27A	1.97	0.47
1:B:190:ARG:HG2	1:B:232:LEU:HD13	1.96	0.47
1:B:486:ILE:HD12	2:B:804:Y01:HAD3	1.96	0.47
1:B:474:MET:HB3	1:C:492:ARG:HD2	1.95	0.46
1:C:53:ALA:O	1:C:91:ASN:ND2	2.47	0.46
1:A:367:LEU:HD13	1:B:516:ASP:HB2	1.97	0.46
3:C:806:POV:H33A	3:C:806:POV:H36A	1.78	0.46
3:D:812:POV:H21A	3:D:812:POV:H21D	1.69	0.46
1:A:33:ARG:O	1:A:37:ASN:ND2	2.49	0.45
1:A:499:VAL:HG11	1:D:466:MET:HG3	1.96	0.45
1:D:107:PHE:HZ	1:D:140:ARG:HG3	1.82	0.45
1:D:486:ILE:HD12	2:D:808:Y01:HAD3	1.98	0.45
1:A:561:ALA:HB2	3:A:816:POV:H21E	1.98	0.45
1:A:377:TYR:OH	1:A:389:GLU:OE1	2.32	0.45
1:B:107:PHE:HZ	1:B:140:ARG:HG3	1.81	0.45
3:C:808:POV:H21A	3:C:808:POV:H21D	1.71	0.45
3:A:806:POV:H27	3:A:806:POV:H24	1.77	0.45
1:C:107:PHE:HZ	1:C:140:ARG:HG3	1.82	0.45
3:C:807:POV:H25	3:C:807:POV:H28	1.78	0.45
3:C:815:POV:H27A	4:D:814:PCW:H19	1.99	0.45
1:A:107:PHE:HZ	1:A:140:ARG:HG3	1.81	0.45
3:C:814:POV:H28	3:C:814:POV:H21A	1.78	0.45
1:B:53:ALA:O	1:B:91:ASN:ND2	2.47	0.45
3:B:815:POV:H27A	4:C:810:PCW:H19	1.99	0.45
1:C:33:ARG:O	1:C:37:ASN:ND2	2.50	0.45
3:A:804:POV:H33A	3:A:804:POV:H36A	1.74	0.45
1:B:33:ARG:O	1:B:37:ASN:ND2	2.49	0.45
3:B:808:POV:H29	3:B:808:POV:H212	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:816:PCW:H242	4:B:816:PCW:H211	1.72	0.45
1:D:33:ARG:O	1:D:37:ASN:ND2	2.50	0.45
3:D:811:POV:H25	3:D:811:POV:H28	1.79	0.45
1:A:350:ARG:HG3	1:A:352:LEU:HD13	1.99	0.44
1:B:286:SER:HA	1:B:615:ARG:HH12	1.83	0.44
1:B:553:PHE:CD1	2:B:801:Y01:HAM1	2.52	0.44
1:D:280:LEU:HD21	1:D:316:LEU:HD13	2.00	0.44
3:D:802:POV:H28	3:D:802:POV:H21A	1.77	0.44
1:A:280:LEU:HD21	1:A:316:LEU:HD13	2.00	0.44
4:D:804:PCW:H211	4:D:804:PCW:H242	1.77	0.44
3:B:814:POV:H39	3:B:814:POV:H36	1.83	0.44
1:C:280:LEU:HD21	1:C:316:LEU:HD13	2.00	0.44
3:C:807:POV:H31G	3:C:807:POV:H31D	1.82	0.44
1:B:119:THR:H	1:B:122:HIS:CD2	2.35	0.44
1:A:263:ARG:NE	6:A:905:HOH:O	2.43	0.44
3:B:814:POV:H38A	3:B:814:POV:H311	1.82	0.44
4:C:810:PCW:H20	4:C:810:PCW:H232	1.80	0.44
1:D:350:ARG:HG3	1:D:352:LEU:HD13	1.99	0.44
1:A:286:SER:HA	1:A:615:ARG:HH12	1.83	0.44
1:B:350:ARG:HG3	1:B:352:LEU:HD13	1.99	0.43
1:D:119:THR:H	1:D:122:HIS:CD2	2.35	0.43
1:A:53:ALA:O	1:A:91:ASN:ND2	2.47	0.43
3:A:804:POV:H316	3:D:802:POV:H21B	2.00	0.43
1:C:263:ARG:NE	6:C:905:HOH:O	2.42	0.43
3:A:804:POV:H21E	3:A:804:POV:H212	1.84	0.43
1:C:286:SER:HA	1:C:615:ARG:HH12	1.83	0.43
1:D:286:SER:HA	1:D:615:ARG:HH12	1.83	0.43
1:D:377:TYR:OH	1:D:389:GLU:OE1	2.32	0.43
3:D:811:POV:H11	3:D:811:POV:H15B	1.86	0.43
3:D:812:POV:H27	3:D:812:POV:H24	1.84	0.43
1:A:119:THR:H	1:A:122:HIS:CD2	2.35	0.43
3:A:812:POV:H21A	3:A:812:POV:H28	1.79	0.43
3:A:813:POV:H27A	4:B:810:PCW:H19	1.99	0.43
3:C:814:POV:H39	3:C:814:POV:H36	1.82	0.43
1:B:280:LEU:HD21	1:B:316:LEU:HD13	2.00	0.43
3:A:812:POV:H38A	3:A:812:POV:H311	1.82	0.43
1:D:412:VAL:HG13	1:D:413:THR:HG23	2.00	0.43
4:A:808:PCW:H212	4:A:808:PCW:H181	1.83	0.43
3:B:806:POV:H36A	3:B:806:POV:H33A	1.74	0.43
3:B:807:POV:H28	3:B:807:POV:H25	1.78	0.43
1:C:350:ARG:HG3	1:C:352:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:THR:H	1:C:122:HIS:CD2	2.35	0.43
3:D:811:POV:H31G	3:D:811:POV:H31D	1.82	0.42
3:D:812:POV:H29	3:D:812:POV:H212	1.82	0.42
1:A:137:LEU:HD23	1:A:141:ALA:HB3	2.01	0.42
1:A:632:ARG:NH2	1:A:634:GLU:OE1	2.44	0.42
1:B:440:MET:HG3	3:B:808:POV:H27A	2.00	0.42
1:C:632:ARG:NH2	1:C:634:GLU:OE1	2.44	0.42
4:C:810:PCW:H212	4:C:810:PCW:H181	1.82	0.42
3:A:805:POV:H39	3:A:805:POV:H211	2.01	0.42
4:A:814:PCW:H242	4:A:814:PCW:H211	1.76	0.42
1:B:412:VAL:HG13	1:B:413:THR:HG23	2.00	0.42
4:D:801:PCW:H241	4:D:801:PCW:H212	1.86	0.42
1:C:137:LEU:HD23	1:C:141:ALA:HB3	2.01	0.42
3:D:810:POV:H33A	3:D:810:POV:H36A	1.72	0.42
1:B:137:LEU:HD23	1:B:141:ALA:HB3	2.01	0.42
1:D:552:PRO:HA	3:D:806:POV:H15A	2.01	0.42
1:A:440:MET:HG3	3:A:806:POV:H27A	2.01	0.42
1:C:412:VAL:HG13	1:C:413:THR:HG23	2.00	0.42
2:D:808:Y01:HAC3	2:D:808:Y01:HAJ1	1.89	0.42
1:A:459:VAL:CG2	2:A:802:Y01:HAN1	2.49	0.42
3:A:806:POV:H29	3:A:806:POV:H212	1.77	0.42
4:B:810:PCW:H20	4:B:810:PCW:H232	1.80	0.42
1:C:456:PHE:HZ	3:D:806:POV:H28A	1.85	0.42
1:D:440:MET:HG3	3:D:812:POV:H27A	2.01	0.42
1:B:377:TYR:OH	1:B:389:GLU:OE1	2.32	0.42
1:D:137:LEU:HD23	1:D:141:ALA:HB3	2.01	0.42
1:D:150:THR:HA	1:D:153:ARG:HD3	2.02	0.42
1:D:263:ARG:NE	6:D:905:HOH:O	2.42	0.42
1:A:150:THR:HA	1:A:153:ARG:HD3	2.02	0.42
1:B:150:THR:HA	1:B:153:ARG:HD3	2.02	0.42
3:B:814:POV:H28	3:B:814:POV:H21A	1.78	0.42
1:C:150:THR:HA	1:C:153:ARG:HD3	2.02	0.42
1:D:436:VAL:HG13	3:D:812:POV:H21C	2.02	0.42
1:A:431:THR:HG21	3:A:805:POV:H21J	2.02	0.41
3:C:807:POV:H39	3:C:807:POV:H211	2.02	0.41
3:D:811:POV:H39	3:D:811:POV:H211	2.02	0.41
1:A:412:VAL:HG13	1:A:413:THR:HG23	2.00	0.41
4:C:816:PCW:H242	4:C:816:PCW:H211	1.75	0.41
1:A:311:THR:HG23	1:A:312:PRO:HD3	2.02	0.41
1:A:426:HIS:CE1	2:A:801:Y01:HAL1	2.55	0.41
3:A:816:POV:H28A	1:D:456:PHE:HZ	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:THR:HG23	1:D:312:PRO:HD3	2.02	0.41
2:A:802:Y01:HAC3	2:A:802:Y01:HAJ1	1.89	0.41
1:D:426:HIS:CE1	2:D:807:Y01:HAL1	2.56	0.41
1:A:466:MET:HG3	1:B:499:VAL:HG11	2.02	0.41
1:A:341:ILE:HG12	3:B:806:POV:H37A	2.02	0.41
1:A:553:PHE:CD1	2:A:815:Y01:HAM1	2.56	0.41
3:A:805:POV:H15B	3:A:805:POV:H11	1.88	0.41
1:C:311:THR:HG23	1:C:312:PRO:HD3	2.02	0.41
3:C:807:POV:H15B	3:C:807:POV:H11	1.86	0.41
1:D:44:ILE:HD11	1:D:54:LYS:HB2	2.03	0.41
1:D:431:THR:HG21	3:D:811:POV:H21J	2.03	0.41
1:C:426:HIS:CE1	2:C:803:Y01:HAL1	2.56	0.41
2:C:803:Y01:HAU2	2:C:803:Y01:HAC1	2.03	0.41
4:A:811:PCW:H241	4:A:811:PCW:H212	1.84	0.41
1:B:488:GLY:HA3	3:B:807:POV:H15A	2.03	0.41
1:B:543:GLY:HA2	1:B:544:PRO:HD3	1.97	0.41
1:C:431:THR:HG21	3:C:807:POV:H21J	2.03	0.41
2:C:801:Y01:HAA1	2:C:801:Y01:HAJ2	1.86	0.41
2:C:801:Y01:HAJ2	2:C:801:Y01:HAC3	1.97	0.41
3:C:808:POV:H24	3:C:808:POV:H27	1.86	0.41
3:C:814:POV:H21B	3:D:810:POV:H316	2.03	0.41
4:D:814:PCW:H181	4:D:814:PCW:H212	1.82	0.41
1:A:44:ILE:HD11	1:A:54:LYS:HB2	2.03	0.41
1:A:488:GLY:HA3	3:A:805:POV:H15A	2.02	0.41
1:B:426:HIS:CE1	2:B:803:Y01:HAL1	2.55	0.41
1:B:456:PHE:HZ	3:C:802:POV:H28A	1.86	0.41
3:B:815:POV:H27A	3:B:815:POV:H210	1.82	0.41
1:C:44:ILE:HD11	1:C:54:LYS:HB2	2.03	0.41
1:B:535:GLU:HB3	1:B:541:ILE:HG12	2.04	0.40
1:C:488:GLY:HA3	3:C:807:POV:H15A	2.04	0.40
1:A:535:GLU:HB3	1:A:541:ILE:HG12	2.03	0.40
2:B:804:Y01:HAO1	2:B:804:Y01:HAP1	1.86	0.40
1:C:535:GLU:HB3	1:C:541:ILE:HG12	2.03	0.40
1:D:553:PHE:CD1	2:D:805:Y01:HAM1	2.56	0.40
1:C:466:MET:HG3	1:D:499:VAL:HG11	2.02	0.40
2:C:804:Y01:HAO1	2:C:804:Y01:HAP1	1.85	0.40
2:D:807:Y01:HAC1	2:D:807:Y01:HAU2	2.04	0.40
1:B:161:TYR:OH	1:B:193:ASP:OD2	2.36	0.40
1:B:473:GLN:H	3:B:814:POV:H13A	1.87	0.40
1:B:568:LEU:O	1:B:572:ASN:ND2	2.55	0.40
1:C:553:PHE:CD1	2:C:801:Y01:HAM1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:808:POV:H29	3:C:808:POV:H212	1.81	0.40
1:D:568:LEU:O	1:D:572:ASN:ND2	2.55	0.40
3:A:812:POV:H39	3:A:812:POV:H36	1.82	0.40
1:C:436:VAL:HG13	3:C:808:POV:H21C	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	608/765 (80%)	582 (96%)	26 (4%)	0	100	100
1	B	608/765 (80%)	582 (96%)	26 (4%)	0	100	100
1	C	608/765 (80%)	582 (96%)	26 (4%)	0	100	100
1	D	608/765 (80%)	582 (96%)	26 (4%)	0	100	100
All	All	2432/3060 (80%)	2328 (96%)	104 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	529/662 (80%)	521 (98%)	8 (2%)	60	84
1	B	529/662 (80%)	521 (98%)	8 (2%)	60	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	529/662 (80%)	521 (98%)	8 (2%)	60 84
1	D	529/662 (80%)	521 (98%)	8 (2%)	60 84
All	All	2116/2648 (80%)	2084 (98%)	32 (2%)	60 84

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

Mol	Chain	Res	Type
1	A	33	ARG
1	A	174	ASN
1	A	224	ARG
1	A	229	LEU
1	A	311	THR
1	A	358	ASN
1	A	365	ASN
1	A	452	VAL
1	B	33	ARG
1	B	174	ASN
1	B	224	ARG
1	B	229	LEU
1	B	311	THR
1	B	358	ASN
1	B	365	ASN
1	B	452	VAL
1	C	33	ARG
1	C	174	ASN
1	C	224	ARG
1	C	229	LEU
1	C	311	THR
1	C	358	ASN
1	C	365	ASN
1	C	452	VAL
1	D	33	ARG
1	D	174	ASN
1	D	224	ARG
1	D	229	LEU
1	D	311	THR
1	D	358	ASN
1	D	365	ASN
1	D	452	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	118	GLN
1	A	122	HIS
1	A	174	ASN
1	A	238	HIS
1	A	358	ASN
1	A	365	ASN
1	A	369	GLN
1	A	370	GLN
1	B	37	ASN
1	B	118	GLN
1	B	122	HIS
1	B	174	ASN
1	B	238	HIS
1	B	358	ASN
1	B	365	ASN
1	B	369	GLN
1	B	370	GLN
1	C	37	ASN
1	C	118	GLN
1	C	122	HIS
1	C	174	ASN
1	C	238	HIS
1	C	358	ASN
1	C	365	ASN
1	C	369	GLN
1	C	370	GLN
1	D	37	ASN
1	D	118	GLN
1	D	122	HIS
1	D	174	ASN
1	D	238	HIS
1	D	358	ASN
1	D	365	ASN
1	D	369	GLN
1	D	370	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 65 ligands modelled in this entry, 1 is monoatomic - leaving 64 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	$\#\|Z\| > 2$
3	POV	C	815	-	51,51,51	1.08	4 (7%)	57,59,59	0.90	3 (5%)
3	POV	B	809	-	13,13,51	1.14	1 (7%)	13,13,59	0.73	0
2	Y01	B	804	-	38,38,38	0.54	0	57,57,57	0.57	0
2	Y01	C	801	-	38,38,38	0.45	0	57,57,57	0.71	0
3	POV	B	805	-	19,19,51	1.41	2 (10%)	19,19,59	0.91	1 (5%)
3	POV	B	806	-	51,51,51	1.06	3 (5%)	57,59,59	1.00	3 (5%)
3	POV	D	811	-	51,51,51	1.07	3 (5%)	57,59,59	0.91	3 (5%)
4	PCW	A	811	-	12,12,53	0.83	0	11,11,61	0.34	0
4	PCW	C	816	-	14,14,53	0.88	0	13,13,61	0.25	0
3	POV	D	810	-	51,51,51	1.06	3 (5%)	57,59,59	1.00	3 (5%)
3	POV	A	803	-	19,19,51	1.41	2 (10%)	19,19,59	0.92	1 (5%)
3	POV	B	815	-	51,51,51	1.08	4 (7%)	57,59,59	0.90	3 (5%)
3	POV	C	814	-	51,51,51	1.08	4 (7%)	57,59,59	0.91	3 (5%)
2	Y01	D	807	-	38,38,38	0.48	0	57,57,57	0.46	0
2	Y01	C	803	-	38,38,38	0.48	0	57,57,57	0.46	0
3	POV	A	813	-	51,51,51	1.08	3 (5%)	57,59,59	0.91	3 (5%)
3	POV	A	812	-	51,51,51	1.09	4 (7%)	57,59,59	0.90	3 (5%)
3	POV	C	808	-	18,18,51	1.40	2 (11%)	18,18,59	0.92	1 (5%)
3	POV	D	803	-	51,51,51	1.08	4 (7%)	57,59,59	0.90	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PCW	C	811	-	7,7,53	0.90	0	6,6,61	0.33	0
4	PCW	D	801	-	12,12,53	0.83	0	11,11,61	0.35	0
3	POV	B	808	-	18,18,51	1.40	2 (11%)	18,18,59	0.93	1 (5%)
4	PCW	B	811	-	7,7,53	0.90	0	6,6,61	0.32	0
4	PCW	B	813	-	12,12,53	0.82	0	11,11,61	0.35	0
3	POV	C	805	-	19,19,51	1.41	2 (10%)	19,19,59	0.91	1 (5%)
3	POV	C	806	-	51,51,51	1.06	3 (5%)	57,59,59	1.00	3 (5%)
4	PCW	D	815	-	7,7,53	0.90	0	6,6,61	0.32	0
3	POV	D	813	-	13,13,51	1.14	1 (7%)	13,13,59	0.73	0
2	Y01	A	801	-	38,38,38	0.48	0	57,57,57	0.46	0
2	Y01	B	801	-	38,38,38	0.45	0	57,57,57	0.71	0
2	Y01	D	805	-	38,38,38	0.45	0	57,57,57	0.71	0
4	PCW	A	808	-	13,13,53	0.86	0	12,12,61	0.32	0
4	PCW	A	810	-	7,7,53	0.90	0	6,6,61	0.30	0
3	POV	C	802	-	51,51,51	1.09	3 (5%)	57,59,59	0.90	3 (5%)
3	POV	C	807	-	51,51,51	1.07	3 (5%)	57,59,59	0.91	3 (5%)
2	Y01	C	804	-	38,38,38	0.54	0	57,57,57	0.57	0
4	PCW	B	810	-	13,13,53	0.86	0	12,12,61	0.32	0
3	POV	C	809	-	13,13,51	1.14	1 (7%)	13,13,59	0.73	0
3	POV	D	806	-	51,51,51	1.09	3 (5%)	57,59,59	0.90	3 (5%)
4	PCW	C	813	-	12,12,53	0.82	0	11,11,61	0.35	0
4	PCW	D	814	-	13,13,53	0.86	0	12,12,61	0.32	0
3	POV	D	802	-	51,51,51	1.09	4 (7%)	57,59,59	0.90	3 (5%)
2	Y01	A	802	-	38,38,38	0.54	0	57,57,57	0.57	0
4	PCW	B	812	-	7,7,53	0.89	0	6,6,61	0.32	0
3	POV	B	802	-	51,51,51	1.09	3 (5%)	57,59,59	0.90	3 (5%)
3	POV	B	807	-	51,51,51	1.07	3 (5%)	57,59,59	0.91	3 (5%)
4	PCW	D	816	-	7,7,53	0.88	0	6,6,61	0.32	0
4	PCW	C	812	-	7,7,53	0.89	0	6,6,61	0.31	0
3	POV	A	807	-	13,13,51	1.14	1 (7%)	13,13,59	0.73	0
4	PCW	B	816	-	14,14,53	0.88	0	13,13,61	0.22	0
3	POV	A	816	-	51,51,51	1.10	3 (5%)	57,59,59	0.90	3 (5%)
4	PCW	D	804	-	14,14,53	0.88	0	13,13,61	0.26	0
4	PCW	A	809	-	7,7,53	0.90	0	6,6,61	0.32	0
3	POV	B	814	-	51,51,51	1.08	4 (7%)	57,59,59	0.92	3 (5%)
2	Y01	B	803	-	38,38,38	0.48	0	57,57,57	0.45	0
2	Y01	D	808	-	38,38,38	0.54	0	57,57,57	0.57	0
3	POV	A	804	-	51,51,51	1.06	3 (5%)	57,59,59	0.99	3 (5%)
3	POV	D	812	-	18,18,51	1.40	2 (11%)	18,18,59	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PCW	A	814	-	14,14,53	0.88	0	13,13,61	0.28	0
3	POV	A	805	-	51,51,51	1.07	3 (5%)	57,59,59	0.90	4 (7%)
3	POV	A	806	-	18,18,51	1.39	2 (11%)	18,18,59	0.92	1 (5%)
2	Y01	A	815	-	38,38,38	0.45	0	57,57,57	0.72	0
4	PCW	C	810	-	13,13,53	0.86	0	12,12,61	0.32	0
3	POV	D	809	-	19,19,51	1.40	2 (10%)	19,19,59	0.91	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	C	815	-	-	25/55/55/55	-
3	POV	B	809	-	-	6/12/12/55	-
2	Y01	B	804	-	-	7/19/77/77	0/4/4/4
2	Y01	C	801	-	-	5/19/77/77	0/4/4/4
3	POV	B	805	-	-	9/18/18/55	-
3	POV	B	806	-	-	29/55/55/55	-
3	POV	D	811	-	-	21/55/55/55	-
4	PCW	A	811	-	-	6/10/10/57	-
4	PCW	C	816	-	-	8/12/12/57	-
3	POV	D	810	-	-	29/55/55/55	-
3	POV	A	803	-	-	10/18/18/55	-
3	POV	B	815	-	-	25/55/55/55	-
3	POV	C	814	-	-	34/55/55/55	-
2	Y01	D	807	-	-	9/19/77/77	0/4/4/4
2	Y01	C	803	-	-	9/19/77/77	0/4/4/4
3	POV	A	813	-	-	24/55/55/55	-
3	POV	A	812	-	-	32/55/55/55	-
3	POV	C	808	-	-	7/17/17/55	-
3	POV	D	803	-	-	24/55/55/55	-
4	PCW	C	811	-	-	3/5/5/57	-
4	PCW	D	801	-	-	6/10/10/57	-
3	POV	B	808	-	-	6/17/17/55	-
4	PCW	B	811	-	-	3/5/5/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	B	813	-	-	6/10/10/57	-
3	POV	C	805	-	-	10/18/18/55	-
3	POV	C	806	-	-	29/55/55/55	-
4	PCW	D	815	-	-	3/5/5/57	-
3	POV	D	813	-	-	6/12/12/55	-
2	Y01	A	801	-	-	9/19/77/77	0/4/4/4
2	Y01	B	801	-	-	5/19/77/77	0/4/4/4
2	Y01	D	805	-	-	4/19/77/77	0/4/4/4
4	PCW	A	808	-	-	7/11/11/57	-
4	PCW	A	810	-	-	2/5/5/57	-
3	POV	C	802	-	-	31/55/55/55	-
3	POV	C	807	-	-	20/55/55/55	-
2	Y01	C	804	-	-	7/19/77/77	0/4/4/4
4	PCW	B	810	-	-	7/11/11/57	-
3	POV	C	809	-	-	6/12/12/55	-
3	POV	D	806	-	-	30/55/55/55	-
4	PCW	C	813	-	-	6/10/10/57	-
4	PCW	D	814	-	-	7/11/11/57	-
3	POV	D	802	-	-	34/55/55/55	-
2	Y01	A	802	-	-	8/19/77/77	0/4/4/4
4	PCW	B	812	-	-	3/5/5/57	-
3	POV	B	802	-	-	31/55/55/55	-
3	POV	B	807	-	-	21/55/55/55	-
4	PCW	D	816	-	-	2/5/5/57	-
4	PCW	C	812	-	-	2/5/5/57	-
3	POV	A	807	-	-	6/12/12/55	-
4	PCW	B	816	-	-	9/12/12/57	-
3	POV	A	816	-	-	30/55/55/55	-
4	PCW	D	804	-	-	8/12/12/57	-
4	PCW	A	809	-	-	3/5/5/57	-
3	POV	B	814	-	-	34/55/55/55	-
2	Y01	B	803	-	-	9/19/77/77	0/4/4/4
2	Y01	D	808	-	-	7/19/77/77	0/4/4/4
3	POV	A	804	-	-	28/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	D	812	-	-	6/17/17/55	-
4	PCW	A	814	-	-	8/12/12/57	-
3	POV	A	805	-	-	20/55/55/55	-
3	POV	A	806	-	-	7/17/17/55	-
2	Y01	A	815	-	-	5/19/77/77	0/4/4/4
4	PCW	C	810	-	-	7/11/11/57	-
3	POV	D	809	-	-	10/18/18/55	-

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	POV	C29-C210	4.23	1.55	1.31
3	B	805	POV	C29-C210	4.21	1.55	1.31
3	D	809	POV	C29-C210	4.20	1.55	1.31
3	C	805	POV	C29-C210	4.20	1.55	1.31
3	C	808	POV	C29-C210	4.18	1.55	1.31
3	B	808	POV	C29-C210	4.17	1.55	1.31
3	A	806	POV	C29-C210	4.16	1.55	1.31
3	D	812	POV	C29-C210	4.16	1.55	1.31
3	A	812	POV	O21-C21	2.96	1.42	1.34
3	D	802	POV	O21-C21	2.95	1.42	1.34
3	C	814	POV	O21-C21	2.94	1.42	1.34
3	B	814	POV	O21-C21	2.93	1.42	1.34
3	C	802	POV	O21-C21	2.93	1.42	1.34
3	D	806	POV	O21-C21	2.91	1.42	1.34
3	D	803	POV	O21-C21	2.91	1.42	1.34
3	A	816	POV	O21-C21	2.90	1.42	1.34
3	B	802	POV	O21-C21	2.89	1.42	1.34
3	A	813	POV	O21-C21	2.87	1.42	1.34
3	C	815	POV	O21-C21	2.87	1.42	1.34
3	B	815	POV	O21-C21	2.84	1.42	1.34
3	D	802	POV	O31-C31	2.82	1.41	1.33
3	B	814	POV	O31-C31	2.80	1.41	1.33
3	A	812	POV	O31-C31	2.78	1.41	1.33
3	A	816	POV	O31-C31	2.78	1.41	1.33
3	C	814	POV	O31-C31	2.78	1.41	1.33
3	A	805	POV	O31-C31	2.77	1.41	1.33
3	B	807	POV	O31-C31	2.77	1.41	1.33
3	D	811	POV	O31-C31	2.76	1.41	1.33
3	D	811	POV	O21-C21	2.76	1.42	1.34
3	A	805	POV	O21-C21	2.76	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	807	POV	O31-C31	2.75	1.41	1.33
3	C	802	POV	O31-C31	2.75	1.41	1.33
3	C	805	POV	O21-C21	2.74	1.41	1.33
3	B	802	POV	O31-C31	2.74	1.41	1.33
3	D	806	POV	O31-C31	2.74	1.41	1.33
3	D	809	POV	O21-C21	2.73	1.41	1.33
3	C	807	POV	O21-C21	2.73	1.42	1.34
3	D	810	POV	O21-C21	2.72	1.42	1.34
3	B	807	POV	O21-C21	2.72	1.42	1.34
3	A	804	POV	O21-C21	2.72	1.41	1.34
3	B	806	POV	O21-C21	2.72	1.41	1.34
3	B	805	POV	O21-C21	2.71	1.41	1.33
3	A	803	POV	O21-C21	2.71	1.41	1.33
3	C	806	POV	O21-C21	2.71	1.41	1.34
3	A	807	POV	O31-C31	2.69	1.41	1.33
3	C	809	POV	O31-C31	2.69	1.41	1.33
3	B	809	POV	O31-C31	2.69	1.41	1.33
3	D	813	POV	O31-C31	2.69	1.41	1.33
3	B	808	POV	O21-C21	2.68	1.41	1.33
3	D	812	POV	O21-C21	2.65	1.41	1.33
3	C	808	POV	O21-C21	2.65	1.41	1.33
3	B	807	POV	O21-C2	-2.63	1.40	1.46
3	D	811	POV	O21-C2	-2.62	1.40	1.46
3	A	804	POV	O21-C2	-2.62	1.40	1.46
3	A	806	POV	O21-C21	2.61	1.41	1.33
3	C	806	POV	O21-C2	-2.61	1.40	1.46
3	C	807	POV	O21-C2	-2.60	1.40	1.46
3	B	806	POV	O21-C2	-2.60	1.40	1.46
3	D	810	POV	O21-C2	-2.59	1.40	1.46
3	A	805	POV	O21-C2	-2.57	1.40	1.46
3	D	803	POV	O31-C31	2.54	1.40	1.33
3	C	806	POV	O31-C31	2.53	1.40	1.33
3	D	810	POV	O31-C31	2.53	1.40	1.33
3	C	815	POV	O31-C31	2.52	1.40	1.33
3	B	815	POV	O31-C31	2.52	1.40	1.33
3	A	804	POV	O31-C31	2.52	1.40	1.33
3	D	803	POV	O21-C2	-2.51	1.40	1.46
3	A	813	POV	O21-C2	-2.51	1.40	1.46
3	A	813	POV	O31-C31	2.51	1.40	1.33
3	B	806	POV	O31-C31	2.50	1.40	1.33
3	C	815	POV	O21-C2	-2.49	1.40	1.46
3	B	815	POV	O21-C2	-2.46	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	816	POV	O21-C2	-2.46	1.40	1.46
3	B	802	POV	O21-C2	-2.45	1.40	1.46
3	D	806	POV	O21-C2	-2.45	1.40	1.46
3	C	802	POV	O21-C2	-2.45	1.40	1.46
3	C	814	POV	P-O12	2.19	1.68	1.59
3	B	814	POV	P-O12	2.18	1.67	1.59
3	A	812	POV	P-O12	2.18	1.67	1.59
3	D	802	POV	P-O12	2.17	1.67	1.59
3	D	802	POV	O21-C2	-2.08	1.41	1.46
3	C	814	POV	O21-C2	-2.08	1.41	1.46
3	A	812	POV	O21-C2	-2.08	1.41	1.46
3	B	814	POV	O21-C2	-2.04	1.41	1.46
3	B	815	POV	P-O12	2.02	1.67	1.59
3	C	815	POV	P-O12	2.01	1.67	1.59
3	D	803	POV	P-O12	2.00	1.67	1.59

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	813	POV	O21-C21-C22	4.07	120.28	111.48
3	D	803	POV	O21-C21-C22	4.07	120.28	111.48
3	B	815	POV	O21-C21-C22	4.06	120.27	111.48
3	C	815	POV	O21-C21-C22	4.06	120.25	111.48
3	D	806	POV	O21-C21-C22	4.00	120.13	111.48
3	C	802	POV	O21-C21-C22	3.99	120.12	111.48
3	A	816	POV	O21-C21-C22	3.97	120.06	111.48
3	B	802	POV	O21-C21-C22	3.94	120.01	111.48
3	A	804	POV	O21-C21-C22	3.63	119.34	111.48
3	D	810	POV	O21-C21-C22	3.63	119.33	111.48
3	B	807	POV	O21-C21-C22	3.63	119.33	111.48
3	C	806	POV	O21-C21-C22	3.61	119.30	111.48
3	B	806	POV	O21-C21-C22	3.60	119.26	111.48
3	D	811	POV	O21-C21-C22	3.59	119.25	111.48
3	C	807	POV	O21-C21-C22	3.59	119.25	111.48
3	A	805	POV	O21-C21-C22	3.51	119.07	111.48
3	C	814	POV	O21-C21-C22	3.46	118.97	111.48
3	A	812	POV	O21-C21-C22	3.45	118.95	111.48
3	D	802	POV	O21-C21-C22	3.44	118.92	111.48
3	B	814	POV	O21-C21-C22	3.44	118.92	111.48
3	B	806	POV	O31-C31-C32	3.33	121.98	111.83
3	C	806	POV	O31-C31-C32	3.28	121.85	111.83
3	D	810	POV	O31-C31-C32	3.26	121.77	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	804	POV	O31-C31-C32	3.22	121.66	111.83
3	A	816	POV	O31-C31-C32	2.61	119.78	111.83
3	C	807	POV	O31-C31-C32	2.59	119.72	111.83
3	B	802	POV	O31-C31-C32	2.58	119.72	111.83
3	D	806	POV	O31-C31-C32	2.57	119.69	111.83
3	D	811	POV	O31-C31-C32	2.57	119.67	111.83
3	B	807	POV	O31-C31-C32	2.57	119.67	111.83
3	B	814	POV	C14-N-C12	2.56	120.09	109.91
3	C	802	POV	O31-C31-C32	2.56	119.64	111.83
3	A	805	POV	O31-C31-C32	2.56	119.63	111.83
3	D	802	POV	C14-N-C12	2.54	120.01	109.91
3	A	812	POV	C14-N-C12	2.54	119.99	109.91
3	A	803	POV	O21-C21-C22	2.54	119.57	111.83
3	C	814	POV	C14-N-C12	2.52	119.93	109.91
3	B	805	POV	O21-C21-C22	2.48	119.39	111.83
3	B	815	POV	O31-C31-C32	2.47	119.36	111.83
3	D	809	POV	O21-C21-C22	2.47	119.36	111.83
3	C	815	POV	O31-C31-C32	2.46	119.34	111.83
3	C	805	POV	O21-C21-C22	2.46	119.34	111.83
3	D	803	POV	O31-C31-C32	2.46	119.33	111.83
3	A	813	POV	O31-C31-C32	2.42	119.22	111.83
3	B	814	POV	O31-C31-C32	2.37	119.07	111.83
3	B	806	POV	C14-N-C12	2.36	119.30	109.91
3	D	810	POV	C14-N-C12	2.36	119.28	109.91
3	A	804	POV	C14-N-C12	2.35	119.27	109.91
3	A	805	POV	C14-N-C12	2.35	119.26	109.91
3	C	806	POV	C14-N-C12	2.34	119.23	109.91
3	C	814	POV	O31-C31-C32	2.34	118.96	111.83
3	D	811	POV	C14-N-C12	2.34	119.19	109.91
3	B	807	POV	C14-N-C12	2.33	119.19	109.91
3	C	807	POV	C14-N-C12	2.33	119.17	109.91
3	B	802	POV	C14-N-C12	2.33	119.16	109.91
3	C	802	POV	C14-N-C12	2.32	119.12	109.91
3	A	812	POV	O31-C31-C32	2.32	118.89	111.83
3	D	806	POV	C14-N-C12	2.31	119.09	109.91
3	D	802	POV	O31-C31-C32	2.30	118.86	111.83
3	A	816	POV	C14-N-C12	2.26	118.90	109.91
3	B	808	POV	O21-C21-C22	2.22	120.51	112.14
3	D	812	POV	O21-C21-C22	2.20	120.45	112.14
3	C	808	POV	O21-C21-C22	2.19	120.42	112.14
3	B	815	POV	C14-N-C12	2.17	118.55	109.91
3	D	803	POV	C14-N-C12	2.16	118.49	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	806	POV	O21-C21-C22	2.15	120.28	112.14
3	C	815	POV	C14-N-C12	2.15	118.44	109.91
3	A	813	POV	C14-N-C12	2.14	118.42	109.91
3	A	805	POV	C2-O21-C21	-2.01	112.98	117.80

There are no chirality outliers.

All (830) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	804	POV	C1-O11-P-O12
3	A	804	POV	C1-O11-P-O14
3	A	804	POV	C11-O12-P-O11
3	A	804	POV	C11-O12-P-O13
3	A	804	POV	C11-O12-P-O14
3	A	804	POV	O12-C11-C12-N
3	A	804	POV	O22-C21-O21-C2
3	A	805	POV	O22-C21-O21-C2
3	A	812	POV	C11-O12-P-O11
3	A	812	POV	C11-O12-P-O14
3	A	812	POV	C12-C11-O12-P
3	A	813	POV	C11-O12-P-O11
3	A	813	POV	C11-O12-P-O13
3	A	813	POV	O11-C1-C2-O21
3	A	816	POV	C1-O11-P-O12
3	A	816	POV	C1-O11-P-O13
3	A	816	POV	C1-O11-P-O14
3	A	816	POV	C11-O12-P-O14
3	A	816	POV	C22-C21-O21-C2
3	B	802	POV	C1-O11-P-O12
3	B	802	POV	C1-O11-P-O13
3	B	802	POV	C1-O11-P-O14
3	B	802	POV	C11-O12-P-O14
3	B	802	POV	C22-C21-O21-C2
3	B	806	POV	C1-O11-P-O12
3	B	806	POV	C1-O11-P-O14
3	B	806	POV	C11-O12-P-O11
3	B	806	POV	C11-O12-P-O13
3	B	806	POV	C11-O12-P-O14
3	B	806	POV	O12-C11-C12-N
3	B	806	POV	O22-C21-O21-C2
3	B	807	POV	O22-C21-O21-C2
3	B	814	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
3	B	814	POV	C11-O12-P-O14
3	B	814	POV	C12-C11-O12-P
3	B	815	POV	C11-O12-P-O11
3	B	815	POV	C11-O12-P-O13
3	B	815	POV	O11-C1-C2-O21
3	C	802	POV	C1-O11-P-O12
3	C	802	POV	C1-O11-P-O13
3	C	802	POV	C1-O11-P-O14
3	C	802	POV	C11-O12-P-O14
3	C	802	POV	C22-C21-O21-C2
3	C	806	POV	C1-O11-P-O12
3	C	806	POV	C1-O11-P-O14
3	C	806	POV	C11-O12-P-O11
3	C	806	POV	C11-O12-P-O13
3	C	806	POV	C11-O12-P-O14
3	C	806	POV	O12-C11-C12-N
3	C	806	POV	O22-C21-O21-C2
3	C	807	POV	O22-C21-O21-C2
3	C	814	POV	C11-O12-P-O14
3	C	814	POV	C12-C11-O12-P
3	C	815	POV	C11-O12-P-O11
3	C	815	POV	C11-O12-P-O13
3	C	815	POV	O11-C1-C2-O21
3	D	802	POV	C11-O12-P-O11
3	D	802	POV	C11-O12-P-O14
3	D	802	POV	C12-C11-O12-P
3	D	803	POV	C11-O12-P-O11
3	D	803	POV	O11-C1-C2-O21
3	D	806	POV	C1-O11-P-O12
3	D	806	POV	C1-O11-P-O13
3	D	806	POV	C1-O11-P-O14
3	D	806	POV	C22-C21-O21-C2
3	D	810	POV	C1-O11-P-O12
3	D	810	POV	C1-O11-P-O14
3	D	810	POV	C11-O12-P-O11
3	D	810	POV	C11-O12-P-O13
3	D	810	POV	C11-O12-P-O14
3	D	810	POV	O12-C11-C12-N
3	D	810	POV	O22-C21-O21-C2
3	D	811	POV	O22-C21-O21-C2
3	A	807	POV	C32-C31-O31-C3
3	B	809	POV	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
3	C	809	POV	C32-C31-O31-C3
3	D	813	POV	C32-C31-O31-C3
3	A	804	POV	C22-C21-O21-C2
3	A	805	POV	C22-C21-O21-C2
3	B	806	POV	C22-C21-O21-C2
3	B	807	POV	C22-C21-O21-C2
3	C	806	POV	C22-C21-O21-C2
3	C	807	POV	C22-C21-O21-C2
3	D	810	POV	C22-C21-O21-C2
3	D	811	POV	C22-C21-O21-C2
3	A	807	POV	O32-C31-O31-C3
3	B	809	POV	O32-C31-O31-C3
3	C	809	POV	O32-C31-O31-C3
3	D	813	POV	O32-C31-O31-C3
3	A	812	POV	O22-C21-O21-C2
3	A	816	POV	O22-C21-O21-C2
3	B	802	POV	O22-C21-O21-C2
3	C	802	POV	O22-C21-O21-C2
3	C	814	POV	O22-C21-O21-C2
3	D	806	POV	O22-C21-O21-C2
3	A	812	POV	C22-C21-O21-C2
3	B	814	POV	C22-C21-O21-C2
3	C	814	POV	C22-C21-O21-C2
3	D	802	POV	C22-C21-O21-C2
2	B	804	Y01	CAX-CAL-CAM-CAY
3	B	814	POV	O22-C21-O21-C2
3	D	802	POV	O22-C21-O21-C2
3	A	804	POV	C32-C31-O31-C3
3	A	805	POV	C22-C23-C24-C25
3	C	806	POV	C32-C31-O31-C3
3	D	802	POV	C311-C310-C39-C38
3	D	802	POV	C36-C37-C38-C39
3	B	807	POV	C22-C23-C24-C25
3	C	807	POV	C22-C23-C24-C25
3	D	811	POV	C22-C23-C24-C25
2	C	804	Y01	CAX-CAL-CAM-CAY
2	D	808	Y01	CAX-CAL-CAM-CAY
3	A	816	POV	C21-C22-C23-C24
3	C	802	POV	C21-C22-C23-C24
3	D	806	POV	C21-C22-C23-C24
3	B	806	POV	C32-C31-O31-C3
3	D	810	POV	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
3	B	802	POV	C21-C22-C23-C24
2	A	802	Y01	CAX-CAL-CAM-CAY
3	A	812	POV	C36-C37-C38-C39
3	A	803	POV	C21-C22-C23-C24
3	C	805	POV	C21-C22-C23-C24
3	B	805	POV	C21-C22-C23-C24
3	D	809	POV	C21-C22-C23-C24
3	C	806	POV	O32-C31-O31-C3
3	B	814	POV	C36-C37-C38-C39
3	C	814	POV	C36-C37-C38-C39
3	A	804	POV	O32-C31-O31-C3
3	A	803	POV	C211-C210-C29-C28
3	B	805	POV	C211-C210-C29-C28
3	C	805	POV	C211-C210-C29-C28
3	D	809	POV	C211-C210-C29-C28
3	B	806	POV	O32-C31-O31-C3
2	D	805	Y01	CAX-CAL-CAM-CAY
3	D	810	POV	O32-C31-O31-C3
3	B	806	POV	C24-C25-C26-C27
3	C	806	POV	C24-C25-C26-C27
3	D	810	POV	C24-C25-C26-C27
4	A	811	PCW	C21-C22-C23-C24
3	D	812	POV	C211-C212-C213-C214
2	B	804	Y01	CAO-CAJ-CAN-CBA
3	A	816	POV	C32-C31-O31-C3
3	C	802	POV	C32-C31-O31-C3
2	A	815	Y01	CAX-CAL-CAM-CAY
2	B	801	Y01	CAX-CAL-CAM-CAY
2	C	801	Y01	CAX-CAL-CAM-CAY
3	D	803	POV	C39-C310-C311-C312
2	A	802	Y01	CAO-CAJ-CAN-CBA
2	C	804	Y01	CAO-CAJ-CAN-CBA
3	B	815	POV	C39-C310-C311-C312
3	C	808	POV	C211-C212-C213-C214
3	A	813	POV	C39-C310-C311-C312
3	B	808	POV	C211-C212-C213-C214
3	C	815	POV	C39-C310-C311-C312
3	A	804	POV	C24-C25-C26-C27
2	A	801	Y01	CAJ-CAN-CBA-CAA
2	B	803	Y01	CAJ-CAN-CBA-CAB
2	D	807	Y01	CAJ-CAN-CBA-CAA
3	C	807	POV	C39-C310-C311-C312

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Mol	Chain	Res	Type	Atoms
3	A	805	POV	C39-C310-C311-C312
3	D	803	POV	C311-C312-C313-C314
4	A	814	PCW	C15-C16-C17-C18
4	B	812	PCW	C13-C14-C15-C16
4	B	816	PCW	C15-C16-C17-C18
4	C	816	PCW	C15-C16-C17-C18
4	D	804	PCW	C15-C16-C17-C18
4	D	816	PCW	C13-C14-C15-C16
3	D	811	POV	C39-C310-C311-C312
4	C	812	PCW	C13-C14-C15-C16
3	B	802	POV	C23-C24-C25-C26
3	B	807	POV	C39-C310-C311-C312
3	C	802	POV	C23-C24-C25-C26
4	A	810	PCW	C13-C14-C15-C16
4	D	801	PCW	C21-C22-C23-C24
3	A	816	POV	C23-C24-C25-C26
3	D	806	POV	C23-C24-C25-C26
2	A	801	Y01	CAJ-CAN-CBA-CAB
2	B	803	Y01	CAJ-CAN-CBA-CAA
2	C	803	Y01	CAJ-CAN-CBA-CAA
2	C	803	Y01	CAJ-CAN-CBA-CAB
2	D	807	Y01	CAJ-CAN-CBA-CAB
2	D	808	Y01	CAO-CAJ-CAN-CBA
4	B	816	PCW	C23-C24-C25-C26
3	A	803	POV	C24-C25-C26-C27
3	D	802	POV	C39-C310-C311-C312
3	A	812	POV	C24-C25-C26-C27
3	A	813	POV	C311-C312-C313-C314
3	A	813	POV	C36-C37-C38-C39
3	B	815	POV	C36-C37-C38-C39
3	C	815	POV	C311-C312-C313-C314
3	D	802	POV	C24-C25-C26-C27
3	B	805	POV	C24-C25-C26-C27
4	C	816	PCW	C23-C24-C25-C26
2	B	803	Y01	CAX-CAL-CAM-CAY
2	C	803	Y01	CAX-CAL-CAM-CAY
2	D	807	Y01	CAX-CAL-CAM-CAY
3	B	815	POV	C311-C312-C313-C314
3	D	802	POV	C21-C22-C23-C24
3	D	809	POV	C24-C25-C26-C27
4	C	813	PCW	C21-C22-C23-C24
3	A	816	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
3	C	802	POV	O32-C31-O31-C3
3	A	805	POV	C23-C24-C25-C26
3	B	814	POV	C311-C310-C39-C38
3	B	814	POV	C24-C25-C26-C27
3	A	812	POV	C311-C310-C39-C38
3	C	805	POV	C24-C25-C26-C27
3	C	814	POV	C24-C25-C26-C27
3	B	802	POV	C32-C31-O31-C3
3	D	806	POV	C32-C31-O31-C3
3	B	814	POV	C1-C2-C3-O31
3	D	802	POV	C1-C2-C3-O31
3	B	814	POV	C32-C33-C34-C35
3	C	814	POV	C311-C310-C39-C38
3	C	814	POV	C32-C33-C34-C35
3	C	815	POV	C36-C37-C38-C39
4	A	808	PCW	C22-C23-C24-C25
4	A	814	PCW	C23-C24-C25-C26
4	B	810	PCW	C22-C23-C24-C25
4	C	816	PCW	C14-C15-C16-C17
3	A	812	POV	C32-C33-C34-C35
3	B	814	POV	C39-C310-C311-C312
3	C	807	POV	C311-C310-C39-C38
4	B	816	PCW	C14-C15-C16-C17
4	C	810	PCW	C22-C23-C24-C25
4	D	804	PCW	C23-C24-C25-C26
4	D	814	PCW	C22-C23-C24-C25
3	A	805	POV	C311-C310-C39-C38
3	D	802	POV	C32-C33-C34-C35
3	D	802	POV	C35-C36-C37-C38
4	A	814	PCW	C14-C15-C16-C17
4	D	804	PCW	C14-C15-C16-C17
2	B	804	Y01	CAJ-CAO-CBB-CAC
3	A	806	POV	C211-C212-C213-C214
3	C	814	POV	C39-C310-C311-C312
3	D	803	POV	C36-C37-C38-C39
4	B	816	PCW	C21-C22-C23-C24
2	C	803	Y01	CAO-CAJ-CAN-CBA
3	B	814	POV	C213-C214-C215-C216
3	B	807	POV	C311-C310-C39-C38
3	C	807	POV	C23-C24-C25-C26
3	D	811	POV	C311-C310-C39-C38
3	D	811	POV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
3	A	803	POV	C29-C210-C211-C212
3	C	807	POV	C26-C27-C28-C29
2	B	803	Y01	CAO-CAJ-CAN-CBA
2	D	807	Y01	CAO-CAJ-CAN-CBA
3	A	812	POV	C39-C310-C311-C312
3	B	807	POV	C23-C24-C25-C26
3	D	806	POV	C311-C312-C313-C314
3	A	812	POV	C21-C22-C23-C24
3	B	814	POV	C21-C22-C23-C24
3	A	816	POV	C311-C312-C313-C314
3	D	806	POV	O32-C31-O31-C3
3	C	802	POV	C311-C312-C313-C314
3	A	804	POV	C22-C23-C24-C25
3	D	802	POV	C213-C214-C215-C216
3	B	802	POV	C311-C312-C313-C314
3	C	814	POV	C213-C214-C215-C216
3	B	802	POV	C35-C36-C37-C38
3	C	802	POV	C35-C36-C37-C38
3	A	805	POV	C213-C214-C215-C216
3	B	806	POV	C22-C23-C24-C25
4	A	808	PCW	C23-C24-C25-C26
2	A	801	Y01	CAO-CAJ-CAN-CBA
3	C	806	POV	C22-C23-C24-C25
3	D	810	POV	C22-C23-C24-C25
4	B	810	PCW	C23-C24-C25-C26
4	D	814	PCW	C23-C24-C25-C26
3	B	807	POV	C213-C214-C215-C216
3	C	807	POV	C213-C214-C215-C216
3	D	811	POV	C213-C214-C215-C216
4	C	810	PCW	C23-C24-C25-C26
3	B	805	POV	C29-C210-C211-C212
3	D	809	POV	C29-C210-C211-C212
3	C	814	POV	C21-C22-C23-C24
3	A	816	POV	C35-C36-C37-C38
4	B	813	PCW	C21-C22-C23-C24
3	A	813	POV	C34-C35-C36-C37
3	C	815	POV	C34-C35-C36-C37
3	D	806	POV	C35-C36-C37-C38
3	B	807	POV	C26-C27-C28-C29
3	C	808	POV	C26-C27-C28-C29
3	D	811	POV	C26-C27-C28-C29
3	B	806	POV	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
3	A	812	POV	C213-C214-C215-C216
4	B	811	PCW	C14-C15-C16-C17
3	C	806	POV	C211-C212-C213-C214
4	A	809	PCW	C14-C15-C16-C17
4	C	811	PCW	C14-C15-C16-C17
4	D	815	PCW	C14-C15-C16-C17
4	D	815	PCW	C15-C16-C17-C18
3	B	806	POV	C211-C212-C213-C214
3	D	803	POV	C34-C35-C36-C37
4	A	809	PCW	C15-C16-C17-C18
4	B	811	PCW	C15-C16-C17-C18
4	C	811	PCW	C15-C16-C17-C18
3	D	810	POV	C211-C212-C213-C214
3	B	802	POV	O32-C31-O31-C3
3	B	808	POV	C212-C213-C214-C215
3	A	812	POV	C35-C36-C37-C38
3	B	815	POV	C34-C35-C36-C37
3	C	802	POV	C39-C310-C311-C312
3	A	804	POV	C211-C212-C213-C214
3	D	810	POV	C31-C32-C33-C34
3	A	816	POV	C39-C310-C311-C312
3	A	816	POV	C310-C311-C312-C313
3	B	802	POV	C39-C310-C311-C312
3	C	814	POV	C35-C36-C37-C38
3	D	806	POV	C310-C311-C312-C313
3	D	812	POV	C212-C213-C214-C215
3	A	805	POV	C26-C27-C28-C29
3	A	806	POV	C210-C211-C212-C213
3	B	808	POV	C26-C27-C28-C29
3	C	805	POV	C26-C27-C28-C29
3	D	809	POV	C26-C27-C28-C29
3	D	812	POV	C26-C27-C28-C29
3	C	802	POV	C310-C311-C312-C313
3	C	808	POV	C212-C213-C214-C215
3	D	806	POV	C39-C310-C311-C312
3	A	806	POV	C212-C213-C214-C215
3	B	802	POV	C310-C311-C312-C313
3	B	814	POV	C35-C36-C37-C38
3	A	813	POV	C29-C210-C211-C212
3	B	808	POV	C29-C210-C211-C212
3	B	815	POV	C29-C210-C211-C212
3	C	808	POV	C29-C210-C211-C212

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Mol	Chain	Res	Type	Atoms
3	D	812	POV	C29-C210-C211-C212
3	A	813	POV	C33-C34-C35-C36
3	C	807	POV	C36-C37-C38-C39
3	A	805	POV	C36-C37-C38-C39
3	B	815	POV	C33-C34-C35-C36
2	A	801	Y01	CAN-CAJ-CAO-CBB
3	D	811	POV	C36-C37-C38-C39
3	A	806	POV	C29-C210-C211-C212
3	C	805	POV	C29-C210-C211-C212
3	C	815	POV	C29-C210-C211-C212
3	A	803	POV	C26-C27-C28-C29
3	B	802	POV	C26-C27-C28-C29
3	B	805	POV	C26-C27-C28-C29
3	B	808	POV	C210-C211-C212-C213
3	C	808	POV	C210-C211-C212-C213
3	D	806	POV	C26-C27-C28-C29
3	D	812	POV	C210-C211-C212-C213
3	B	807	POV	C36-C37-C38-C39
3	D	811	POV	C312-C313-C314-C315
3	A	812	POV	O11-C1-C2-C3
3	A	813	POV	O11-C1-C2-C3
3	B	814	POV	O11-C1-C2-C3
3	B	815	POV	O11-C1-C2-C3
3	C	814	POV	O11-C1-C2-C3
3	C	815	POV	O11-C1-C2-C3
3	D	802	POV	O11-C1-C2-C3
3	D	803	POV	O11-C1-C2-C3
3	D	803	POV	C33-C34-C35-C36
3	D	810	POV	C33-C34-C35-C36
3	B	807	POV	C312-C313-C314-C315
3	C	807	POV	C312-C313-C314-C315
2	A	802	Y01	CAJ-CAO-CBB-CAC
3	C	815	POV	C33-C34-C35-C36
3	D	803	POV	C24-C25-C26-C27
3	B	807	POV	C311-C312-C313-C314
3	D	811	POV	C311-C312-C313-C314
3	D	803	POV	C29-C210-C211-C212
3	D	806	POV	C36-C37-C38-C39
3	C	802	POV	C36-C37-C38-C39
3	A	812	POV	C1-C2-C3-O31
3	B	806	POV	C1-C2-C3-O31
3	C	814	POV	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
3	D	810	POV	C1-C2-C3-O31
3	C	806	POV	C33-C34-C35-C36
3	C	802	POV	C26-C27-C28-C29
3	A	805	POV	C311-C312-C313-C314
3	B	802	POV	C36-C37-C38-C39
3	A	816	POV	C36-C37-C38-C39
3	C	815	POV	C24-C25-C26-C27
3	A	805	POV	C312-C313-C314-C315
3	C	807	POV	C311-C312-C313-C314
3	A	813	POV	C24-C25-C26-C27
3	B	815	POV	C24-C25-C26-C27
3	A	804	POV	C31-C32-C33-C34
3	A	816	POV	C311-C310-C39-C38
4	C	816	PCW	C21-C22-C23-C24
2	A	801	Y01	CAX-CAL-CAM-CAY
3	B	802	POV	C312-C313-C314-C315
3	B	809	POV	C33-C34-C35-C36
3	C	802	POV	C311-C310-C39-C38
3	D	806	POV	C311-C310-C39-C38
3	A	816	POV	C312-C313-C314-C315
3	C	809	POV	C33-C34-C35-C36
3	D	813	POV	C33-C34-C35-C36
3	A	807	POV	C33-C34-C35-C36
3	D	806	POV	C312-C313-C314-C315
3	B	802	POV	C311-C310-C39-C38
3	C	802	POV	C312-C313-C314-C315
3	B	806	POV	C31-C32-C33-C34
3	C	806	POV	C31-C32-C33-C34
2	C	804	Y01	CAJ-CAO-CBB-CAC
3	A	806	POV	C26-C27-C28-C29
3	A	816	POV	C26-C27-C28-C29
3	B	809	POV	C36-C37-C38-C39
2	A	801	Y01	CAJ-CAO-CBB-CBE
3	A	807	POV	C36-C37-C38-C39
3	C	809	POV	C36-C37-C38-C39
3	A	804	POV	C311-C310-C39-C38
3	D	813	POV	C36-C37-C38-C39
3	A	813	POV	C215-C216-C217-C218
3	B	815	POV	C215-C216-C217-C218
4	B	816	PCW	C13-C14-C15-C16
4	C	816	PCW	C13-C14-C15-C16
3	B	802	POV	C37-C38-C39-C310

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Mol	Chain	Res	Type	Atoms
3	C	802	POV	C37-C38-C39-C310
3	A	816	POV	C37-C38-C39-C310
3	B	806	POV	C311-C310-C39-C38
3	C	815	POV	C215-C216-C217-C218
4	A	814	PCW	C13-C14-C15-C16
4	D	804	PCW	C13-C14-C15-C16
3	C	806	POV	C311-C310-C39-C38
3	D	806	POV	C37-C38-C39-C310
3	B	808	POV	C213-C214-C215-C216
3	D	810	POV	C311-C310-C39-C38
3	D	803	POV	C215-C216-C217-C218
3	D	802	POV	C210-C211-C212-C213
3	B	807	POV	C21-C22-C23-C24
4	D	814	PCW	C15-C16-C17-C18
3	B	802	POV	C313-C314-C315-C316
3	D	806	POV	C313-C314-C315-C316
3	B	814	POV	C211-C212-C213-C214
3	A	816	POV	C313-C314-C315-C316
3	C	802	POV	C313-C314-C315-C316
3	A	807	POV	C311-C310-C39-C38
3	D	802	POV	C211-C212-C213-C214
3	D	810	POV	C34-C35-C36-C37
4	D	814	PCW	C21-C22-C23-C24
4	B	810	PCW	C15-C16-C17-C18
4	C	810	PCW	C21-C22-C23-C24
4	A	808	PCW	C21-C22-C23-C24
4	B	810	PCW	C21-C22-C23-C24
4	C	810	PCW	C15-C16-C17-C18
4	D	804	PCW	C21-C22-C23-C24
2	D	807	Y01	CAN-CAJ-CAO-CBB
3	A	812	POV	C2-C1-O11-P
3	B	814	POV	C2-C1-O11-P
3	C	814	POV	C2-C1-O11-P
3	D	802	POV	C2-C1-O11-P
3	C	814	POV	C313-C314-C315-C316
3	B	814	POV	C313-C314-C315-C316
4	A	808	PCW	C15-C16-C17-C18
3	A	805	POV	O11-C1-C2-C3
3	B	807	POV	O11-C1-C2-C3
3	C	807	POV	O11-C1-C2-C3
3	D	811	POV	O11-C1-C2-C3
3	D	809	POV	C213-C214-C215-C216

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Mol	Chain	Res	Type	Atoms
4	D	815	PCW	C16-C17-C18-C19
3	A	804	POV	C33-C34-C35-C36
3	C	815	POV	C25-C26-C27-C28
2	C	803	Y01	CAN-CAJ-CAO-CBB
3	B	805	POV	C213-C214-C215-C216
4	A	809	PCW	C16-C17-C18-C19
4	B	811	PCW	C16-C17-C18-C19
4	C	811	PCW	C16-C17-C18-C19
3	D	802	POV	C23-C24-C25-C26
3	D	811	POV	C21-C22-C23-C24
3	A	812	POV	C313-C314-C315-C316
3	D	802	POV	C313-C314-C315-C316
3	A	813	POV	C25-C26-C27-C28
4	C	813	PCW	C15-C16-C17-C18
3	C	805	POV	C213-C214-C215-C216
4	B	813	PCW	C15-C16-C17-C18
4	D	801	PCW	C15-C16-C17-C18
3	A	806	POV	C213-C214-C215-C216
4	A	811	PCW	C15-C16-C17-C18
3	C	814	POV	C211-C212-C213-C214
3	A	803	POV	C213-C214-C215-C216
2	B	803	Y01	CAN-CAJ-CAO-CBB
3	B	814	POV	C210-C211-C212-C213
3	C	814	POV	C210-C211-C212-C213
3	C	815	POV	C312-C313-C314-C315
3	B	815	POV	C25-C26-C27-C28
3	B	814	POV	C23-C24-C25-C26
3	C	805	POV	C25-C26-C27-C28
3	A	804	POV	C1-C2-C3-O31
3	C	806	POV	C1-C2-C3-O31
3	C	807	POV	C31-C32-C33-C34
3	D	811	POV	C31-C32-C33-C34
3	A	804	POV	C313-C314-C315-C316
3	B	806	POV	C313-C314-C315-C316
3	C	808	POV	C213-C214-C215-C216
3	D	810	POV	C313-C314-C315-C316
3	A	813	POV	C312-C313-C314-C315
3	C	806	POV	C310-C311-C312-C313
3	B	806	POV	C310-C311-C312-C313
3	C	815	POV	C214-C215-C216-C217
3	D	810	POV	C310-C311-C312-C313
3	C	807	POV	C313-C314-C315-C316

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Mol	Chain	Res	Type	Atoms
3	D	809	POV	C25-C26-C27-C28
2	A	801	Y01	CAJ-CAO-CBB-CAC
3	B	807	POV	C313-C314-C315-C316
3	B	805	POV	C25-C26-C27-C28
3	C	806	POV	C313-C314-C315-C316
3	B	807	POV	C31-C32-C33-C34
3	D	811	POV	C313-C314-C315-C316
3	C	807	POV	C21-C22-C23-C24
3	A	803	POV	C25-C26-C27-C28
3	A	813	POV	C214-C215-C216-C217
3	B	815	POV	C214-C215-C216-C217
3	D	813	POV	C311-C310-C39-C38
3	A	804	POV	C310-C311-C312-C313
3	A	812	POV	C23-C24-C25-C26
4	A	814	PCW	C21-C22-C23-C24
3	C	814	POV	C23-C24-C25-C26
3	A	805	POV	C31-C32-C33-C34
3	B	814	POV	C215-C216-C217-C218
3	C	814	POV	C215-C216-C217-C218
3	B	815	POV	C312-C313-C314-C315
3	D	803	POV	C312-C313-C314-C315
3	D	803	POV	C214-C215-C216-C217
3	D	802	POV	C215-C216-C217-C218
3	A	807	POV	C32-C33-C34-C35
3	C	809	POV	C311-C310-C39-C38
3	C	809	POV	C32-C33-C34-C35
3	B	809	POV	C32-C33-C34-C35
3	D	813	POV	C32-C33-C34-C35
3	A	804	POV	C23-C24-C25-C26
4	B	816	PCW	C20-C21-C22-C23
3	D	812	POV	C213-C214-C215-C216
3	D	803	POV	C27-C28-C29-C210
3	A	812	POV	C215-C216-C217-C218
3	B	806	POV	C34-C35-C36-C37
3	D	803	POV	C25-C26-C27-C28
3	A	812	POV	C3-C2-O21-C21
3	B	814	POV	C3-C2-O21-C21
3	C	814	POV	C3-C2-O21-C21
3	D	802	POV	C3-C2-O21-C21
3	A	805	POV	C313-C314-C315-C316
3	C	802	POV	C31-C32-C33-C34
2	D	808	Y01	CAJ-CAO-CBB-CAC

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Mol	Chain	Res	Type	Atoms
3	A	805	POV	O11-C1-C2-O21
3	B	807	POV	O11-C1-C2-O21
3	C	807	POV	O11-C1-C2-O21
3	D	811	POV	O11-C1-C2-O21
3	B	806	POV	C23-C24-C25-C26
3	B	806	POV	C215-C216-C217-C218
3	A	805	POV	C21-C22-C23-C24
3	A	804	POV	C34-C35-C36-C37
3	A	804	POV	O21-C2-C3-O31
3	A	812	POV	O21-C2-C3-O31
3	A	812	POV	C210-C211-C212-C213
3	B	806	POV	O21-C2-C3-O31
3	B	814	POV	O21-C2-C3-O31
3	C	806	POV	O21-C2-C3-O31
3	C	814	POV	O21-C2-C3-O31
3	D	802	POV	O21-C2-C3-O31
3	D	810	POV	O21-C2-C3-O31
3	B	809	POV	C311-C310-C39-C38
4	A	810	PCW	C16-C17-C18-C19
4	D	814	PCW	C24-C25-C26-C27
3	C	806	POV	C23-C24-C25-C26
4	B	810	PCW	C24-C25-C26-C27
4	C	810	PCW	C24-C25-C26-C27
3	C	806	POV	C37-C38-C39-C310
4	A	808	PCW	C24-C25-C26-C27
3	C	802	POV	C213-C214-C215-C216
3	D	802	POV	C311-C312-C313-C314
2	D	805	Y01	CAJ-CAN-CBA-CAA
3	D	810	POV	C215-C216-C217-C218
3	A	813	POV	O12-C11-C12-N
3	A	816	POV	O12-C11-C12-N
3	B	802	POV	O12-C11-C12-N
3	B	815	POV	O12-C11-C12-N
3	C	802	POV	O12-C11-C12-N
3	C	815	POV	O12-C11-C12-N
3	D	803	POV	O12-C11-C12-N
3	D	806	POV	O12-C11-C12-N
2	A	815	Y01	CAJ-CAN-CBA-CAA
2	C	801	Y01	CAJ-CAN-CBA-CAA
3	A	812	POV	C211-C212-C213-C214
3	A	813	POV	C27-C28-C29-C210
3	B	815	POV	C27-C28-C29-C210

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Mol	Chain	Res	Type	Atoms
3	C	806	POV	C215-C216-C217-C218
2	B	801	Y01	CAJ-CAN-CBA-CAA
3	D	811	POV	C25-C26-C27-C28
3	A	816	POV	C213-C214-C215-C216
3	C	807	POV	C25-C26-C27-C28
3	D	806	POV	C213-C214-C215-C216
4	C	812	PCW	C16-C17-C18-C19
3	D	810	POV	C23-C24-C25-C26
3	B	815	POV	O22-C21-O21-C2
3	C	815	POV	O22-C21-O21-C2
3	A	816	POV	C31-C32-C33-C34
3	D	806	POV	C31-C32-C33-C34
2	D	807	Y01	CAJ-CAO-CBB-CBE
3	B	802	POV	C211-C212-C213-C214
3	B	802	POV	C213-C214-C215-C216
3	C	815	POV	C27-C28-C29-C210
3	B	806	POV	C37-C38-C39-C310
3	B	807	POV	C25-C26-C27-C28
3	A	812	POV	O11-C1-C2-O21
3	B	814	POV	O11-C1-C2-O21
3	C	814	POV	O11-C1-C2-O21
3	D	802	POV	O11-C1-C2-O21
4	A	808	PCW	C20-C21-C22-C23
4	B	810	PCW	C20-C21-C22-C23
4	C	810	PCW	C20-C21-C22-C23
4	D	814	PCW	C20-C21-C22-C23
3	A	816	POV	C211-C212-C213-C214
3	D	806	POV	C211-C212-C213-C214
3	A	804	POV	C214-C215-C216-C217
3	A	804	POV	C37-C38-C39-C310
3	C	802	POV	C211-C212-C213-C214
3	A	804	POV	C215-C216-C217-C218
4	B	812	PCW	C16-C17-C18-C19
3	A	804	POV	C212-C213-C214-C215
4	C	813	PCW	C16-C17-C18-C19
3	C	815	POV	C22-C21-O21-C2
3	A	812	POV	C311-C312-C313-C314
3	C	814	POV	C22-C23-C24-C25
3	A	813	POV	C11-O12-P-O14
3	B	815	POV	C11-O12-P-O14
3	C	814	POV	C11-O12-P-O11
3	C	815	POV	C11-O12-P-O14

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Mol	Chain	Res	Type	Atoms
3	D	803	POV	C11-O12-P-O14
3	D	806	POV	C11-O12-P-O14
3	B	802	POV	C31-C32-C33-C34
2	C	803	Y01	CAJ-CAO-CBB-CBE
3	C	814	POV	C311-C312-C313-C314
3	C	805	POV	C22-C23-C24-C25
3	B	814	POV	C311-C312-C313-C314
3	C	806	POV	C214-C215-C216-C217
4	D	816	PCW	C16-C17-C18-C19
3	D	803	POV	C313-C314-C315-C316
3	B	814	POV	C34-C35-C36-C37
4	B	816	PCW	C22-C23-C24-C25
3	C	805	POV	C27-C28-C29-C210
3	A	812	POV	C22-C23-C24-C25
3	C	806	POV	C34-C35-C36-C37
3	A	812	POV	C34-C35-C36-C37
4	B	813	PCW	C16-C17-C18-C19
3	D	809	POV	C22-C23-C24-C25
3	C	814	POV	C34-C35-C36-C37
3	A	813	POV	O22-C21-O21-C2
3	D	810	POV	C214-C215-C216-C217
3	B	815	POV	C22-C21-O21-C2
3	A	813	POV	C21-C22-C23-C24
2	C	801	Y01	CAN-CAJ-CAO-CBB
4	D	814	PCW	C14-C15-C16-C17
3	A	803	POV	C22-C23-C24-C25
2	D	805	Y01	CAN-CAJ-CAO-CBB
4	A	808	PCW	C14-C15-C16-C17
4	C	810	PCW	C14-C15-C16-C17
2	B	803	Y01	CAJ-CAO-CBB-CBE
3	A	813	POV	C22-C21-O21-C2
2	B	801	Y01	OAG-CAY-OAW-CBC
3	A	803	POV	C27-C28-C29-C210
3	B	805	POV	C27-C28-C29-C210
3	D	809	POV	C27-C28-C29-C210
3	D	802	POV	O31-C31-C32-C33
3	B	815	POV	C313-C314-C315-C316
3	C	815	POV	C212-C213-C214-C215
2	B	801	Y01	CAN-CAJ-CAO-CBB
3	C	815	POV	C21-C22-C23-C24
3	B	805	POV	C22-C23-C24-C25
3	D	803	POV	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
3	D	802	POV	C22-C23-C24-C25
4	B	810	PCW	C14-C15-C16-C17
3	D	803	POV	O22-C21-O21-C2
3	B	815	POV	C21-C22-C23-C24
3	B	814	POV	C22-C23-C24-C25
3	C	802	POV	C24-C25-C26-C27
3	A	813	POV	C212-C213-C214-C215
3	B	815	POV	C212-C213-C214-C215
2	A	815	Y01	CAN-CAJ-CAO-CBB
4	A	811	PCW	C20-C21-C22-C23
3	B	814	POV	O31-C31-C32-C33
3	D	803	POV	C21-C22-C23-C24
3	B	806	POV	C214-C215-C216-C217
3	A	812	POV	O31-C31-C32-C33
3	C	814	POV	O31-C31-C32-C33
3	D	806	POV	C24-C25-C26-C27
3	A	813	POV	C313-C314-C315-C316
3	A	806	POV	C24-C25-C26-C27
3	D	810	POV	C37-C38-C39-C310
3	B	802	POV	C24-C25-C26-C27
3	D	802	POV	C34-C35-C36-C37
3	C	815	POV	C313-C314-C315-C316
3	B	814	POV	C310-C311-C312-C313
2	D	807	Y01	CAJ-CAO-CBB-CAC
3	B	802	POV	C215-C216-C217-C218
3	A	812	POV	C214-C215-C216-C217
3	A	816	POV	C24-C25-C26-C27
4	D	801	PCW	C16-C17-C18-C19
3	A	805	POV	C25-C26-C27-C28
3	D	803	POV	C212-C213-C214-C215
3	A	816	POV	C215-C216-C217-C218
3	A	812	POV	C310-C311-C312-C313
3	C	815	POV	C32-C33-C34-C35
3	C	814	POV	C310-C311-C312-C313
3	D	806	POV	C215-C216-C217-C218
3	C	815	POV	C23-C24-C25-C26
3	A	816	POV	C25-C26-C27-C28
3	A	813	POV	C23-C24-C25-C26
2	C	801	Y01	OAG-CAY-OAW-CBC
3	B	815	POV	C23-C24-C25-C26
3	C	802	POV	C215-C216-C217-C218
2	C	803	Y01	CAJ-CAO-CBB-CAC

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Mol	Chain	Res	Type	Atoms
3	B	802	POV	C25-C26-C27-C28
3	D	806	POV	C25-C26-C27-C28
4	C	816	PCW	C20-C21-C22-C23
4	D	804	PCW	C20-C21-C22-C23
3	D	802	POV	C214-C215-C216-C217
3	B	814	POV	C11-C12-N-C14
2	A	815	Y01	OAG-CAY-OAW-CBC
3	B	815	POV	C32-C33-C34-C35
2	B	804	Y01	CAO-CBB-CBE-CAP
3	C	805	POV	C212-C213-C214-C215
4	A	814	PCW	C20-C21-C22-C23
3	A	803	POV	C212-C213-C214-C215
3	B	814	POV	C212-C213-C214-C215
4	C	816	PCW	C22-C23-C24-C25
3	D	803	POV	C22-C21-O21-C2
3	C	802	POV	C25-C26-C27-C28
4	B	816	PCW	C24-C25-C26-C27
3	C	814	POV	C212-C213-C214-C215
3	D	809	POV	C212-C213-C214-C215
3	D	803	POV	C23-C24-C25-C26
3	D	806	POV	C34-C35-C36-C37
4	A	811	PCW	C16-C17-C18-C19
3	D	802	POV	C212-C213-C214-C215
3	A	812	POV	C212-C213-C214-C215
2	B	803	Y01	CAJ-CAO-CBB-CAC
4	C	813	PCW	C20-C21-C22-C23
4	D	801	PCW	C20-C21-C22-C23
3	A	805	POV	C27-C28-C29-C210
4	D	801	PCW	C17-C18-C19-C20
2	A	802	Y01	CAO-CBB-CBE-CAP
4	D	804	PCW	C22-C23-C24-C25
3	C	802	POV	C29-C210-C211-C212
4	B	813	PCW	C17-C18-C19-C20
4	C	813	PCW	C17-C18-C19-C20
3	B	802	POV	C34-C35-C36-C37
3	A	804	POV	C312-C313-C314-C315
4	A	811	PCW	C17-C18-C19-C20
3	A	816	POV	C32-C33-C34-C35
3	A	816	POV	C29-C210-C211-C212
3	B	802	POV	C29-C210-C211-C212
3	C	807	POV	C27-C28-C29-C210
3	D	806	POV	C29-C210-C211-C212

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Mol	Chain	Res	Type	Atoms
4	A	814	PCW	C17-C18-C19-C20
4	B	816	PCW	C17-C18-C19-C20
4	C	816	PCW	C17-C18-C19-C20
3	D	810	POV	C312-C313-C314-C315
3	C	814	POV	C214-C215-C216-C217
2	B	804	Y01	CAC-CBB-CBE-CBI
3	B	807	POV	C27-C28-C29-C210
3	D	811	POV	C27-C28-C29-C210
4	D	804	PCW	C17-C18-C19-C20
3	C	814	POV	C11-C12-N-C14
3	D	802	POV	C11-C12-N-C14
3	C	806	POV	C312-C313-C314-C315
2	B	801	Y01	CAM-CAY-OAW-CBC
3	C	802	POV	O21-C21-C22-C23
2	D	805	Y01	OAG-CAY-OAW-CBC
2	C	804	Y01	CAO-CBB-CBE-CAP
3	A	816	POV	O21-C21-C22-C23
3	B	802	POV	O21-C21-C22-C23
4	A	814	PCW	C22-C23-C24-C25
2	C	804	Y01	CAM-CAL-CAX-OAF
2	A	802	Y01	CAC-CBB-CBE-CBI
3	B	806	POV	C312-C313-C314-C315
3	C	802	POV	C34-C35-C36-C37
2	B	804	Y01	CAM-CAL-CAX-OAF
3	D	802	POV	C310-C311-C312-C313
3	D	806	POV	O21-C21-C22-C23
3	B	802	POV	C32-C33-C34-C35
3	B	814	POV	C11-C12-N-C15
2	A	802	Y01	CAM-CAL-CAX-OAH
2	D	808	Y01	CAM-CAL-CAX-OAF
2	C	801	Y01	CAM-CAY-OAW-CBC
3	B	814	POV	C214-C215-C216-C217
3	B	814	POV	C11-C12-N-C13
3	B	807	POV	C215-C216-C217-C218
3	C	806	POV	O21-C21-C22-C23
2	A	802	Y01	CAM-CAL-CAX-OAF
3	A	804	POV	O21-C21-C22-C23
3	D	810	POV	O21-C21-C22-C23
3	B	806	POV	O21-C21-C22-C23
2	A	815	Y01	CAM-CAY-OAW-CBC
2	B	803	Y01	CAM-CAL-CAX-OAF
2	D	808	Y01	CAM-CAL-CAX-OAH

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Mol	Chain	Res	Type	Atoms
2	B	803	Y01	CAM-CAL-CAX-OAH
2	C	803	Y01	CAM-CAL-CAX-OAF
2	D	807	Y01	CAM-CAL-CAX-OAF
2	C	804	Y01	CAC-CBB-CBE-CBI
2	B	804	Y01	CAM-CAL-CAX-OAH
2	C	804	Y01	CAM-CAL-CAX-OAH
2	A	801	Y01	CAM-CAL-CAX-OAF
3	C	802	POV	C32-C33-C34-C35
3	D	811	POV	C35-C36-C37-C38
3	A	812	POV	C11-C12-N-C14
3	C	814	POV	C11-C12-N-C15
3	D	802	POV	C11-C12-N-C15
3	B	807	POV	C35-C36-C37-C38
4	A	811	PCW	C24-C25-C26-C27
4	C	813	PCW	C24-C25-C26-C27
4	D	801	PCW	C24-C25-C26-C27
2	C	803	Y01	CAM-CAL-CAX-OAH
3	C	808	POV	C211-C210-C29-C28
3	C	814	POV	C11-C12-N-C13
3	D	802	POV	C11-C12-N-C13
4	B	812	PCW	C12-C13-C14-C15
2	D	807	Y01	CAM-CAL-CAX-OAH
3	B	806	POV	O22-C21-C22-C23
2	A	802	Y01	CAV-CBC-OAW-CAY
2	D	808	Y01	CAV-CBC-OAW-CAY
3	C	807	POV	C35-C36-C37-C38
3	A	805	POV	C29-C210-C211-C212
3	B	807	POV	C29-C210-C211-C212
3	A	805	POV	C35-C36-C37-C38
3	C	806	POV	C212-C213-C214-C215
3	C	806	POV	O22-C21-C22-C23
3	D	810	POV	O22-C21-C22-C23
4	B	813	PCW	C24-C25-C26-C27
3	B	806	POV	C212-C213-C214-C215
2	D	808	Y01	CAO-CBB-CBE-CAP
2	A	801	Y01	CAM-CAL-CAX-OAH
4	B	813	PCW	C20-C21-C22-C23
3	D	810	POV	C212-C213-C214-C215
3	D	811	POV	C29-C210-C211-C212
3	C	807	POV	C215-C216-C217-C218
3	D	811	POV	C215-C216-C217-C218

There are no ring outliers.

46 monomers are involved in 110 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	815	POV	2	0
2	B	804	Y01	3	0
2	C	801	Y01	3	0
3	B	806	POV	4	0
3	D	811	POV	5	0
4	A	811	PCW	1	0
4	C	816	PCW	1	0
3	D	810	POV	4	0
3	B	815	POV	3	0
3	C	814	POV	3	0
2	D	807	Y01	3	0
2	C	803	Y01	3	0
3	A	813	POV	2	0
3	A	812	POV	3	0
3	C	808	POV	5	0
3	D	803	POV	1	0
4	D	801	PCW	1	0
3	B	808	POV	2	0
3	C	806	POV	3	0
2	A	801	Y01	2	0
2	B	801	Y01	1	0
2	D	805	Y01	1	0
4	A	808	PCW	2	0
3	C	802	POV	2	0
3	C	807	POV	6	0
2	C	804	Y01	3	0
4	B	810	PCW	3	0
3	D	806	POV	3	0
4	D	814	PCW	3	0
3	D	802	POV	2	0
2	A	802	Y01	3	0
3	B	802	POV	1	0
3	B	807	POV	2	0
4	B	816	PCW	1	0
3	A	816	POV	3	0
4	D	804	PCW	1	0
3	B	814	POV	4	0
2	B	803	Y01	2	0
2	D	808	Y01	3	0
3	A	804	POV	5	0
3	D	812	POV	5	0
4	A	814	PCW	1	0

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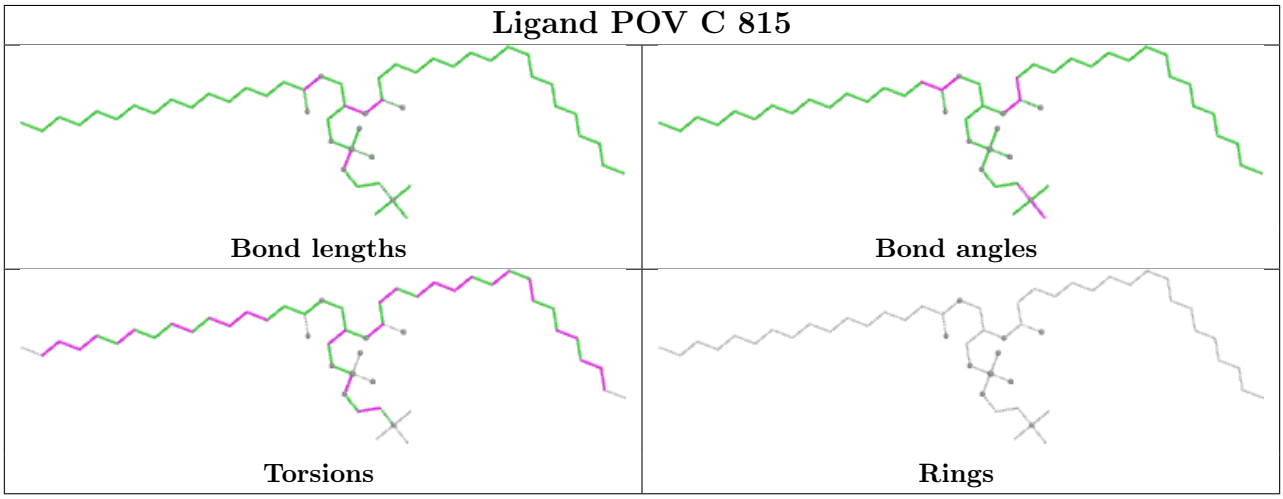
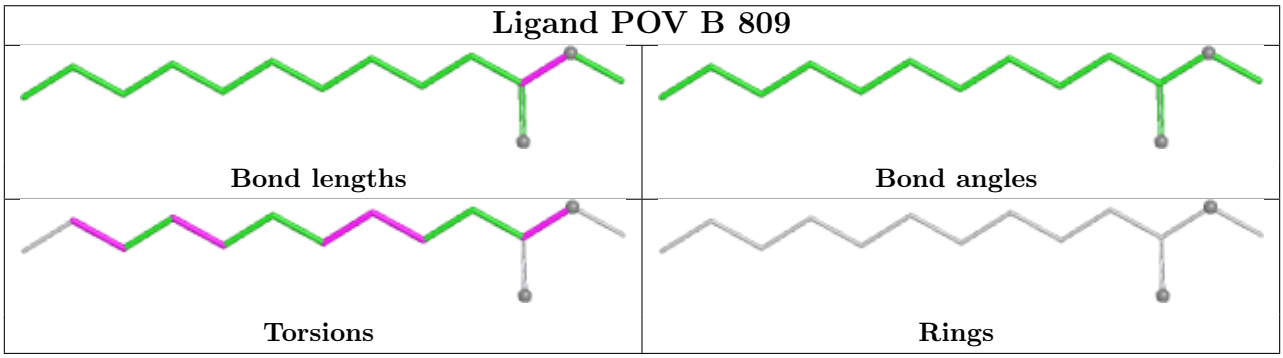
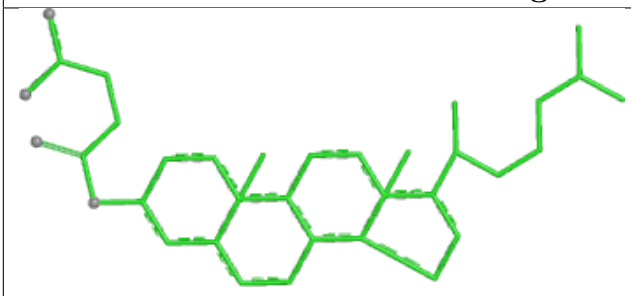
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	805	POV	4	0
3	A	806	POV	3	0
2	A	815	Y01	1	0
4	C	810	PCW	4	0

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

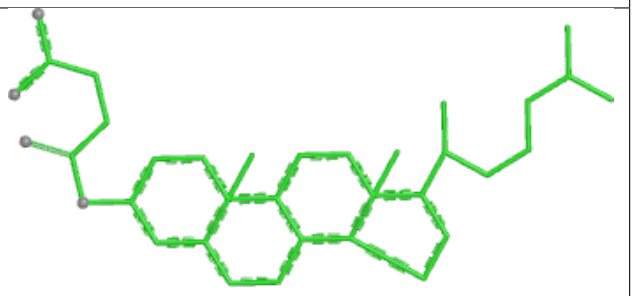




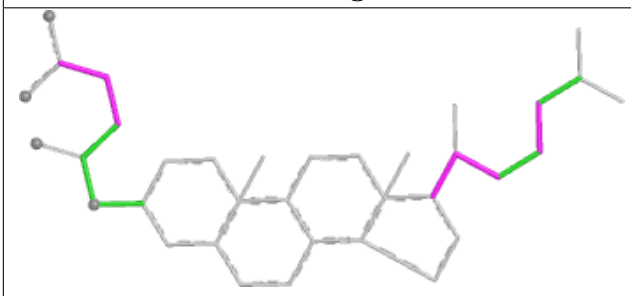
Ligand Y01 B 804



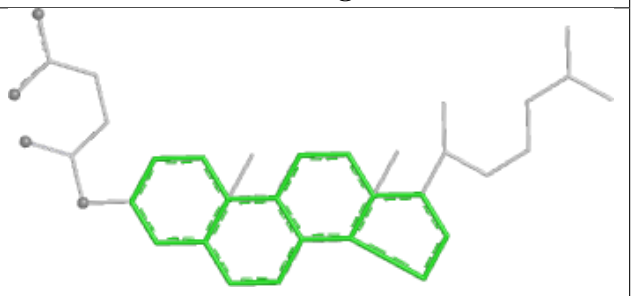
Bond lengths



Bond angles

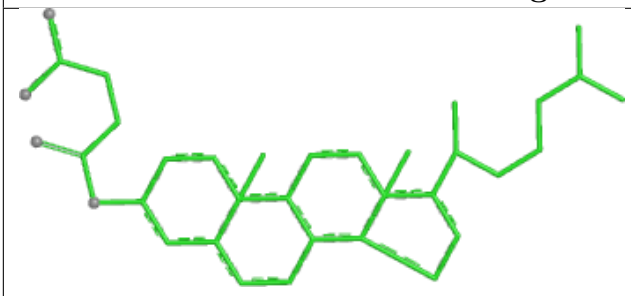


Torsions

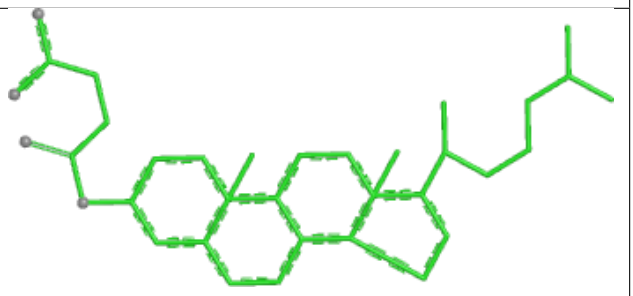


Rings

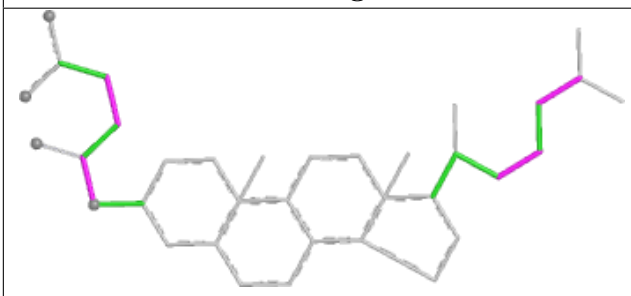
Ligand Y01 C 801



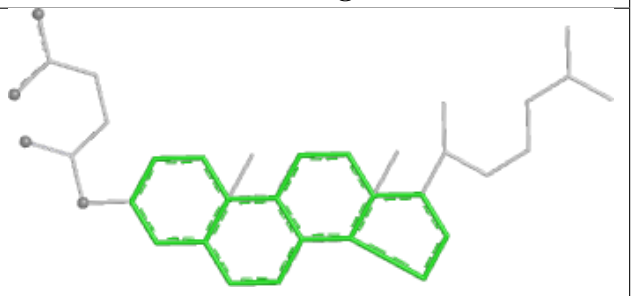
Bond lengths



Bond angles

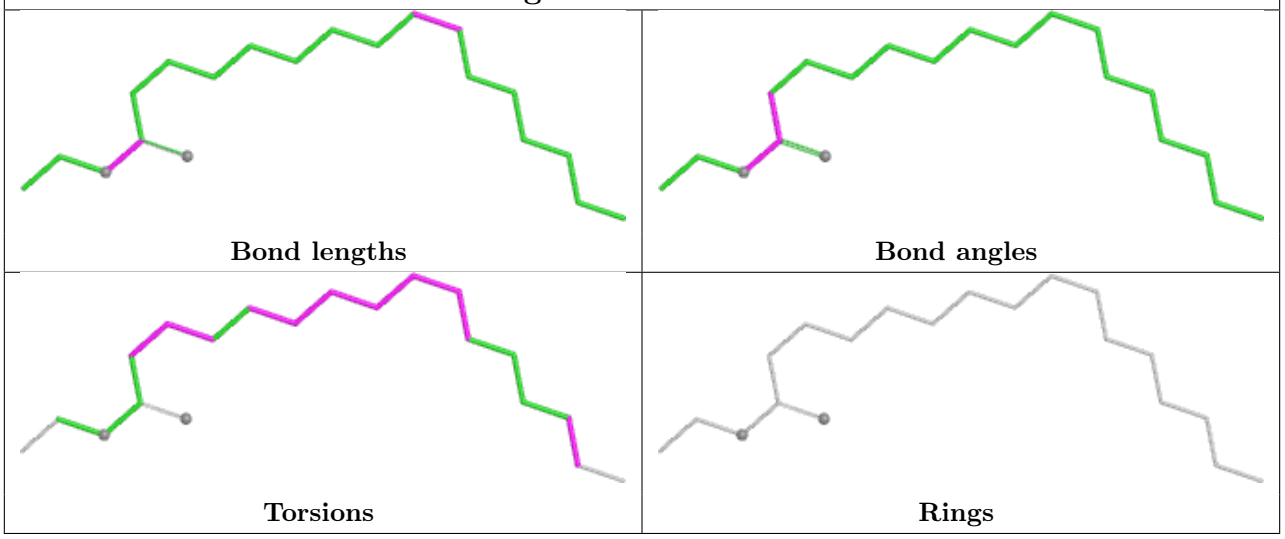


Torsions

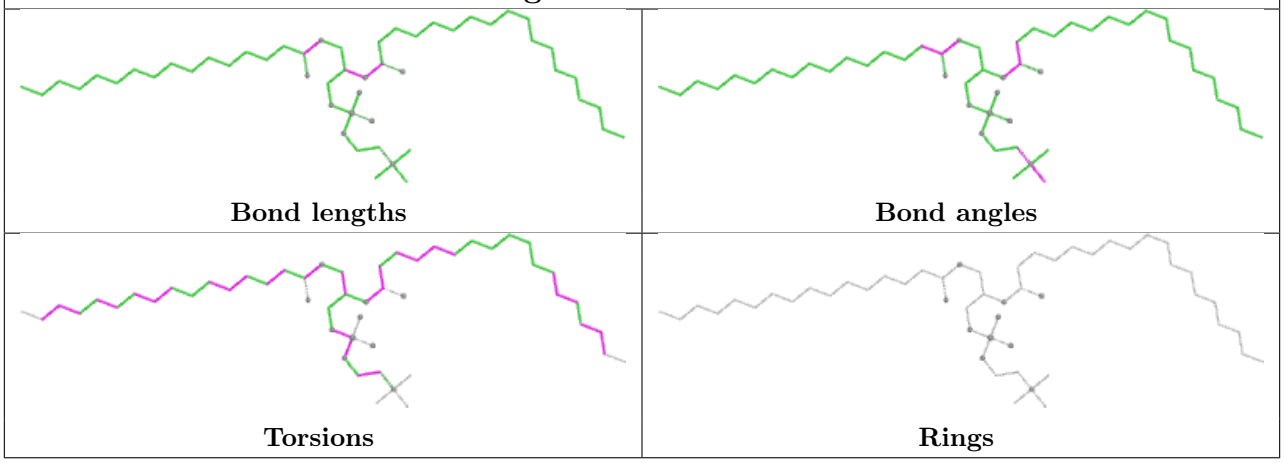


Rings

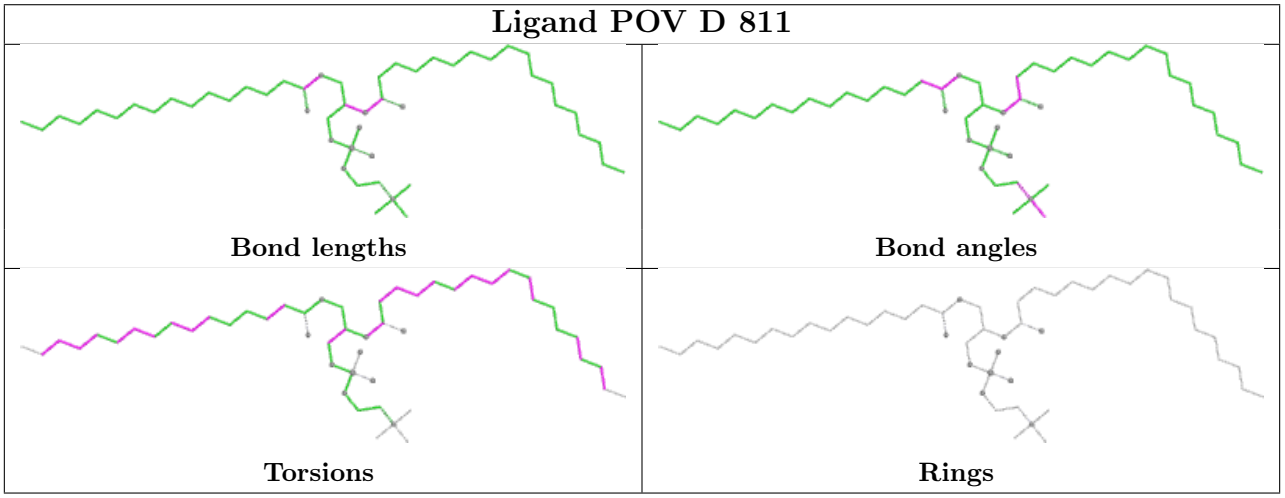
Ligand POV B 805



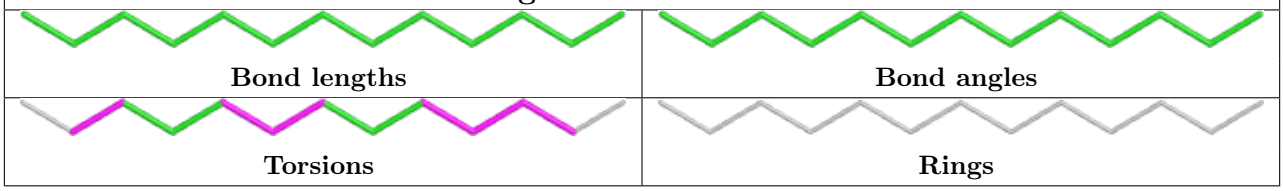
Ligand POV B 806



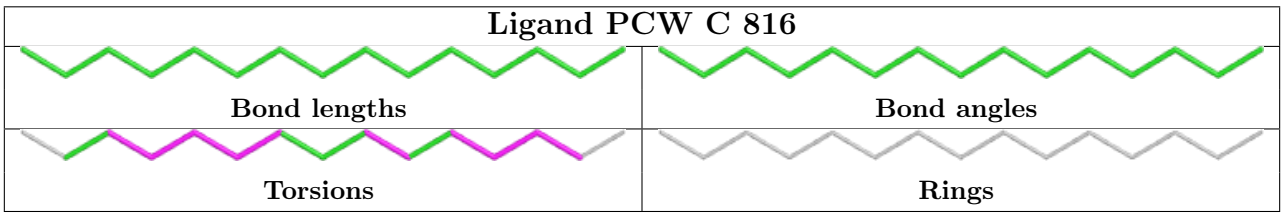
Ligand POV D 811



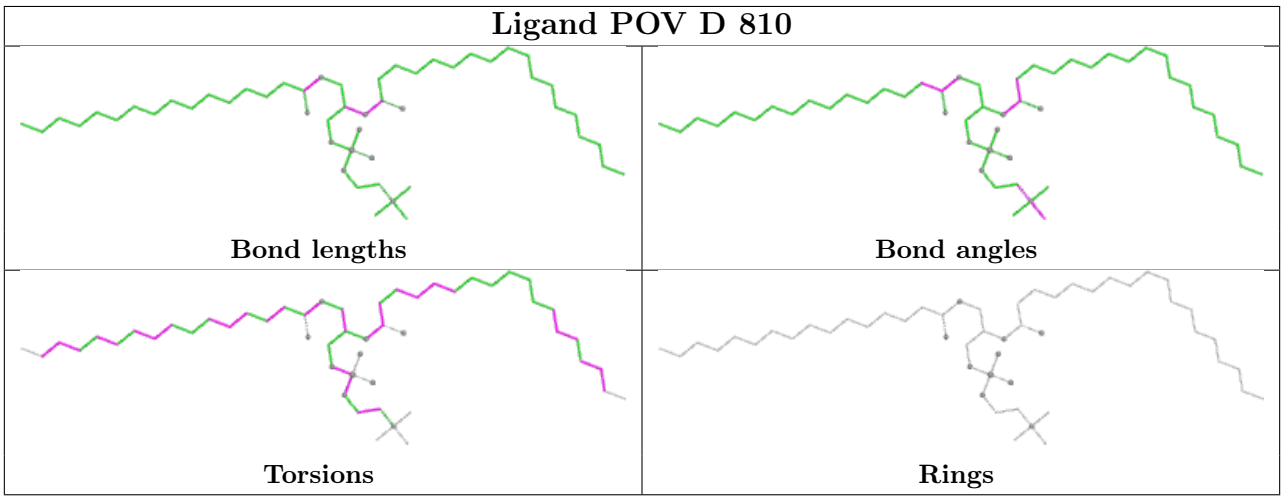
Ligand PCW A 811



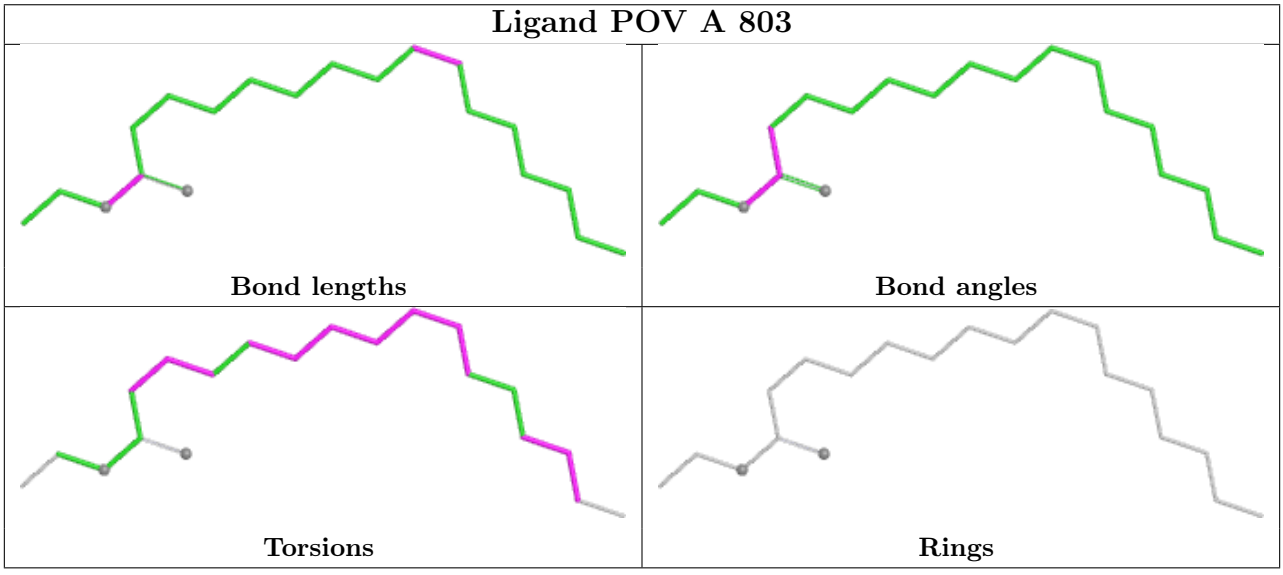
Ligand PCW C 816



Ligand POV D 810



Ligand POV A 803



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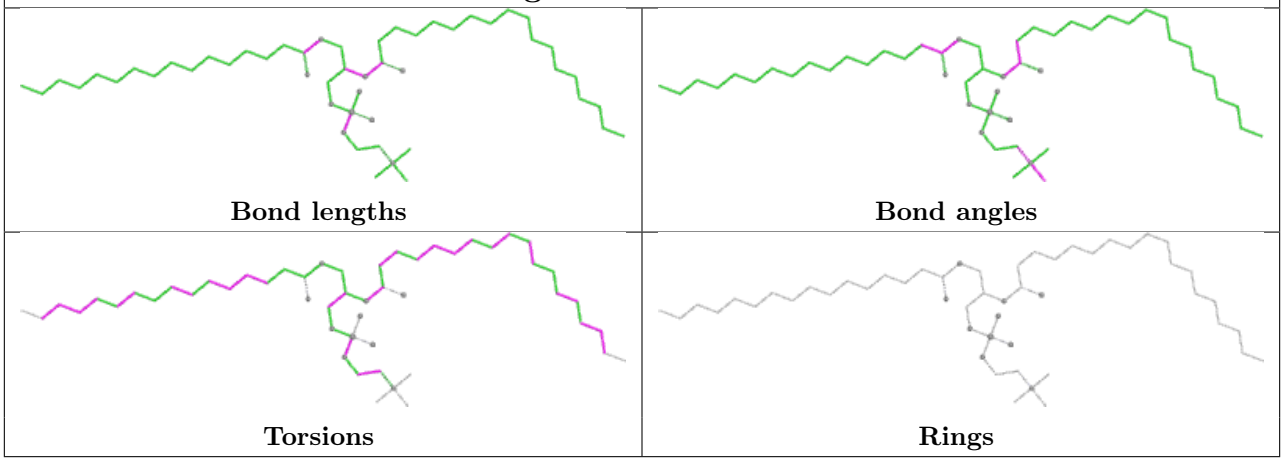
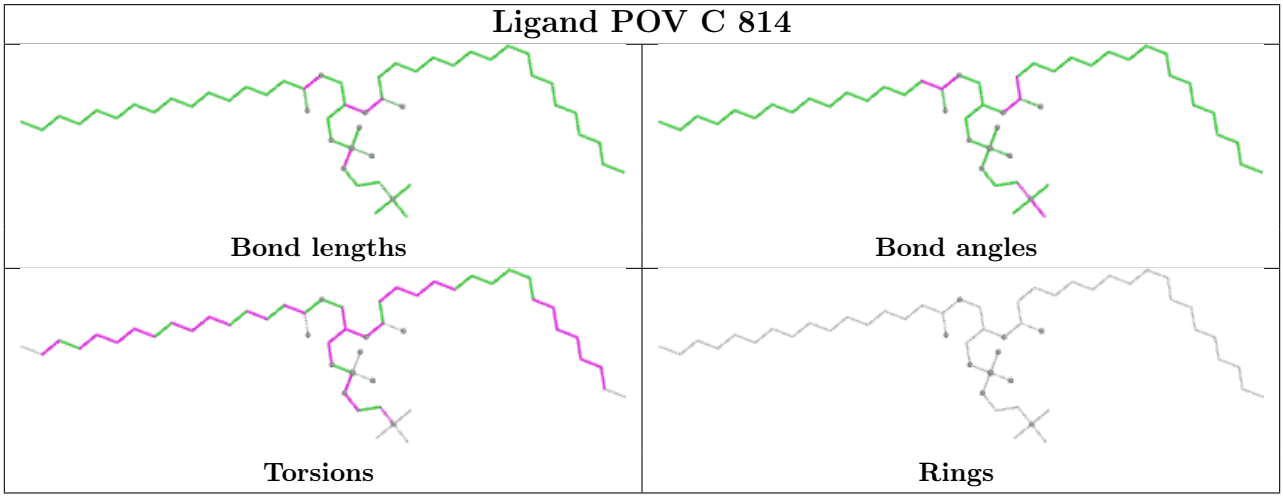
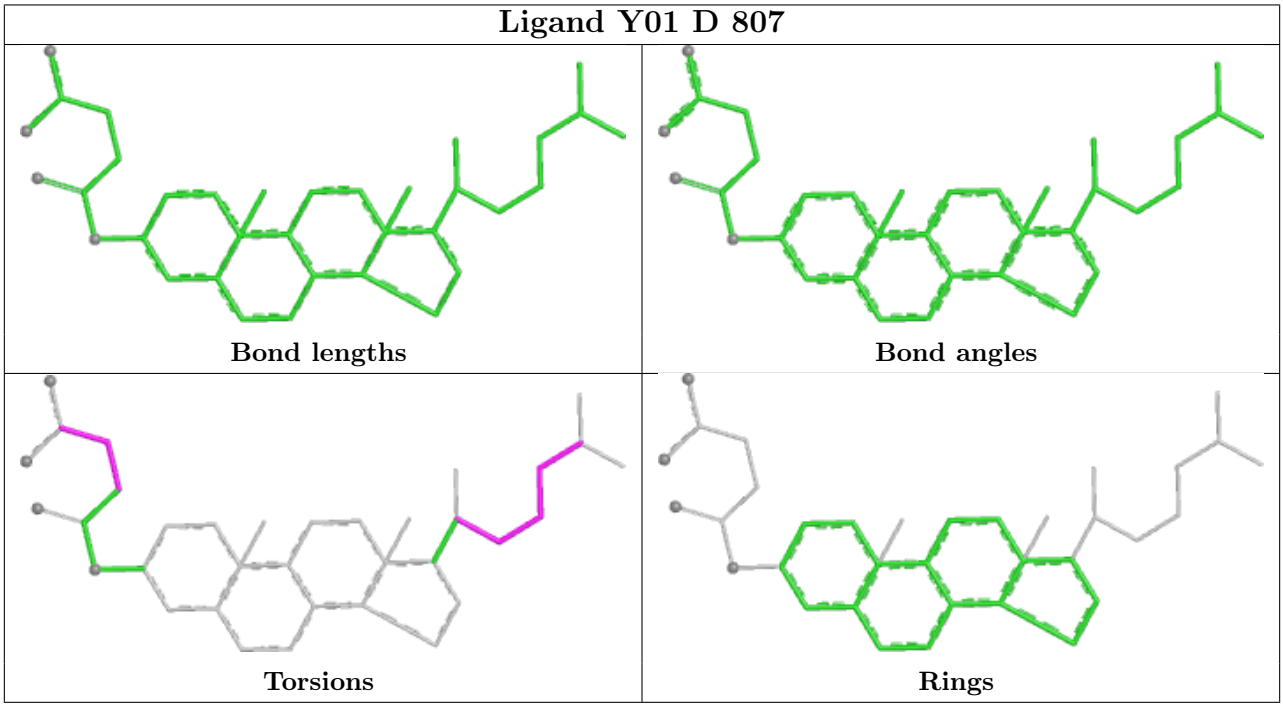


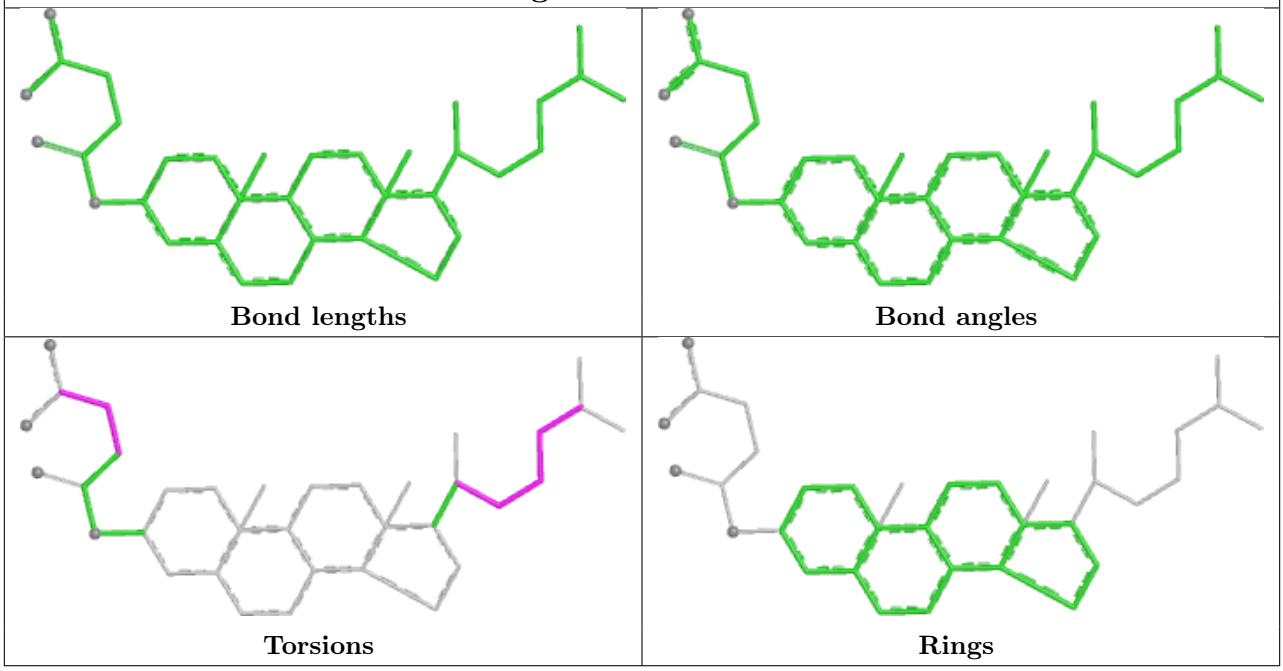
Ligand POV C 814



Ligand Y01 D 807



Ligand Y01 C 803



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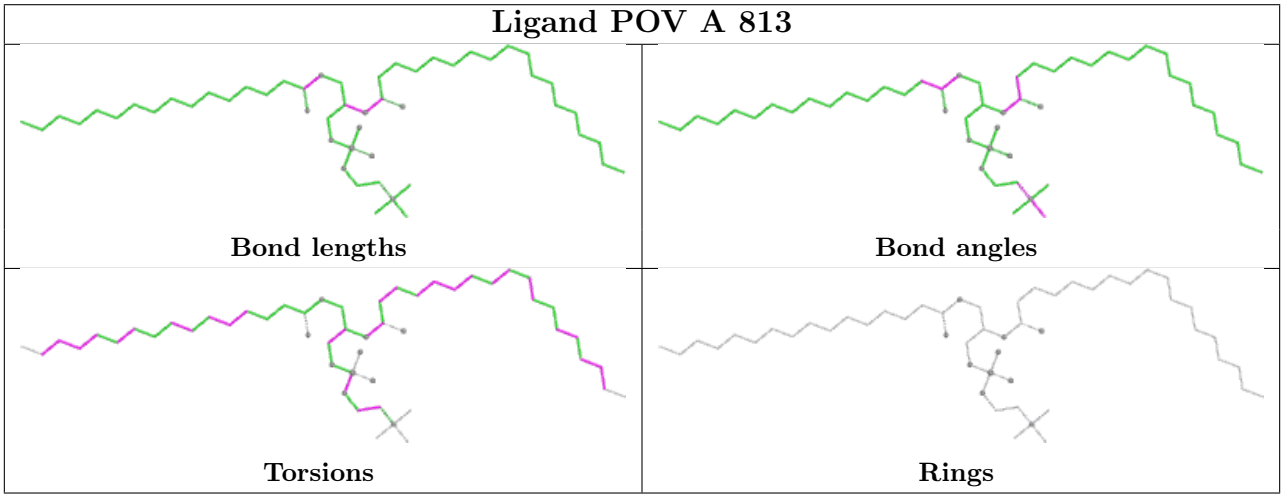
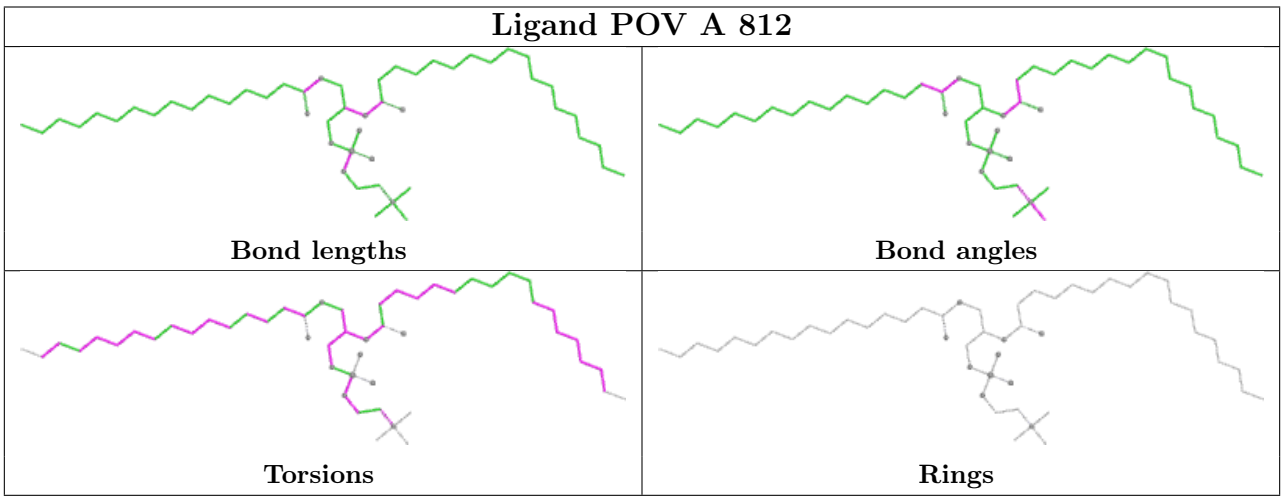
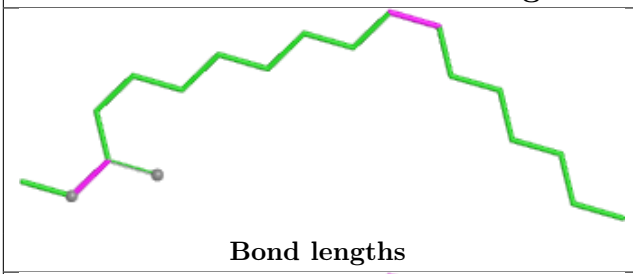
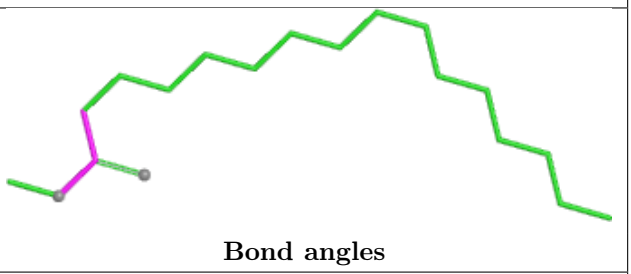


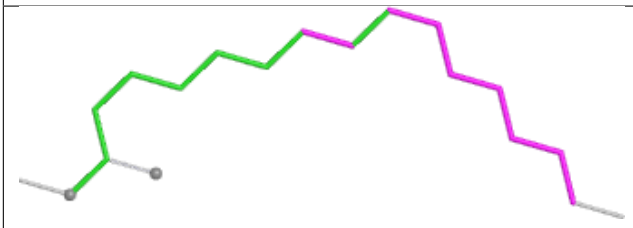
Ligand POV A 812

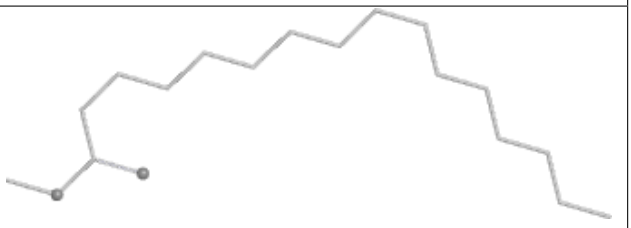


Ligand POV C 808

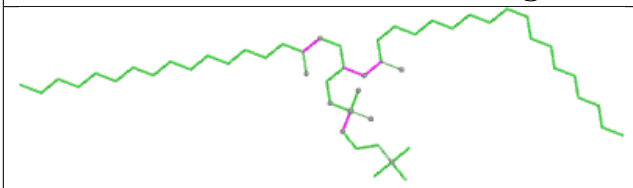

Bond lengths

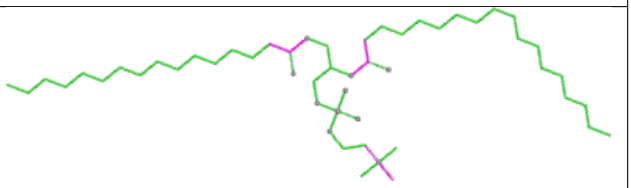

Bond angles

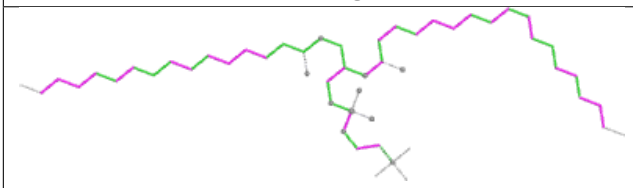

Torsions

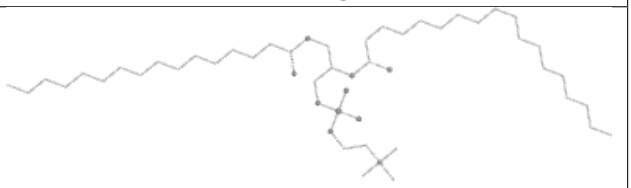

Rings

Ligand POV D 803


Bond lengths

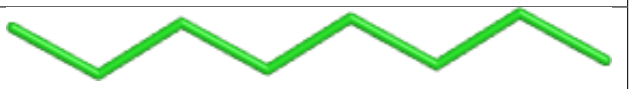

Bond angles

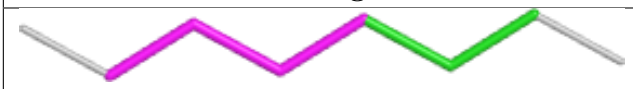

Torsions


Rings

Ligand PCW C 811


Bond lengths


Bond angles

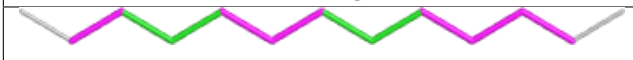

Torsions


Rings

Ligand PCW D 801

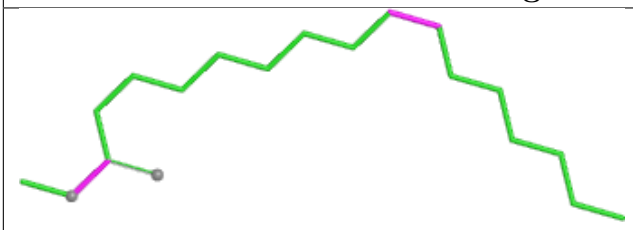

Bond lengths

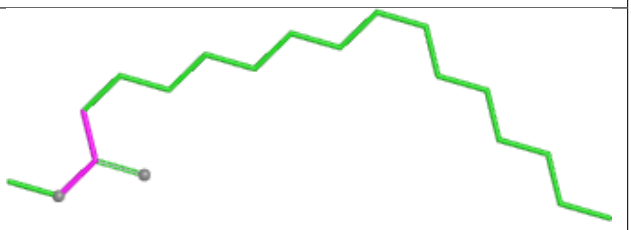

Bond angles

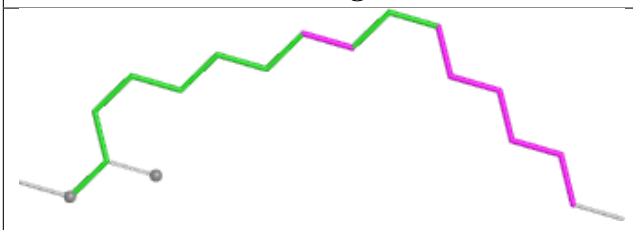

Torsions

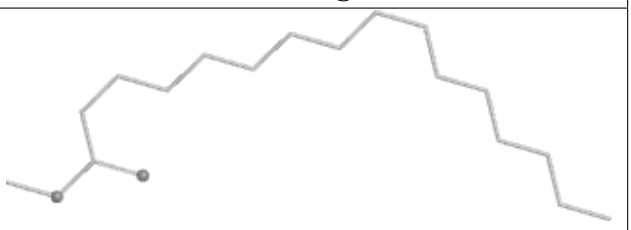

Rings

Ligand POV B 808


Bond lengths

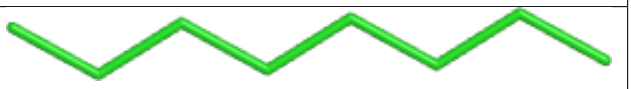

Bond angles


Torsions


Rings

Ligand PCW B 811


Bond lengths


Bond angles


Torsions


Rings

Ligand PCW B 813

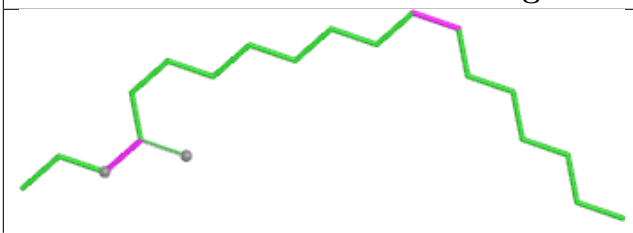

Bond lengths

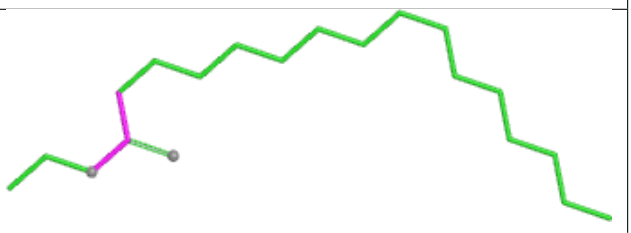

Bond angles

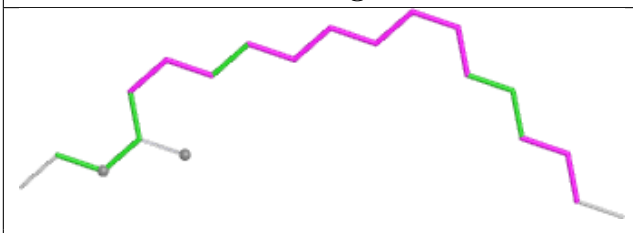

Torsions

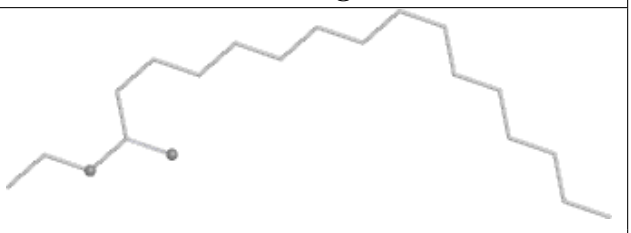

Rings

Ligand POV C 805

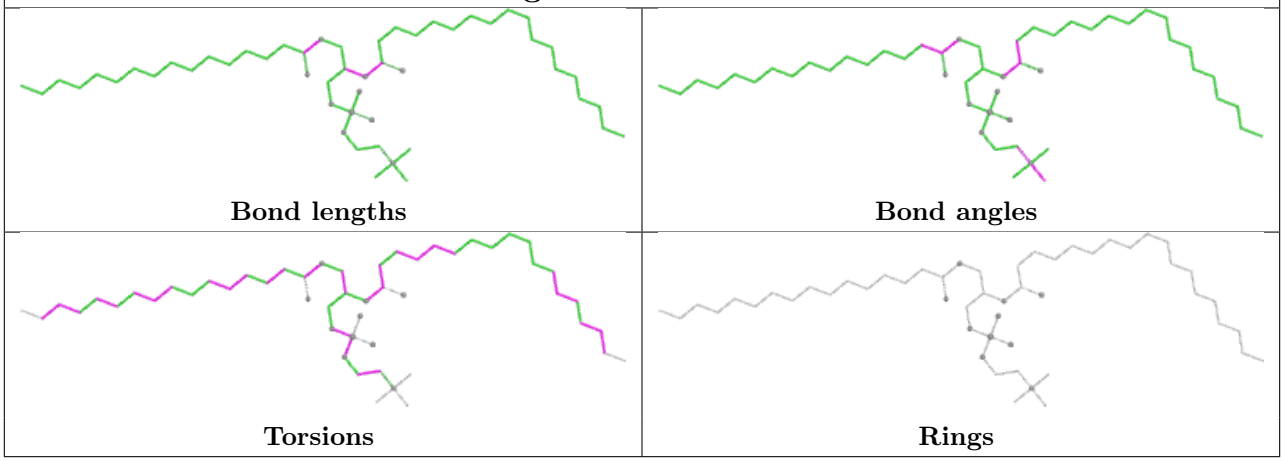

Bond lengths


Bond angles

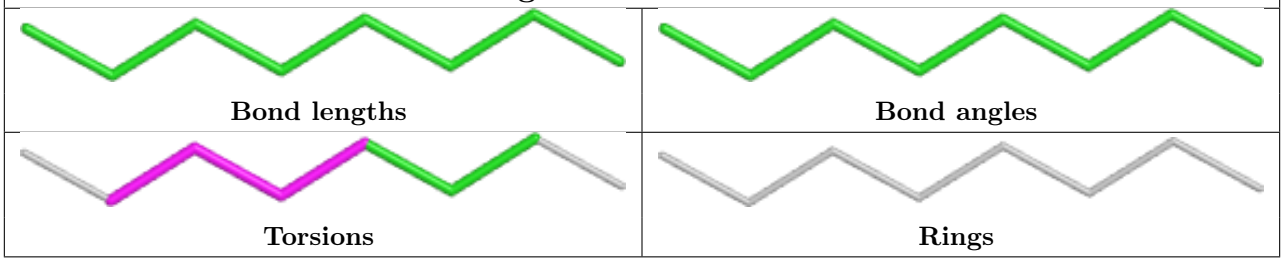

Torsions


Rings

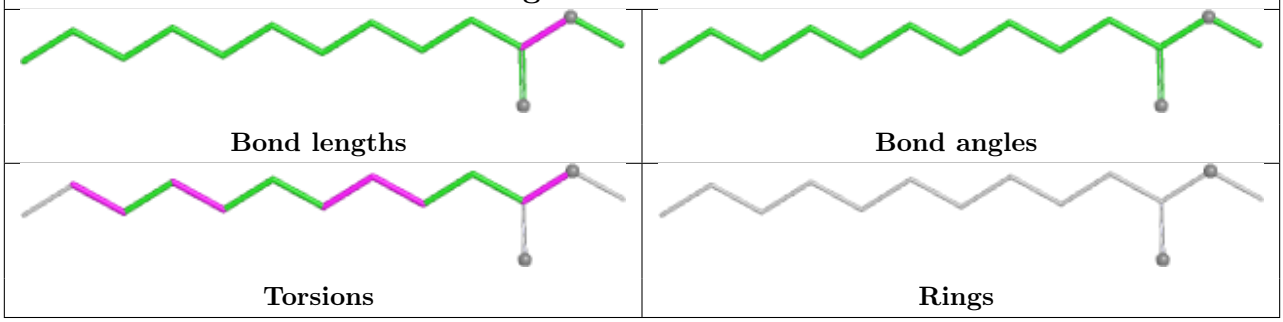
Ligand POV C 806



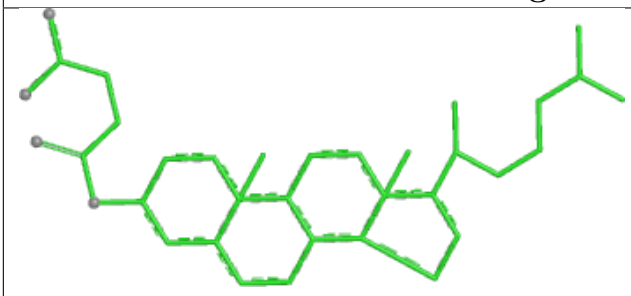
Ligand PCW D 815



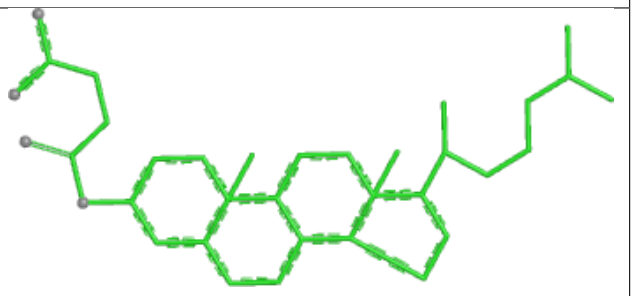
Ligand POV D 813



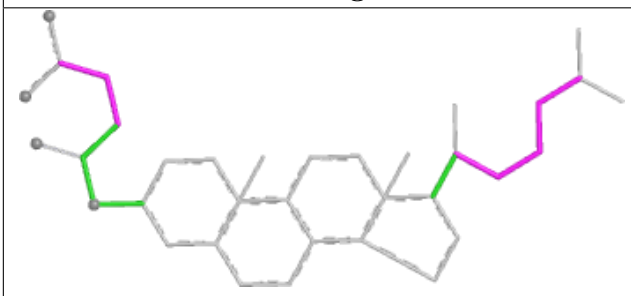
Ligand Y01 A 801



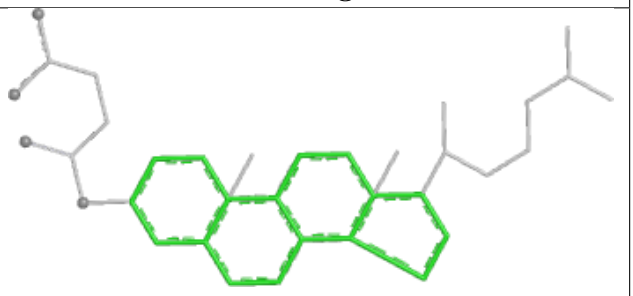
Bond lengths



Bond angles

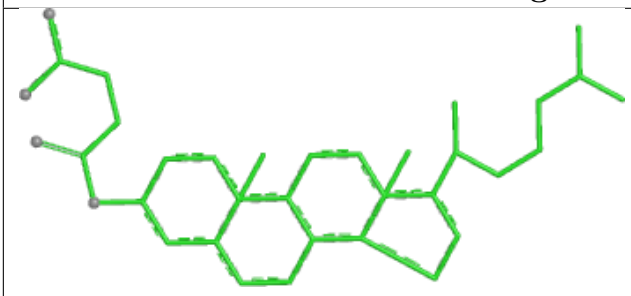


Torsions

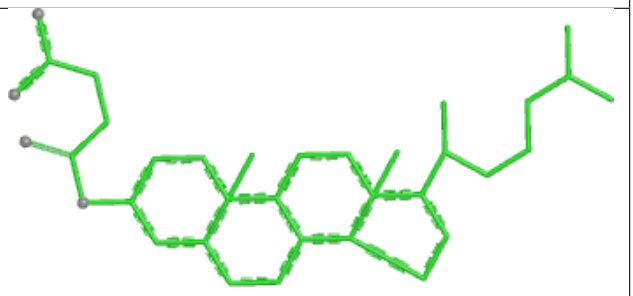


Rings

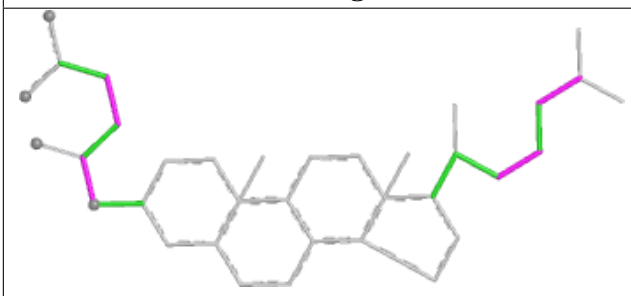
Ligand Y01 B 801



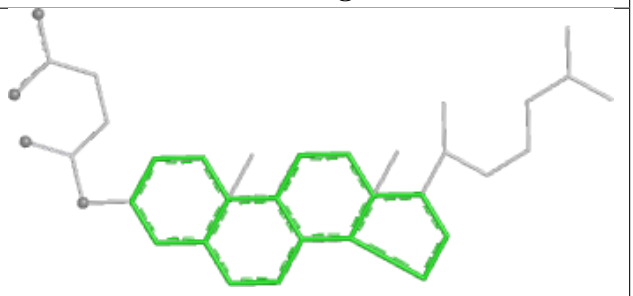
Bond lengths



Bond angles

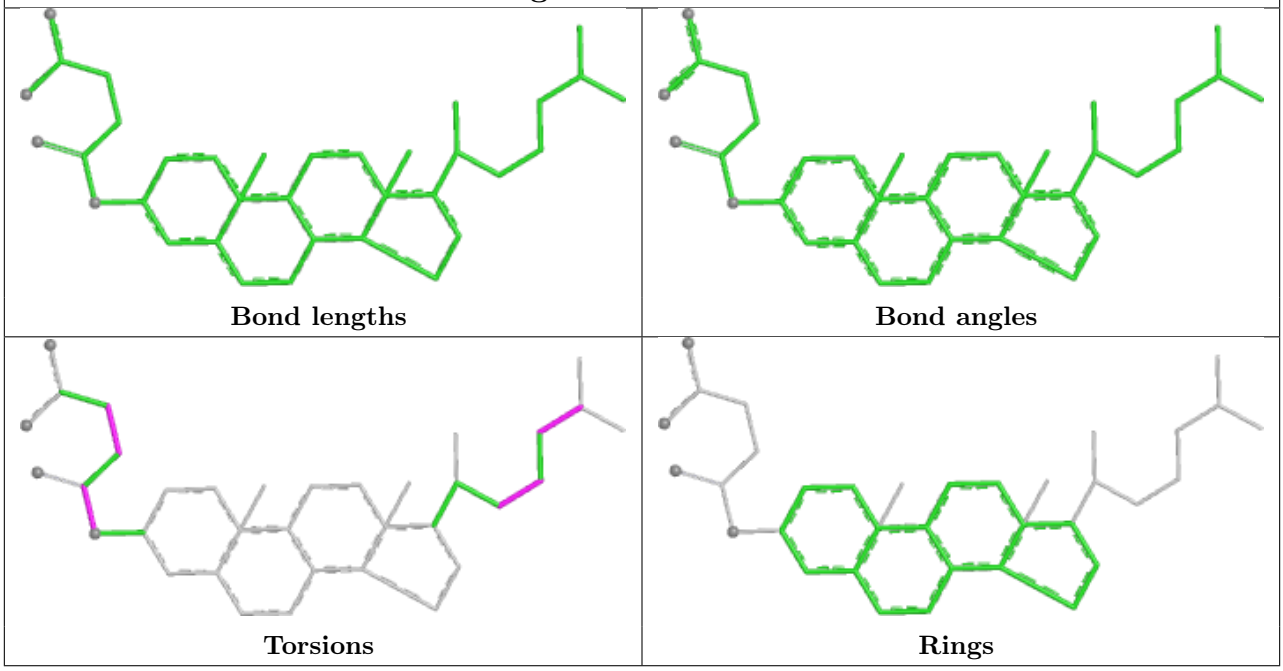


Torsions

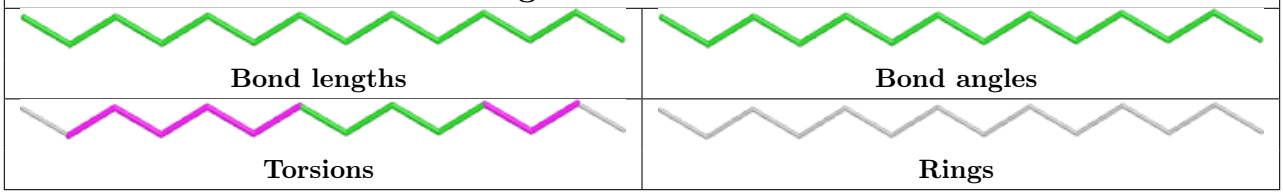


Rings

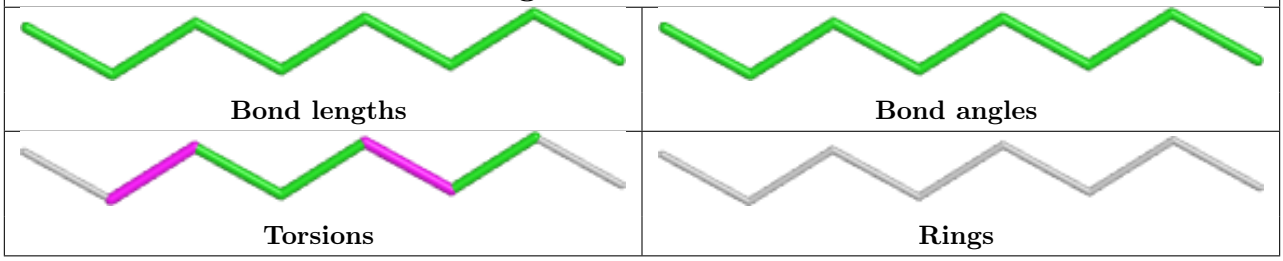
Ligand Y01 D 805



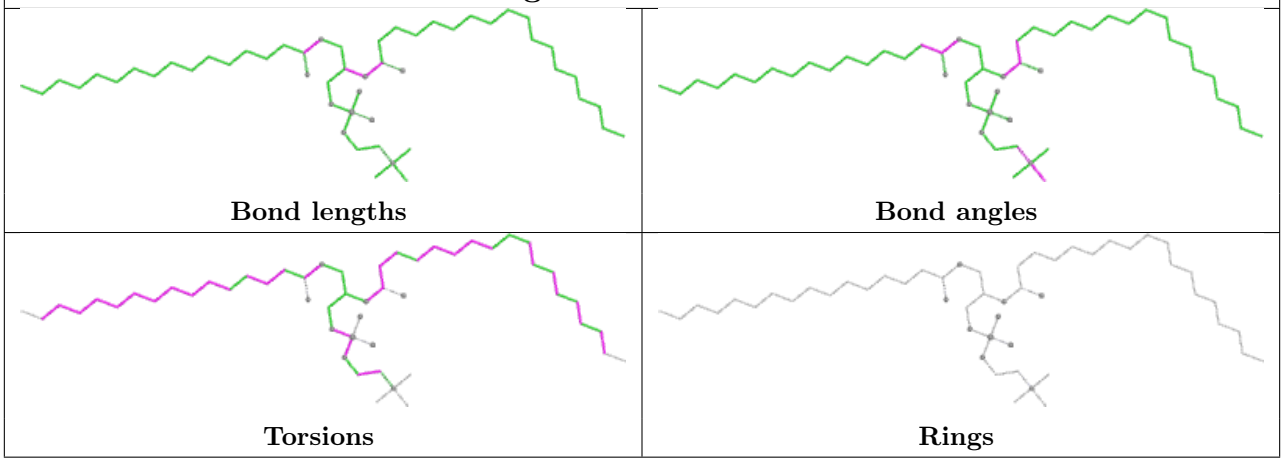
Ligand PCW A 808



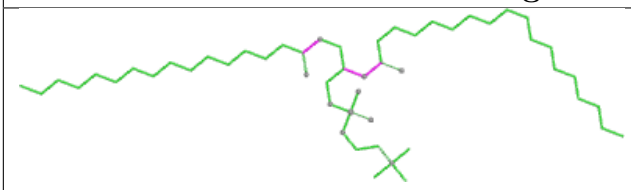
Ligand PCW A 810



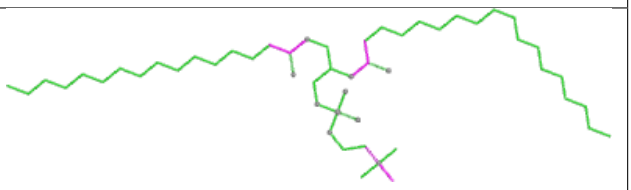
Ligand POV C 802



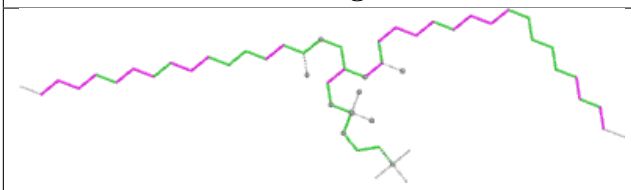
Ligand POV C 807



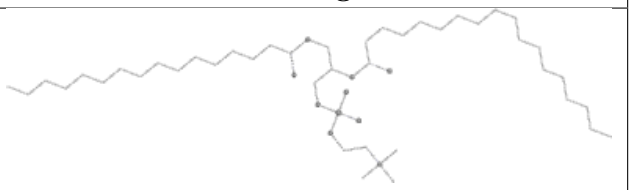
Bond lengths



Bond angles

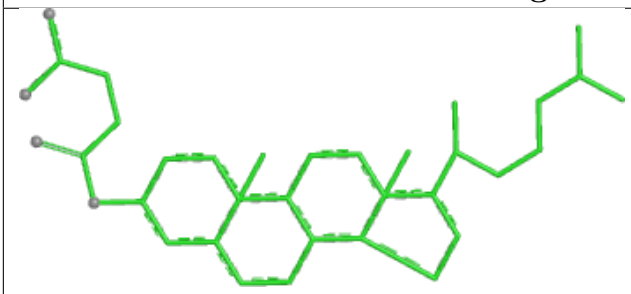


Torsions



Rings

Ligand Y01 C 804



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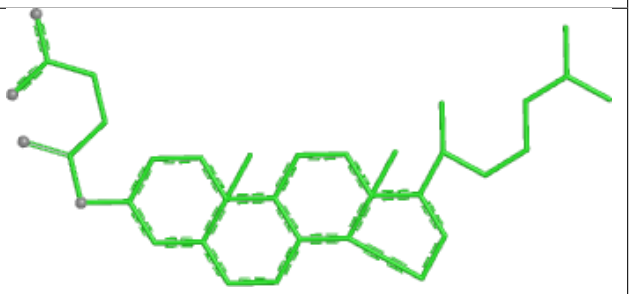
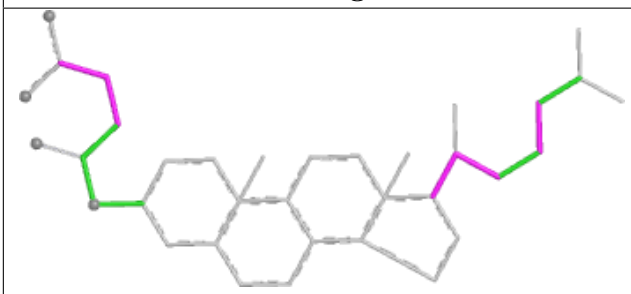


Bond angles



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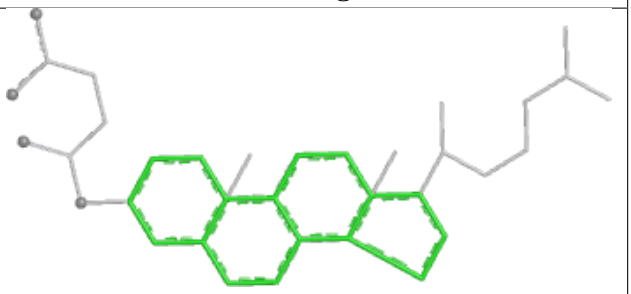
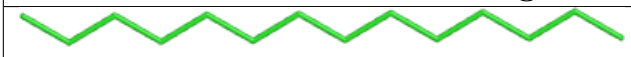


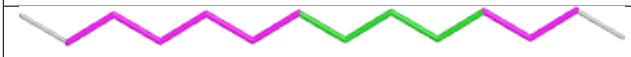
Rings

Ligand PCW B 810



Bond lengths

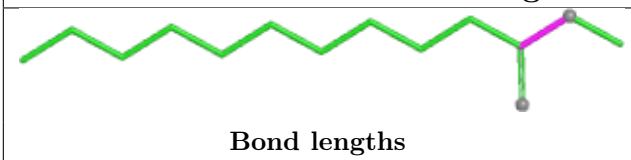
Bond angles

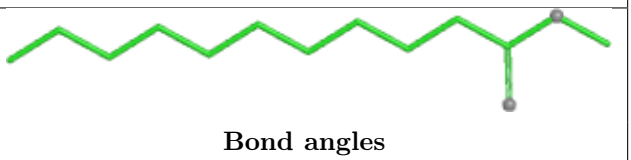


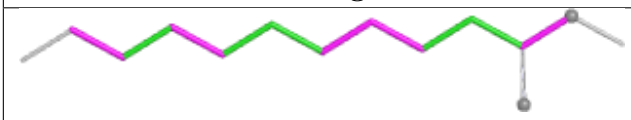
Torsions

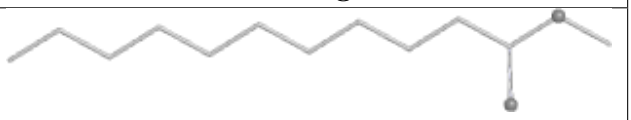
Rings

Ligand POV C 809

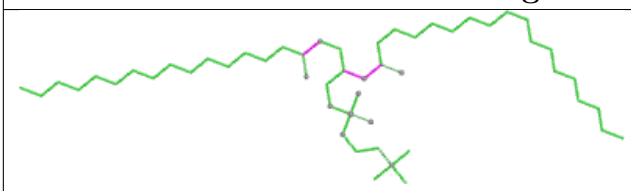

Bond lengths

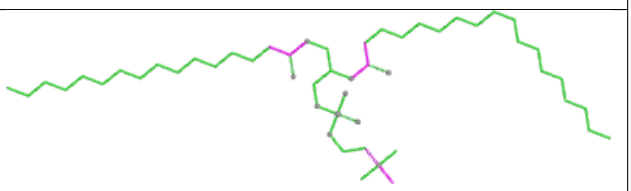

Bond angles

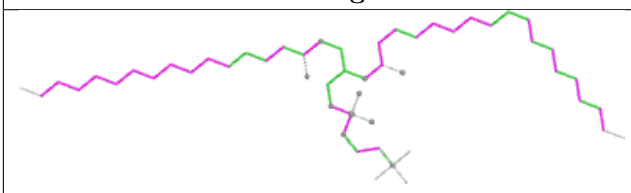

Torsions

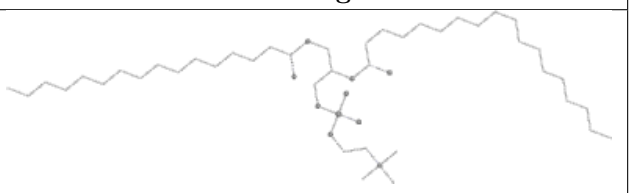

Rings

Ligand POV D 806

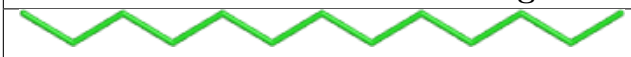

Bond lengths

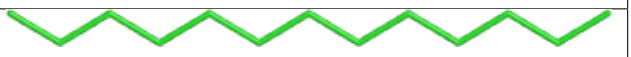

Bond angles

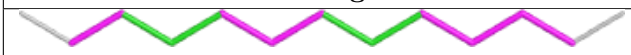

Torsions

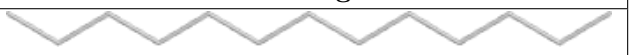

Rings

Ligand PCW C 813


Bond lengths


Bond angles

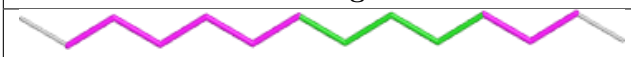

Torsions


Rings

Ligand PCW D 814

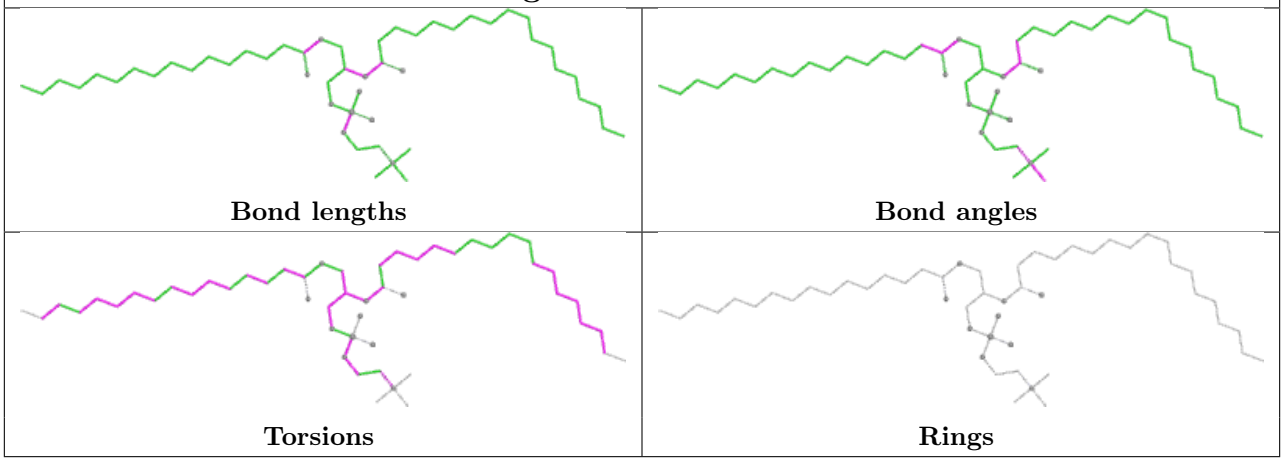

Bond lengths


Bond angles

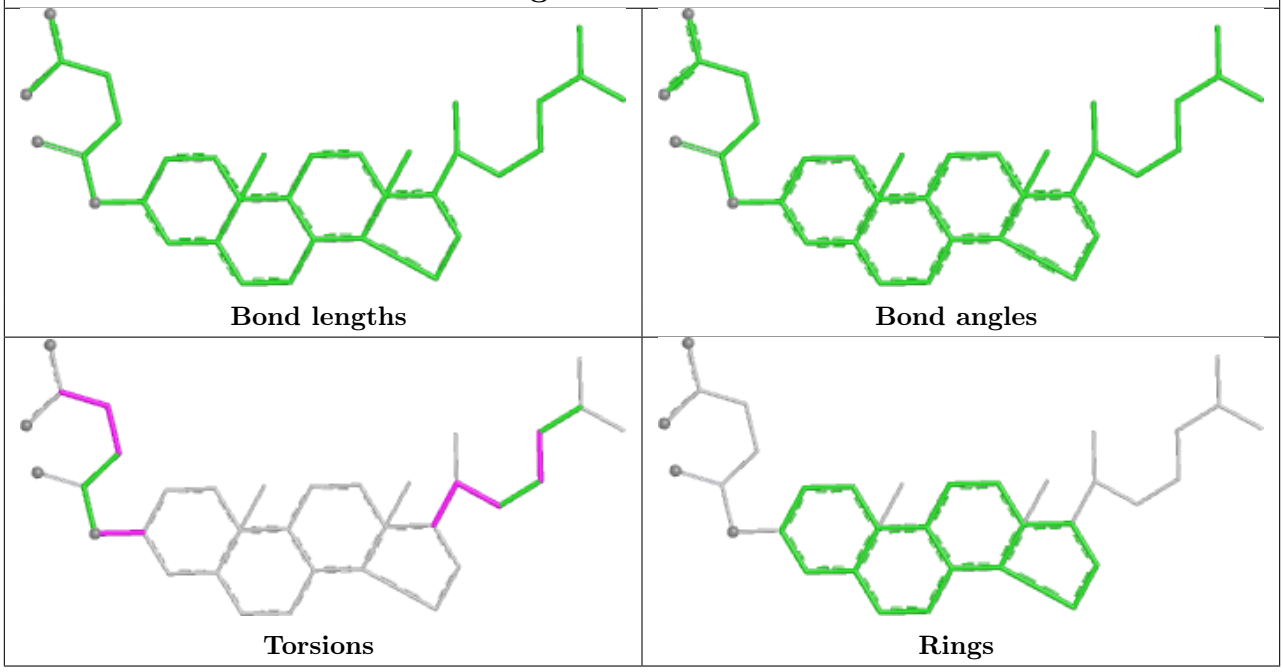

Torsions


Rings

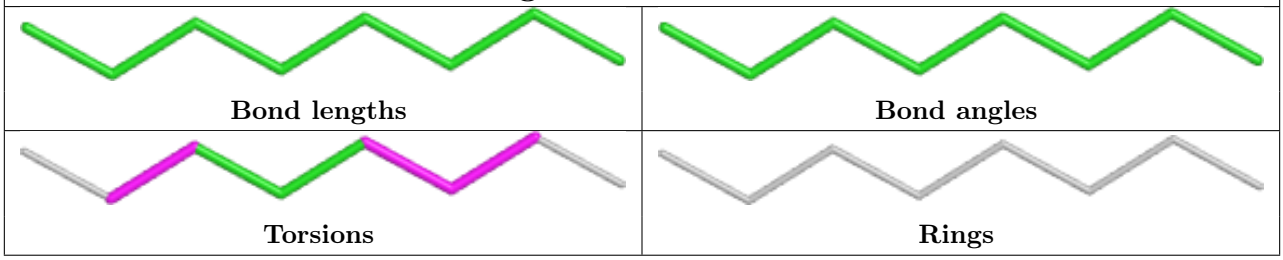
Ligand POV D 802



Ligand Y01 A 802



Ligand PCW B 812



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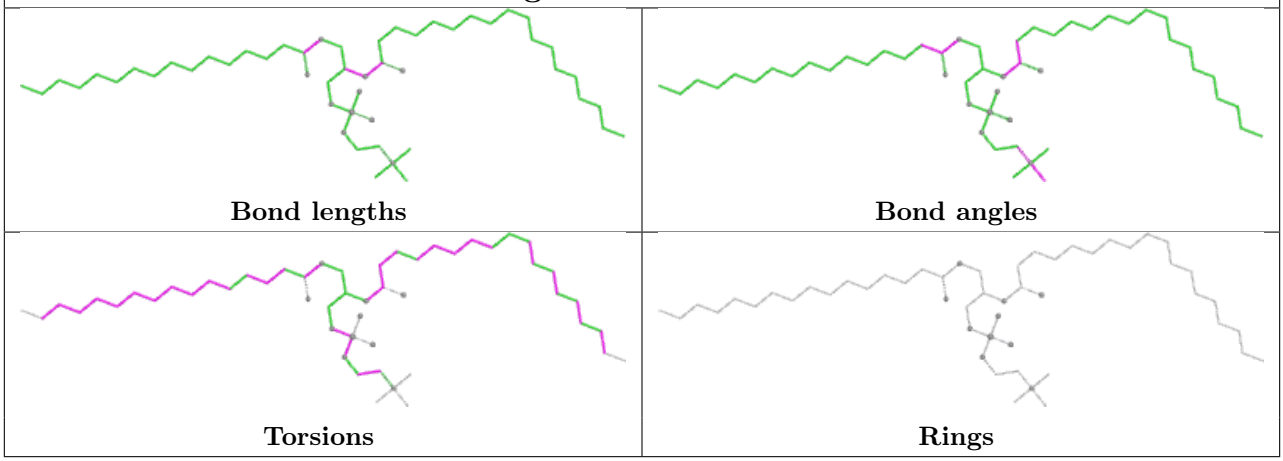
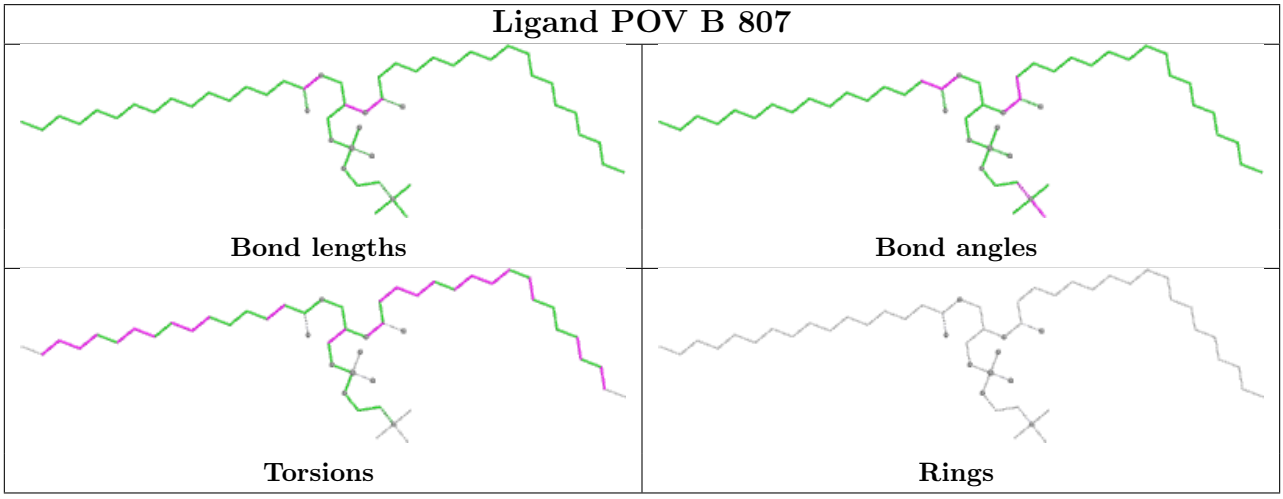
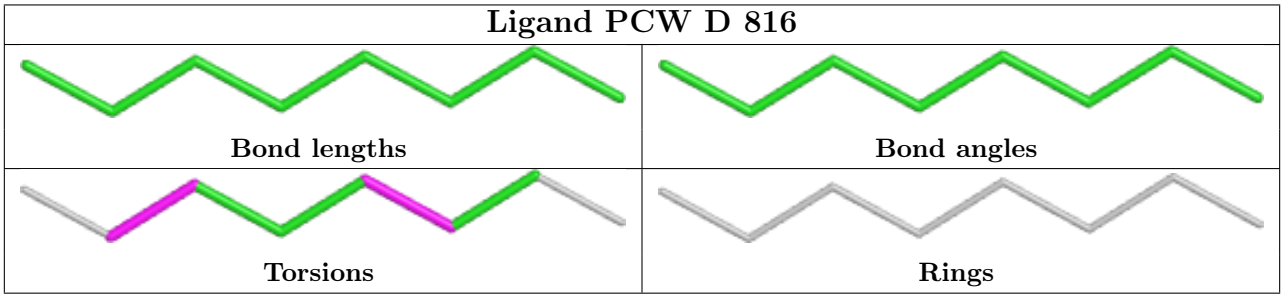


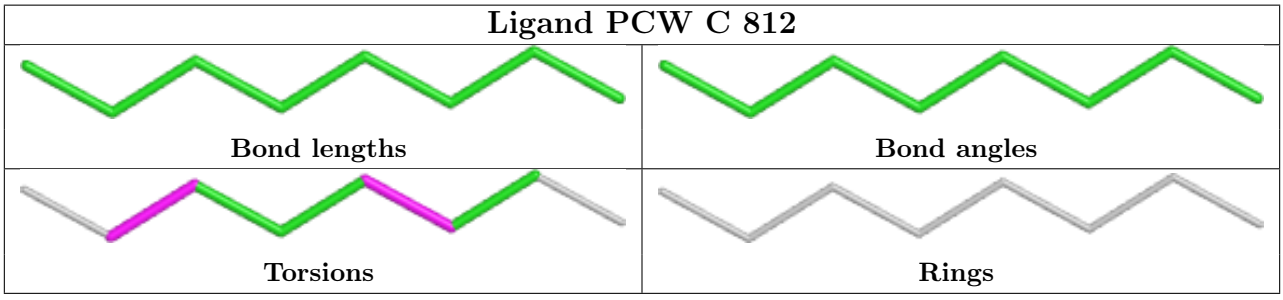
Ligand POV B 807



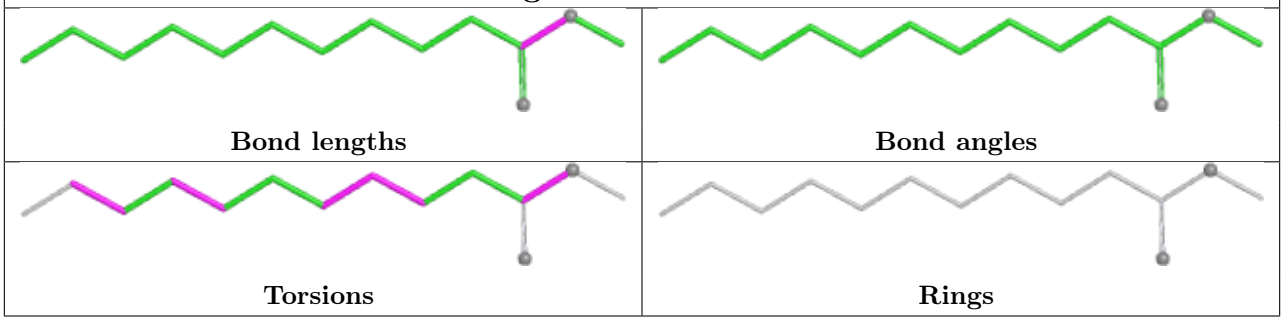
Ligand PCW D 816



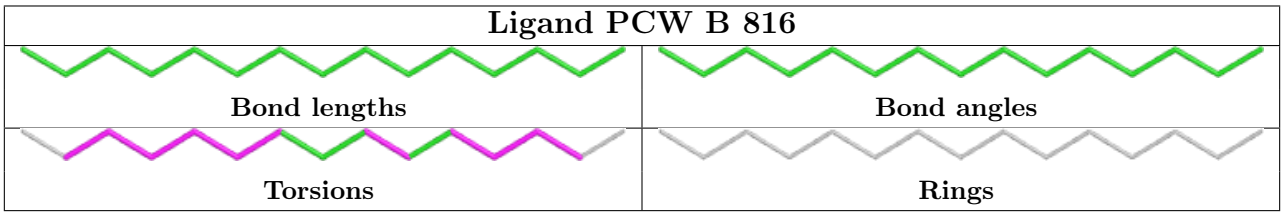
Ligand PCW C 812



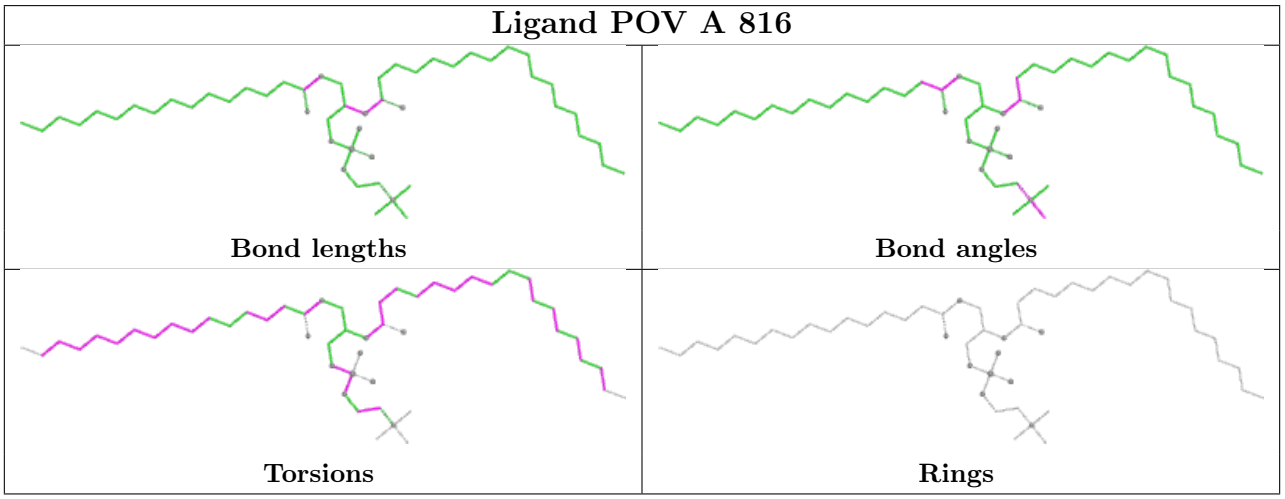
Ligand POV A 807



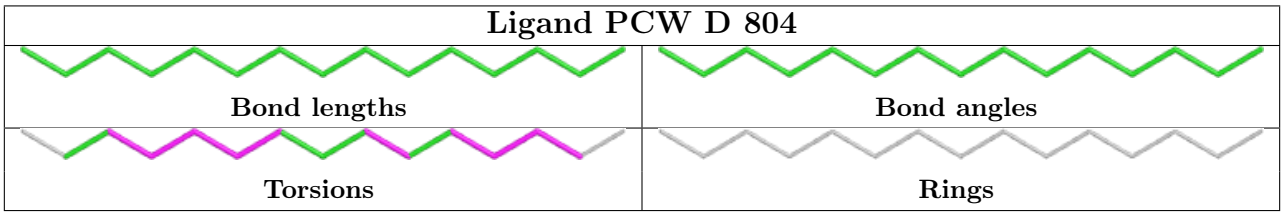
Ligand PCW B 816



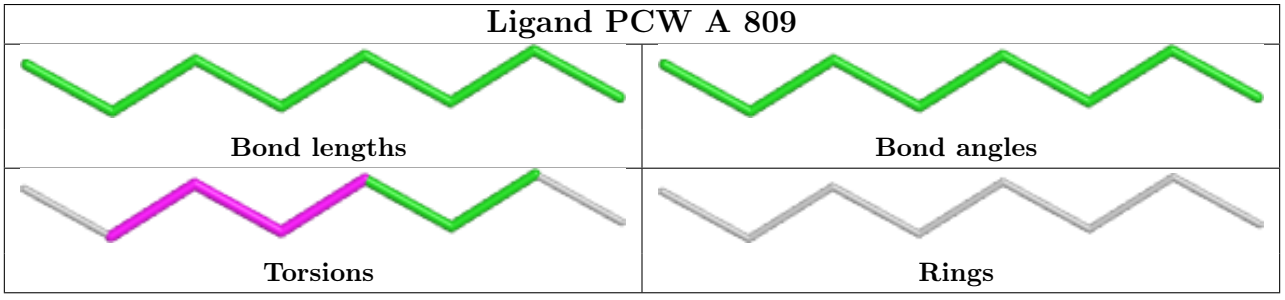
Ligand POV A 816



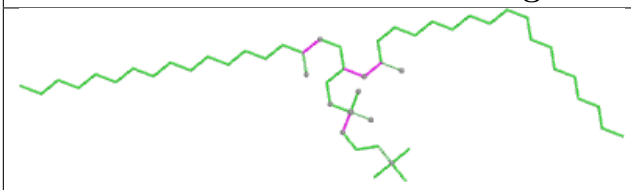
Ligand PCW D 804



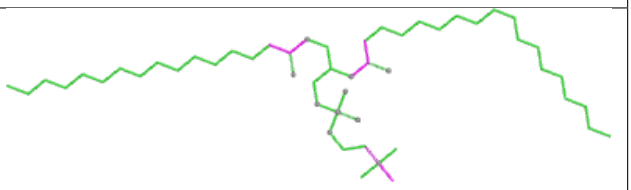
Ligand PCW A 809



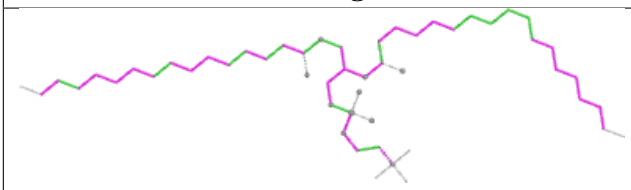
Ligand POV B 814



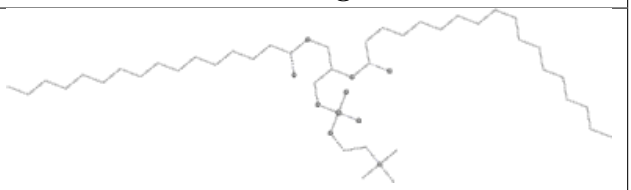
Bond lengths



Bond angles

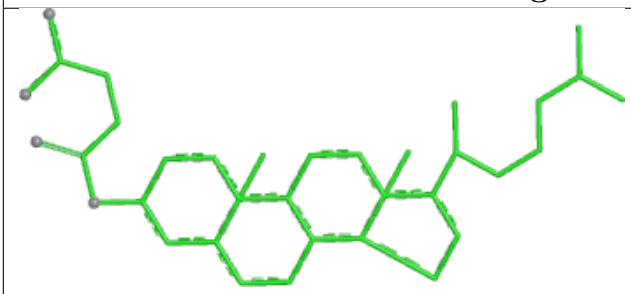


Torsions

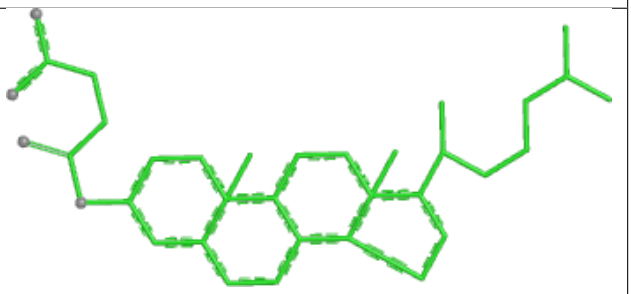


Rings

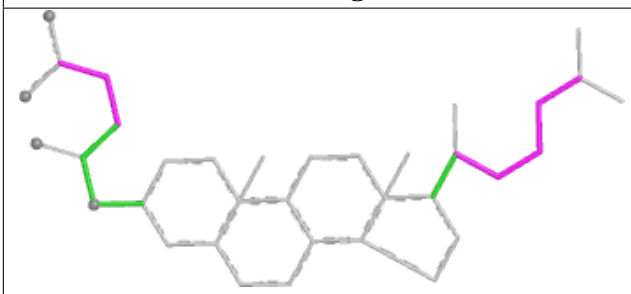
Ligand Y01 B 803



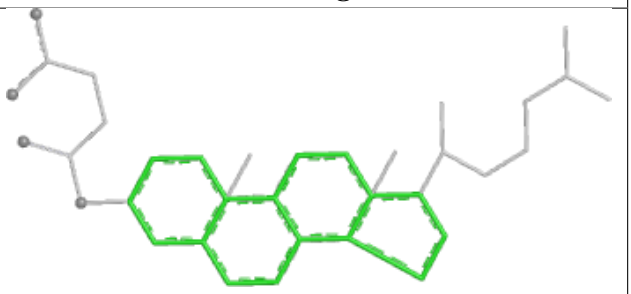
Bond lengths



Bond angles

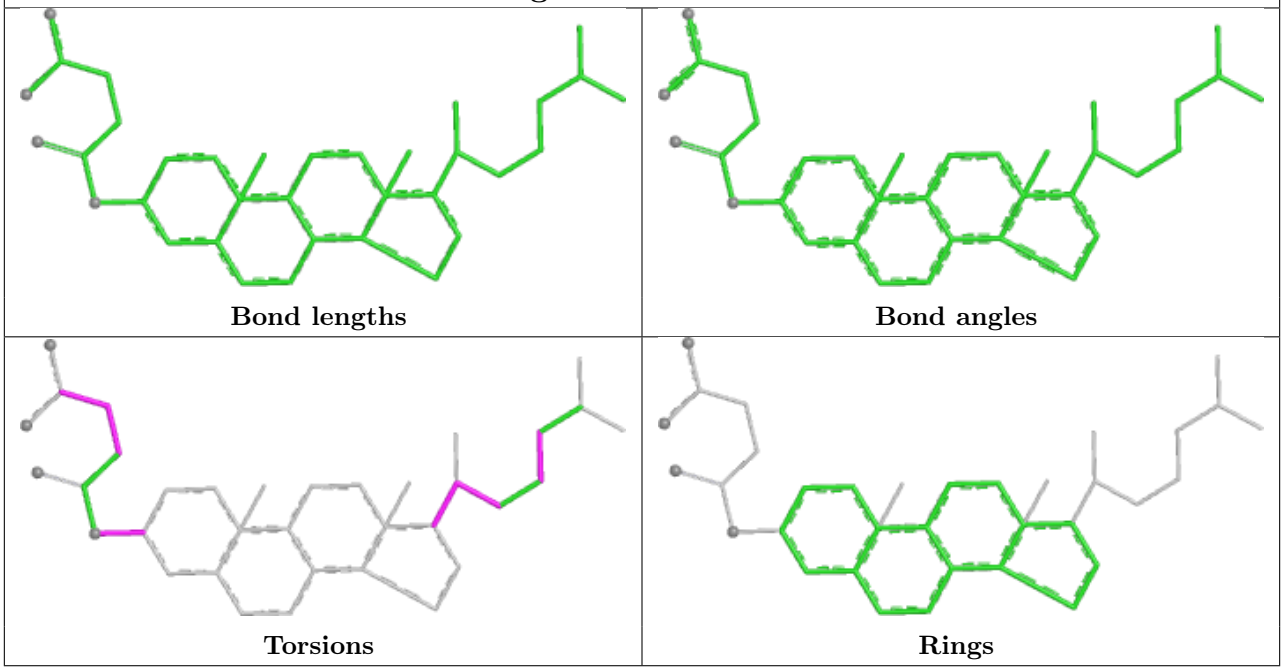


Torsions

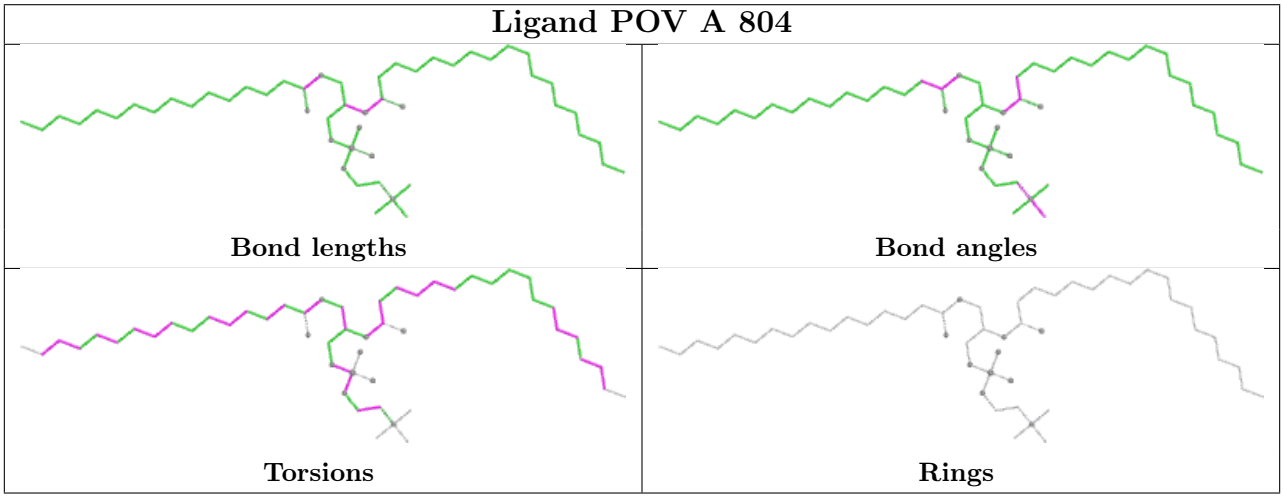


Rings

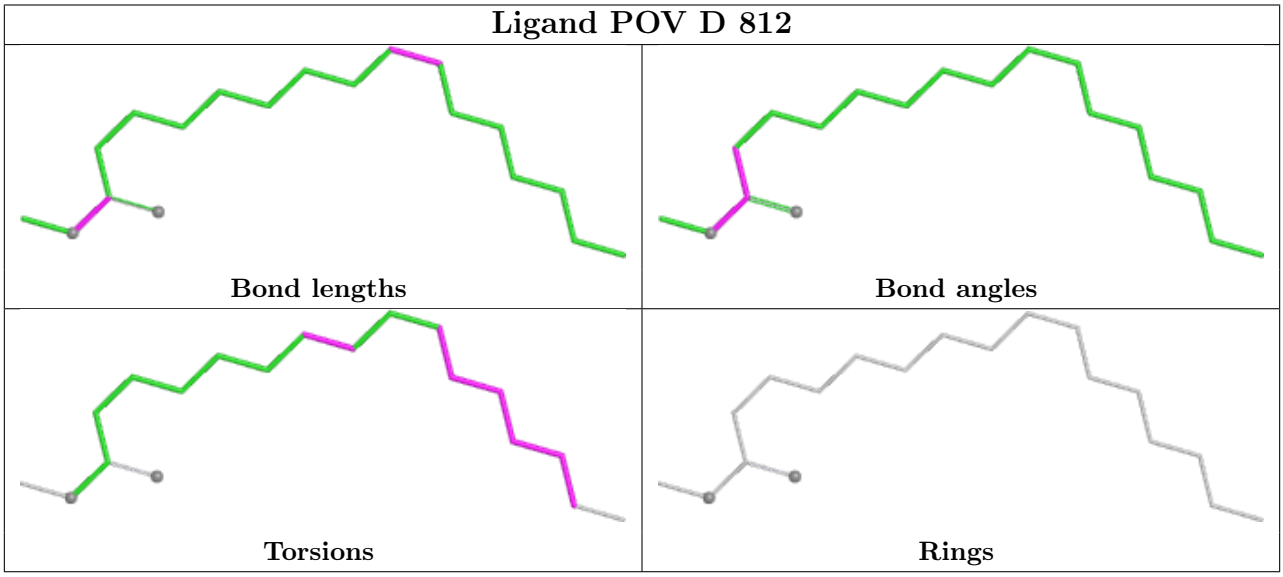
Ligand Y01 D 808



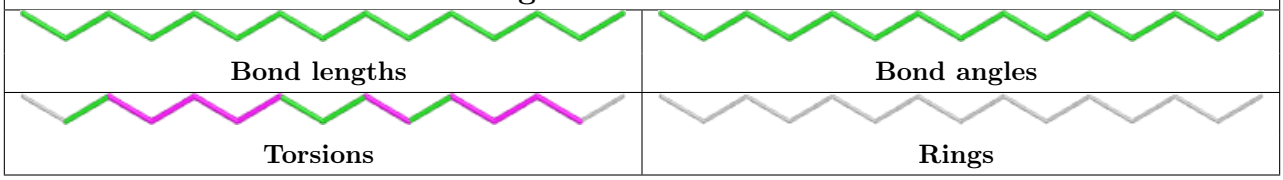
Ligand POV A 804



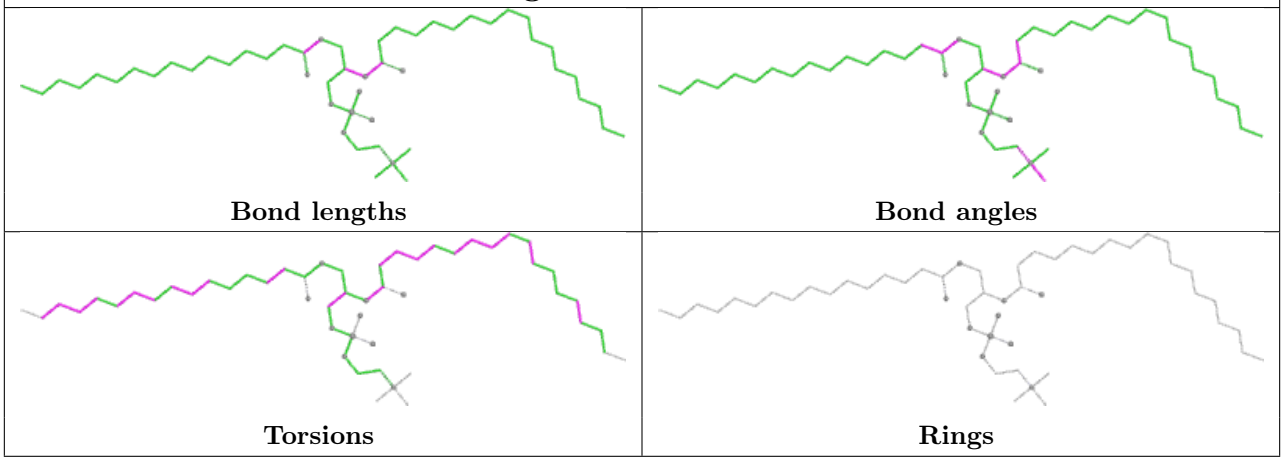
Ligand POV D 812



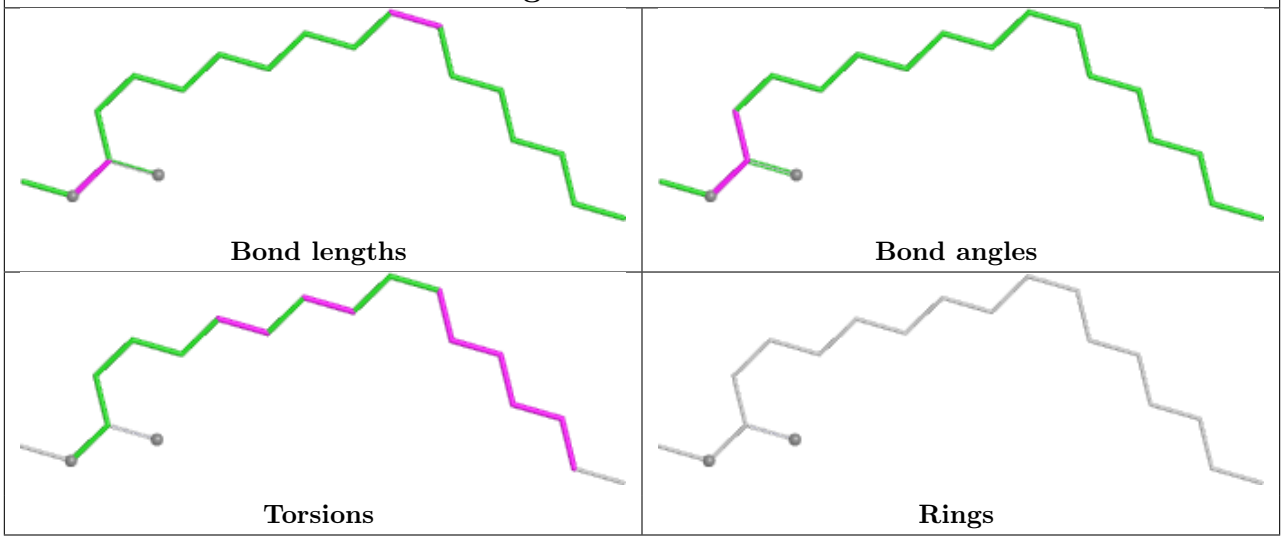
Ligand PCW A 814



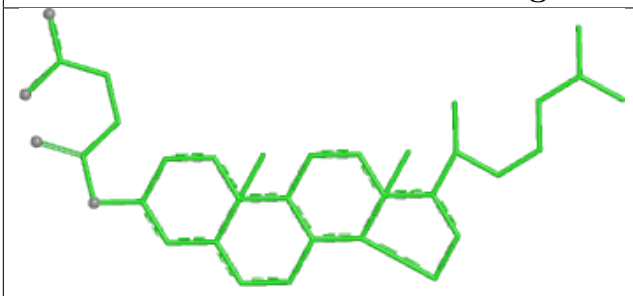
Ligand POV A 805



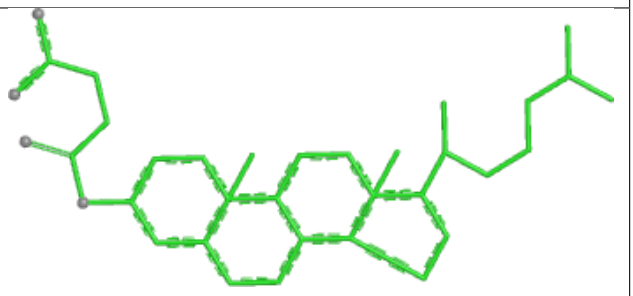
Ligand POV A 806



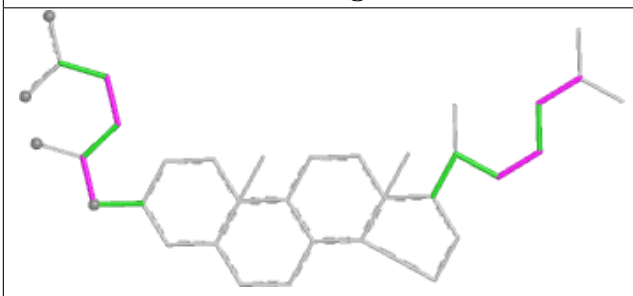
Ligand Y01 A 815



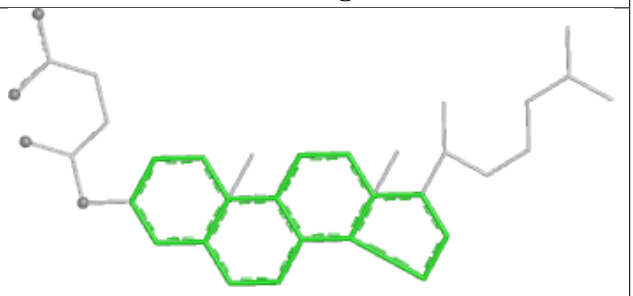
Bond lengths



Bond angles



Torsions

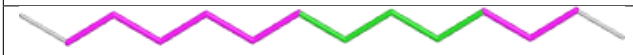


Rings

Ligand PCW C 810

Bond lengths

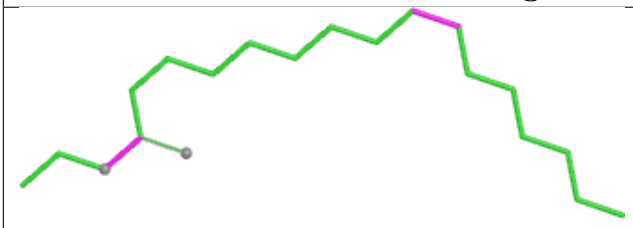
Bond angles



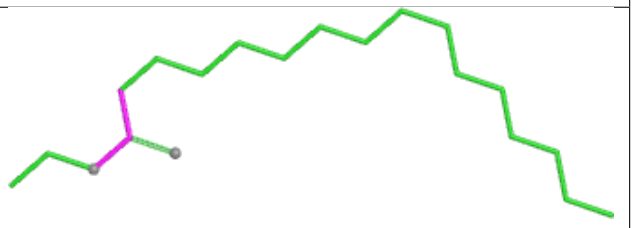
Torsions

Rings

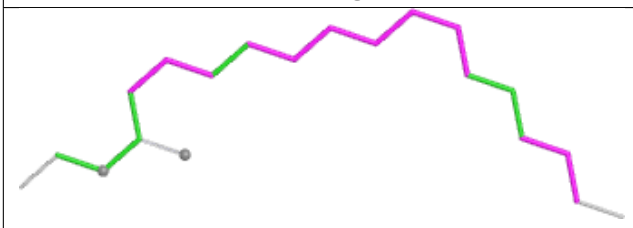
Ligand POV D 809



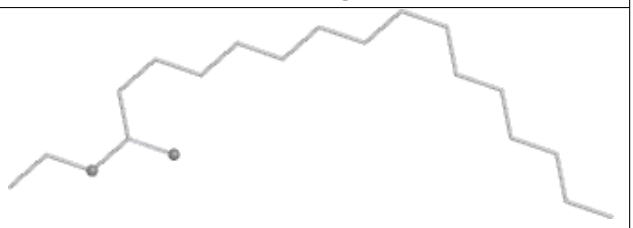
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

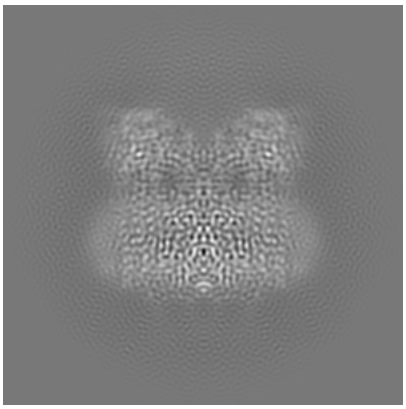
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45935. These allow visual inspection of the internal detail of the map and identification of artifacts.

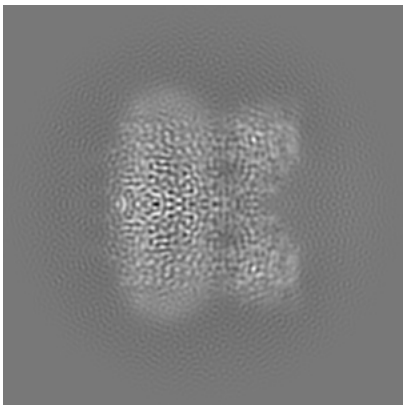
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

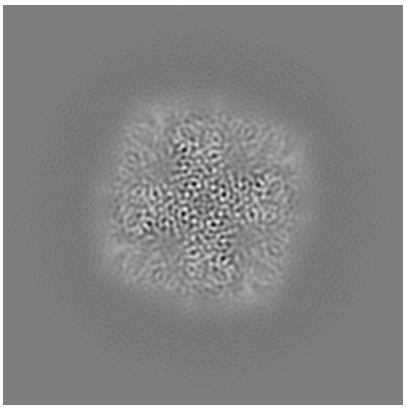
6.1.1 Primary map



X

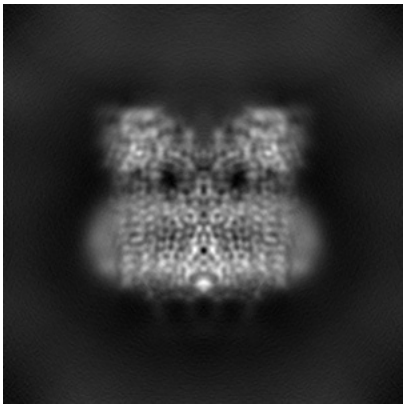


Y

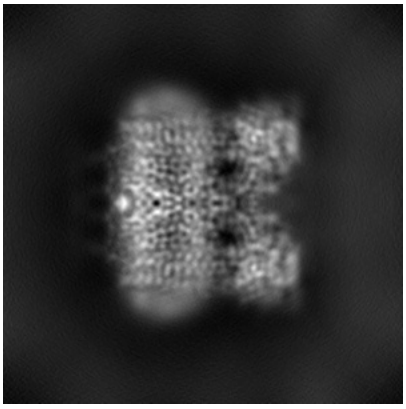


Z

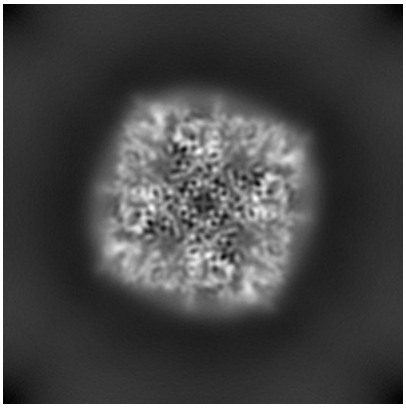
6.1.2 Raw map



X



Y

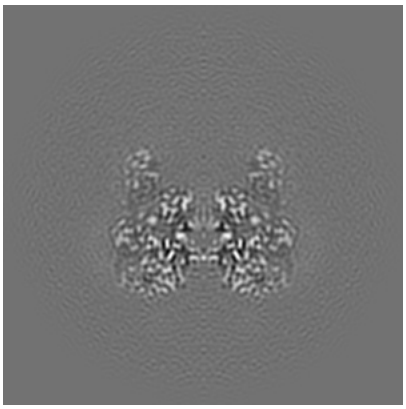


Z

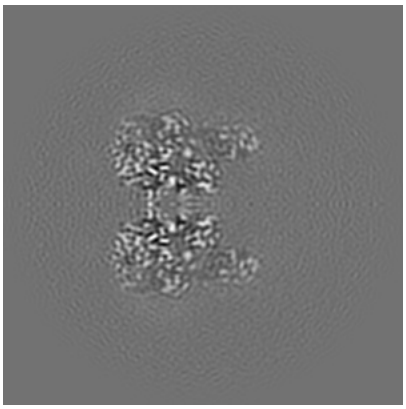
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

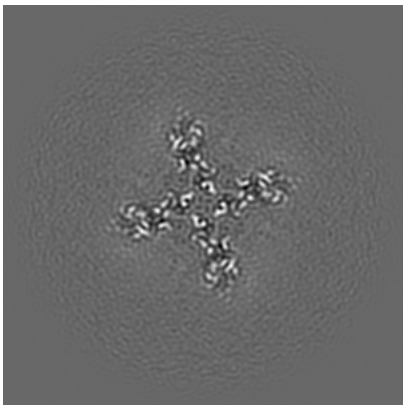
6.2.1 Primary map



X Index: 128

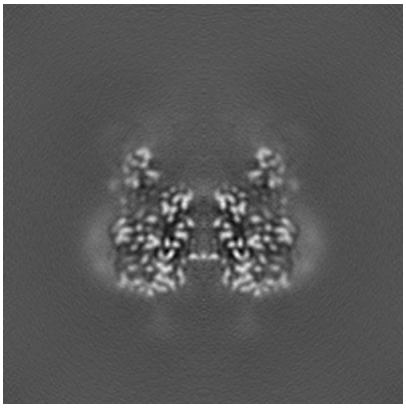


Y Index: 128

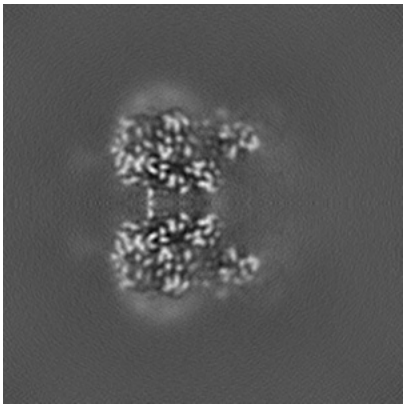


Z Index: 128

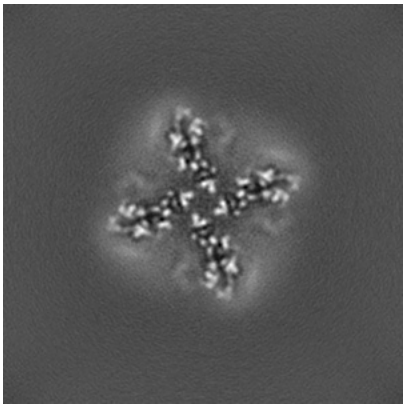
6.2.2 Raw map



X Index: 128



Y Index: 128

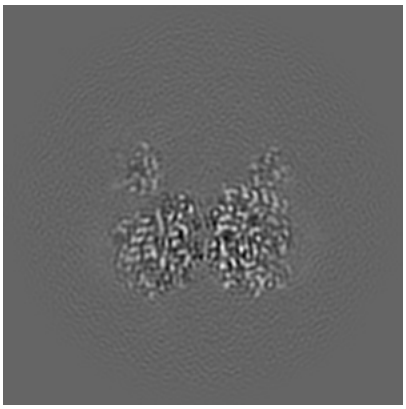


Z Index: 128

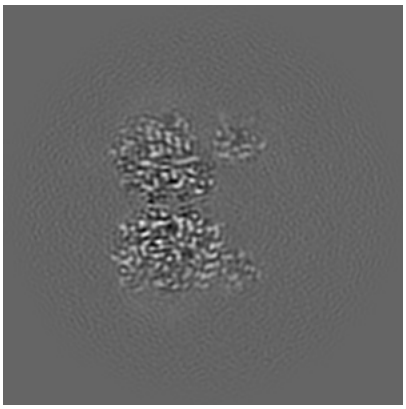
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

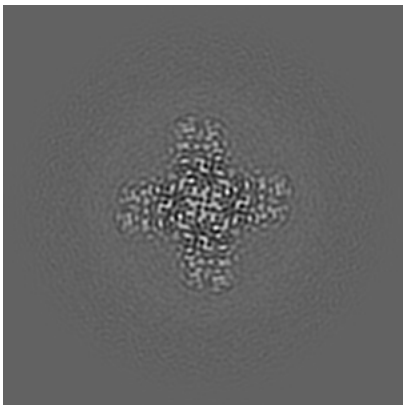
6.3.1 Primary map



X Index: 125

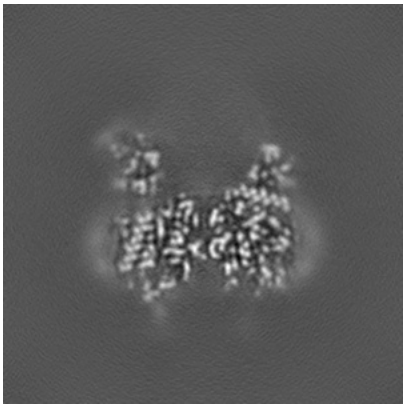


Y Index: 125

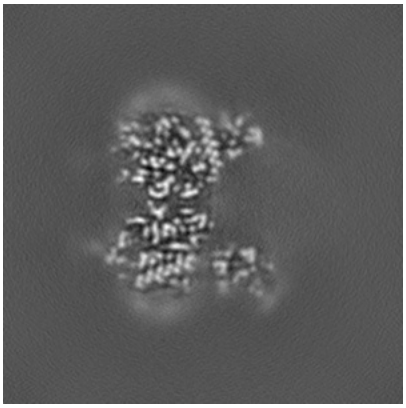


Z Index: 94

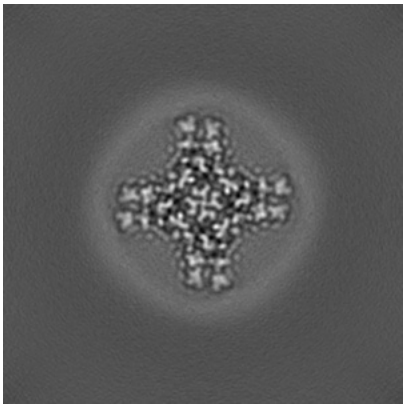
6.3.2 Raw map



X Index: 123



Y Index: 133

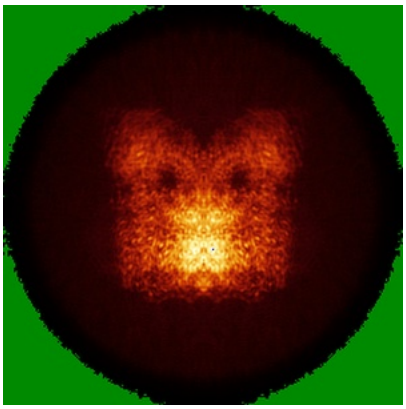


Z Index: 94

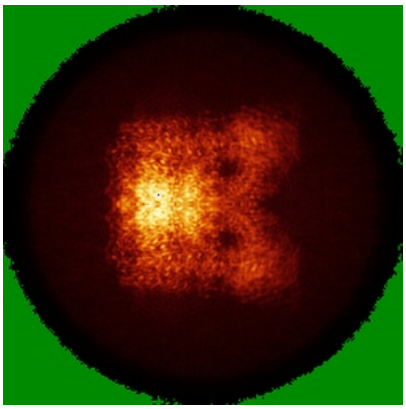
The images above show the largest variance slices of the map in three orthogonal directions.

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

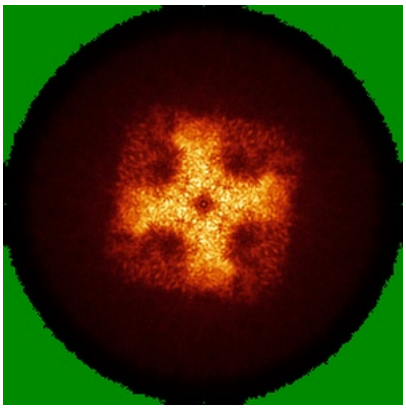
6.4.1 Primary map



X

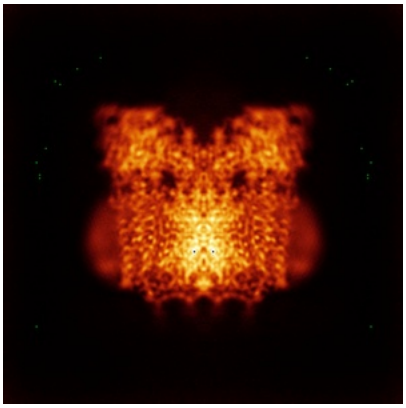


Y

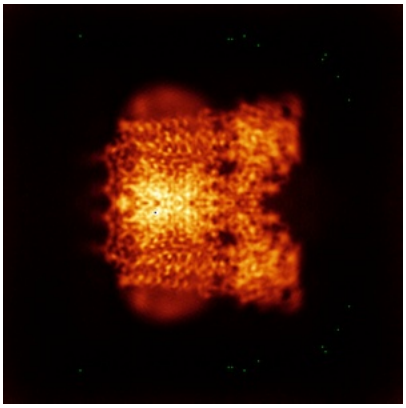


Z

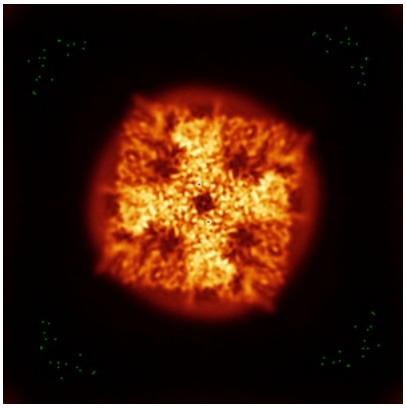
6.4.2 Raw map



X



Y

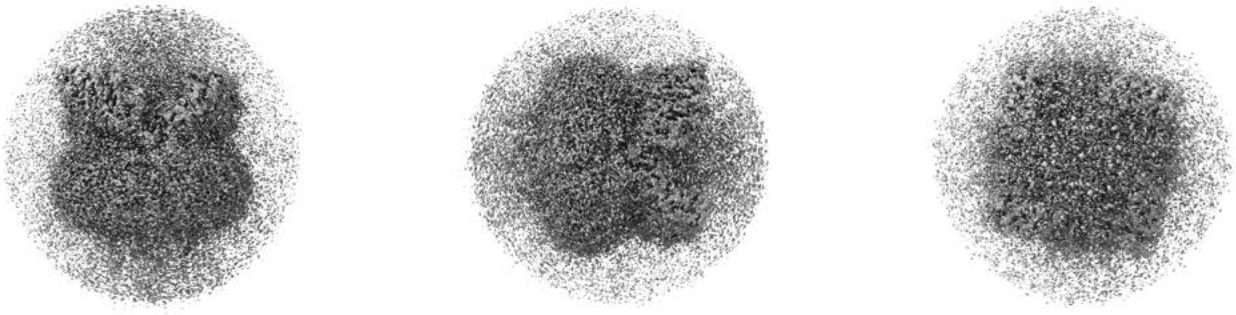


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

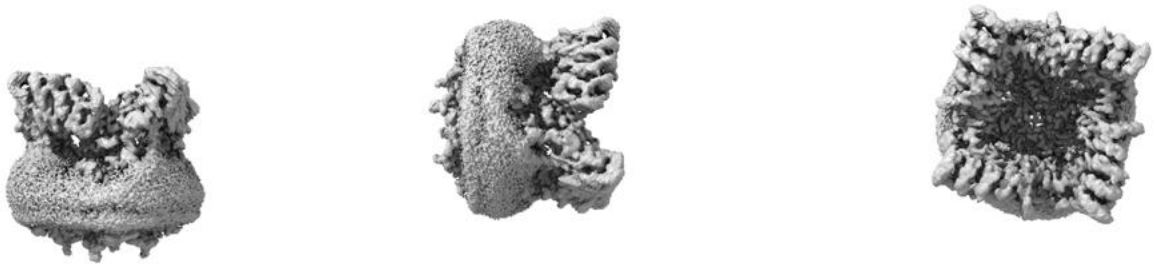
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0959. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

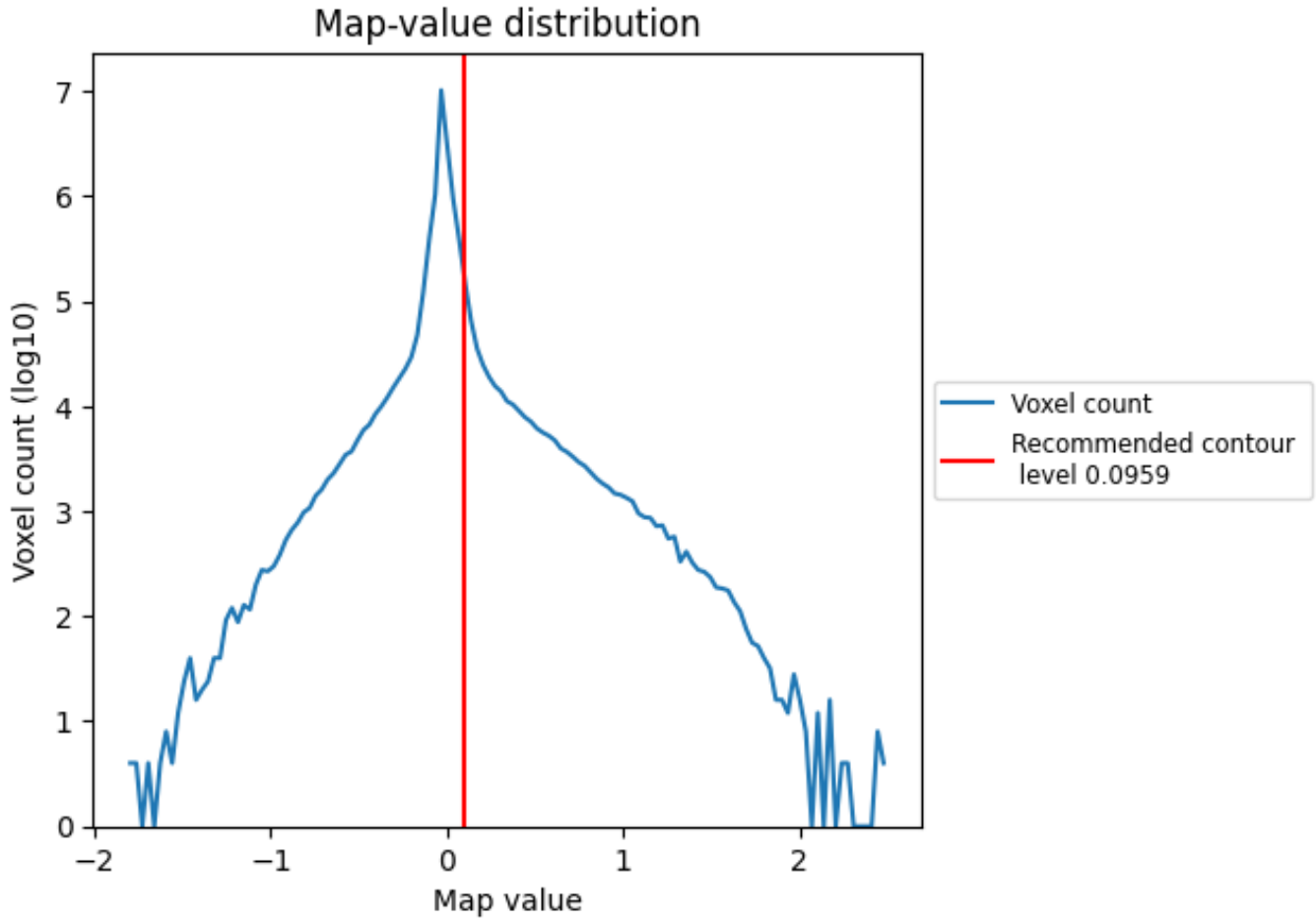
6.6 Mask visualisation (i)

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

7 Map analysis

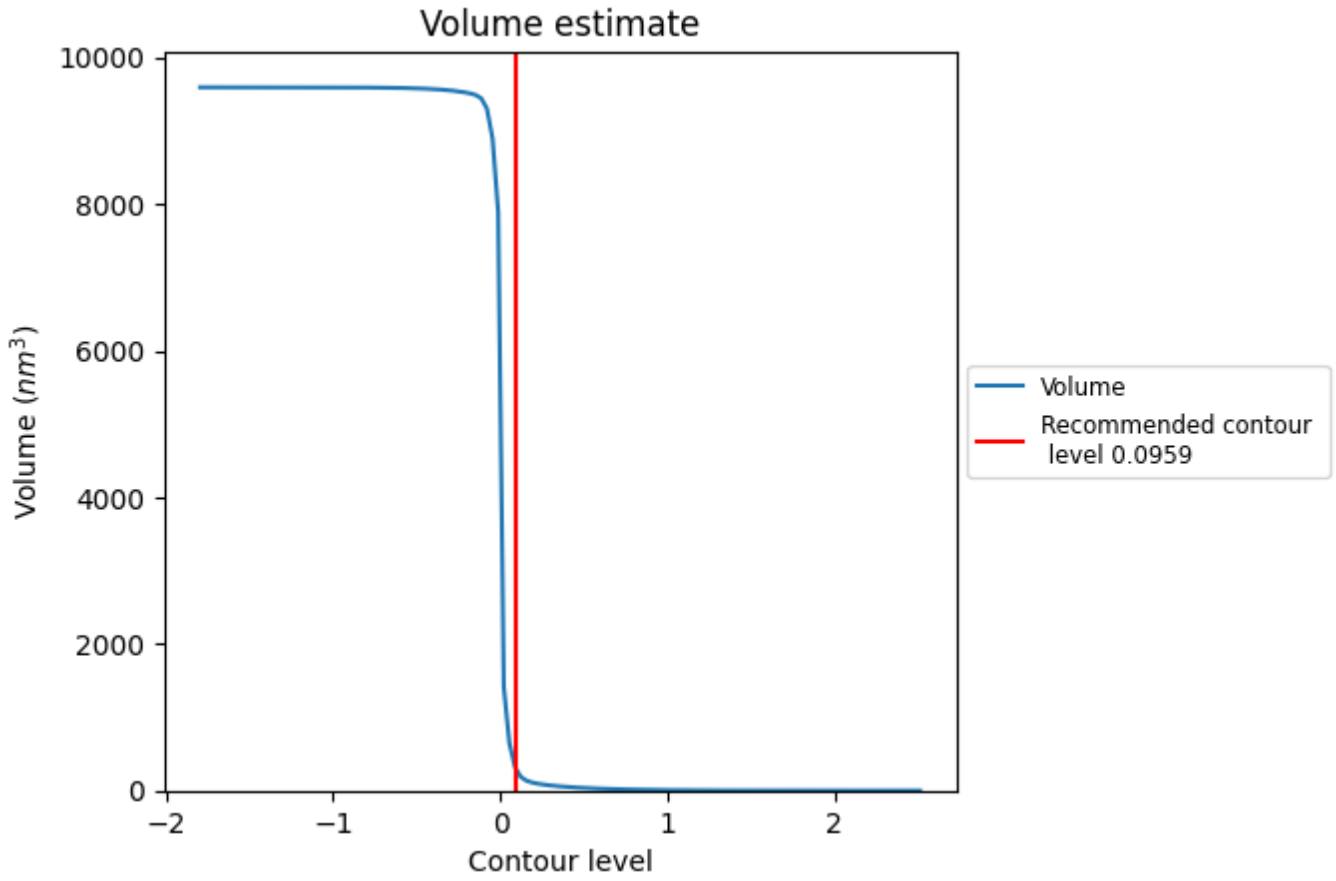
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

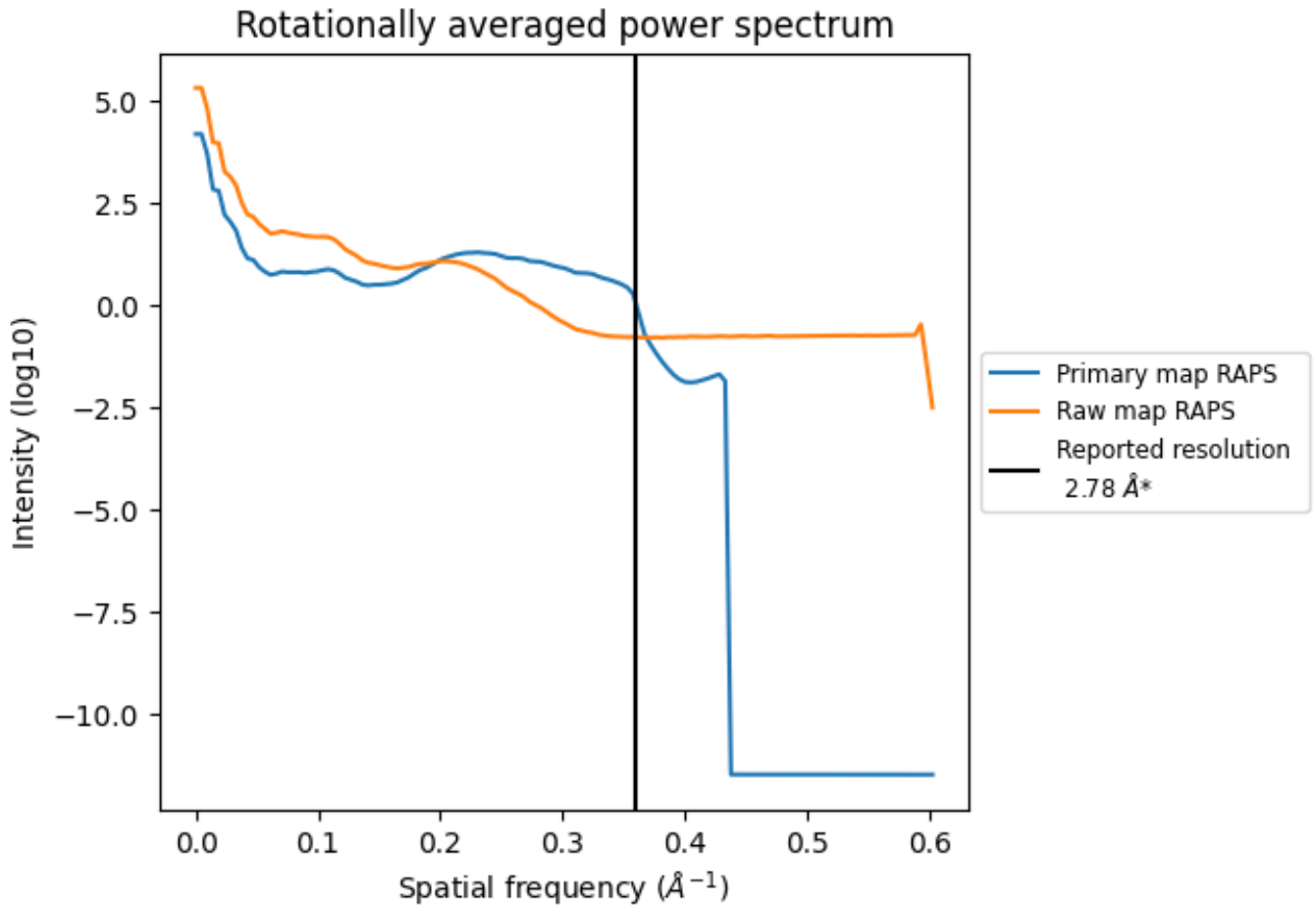
7.2 Volume estimate



The volume at the recommended contour level is 289 nm^3; this corresponds to an approximate mass of 261 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)

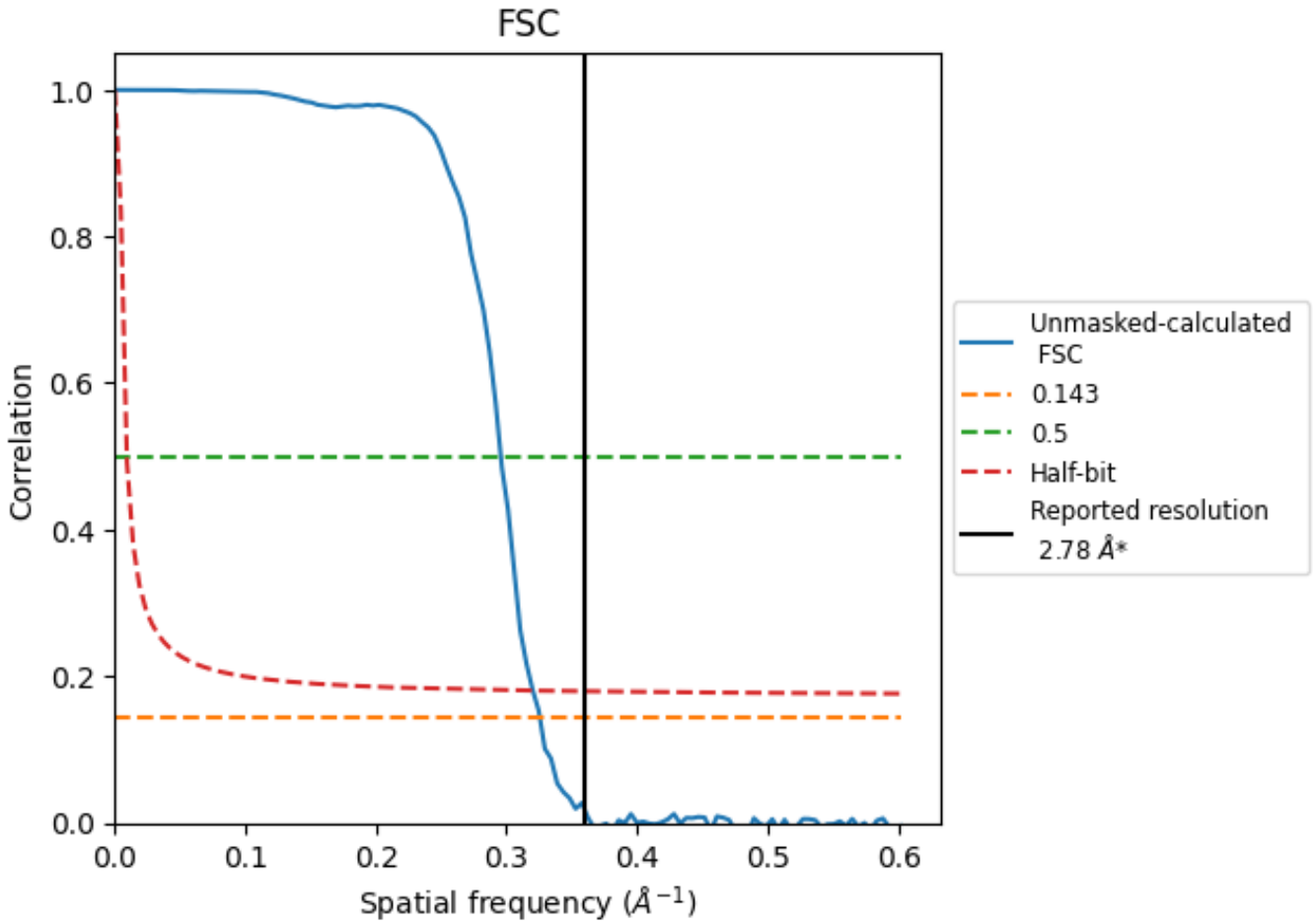


*Reported resolution corresponds to spatial frequency of 0.360 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.360 Å^{-1}

8.2 Resolution estimates (i)

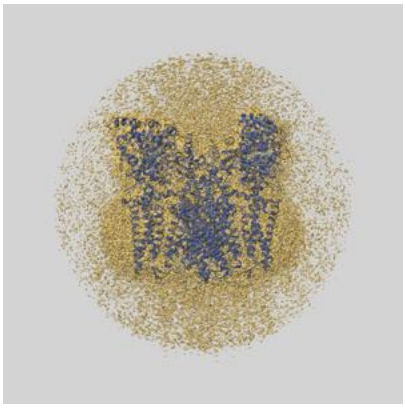
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.07	3.38	3.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.07 differs from the reported value 2.78 by more than 10 %

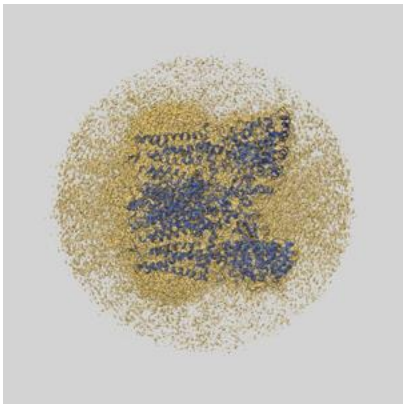
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45935 and PDB model 9CUJ. Per-residue inclusion information can be found in section 3 on page 9.

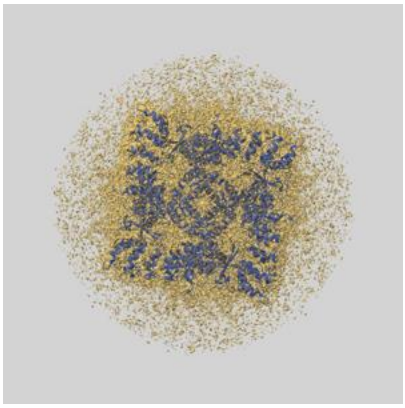
9.1 Map-model overlay



X



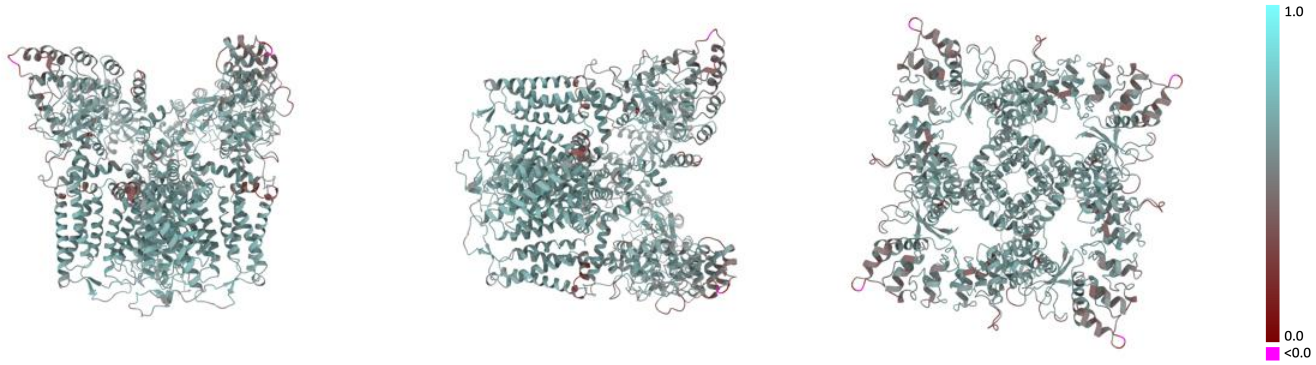
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0959 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.

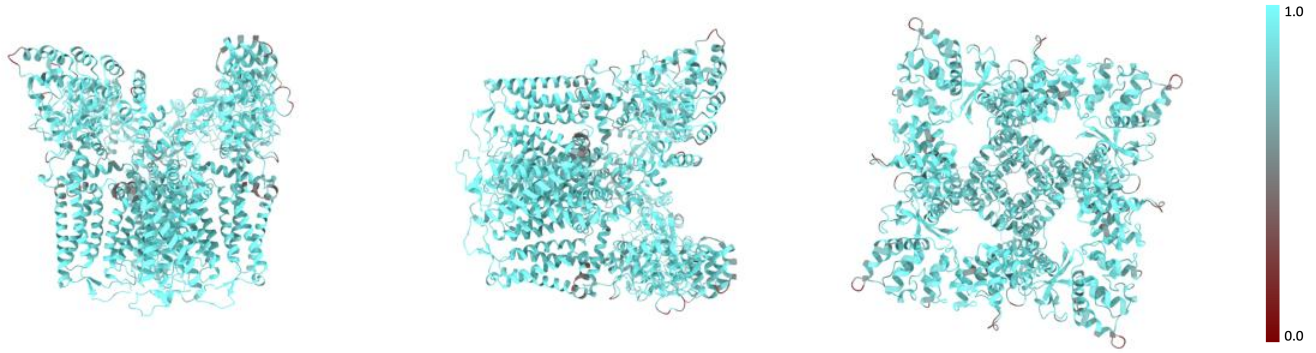
9.2 Q-score mapped to coordinate model (i)



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.

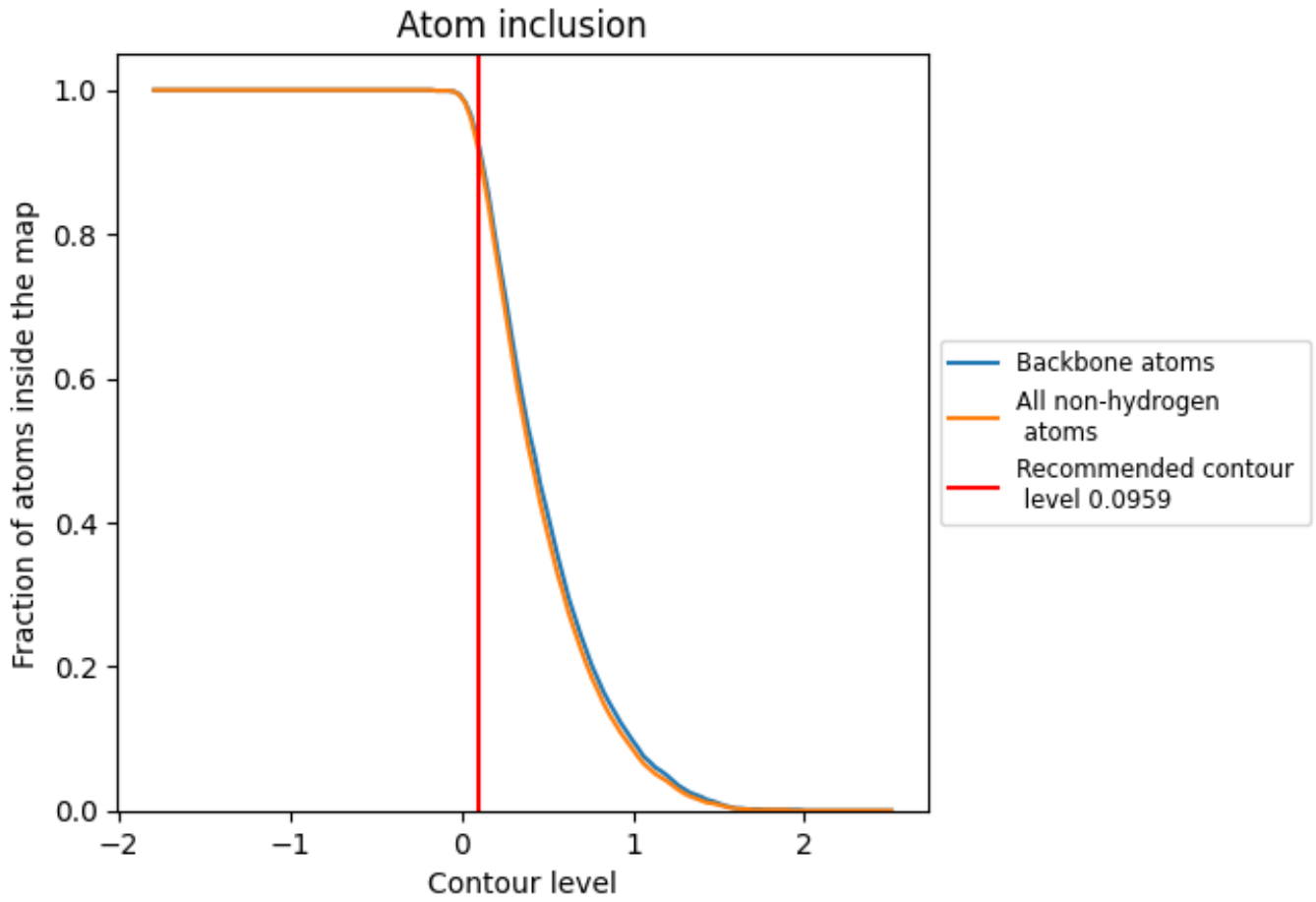
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0959).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0959) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9200	0.5690
A	0.9230	0.5690
B	0.9230	0.5700
C	0.9220	0.5700
D	0.9230	0.5690