Full wwPDB EM Validation Report ⓘ

May 15, 2023 – 03:09 PM EDT

PDB ID	:	8FOA
EMDB ID	:	EMD-29343
Title	:	Cryo-EM structure of human TRPV6 in complex with the natural phytoestrogen genistein
Authors	:	Neuberger, A.; Yelshanskaya, M.V.; Nadezhdin, K.D.; Sobolevsky, A.I.
Deposited on	:	2022-12-30
Resolution	:	2.66 Å(reported)
Based on initial model	:	7MIJ

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:

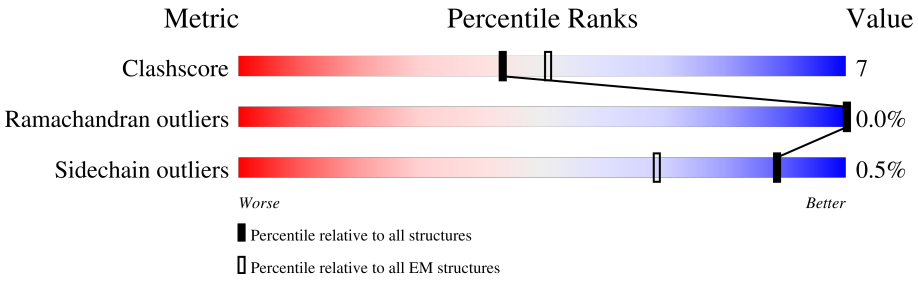
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.66 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	725	8% 77% 7% 16%
1	B	725	10% 76% 8% 16%
1	C	725	12% 75% 9% 16%
1	D	725	12% 76% 8% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	Y01	A	801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	Y01	A	802	X	-	-	-
2	Y01	A	803	X	-	-	-
2	Y01	A	812	X	-	-	-
2	Y01	B	802	X	-	-	-
2	Y01	B	803	X	-	-	-
2	Y01	B	804	X	-	-	-
2	Y01	C	802	X	-	-	-
2	Y01	C	803	X	-	-	-
2	Y01	C	804	X	-	-	-
2	Y01	D	804	X	-	-	-
2	Y01	D	805	X	-	-	-

2 Entry composition

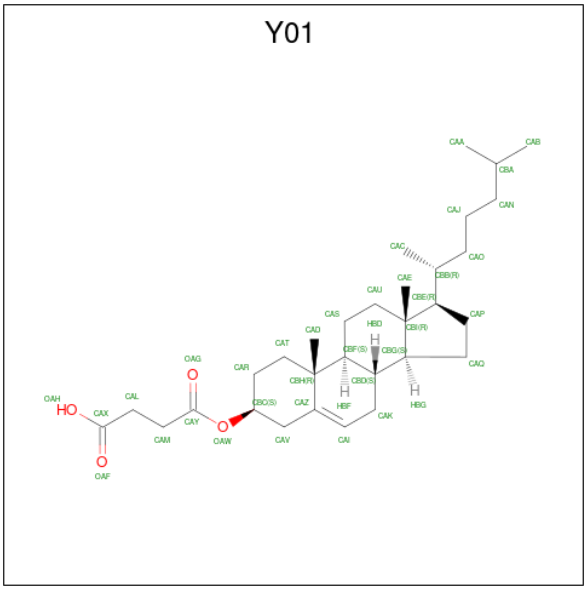
There are 6 unique types of molecules in this entry. The entry contains 21287 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	612	Total	C	N	O	S	0	0
			4912	3173	831	868	40		
1	B	612	Total	C	N	O	S	0	0
			4912	3173	831	868	40		
1	C	612	Total	C	N	O	S	0	0
			4912	3173	831	868	40		
1	D	612	Total	C	N	O	S	0	0
			4912	3173	831	868	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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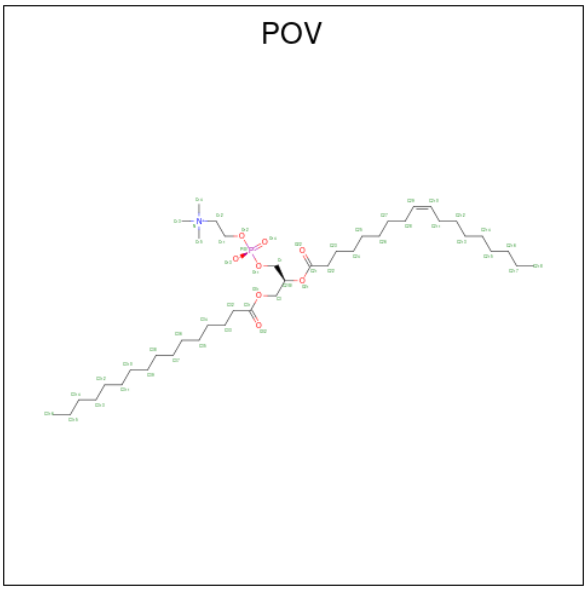
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C O 35 31 4	0
2	A	1	Total C O 35 31 4	0
2	B	1	Total C O 35 31 4	0
2	B	1	Total C O 35 31 4	0
2	B	1	Total C O 35 31 4	0
2	C	1	Total C O 35 31 4	0
2	C	1	Total C O 35 31 4	0
2	C	1	Total C O 35 31 4	0
2	D	1	Total C O 35 31 4	0
2	D	1	Total C O 35 31 4	0

- 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 13 13	0

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Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O P 52 42 1 8 1	0
3	A	1	Total C N O P 52 42 1 8 1	0
3	A	1	Total C 13 13	0
3	A	1	Total C O 19 17 2	0
3	A	1	Total C 13 13	0
3	A	1	Total C N O P 52 42 1 8 1	0
3	A	1	Total C N O P 52 42 1 8 1	0
3	A	1	Total C N O P 46 36 1 8 1	0
3	B	1	Total C 13 13	0
3	B	1	Total C 13 13	0
3	B	1	Total C N O P 46 36 1 8 1	0
3	B	1	Total C N O P 52 42 1 8 1	0
3	B	1	Total C 13 13	0
3	B	1	Total C O 19 17 2	0
3	B	1	Total C 13 13	0
3	B	1	Total C N O P 52 42 1 8 1	0
3	B	1	Total C N O P 52 42 1 8 1	0
3	B	1	Total C N O P 52 42 1 8 1	0
3	C	1	Total C N O P 46 36 1 8 1	0
3	C	1	Total C 13 13	0
3	C	1	Total C N O P 52 42 1 8 1	0

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Mol	Chain	Residues	Atoms	AltConf
3	C	1	Total C 13 13	0
3	C	1	Total C O 19 17 2	0
3	C	1	Total C 13 13	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 13 13	0
3	D	1	Total C N O P 52 42 1 8 1	0
3	D	1	Total C 13 13	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 13 13	0
3	D	1	Total C O 19 17 2	0
3	D	1	Total C 13 13	0

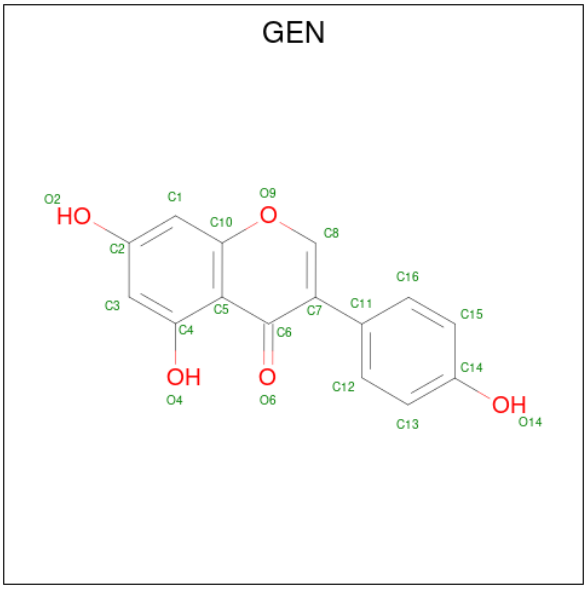
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Zn 1 1	0
4	C	1	Total Zn 1 1	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 GENISTEIN (three-letter code: GEN) (formula: $C_{15}H_{10}O_5$) (labeled as "Ligand of Interest" by depositor).



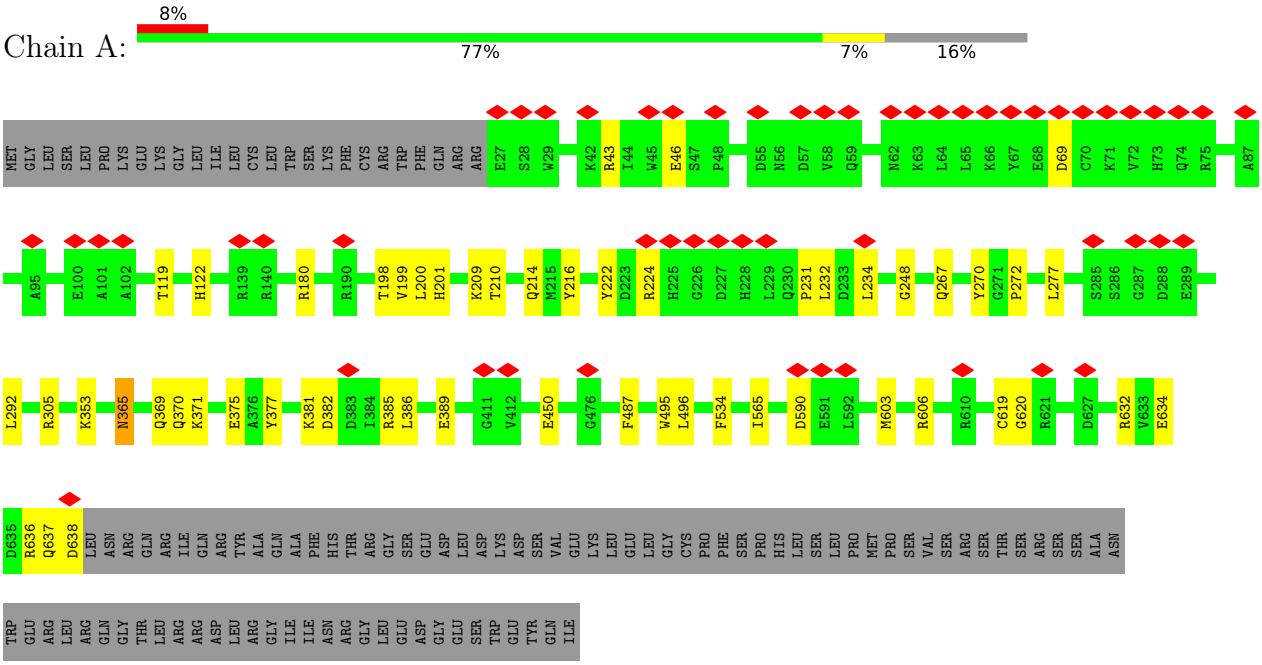
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C O 20 15 5	0
6	D	1	Total C O 20 15 5	0

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.

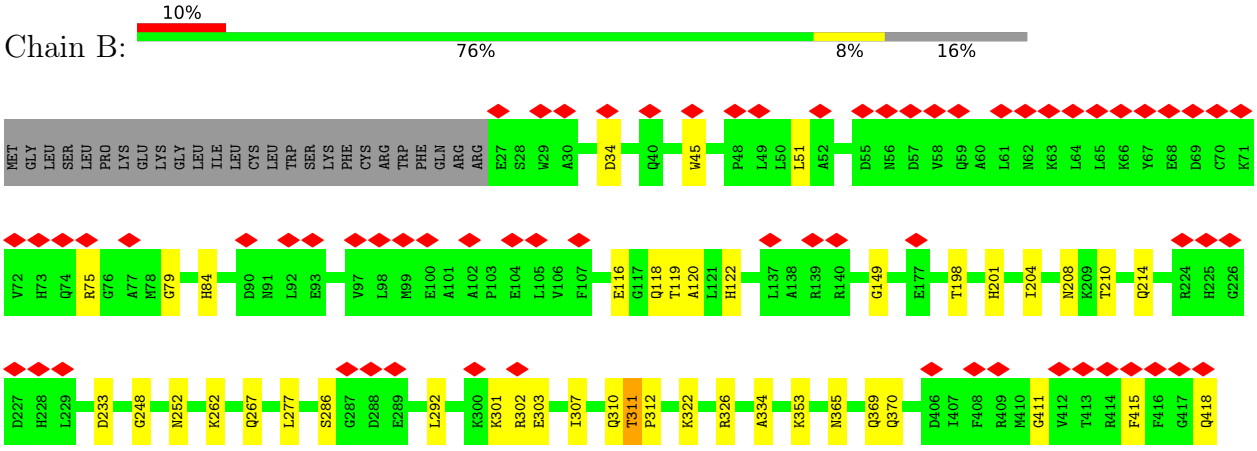
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

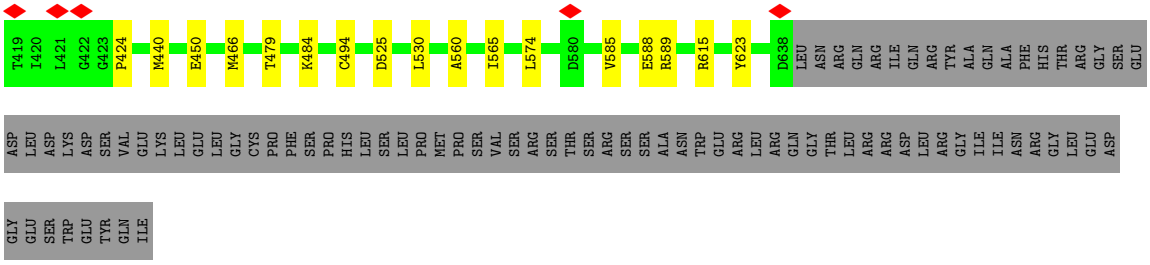
Chain A:



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

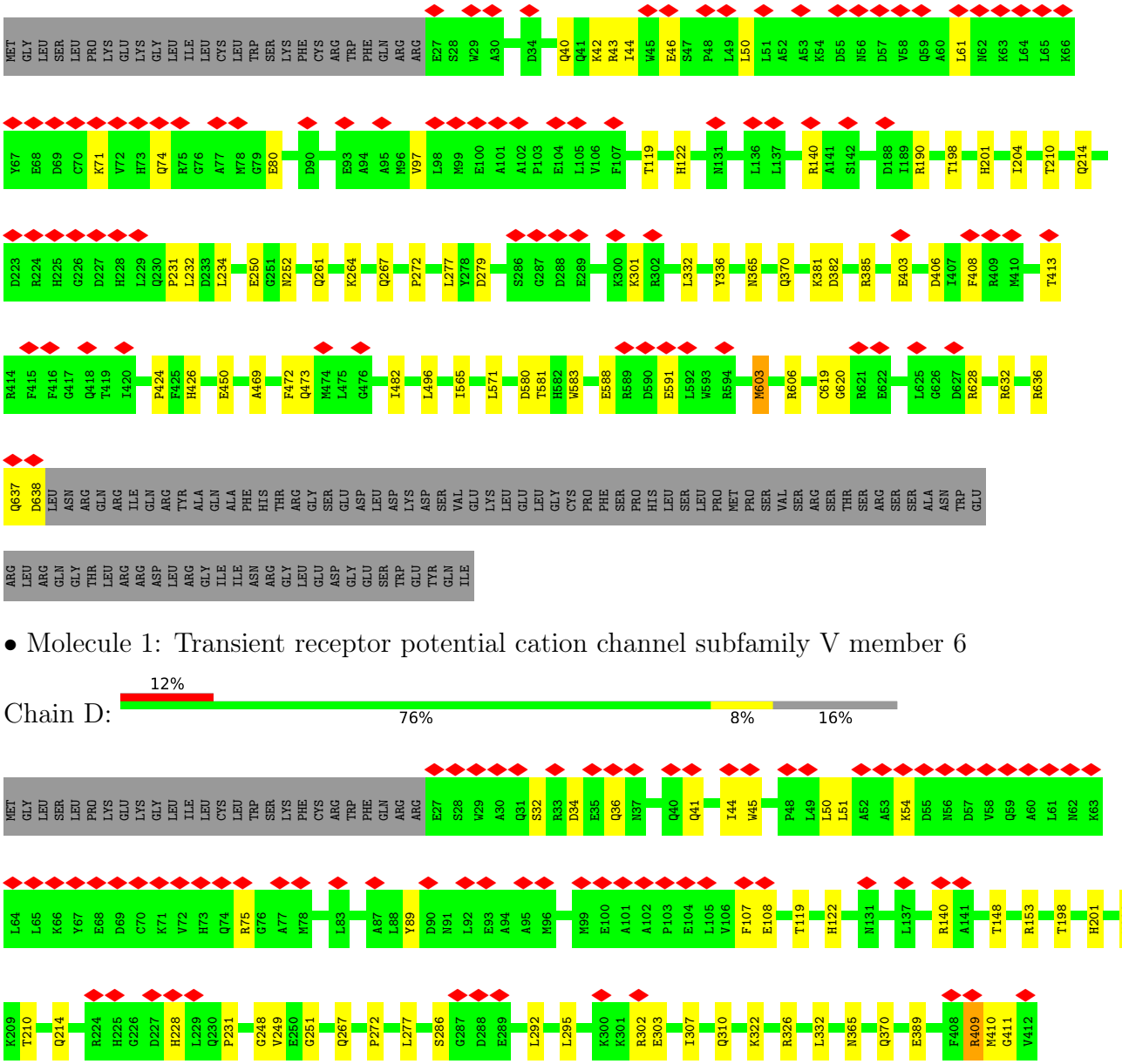
Chain B:





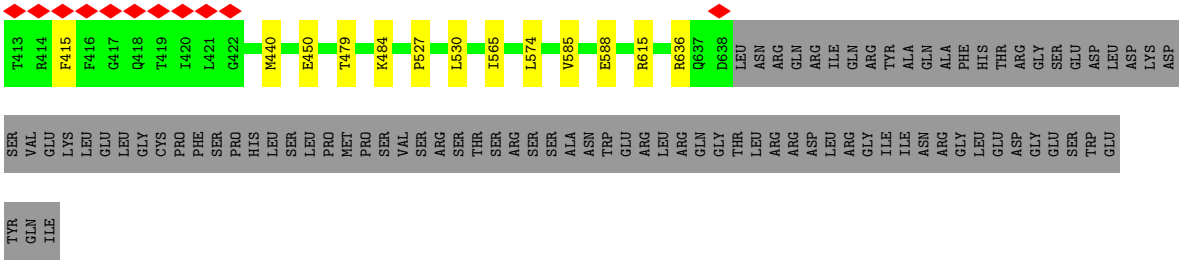
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

Chain C:



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

Chain D:


T413 R414 F415 F416 G417 Q418 T419 I420 L421 G422 M440 E450 T479 K484 P527 L530 I565 L574 V585 E588 R615 R636 Q637 D638
LEU ASN ARG GLN ARG ILE GLN ARG TYR ALA GLN ALA PHE HIS THR ARG GLY SER GLU ASP LEU ASP LYS ASP
SER VAL GLU LYS LEU GLU LEU GLY CYS PRO PHE SER PRO HIS LEU SER LEU PRO MET PRO SER VAL SER ARG SER THR SER ARG SER SER ALA ASN TRP GLU ARG LEU ARG GLN GLY THR LEU ARG ARG ASP LEU ARG GLY ILE ILE ASN ARG GLY LEU GLU ASP GLY GLU SER TRP GLU
TYR GLN ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	196340	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.727	Depositor
Minimum map value	-1.940	Depositor
Average map value	0.040	Depositor
Map value standard deviation	0.141	Depositor
Recommended contour level	0.537	Depositor
Map size (Å)	215.04, 215.04, 215.04	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/5025	0.54	0/6818
1	B	0.31	0/5025	0.53	0/6818
1	C	0.30	0/5025	0.55	0/6818
1	D	0.31	0/5025	0.53	0/6818
All	All	0.31	0/20100	0.54	0/27272

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Peptide
1	A	69	ASP	Peptide
1	C	408	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4912	0	4964	33	0
1	B	4912	0	4964	38	0
1	C	4912	0	4964	40	0
1	D	4912	0	4964	37	0
2	A	140	0	180	48	0
2	B	105	0	135	38	0
2	C	105	0	135	34	0
2	D	70	0	89	23	0
3	A	312	0	487	11	0
3	B	325	0	509	15	0
3	C	208	0	323	13	0
3	D	331	0	524	17	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0
6	A	20	0	9	1	0
6	D	20	0	9	0	0
All	All	21287	0	22256	304	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 7.

All (304) 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)
2:B:802:Y01:CBH	2:B:802:Y01:CAT	1.79	1.60
2:A:801:Y01:CBH	2:A:801:Y01:CAT	1.80	1.59
2:B:804:Y01:CBH	2:B:804:Y01:CAT	1.80	1.59
2:A:803:Y01:CBH	2:A:803:Y01:CAT	1.80	1.59
2:D:805:Y01:CBH	2:D:805:Y01:CAT	1.80	1.58
2:B:803:Y01:CBH	2:B:803:Y01:CAT	1.79	1.56
2:C:803:Y01:CBH	2:C:803:Y01:CAT	1.80	1.56
2:D:804:Y01:CBH	2:D:804:Y01:CAT	1.79	1.55
2:A:812:Y01:CBH	2:A:812:Y01:CAT	1.79	1.54
2:C:802:Y01:CBH	2:C:802:Y01:CAT	1.79	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:802:Y01:CBH	2:A:802:Y01:CAT	1.79	1.53
2:C:804:Y01:CBH	2:C:804:Y01:CAT	1.80	1.53
2:B:802:Y01:CAV	2:B:802:Y01:CAZ	1.90	1.49
2:C:804:Y01:CAV	2:C:804:Y01:CAZ	1.91	1.48
2:A:803:Y01:CAV	2:A:803:Y01:CAZ	1.91	1.48
2:C:802:Y01:CAZ	2:C:802:Y01:CAV	1.91	1.47
2:D:804:Y01:CAZ	2:D:804:Y01:CAV	1.91	1.46
2:C:803:Y01:CAZ	2:C:803:Y01:CAV	1.92	1.45
2:B:803:Y01:CAZ	2:B:803:Y01:CAV	1.92	1.45
2:A:812:Y01:CAZ	2:A:812:Y01:CAV	1.91	1.44
2:A:801:Y01:CAV	2:A:801:Y01:CAZ	1.91	1.44
2:B:804:Y01:CAZ	2:B:804:Y01:CAV	1.92	1.44
2:D:805:Y01:CAV	2:D:805:Y01:CAZ	1.93	1.44
2:A:802:Y01:CAZ	2:A:802:Y01:CAV	1.91	1.44
2:A:802:Y01:CAT	2:A:802:Y01:CAZ	2.41	0.96
2:D:804:Y01:CAT	2:D:804:Y01:CAZ	2.45	0.93
2:B:802:Y01:CAT	2:B:802:Y01:CAZ	2.46	0.92
2:A:812:Y01:CAT	2:A:812:Y01:CAZ	2.49	0.91
2:C:803:Y01:CAT	2:C:803:Y01:CAZ	2.47	0.91
2:A:801:Y01:CAT	2:A:801:Y01:CAZ	2.48	0.91
2:B:803:Y01:CAT	2:B:803:Y01:CAZ	2.48	0.89
2:C:802:Y01:CAT	2:C:802:Y01:CAZ	2.49	0.89
2:A:803:Y01:CAT	2:A:803:Y01:CAZ	2.49	0.89
2:B:804:Y01:CAT	2:B:804:Y01:CAZ	2.51	0.87
2:D:805:Y01:CAT	2:D:805:Y01:CAZ	2.52	0.87
2:C:804:Y01:CAT	2:C:804:Y01:CAZ	2.51	0.87
2:C:802:Y01:CAT	2:C:802:Y01:CBF	2.55	0.84
2:A:801:Y01:CAT	2:A:801:Y01:CBF	2.56	0.83
2:C:803:Y01:CAT	2:C:803:Y01:CBF	2.58	0.81
2:B:802:Y01:CAT	2:B:802:Y01:CBF	2.60	0.80
2:D:804:Y01:CBH	2:D:804:Y01:CAV	2.60	0.80
2:B:803:Y01:CAT	2:B:803:Y01:CBF	2.59	0.79
2:D:804:Y01:CAT	2:D:804:Y01:CBF	2.58	0.79
2:D:805:Y01:CAT	2:D:805:Y01:CBF	2.62	0.78
2:A:802:Y01:CAT	2:A:802:Y01:CBF	2.62	0.77
2:C:802:Y01:CBH	2:C:802:Y01:CAV	2.62	0.74
2:B:804:Y01:CAT	2:B:804:Y01:CBF	2.64	0.74
2:A:802:Y01:HAD3	1:B:565:ILE:HG12	1.69	0.73
2:A:803:Y01:CAT	2:A:803:Y01:CBF	2.66	0.73
2:C:804:Y01:CAT	2:C:804:Y01:CBF	2.66	0.72
2:B:802:Y01:CBH	2:B:802:Y01:CAV	2.60	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:812:Y01:CAT	2:A:812:Y01:CBF	2.66	0.71
1:A:370:GLN:HE22	1:A:450:GLU:H	1.39	0.70
2:A:812:Y01:CAT	2:A:812:Y01:CAD	2.71	0.68
2:C:804:Y01:CAT	2:C:804:Y01:CAD	2.73	0.66
1:D:409:ARG:HD3	1:D:410:MET:HG3	1.78	0.65
1:B:119:THR:H	1:B:122:HIS:HD2	1.46	0.64
2:A:802:Y01:CBH	2:A:802:Y01:CAV	2.65	0.64
1:C:370:GLN:HE22	1:C:450:GLU:H	1.45	0.64
2:A:801:Y01:CBH	2:A:801:Y01:CAV	2.63	0.64
2:C:804:Y01:CAV	2:C:804:Y01:CAI	2.74	0.63
6:A:816:GEN:H8	1:D:574:LEU:HD11	1.80	0.63
3:A:813:POV:H1	3:D:807:POV:H33	1.80	0.63
2:C:804:Y01:CAZ	2:C:804:Y01:CBC	2.76	0.62
2:A:812:Y01:CAV	2:A:812:Y01:CAI	2.73	0.62
2:C:802:Y01:CAT	2:C:802:Y01:CAD	2.76	0.62
2:B:803:Y01:CAT	2:B:803:Y01:CAD	2.75	0.62
2:A:803:Y01:CAV	2:A:803:Y01:CAI	2.74	0.62
1:D:119:THR:H	1:D:122:HIS:HD2	1.46	0.61
2:D:805:Y01:CAT	2:D:805:Y01:CAS	2.79	0.61
1:A:200:LEU:HD23	1:A:232:LEU:HD22	1.82	0.61
1:B:322:LYS:HD3	1:B:326:ARG:HH22	1.65	0.61
1:D:32:SER:O	1:D:36:GLN:NE2	2.34	0.61
2:A:801:Y01:CAT	2:A:801:Y01:HAS1	2.31	0.61
2:D:804:Y01:CAT	2:D:804:Y01:CAD	2.75	0.61
1:B:411:GLY:HA3	1:B:415:PHE:HB2	1.83	0.60
1:C:619:CYS:SG	1:C:620:GLY:N	2.75	0.60
1:C:119:THR:H	1:C:122:HIS:HD2	1.50	0.60
1:D:484:LYS:HG2	1:D:585:VAL:HG21	1.84	0.60
1:A:119:THR:H	1:A:122:HIS:HD2	1.49	0.60
1:C:473:GLN:HG2	3:D:806:POV:H3A	1.82	0.59
2:B:804:Y01:CAT	2:B:804:Y01:CAD	2.77	0.59
1:B:370:GLN:HE22	1:B:450:GLU:H	1.48	0.59
2:B:802:Y01:CAT	2:B:802:Y01:CAD	2.73	0.59
2:B:803:Y01:CAT	2:B:803:Y01:CAS	2.81	0.59
2:A:803:Y01:CAT	2:A:803:Y01:CAD	2.75	0.59
2:B:804:Y01:CAT	2:B:804:Y01:CAS	2.81	0.58
1:D:210:THR:O	1:D:214:GLN:NE2	2.37	0.58
1:D:370:GLN:HE22	1:D:450:GLU:H	1.50	0.58
2:A:801:Y01:CAT	2:A:801:Y01:CAS	2.81	0.57
1:A:603:MET:SD	1:A:606:ARG:NH2	2.77	0.57
2:B:803:Y01:HAS1	2:B:803:Y01:HAT2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:804:Y01:CAT	2:D:804:Y01:CAS	2.82	0.57
1:A:565:ILE:HD11	2:D:805:Y01:HAE3	1.86	0.57
1:C:250:GLU:OE1	1:C:301:LYS:NZ	2.37	0.57
2:B:803:Y01:CBH	2:B:803:Y01:CAR	2.77	0.57
2:A:812:Y01:CAT	2:A:812:Y01:CAS	2.83	0.56
2:C:803:Y01:CBH	2:C:803:Y01:CAV	2.68	0.56
1:A:381:LYS:NZ	3:A:811:POV:O14	2.37	0.56
1:C:403:GLU:OE2	1:C:426:HIS:ND1	2.33	0.56
1:C:424:PRO:HG3	3:C:806:POV:H38A	1.88	0.56
1:C:44:ILE:HG13	1:C:50:LEU:HB3	1.87	0.56
1:B:334:ALA:HB1	3:B:811:POV:H216	1.87	0.56
1:A:495:TRP:HE1	3:A:806:POV:H28	1.70	0.56
1:D:75:ARG:NH1	1:D:108:GLU:OE1	2.39	0.56
1:C:198:THR:H	1:C:201:HIS:HD2	1.53	0.56
2:C:803:Y01:HAD3	1:D:565:ILE:HG12	1.87	0.55
2:B:803:Y01:CAS	2:B:803:Y01:HAT2	2.37	0.55
2:C:804:Y01:CAT	2:C:804:Y01:CAS	2.85	0.55
2:A:803:Y01:CAT	2:A:803:Y01:CAS	2.84	0.55
2:A:812:Y01:HAB1	3:D:809:POV:H31D	1.89	0.54
2:D:804:Y01:CAT	2:D:804:Y01:HAS1	2.36	0.54
1:D:322:LYS:HD3	1:D:326:ARG:HH22	1.73	0.54
1:B:198:THR:H	1:B:201:HIS:HD2	1.55	0.54
2:A:802:Y01:CAT	2:A:802:Y01:CAD	2.79	0.54
2:D:805:Y01:CAT	2:D:805:Y01:CAD	2.79	0.54
1:C:61:LEU:HB3	1:C:97:VAL:HG11	1.90	0.54
1:D:198:THR:H	1:D:201:HIS:HD2	1.57	0.53
1:A:371:LYS:HB3	1:A:375:GLU:HG3	1.90	0.53
1:C:210:THR:O	1:C:214:GLN:NE2	2.42	0.53
1:C:279:ASP:OD2	1:C:628:ARG:NH1	2.41	0.53
2:C:802:Y01:CAT	2:C:802:Y01:CAS	2.86	0.53
2:C:802:Y01:CAT	2:C:802:Y01:HAS1	2.39	0.53
1:B:479:THR:HG23	1:C:496:LEU:HD21	1.90	0.53
2:C:803:Y01:CAT	2:C:803:Y01:CAS	2.87	0.53
1:C:424:PRO:HB3	3:C:806:POV:H310	1.92	0.52
1:A:210:THR:O	1:A:214:GLN:NE2	2.41	0.52
2:A:801:Y01:CAT	2:A:801:Y01:CAD	2.80	0.52
2:B:802:Y01:CAT	2:B:802:Y01:CAS	2.88	0.52
1:D:267:GLN:HE21	1:D:277:LEU:HD22	1.74	0.52
1:C:632:ARG:NH1	1:D:34:ASP:OD1	2.42	0.52
2:C:803:Y01:CAZ	2:C:803:Y01:CBC	2.82	0.52
1:B:233:ASP:OD2	1:B:262:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:804:Y01:CAV	2:B:804:Y01:CAI	2.82	0.51
2:A:803:Y01:CAZ	2:A:803:Y01:CBC	2.79	0.51
1:C:43:ARG:HA	1:C:46:GLU:HG2	1.92	0.51
1:A:248:GLY:HA3	1:A:292:LEU:HD11	1.92	0.51
1:A:386:LEU:HD11	3:A:808:POV:H25	1.93	0.51
1:D:44:ILE:HG21	1:D:54:LYS:HE3	1.93	0.51
1:B:424:PRO:HG3	2:B:803:Y01:HAR1	1.93	0.50
1:B:440:MET:HA	3:B:809:POV:H210	1.93	0.50
1:C:583:TRP:NE1	1:C:588:GLU:OE2	2.45	0.50
1:B:494:CYS:HB3	2:B:804:Y01:HAN2	1.92	0.50
1:A:198:THR:HG22	1:A:201:HIS:HD2	1.77	0.50
1:B:466:MET:HA	3:B:811:POV:H31G	1.93	0.49
1:B:530:LEU:HB3	2:B:804:Y01:HAI	1.92	0.49
1:D:45:TRP:HA	1:D:51:LEU:HD12	1.94	0.49
1:A:272:PRO:O	1:A:637:GLN:NE2	2.44	0.49
2:B:804:Y01:CAZ	2:B:804:Y01:CBC	2.83	0.49
1:C:272:PRO:O	1:C:637:GLN:NE2	2.45	0.49
1:D:286:SER:HA	1:D:615:ARG:HH22	1.78	0.49
2:B:803:Y01:CAT	2:B:803:Y01:HAS1	2.43	0.49
1:C:381:LYS:NZ	3:C:810:POV:O14	2.40	0.49
3:C:806:POV:H35A	3:C:806:POV:H3A	1.95	0.49
1:D:440:MET:HA	3:D:811:POV:H211	1.94	0.48
2:A:812:Y01:CBH	2:A:812:Y01:CAR	2.85	0.48
1:D:107:PHE:HZ	1:D:140:ARG:HG3	1.79	0.48
1:A:270:TYR:OH	1:B:118:GLN:NE2	2.46	0.48
1:A:496:LEU:HD21	1:D:479:THR:HG23	1.96	0.48
2:B:803:Y01:HAE3	1:C:565:ILE:HD11	1.96	0.48
1:B:415:PHE:HA	1:B:418:GLN:HB3	1.95	0.48
2:D:805:Y01:HAE2	2:D:805:Y01:HBB	1.72	0.48
3:D:812:POV:H37A	3:D:812:POV:H34	1.67	0.48
1:B:302:ARG:NH2	1:B:588:GLU:OE2	2.36	0.48
2:C:802:Y01:HBB	2:C:802:Y01:HAE2	1.74	0.48
1:B:267:GLN:HE21	1:B:277:LEU:HD22	1.78	0.47
2:B:803:Y01:CAV	2:B:803:Y01:CAI	2.82	0.47
1:A:305:ARG:NH1	1:A:590:ASP:OD2	2.44	0.47
1:D:248:GLY:HA3	1:D:292:LEU:HD11	1.96	0.47
1:C:267:GLN:HE21	1:C:277:LEU:HD22	1.79	0.47
1:A:198:THR:HG22	1:A:201:HIS:CD2	2.50	0.47
1:B:45:TRP:HA	1:B:51:LEU:HD12	1.96	0.47
1:B:484:LYS:HG2	1:B:585:VAL:HG21	1.95	0.47
1:B:574:LEU:HD21	1:C:571:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:803:Y01:CAV	2:C:803:Y01:CAI	2.83	0.47
1:C:71:LYS:O	1:C:74:GLN:NE2	2.47	0.47
1:D:148:THR:HG22	1:D:153:ARG:HH11	1.79	0.46
1:A:199:VAL:HG23	1:A:200:LEU:HD22	1.96	0.46
2:A:812:Y01:CAZ	2:A:812:Y01:CBC	2.82	0.46
1:B:589:ARG:NH2	1:C:580:ASP:OD1	2.48	0.46
2:D:805:Y01:CAZ	2:D:805:Y01:CBC	2.82	0.46
2:A:812:Y01:HAU2	3:D:809:POV:H314	1.97	0.46
1:A:267:GLN:HE21	1:A:277:LEU:HD22	1.81	0.46
1:B:307:ILE:HA	1:B:310:GLN:HG2	1.98	0.46
1:B:204:ILE:HG23	1:B:252:ASN:HD22	1.80	0.46
2:A:802:Y01:HAE2	2:A:802:Y01:HBB	1.70	0.46
1:C:482:ILE:HD12	1:C:581:THR:HG23	1.98	0.46
2:A:802:Y01:HAE1	1:B:565:ILE:HD11	1.98	0.45
1:B:311:THR:HG23	1:B:312:PRO:HD3	1.99	0.45
1:C:198:THR:HG22	1:C:201:HIS:CD2	2.51	0.45
1:A:636:ARG:NE	1:A:638:ASP:OD1	2.50	0.45
1:D:302:ARG:NH2	1:D:588:GLU:OE2	2.41	0.45
1:A:382:ASP:OD1	1:A:385:ARG:NH2	2.48	0.45
3:C:806:POV:H33	3:C:806:POV:H22A	1.98	0.45
2:B:802:Y01:HAE2	2:B:802:Y01:HBB	1.73	0.45
3:B:807:POV:H214	3:B:807:POV:H217	1.78	0.45
1:B:301:LYS:NZ	1:B:303:GLU:OE2	2.48	0.45
1:C:190:ARG:HG2	1:C:232:LEU:HD13	1.99	0.45
1:D:41:GLN:OE1	1:D:54:LYS:NZ	2.42	0.45
3:C:801:POV:H1A	3:C:801:POV:H14B	1.98	0.44
2:D:804:Y01:CAV	2:D:804:Y01:HAD1	2.47	0.44
1:A:632:ARG:NH2	1:A:634:GLU:OE1	2.45	0.44
3:A:813:POV:H34A	3:A:813:POV:H37A	1.81	0.44
1:A:180:ARG:NH2	1:A:222:TYR:OH	2.51	0.44
1:A:377:TYR:OH	1:A:389:GLU:OE1	2.31	0.44
3:B:812:POV:H216	2:C:804:Y01:HAC2	1.99	0.44
3:B:813:POV:H23	3:B:813:POV:H26A	1.69	0.44
1:C:336:TYR:HB2	2:C:802:Y01:HAQ1	1.98	0.44
3:B:812:POV:H36A	3:B:812:POV:H33	1.78	0.44
1:A:353:LYS:HE3	1:A:369:GLN:HE21	1.82	0.44
1:B:623:TYR:HA	1:C:42:LYS:HD2	2.00	0.44
1:B:75:ARG:HB3	1:B:79:GLY:HA2	1.99	0.43
3:B:811:POV:H26	3:B:811:POV:H23A	1.88	0.43
1:A:487:PHE:CE1	2:A:802:Y01:HAT2	2.53	0.43
1:C:406:ASP:HB3	1:C:413:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:THR:H	1:D:122:HIS:CD2	2.32	0.43
1:D:228:HIS:HE1	1:D:231:PRO:HA	1.83	0.43
1:D:332:LEU:HD12	2:D:804:Y01:HAU2	2.00	0.43
3:D:801:POV:H28A	3:D:801:POV:H21A	1.83	0.43
3:D:801:POV:H39	3:D:801:POV:H312	1.68	0.43
1:A:365:ASN:HD22	1:A:365:ASN:HA	1.57	0.43
2:B:802:Y01:CAV	2:B:802:Y01:CAI	2.84	0.43
2:B:803:Y01:CBH	2:B:803:Y01:CAV	2.71	0.43
1:B:116:GLU:HB3	1:B:149:GLY:HA2	2.00	0.43
2:B:802:Y01:HAO1	2:B:802:Y01:HAP1	1.86	0.43
1:C:231:PRO:HD2	1:C:234:LEU:HD12	1.99	0.43
1:A:534:PHE:HE1	2:A:803:Y01:HAB3	1.82	0.43
3:D:806:POV:H29	3:D:806:POV:H26	1.76	0.43
3:D:808:POV:H32A	3:D:808:POV:H35	1.73	0.43
1:A:43:ARG:HA	1:A:46:GLU:HG2	2.00	0.43
3:D:801:POV:H35	3:D:801:POV:H213	2.00	0.43
3:A:813:POV:H31A	3:A:813:POV:H31D	1.80	0.43
1:B:353:LYS:HE3	1:B:369:GLN:HE21	1.84	0.43
1:D:307:ILE:HA	1:D:310:GLN:HG2	2.00	0.43
3:A:811:POV:H21A	3:A:811:POV:H28	1.83	0.43
1:B:210:THR:O	1:B:214:GLN:NE2	2.52	0.43
1:B:286:SER:HA	1:B:615:ARG:HH22	1.82	0.43
1:D:527:PRO:HG3	3:D:808:POV:H23A	2.00	0.43
3:C:810:POV:H24	3:C:810:POV:H27	1.71	0.43
1:D:272:PRO:HB2	1:D:636:ARG:HG3	2.00	0.43
2:A:812:Y01:HAC2	3:D:808:POV:H216	2.00	0.43
3:B:801:POV:H32	3:B:801:POV:H35A	1.84	0.43
1:C:204:ILE:HG23	1:C:252:ASN:HD22	1.83	0.43
1:C:603:MET:HG3	1:C:606:ARG:HH11	1.84	0.43
1:D:389:GLU:HG2	3:D:811:POV:H215	2.01	0.42
2:C:803:Y01:HAP1	2:C:803:Y01:HAO1	1.65	0.42
2:A:801:Y01:CAZ	2:A:801:Y01:CAR	2.97	0.42
3:B:813:POV:H215	3:B:813:POV:H212	1.82	0.42
2:A:801:Y01:HAS1	2:A:801:Y01:HAT1	2.01	0.42
1:B:248:GLY:HA3	1:B:292:LEU:HD11	2.01	0.42
2:C:804:Y01:CBH	2:C:804:Y01:CAV	2.71	0.42
2:A:802:Y01:HAJ2	2:A:802:Y01:HAC3	1.81	0.42
1:B:84:HIS:HD2	1:B:120:ALA:HB2	1.85	0.42
1:C:40:GLN:NE2	1:C:80:GLU:OE2	2.53	0.42
1:D:198:THR:H	1:D:201:HIS:CD2	2.36	0.42
1:D:251:GLY:HA3	1:D:303:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:813:POV:H28	3:B:813:POV:H21A	1.80	0.42
1:C:469:ALA:HA	1:C:472:PHE:HD2	1.84	0.42
1:A:200:LEU:HD12	1:A:216:TYR:CD1	2.54	0.42
3:B:811:POV:H32	3:B:811:POV:H24A	2.02	0.42
1:C:119:THR:H	1:C:122:HIS:CD2	2.33	0.42
2:C:803:Y01:HAE2	2:C:803:Y01:HBB	1.79	0.42
3:C:810:POV:H32A	3:C:810:POV:H35	1.87	0.42
2:D:804:Y01:HAD1	2:D:804:Y01:HAV1	2.01	0.42
2:A:803:Y01:HAE1	1:B:560:ALA:HB1	2.02	0.42
2:B:802:Y01:CAT	2:B:802:Y01:HAS1	2.49	0.42
3:A:813:POV:H22	3:A:813:POV:H2	1.80	0.42
1:B:525:ASP:HB3	3:B:806:POV:H15B	2.01	0.42
3:B:813:POV:H28A	3:B:813:POV:H25	1.81	0.42
1:C:261:GLN:HG3	1:C:264:LYS:HE2	2.02	0.42
1:C:636:ARG:NE	1:C:638:ASP:OD1	2.53	0.42
1:A:632:ARG:NH1	1:B:34:ASP:OD1	2.49	0.41
3:C:809:POV:H35A	3:C:809:POV:H32	1.85	0.41
2:A:802:Y01:CAV	2:A:802:Y01:CAI	2.83	0.41
1:D:41:GLN:HE22	1:D:89:TYR:HH	1.63	0.41
1:D:411:GLY:HA3	1:D:415:PHE:HB2	2.01	0.41
3:A:810:POV:H316	3:A:811:POV:H21H	2.02	0.41
1:D:44:ILE:HG23	1:D:50:LEU:HB3	2.02	0.41
3:D:809:POV:H312	3:D:809:POV:H315	1.89	0.41
3:A:809:POV:H34	3:A:809:POV:H37A	1.49	0.41
2:A:812:Y01:CAS	2:A:812:Y01:HAT2	2.50	0.41
2:B:804:Y01:CBH	2:B:804:Y01:CAV	2.70	0.41
2:D:804:Y01:CAV	2:D:804:Y01:CAD	2.98	0.41
1:A:619:CYS:SG	1:A:620:GLY:N	2.94	0.41
1:C:382:ASP:OD1	1:C:385:ARG:NH2	2.46	0.41
3:C:810:POV:H11	3:C:810:POV:H15A	1.89	0.41
2:C:802:Y01:CAZ	2:C:802:Y01:CAR	2.97	0.41
1:C:332:LEU:HD12	2:C:802:Y01:HAQ2	2.03	0.41
3:D:811:POV:H215	3:D:811:POV:H212	1.85	0.41
3:C:807:POV:H33	3:C:807:POV:H36A	1.83	0.41
1:A:231:PRO:HD2	1:A:234:LEU:HD12	2.03	0.41
3:C:806:POV:H35	3:C:806:POV:H32A	1.92	0.41
1:D:249:VAL:HG22	1:D:295:LEU:HB3	2.02	0.41
2:D:805:Y01:CAS	2:D:805:Y01:HAT2	2.50	0.41
2:A:812:Y01:HAM2	2:A:812:Y01:HBC	1.89	0.40
2:B:802:Y01:CAZ	2:B:802:Y01:CAR	2.99	0.40
2:B:804:Y01:HAJ2	2:B:804:Y01:HAC2	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:812:POV:H21H	3:C:806:POV:H216	2.02	0.40
2:C:802:Y01:CAZ	2:C:802:Y01:CBC	2.87	0.40
3:D:809:POV:H34	3:D:809:POV:H37	1.67	0.40
3:A:810:POV:H11	3:A:810:POV:H15A	1.90	0.40
2:A:812:Y01:HAI	1:D:530:LEU:HB3	2.03	0.40
2:D:805:Y01:HAT2	2:D:805:Y01:HAS2	2.03	0.40
2:A:812:Y01:HAJ2	2:A:812:Y01:HAC3	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	610/725 (84%)	579 (95%)	31 (5%)	0	100	100
1	B	610/725 (84%)	581 (95%)	29 (5%)	0	100	100
1	C	610/725 (84%)	572 (94%)	37 (6%)	1 (0%)	47	64
1	D	610/725 (84%)	579 (95%)	31 (5%)	0	100	100
All	All	2440/2900 (84%)	2311 (95%)	128 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	591	GLU

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	531/633 (84%)	529 (100%)	2 (0%)	91	95
1	B	531/633 (84%)	528 (99%)	3 (1%)	86	92
1	C	531/633 (84%)	528 (99%)	3 (1%)	86	92
1	D	531/633 (84%)	528 (99%)	3 (1%)	86	92
All	All	2124/2532 (84%)	2113 (100%)	11 (0%)	89	94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	LYS
1	A	365	ASN
1	B	208	ASN
1	B	311	THR
1	B	365	ASN
1	C	140	ARG
1	C	365	ASN
1	C	603	MET
1	D	208	ASN
1	D	365	ASN
1	D	409	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	122	HIS
1	A	201	HIS
1	A	206	GLN
1	A	365	ASN
1	A	369	GLN
1	A	370	GLN
1	A	522	HIS
1	A	637	GLN
1	B	84	HIS
1	B	91	ASN
1	B	118	GLN
1	B	122	HIS
1	B	197	ASN

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Mol	Chain	Res	Type
1	B	201	HIS
1	B	206	GLN
1	B	208	ASN
1	B	267	GLN
1	B	365	ASN
1	B	369	GLN
1	B	370	GLN
1	B	637	GLN
1	C	118	GLN
1	C	122	HIS
1	C	127	ASN
1	C	201	HIS
1	C	206	GLN
1	C	217	ASN
1	C	267	GLN
1	C	365	ASN
1	C	370	GLN
1	C	637	GLN
1	D	36	GLN
1	D	91	ASN
1	D	118	GLN
1	D	122	HIS
1	D	197	ASN
1	D	201	HIS
1	D	206	GLN
1	D	208	ASN
1	D	214	GLN
1	D	267	GLN
1	D	365	ASN
1	D	369	GLN
1	D	370	GLN
1	D	522	HIS
1	D	637	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 53 ligands modelled in this entry, 3 are monoatomic - leaving 50 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	807	-	12,12,51	0.66	0	11,11,59	0.36	0
3	POV	B	809	-	18,18,51	1.39	2 (11%)	18,18,59	0.83	0
3	POV	A	807	-	12,12,51	0.66	0	11,11,59	0.31	0
2	Y01	A	803	-	38,38,38	7.48	19 (50%)	57,57,57	3.28	22 (38%)
3	POV	A	804	-	12,12,51	0.62	0	11,11,59	0.43	0
3	POV	B	801	-	12,12,51	0.64	0	11,11,59	0.39	0
3	POV	B	810	-	12,12,51	0.64	0	11,11,59	0.40	0
3	POV	D	807	-	12,12,51	0.62	0	11,11,59	0.42	0
3	POV	C	801	-	45,45,51	1.12	3 (6%)	50,53,59	0.99	3 (6%)
2	Y01	A	812	-	38,38,38	7.44	19 (50%)	57,57,57	3.13	21 (36%)
2	Y01	C	804	-	38,38,38	7.49	19 (50%)	57,57,57	3.28	22 (38%)
3	POV	A	810	-	51,51,51	1.07	2 (3%)	57,59,59	0.90	3 (5%)
3	POV	A	806	-	51,51,51	1.07	3 (5%)	57,59,59	0.93	3 (5%)
3	POV	D	808	-	51,51,51	1.05	3 (5%)	57,59,59	0.91	3 (5%)
3	POV	D	812	-	12,12,51	0.64	0	11,11,59	0.39	0
3	POV	B	807	-	51,51,51	1.07	3 (5%)	57,59,59	0.90	3 (5%)
2	Y01	C	803	-	38,38,38	7.54	21 (55%)	57,57,57	3.61	25 (43%)
3	POV	C	805	-	12,12,51	0.63	0	11,11,59	0.41	0
3	POV	D	801	-	51,51,51	1.06	3 (5%)	57,59,59	0.89	4 (7%)
3	POV	B	806	-	45,45,51	1.09	3 (6%)	50,53,59	0.92	3 (6%)
3	POV	C	806	-	51,51,51	1.06	3 (5%)	57,59,59	0.92	3 (5%)
2	Y01	B	804	-	38,38,38	7.44	22 (57%)	57,57,57	3.26	24 (42%)
3	POV	B	811	-	51,51,51	1.06	3 (5%)	57,59,59	0.90	2 (3%)
3	POV	D	803	-	12,12,51	0.63	0	11,11,59	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GEN	D	813	-	18,22,22	2.89	6 (33%)	22,32,32	1.07	3 (13%)
3	POV	B	813	-	51,51,51	1.06	3 (5%)	57,59,59	0.90	3 (5%)
3	POV	A	811	-	51,51,51	1.07	3 (5%)	57,59,59	0.86	3 (5%)
2	Y01	D	805	-	38,38,38	7.45	21 (55%)	57,57,57	3.42	26 (45%)
3	POV	B	808	-	12,12,51	0.65	0	11,11,59	0.39	0
3	POV	C	808	-	18,18,51	1.39	2 (11%)	18,18,59	0.83	0
2	Y01	B	802	-	38,38,38	7.44	21 (55%)	57,57,57	2.97	25 (43%)
3	POV	B	805	-	12,12,51	0.63	0	11,11,59	0.39	0
6	GEN	A	816	-	18,22,22	2.87	5 (27%)	22,32,32	1.00	2 (9%)
2	Y01	C	802	-	38,38,38	7.56	22 (57%)	57,57,57	3.00	25 (43%)
2	Y01	A	801	-	38,38,38	7.56	21 (55%)	57,57,57	3.10	24 (42%)
2	Y01	A	802	-	38,38,38	7.52	19 (50%)	57,57,57	3.16	30 (52%)
3	POV	C	809	-	12,12,51	0.64	0	11,11,59	0.34	0
2	Y01	B	803	-	38,38,38	7.49	20 (52%)	57,57,57	3.22	25 (43%)
3	POV	A	808	-	18,18,51	1.40	2 (11%)	18,18,59	0.81	0
3	POV	C	810	-	51,51,51	1.07	3 (5%)	57,59,59	0.85	2 (3%)
3	POV	D	811	-	18,18,51	1.39	2 (11%)	18,18,59	0.85	0
3	POV	A	813	-	45,45,51	1.13	3 (6%)	50,53,59	1.09	4 (8%)
3	POV	A	809	-	12,12,51	0.66	0	11,11,59	0.31	0
3	POV	B	812	-	51,51,51	1.05	3 (5%)	57,59,59	0.87	2 (3%)
3	POV	D	809	-	51,51,51	1.06	2 (3%)	57,59,59	0.87	3 (5%)
3	POV	D	810	-	12,12,51	0.64	0	11,11,59	0.41	0
3	POV	D	806	-	51,51,51	1.08	3 (5%)	57,59,59	0.90	3 (5%)
3	POV	A	805	-	51,51,51	1.04	3 (5%)	57,59,59	0.87	2 (3%)
2	Y01	D	804	-	38,38,38	7.48	21 (55%)	57,57,57	2.95	27 (47%)
3	POV	D	802	-	51,51,51	1.06	3 (5%)	57,59,59	0.88	3 (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	807	-	-	4/10/10/55	-
3	POV	B	809	-	-	7/17/17/55	-
3	POV	A	807	-	-	8/10/10/55	-
2	Y01	A	803	-	4/4/12/13	5/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	A	804	-	-	5/10/10/55	-
3	POV	B	801	-	-	5/10/10/55	-
3	POV	B	810	-	-	9/10/10/55	-
3	POV	D	807	-	-	6/10/10/55	-
3	POV	C	801	-	-	27/49/49/55	-
2	Y01	A	812	-	4/4/12/13	13/19/77/77	0/4/4/4
2	Y01	C	804	-	4/4/12/13	10/19/77/77	0/4/4/4
3	POV	A	810	-	-	29/55/55/55	-
3	POV	A	806	-	-	32/55/55/55	-
3	POV	D	808	-	-	31/55/55/55	-
3	POV	D	812	-	-	5/10/10/55	-
3	POV	B	807	-	-	31/55/55/55	-
2	Y01	C	803	-	4/4/12/13	10/19/77/77	0/4/4/4
3	POV	C	805	-	-	4/10/10/55	-
3	POV	D	801	-	-	27/55/55/55	-
3	POV	B	806	-	-	24/49/49/55	-
3	POV	C	806	-	-	28/55/55/55	-
2	Y01	B	804	-	4/4/12/13	12/19/77/77	0/4/4/4
3	POV	B	811	-	-	23/55/55/55	-
3	POV	D	803	-	-	7/10/10/55	-
6	GEN	D	813	-	-	0/0/4/4	0/3/3/3
3	POV	B	813	-	-	26/55/55/55	-
3	POV	A	811	-	-	20/55/55/55	-
2	Y01	D	805	-	4/4/12/13	12/19/77/77	0/4/4/4
3	POV	B	808	-	-	6/10/10/55	-
3	POV	C	808	-	-	7/17/17/55	-
2	Y01	B	802	-	4/4/12/13	8/19/77/77	0/4/4/4
3	POV	B	805	-	-	5/10/10/55	-
6	GEN	A	816	-	-	0/0/4/4	0/3/3/3
2	Y01	C	802	-	4/4/12/13	11/19/77/77	0/4/4/4
2	Y01	A	801	-	4/4/12/13	11/19/77/77	0/4/4/4
2	Y01	A	802	-	4/4/12/13	16/19/77/77	0/4/4/4
3	POV	C	809	-	-	8/10/10/55	-
2	Y01	B	803	-	4/4/12/13	6/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	A	808	-	-	12/17/17/55	-
3	POV	C	810	-	-	26/55/55/55	-
3	POV	D	811	-	-	7/17/17/55	-
3	POV	A	813	-	-	24/49/49/55	-
3	POV	A	809	-	-	7/10/10/55	-
3	POV	B	812	-	-	28/55/55/55	-
3	POV	D	809	-	-	32/55/55/55	-
3	POV	D	810	-	-	9/10/10/55	-
3	POV	D	806	-	-	39/55/55/55	-
3	POV	A	805	-	-	26/55/55/55	-
2	Y01	D	804	-	4/4/12/13	13/19/77/77	0/4/4/4
3	POV	D	802	-	-	23/55/55/55	-

All (316) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	804	Y01	CAK-CBD	-21.56	1.16	1.53
2	A	812	Y01	CAK-CBD	-21.44	1.16	1.53
2	A	803	Y01	CAK-CBD	-21.42	1.16	1.53
2	C	803	Y01	CAK-CBD	-21.15	1.17	1.53
2	C	802	Y01	CBD-CBG	-21.09	1.13	1.53
2	B	803	Y01	CAK-CBD	-21.08	1.17	1.53
2	A	802	Y01	CAK-CBD	-21.02	1.17	1.53
2	C	802	Y01	CAK-CBD	-20.99	1.17	1.53
2	A	801	Y01	CAK-CBD	-20.97	1.17	1.53
2	B	802	Y01	CAK-CBD	-20.88	1.17	1.53
2	B	804	Y01	CAK-CBD	-20.82	1.17	1.53
2	D	805	Y01	CAK-CBD	-20.76	1.18	1.53
2	A	801	Y01	CBD-CBG	-20.70	1.14	1.53
2	D	804	Y01	CAK-CBD	-20.70	1.18	1.53
2	A	802	Y01	CBD-CBG	-20.59	1.14	1.53
2	D	804	Y01	CBD-CBG	-20.45	1.14	1.53
2	C	804	Y01	CBD-CBG	-20.44	1.14	1.53
2	A	803	Y01	CBD-CBG	-20.29	1.14	1.53
2	B	803	Y01	CBD-CBG	-20.21	1.15	1.53
2	B	802	Y01	CBD-CBG	-20.16	1.15	1.53
2	A	812	Y01	CBD-CBG	-20.13	1.15	1.53
2	C	803	Y01	CBD-CBG	-19.87	1.15	1.53
2	B	804	Y01	CBD-CBG	-19.67	1.16	1.53
2	D	805	Y01	CBD-CBG	-19.52	1.16	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	805	Y01	CAV-CAZ	19.01	1.93	1.51
2	C	803	Y01	CAV-CAZ	18.95	1.92	1.51
2	B	803	Y01	CAV-CAZ	18.95	1.92	1.51
2	B	804	Y01	CAV-CAZ	18.75	1.92	1.51
2	A	802	Y01	CAV-CAZ	18.46	1.91	1.51
2	A	801	Y01	CAV-CAZ	18.37	1.91	1.51
2	A	803	Y01	CAV-CAZ	18.22	1.91	1.51
2	C	802	Y01	CAV-CAZ	18.21	1.91	1.51
2	A	812	Y01	CAV-CAZ	18.17	1.91	1.51
2	C	804	Y01	CAV-CAZ	18.17	1.91	1.51
2	D	804	Y01	CAV-CAZ	18.07	1.91	1.51
2	B	802	Y01	CAV-CAZ	17.97	1.90	1.51
2	B	802	Y01	CBH-CAZ	-16.19	1.20	1.52
2	D	804	Y01	CBH-CAZ	-16.18	1.20	1.52
2	A	802	Y01	CBH-CAZ	-15.87	1.21	1.52
2	A	801	Y01	CBH-CAZ	-15.65	1.21	1.52
2	C	802	Y01	CBH-CAZ	-15.61	1.21	1.52
2	C	803	Y01	CBH-CAZ	-15.28	1.22	1.52
2	B	804	Y01	CBH-CAZ	-14.98	1.23	1.52
2	A	812	Y01	CBH-CAZ	-14.95	1.23	1.52
2	D	805	Y01	CBH-CAZ	-14.81	1.23	1.52
2	A	803	Y01	CBH-CAZ	-14.80	1.23	1.52
2	B	803	Y01	CBH-CAZ	-14.80	1.23	1.52
2	C	804	Y01	CBH-CAZ	-14.62	1.23	1.52
2	D	805	Y01	CAT-CBH	14.04	1.80	1.54
2	C	803	Y01	CAT-CBH	13.90	1.80	1.54
2	B	804	Y01	CAT-CBH	13.82	1.80	1.54
2	A	803	Y01	CAT-CBH	13.82	1.80	1.54
2	C	804	Y01	CAT-CBH	13.74	1.80	1.54
2	A	801	Y01	CAT-CBH	13.65	1.80	1.54
2	A	801	Y01	CAU-CBI	-13.63	1.29	1.54
2	A	812	Y01	CAT-CBH	13.48	1.79	1.54
2	C	802	Y01	CAT-CBH	13.48	1.79	1.54
2	C	802	Y01	CAU-CBI	-13.45	1.30	1.54
2	D	804	Y01	CAT-CBH	13.24	1.79	1.54
2	B	803	Y01	CAU-CBI	-13.19	1.30	1.54
2	B	802	Y01	CAT-CBH	13.15	1.79	1.54
2	D	804	Y01	CAU-CBI	-13.13	1.30	1.54
2	A	802	Y01	CAT-CBH	13.12	1.79	1.54
2	B	803	Y01	CAT-CBH	13.10	1.79	1.54
2	D	805	Y01	CAU-CBI	-12.99	1.30	1.54
2	C	803	Y01	CAU-CBI	-12.86	1.31	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	Y01	CAU-CBI	-12.86	1.31	1.54
2	C	804	Y01	CAU-CBI	-12.84	1.31	1.54
2	A	812	Y01	CAU-CBI	-12.83	1.31	1.54
2	A	803	Y01	CAU-CBI	-12.83	1.31	1.54
2	B	802	Y01	CAU-CBI	-12.80	1.31	1.54
2	B	804	Y01	CAU-CBI	-12.47	1.31	1.54
6	D	813	GEN	O6-C6	8.88	1.38	1.23
6	A	816	GEN	O6-C6	8.80	1.38	1.23
2	B	804	Y01	CBI-CBE	8.39	1.71	1.55
2	A	803	Y01	CBI-CBE	8.24	1.70	1.55
2	B	803	Y01	CBI-CBE	8.22	1.70	1.55
2	C	804	Y01	CBI-CBE	8.14	1.70	1.55
2	C	803	Y01	CBI-CBE	7.92	1.70	1.55
2	A	801	Y01	CBI-CBE	7.81	1.69	1.55
2	A	802	Y01	CBI-CBE	7.73	1.69	1.55
2	D	805	Y01	CBI-CBE	7.70	1.69	1.55
2	A	812	Y01	CBI-CBE	7.53	1.69	1.55
2	C	802	Y01	CBI-CBE	7.48	1.69	1.55
2	B	802	Y01	CBI-CBE	7.45	1.69	1.55
2	A	802	Y01	CAQ-CAP	7.45	1.74	1.54
2	D	804	Y01	CAQ-CAP	7.35	1.74	1.54
2	C	802	Y01	CAQ-CAP	7.34	1.74	1.54
2	D	804	Y01	CBI-CBE	7.33	1.69	1.55
2	C	803	Y01	CAQ-CAP	7.33	1.74	1.54
2	D	805	Y01	CAQ-CAP	7.28	1.74	1.54
2	B	802	Y01	CAQ-CAP	7.21	1.73	1.54
2	B	803	Y01	CAQ-CAP	7.20	1.73	1.54
2	A	801	Y01	CAQ-CAP	7.19	1.73	1.54
2	A	812	Y01	CAQ-CAP	7.11	1.73	1.54
2	C	804	Y01	CAQ-CAP	7.08	1.73	1.54
2	B	804	Y01	CBI-CBG	7.07	1.68	1.55
2	B	804	Y01	CAQ-CAP	7.03	1.73	1.54
2	A	803	Y01	CAQ-CAP	7.02	1.73	1.54
2	D	805	Y01	CBI-CBG	7.01	1.68	1.55
2	C	803	Y01	CBI-CBG	6.81	1.68	1.55
2	B	803	Y01	CBI-CBG	6.73	1.67	1.55
2	A	802	Y01	CBI-CBG	6.67	1.67	1.55
2	C	804	Y01	CBI-CBG	6.48	1.67	1.55
2	A	803	Y01	CBI-CBG	6.41	1.67	1.55
2	A	812	Y01	CBI-CBG	6.34	1.67	1.55
2	B	802	Y01	CBI-CBG	6.27	1.66	1.55
2	A	801	Y01	CBI-CBG	6.14	1.66	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	804	Y01	CBI-CBG	6.10	1.66	1.55
2	C	802	Y01	CBI-CBG	6.05	1.66	1.55
2	A	812	Y01	CAQ-CBG	5.73	1.66	1.54
2	B	802	Y01	CAQ-CBG	5.48	1.65	1.54
2	A	803	Y01	CAQ-CBG	5.39	1.65	1.54
6	A	816	GEN	C5-C10	-5.36	1.34	1.41
2	A	801	Y01	CAU-CAS	-5.36	1.42	1.53
2	D	805	Y01	CAQ-CBG	5.33	1.65	1.54
2	C	802	Y01	CAI-CAZ	5.33	1.44	1.33
2	B	804	Y01	CAQ-CBG	5.30	1.65	1.54
2	C	802	Y01	CAU-CAS	-5.28	1.42	1.53
2	C	804	Y01	CAQ-CBG	5.27	1.65	1.54
2	D	804	Y01	CAU-CAS	-5.27	1.42	1.53
6	D	813	GEN	C5-C10	-5.27	1.34	1.41
2	D	804	Y01	CAQ-CBG	5.24	1.65	1.54
2	B	803	Y01	CAQ-CBG	5.18	1.65	1.54
2	C	803	Y01	CAQ-CBG	5.13	1.65	1.54
2	A	801	Y01	CAQ-CBG	5.11	1.65	1.54
2	A	801	Y01	CAI-CAZ	5.08	1.44	1.33
2	B	803	Y01	CAI-CAZ	5.07	1.44	1.33
2	A	802	Y01	CAI-CAZ	5.06	1.44	1.33
2	D	805	Y01	CAI-CAZ	5.05	1.44	1.33
2	C	802	Y01	CAQ-CBG	5.04	1.64	1.54
2	A	802	Y01	CAQ-CBG	4.93	1.64	1.54
2	B	803	Y01	CAU-CAS	-4.92	1.42	1.53
2	A	802	Y01	CAU-CAS	-4.91	1.42	1.53
2	D	804	Y01	CAI-CAZ	4.91	1.43	1.33
2	B	802	Y01	CAI-CAZ	4.84	1.43	1.33
2	B	804	Y01	CAU-CAS	-4.83	1.43	1.53
2	C	803	Y01	CAI-CAZ	4.82	1.43	1.33
2	B	802	Y01	CAU-CAS	-4.78	1.43	1.53
2	C	804	Y01	CAU-CAS	-4.75	1.43	1.53
2	A	812	Y01	CAU-CAS	-4.72	1.43	1.53
2	C	803	Y01	CAU-CAS	-4.72	1.43	1.53
2	A	812	Y01	CBB-CBE	-4.68	1.46	1.54
2	B	804	Y01	CAI-CAZ	4.67	1.43	1.33
2	B	802	Y01	CBB-CBE	-4.58	1.46	1.54
2	A	803	Y01	CAU-CAS	-4.56	1.43	1.53
2	D	805	Y01	CAU-CAS	-4.56	1.43	1.53
2	C	804	Y01	CAI-CAZ	4.55	1.43	1.33
2	A	803	Y01	CAI-CAZ	4.53	1.42	1.33
2	D	804	Y01	CBB-CBE	-4.48	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	Y01	CBB-CBE	-4.48	1.46	1.54
2	C	804	Y01	CBB-CBE	-4.47	1.46	1.54
2	C	802	Y01	CBB-CBE	-4.46	1.46	1.54
2	A	803	Y01	OAW-CAY	4.43	1.46	1.34
2	C	804	Y01	OAW-CAY	4.40	1.46	1.34
2	A	812	Y01	OAW-CAY	4.38	1.46	1.34
2	C	803	Y01	CBH-CBF	-4.37	1.48	1.56
2	A	812	Y01	CAI-CAZ	4.37	1.42	1.33
2	B	803	Y01	CBB-CBE	-4.36	1.46	1.54
2	C	803	Y01	CBB-CBE	-4.34	1.46	1.54
2	D	805	Y01	CBB-CBE	-4.32	1.46	1.54
2	A	803	Y01	CBB-CBE	-4.29	1.46	1.54
2	B	803	Y01	OAW-CAY	4.27	1.46	1.34
2	A	802	Y01	OAW-CAY	4.21	1.46	1.34
2	C	803	Y01	OAW-CAY	4.19	1.46	1.34
2	A	802	Y01	CBB-CBE	-4.19	1.47	1.54
3	A	808	POV	C29-C210	4.12	1.55	1.31
2	D	804	Y01	OAW-CAY	4.12	1.45	1.34
3	B	809	POV	C29-C210	4.11	1.55	1.31
3	C	808	POV	C29-C210	4.10	1.55	1.31
3	D	811	POV	C29-C210	4.09	1.55	1.31
2	C	803	Y01	CBD-CBF	-4.08	1.45	1.53
2	C	802	Y01	CBH-CBF	-4.05	1.49	1.56
2	B	802	Y01	CBH-CBF	-4.02	1.49	1.56
2	D	805	Y01	OAW-CAY	3.99	1.45	1.34
2	A	803	Y01	CAT-CAR	3.98	1.61	1.53
2	C	802	Y01	OAW-CAY	3.97	1.45	1.34
2	C	804	Y01	CAT-CAR	3.94	1.61	1.53
2	A	801	Y01	OAW-CAY	3.93	1.45	1.34
2	B	804	Y01	OAW-CAY	3.91	1.45	1.34
2	A	802	Y01	CBH-CBF	-3.91	1.49	1.56
2	A	801	Y01	CBH-CBF	-3.89	1.49	1.56
2	B	803	Y01	CBH-CBF	-3.85	1.49	1.56
2	D	804	Y01	CBH-CBF	-3.83	1.49	1.56
2	B	802	Y01	OAW-CAY	3.82	1.45	1.34
2	B	804	Y01	CBB-CBE	-3.81	1.47	1.54
2	D	805	Y01	CBH-CBF	-3.80	1.49	1.56
2	A	802	Y01	CAT-CAR	3.80	1.61	1.53
2	A	812	Y01	CAT-CAR	3.75	1.61	1.53
2	B	804	Y01	CBD-CBF	-3.70	1.46	1.53
2	B	804	Y01	CBH-CBF	-3.67	1.49	1.56
2	C	803	Y01	CAT-CAR	3.67	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	802	Y01	CBD-CBF	-3.63	1.46	1.53
2	A	802	Y01	CBD-CBF	-3.62	1.46	1.53
2	A	801	Y01	CBD-CBF	-3.59	1.46	1.53
2	D	805	Y01	CBD-CBF	-3.59	1.46	1.53
2	B	802	Y01	CBD-CBF	-3.56	1.46	1.53
2	B	803	Y01	CBD-CBF	-3.56	1.46	1.53
2	B	804	Y01	CAT-CAR	3.50	1.60	1.53
2	D	805	Y01	CAT-CAR	3.46	1.60	1.53
2	D	804	Y01	CBD-CBF	-3.45	1.47	1.53
2	C	804	Y01	CBH-CBF	-3.45	1.50	1.56
2	B	802	Y01	CAT-CAR	3.44	1.60	1.53
2	A	812	Y01	CBH-CBF	-3.41	1.50	1.56
2	A	812	Y01	CBD-CBF	-3.39	1.47	1.53
2	C	804	Y01	CBD-CBF	-3.37	1.47	1.53
2	A	803	Y01	CBD-CBF	-3.31	1.47	1.53
2	D	804	Y01	CAT-CAR	3.29	1.60	1.53
2	C	802	Y01	CAT-CAR	3.17	1.60	1.53
2	A	803	Y01	CBH-CBF	-3.17	1.50	1.56
2	A	801	Y01	CAT-CAR	3.13	1.60	1.53
3	A	810	POV	O21-C21	3.06	1.42	1.34
3	A	813	POV	O21-C21	3.03	1.42	1.34
2	B	803	Y01	CAT-CAR	3.03	1.59	1.53
3	C	810	POV	O21-C21	3.00	1.42	1.34
3	D	809	POV	O21-C21	2.97	1.42	1.34
6	D	813	GEN	C1-C10	2.96	1.43	1.37
3	A	811	POV	O31-C31	2.83	1.41	1.33
3	D	809	POV	O31-C31	2.83	1.41	1.33
3	D	806	POV	O31-C31	2.83	1.41	1.33
2	C	804	Y01	CAV-CBC	-2.83	1.45	1.52
3	B	811	POV	O21-C21	2.82	1.42	1.34
3	A	811	POV	O21-C21	2.82	1.42	1.34
3	B	807	POV	O21-C21	2.82	1.42	1.34
3	C	801	POV	O31-C31	2.81	1.41	1.33
3	D	802	POV	O21-C21	2.80	1.42	1.34
3	C	806	POV	O31-C31	2.80	1.41	1.33
6	A	816	GEN	O14-C14	2.79	1.43	1.37
3	B	813	POV	O21-C21	2.79	1.42	1.34
3	D	806	POV	O21-C21	2.79	1.42	1.34
3	B	807	POV	O31-C31	2.79	1.41	1.33
3	C	810	POV	O31-C31	2.77	1.41	1.33
3	A	806	POV	O21-C21	2.77	1.42	1.34
2	C	802	Y01	CAK-CAI	2.76	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	806	POV	O31-C31	2.76	1.41	1.33
2	A	803	Y01	CAV-CBC	-2.75	1.45	1.52
3	B	811	POV	O31-C31	2.74	1.41	1.33
3	D	808	POV	O21-C21	2.74	1.42	1.34
6	A	816	GEN	C1-C10	2.73	1.43	1.37
6	D	813	GEN	O14-C14	2.73	1.43	1.37
3	D	801	POV	O31-C31	2.72	1.41	1.33
3	A	805	POV	O31-C31	2.72	1.41	1.33
3	A	810	POV	O31-C31	2.71	1.41	1.33
3	A	805	POV	O21-C21	2.71	1.41	1.34
3	B	813	POV	O31-C31	2.70	1.41	1.33
3	B	812	POV	O21-C21	2.69	1.41	1.34
3	B	806	POV	O31-C31	2.69	1.41	1.33
3	C	808	POV	O21-C21	2.69	1.41	1.33
3	D	801	POV	O21-C21	2.68	1.41	1.34
3	B	806	POV	O21-C21	2.68	1.41	1.34
3	C	806	POV	O21-C21	2.68	1.41	1.34
3	B	812	POV	O31-C31	2.67	1.41	1.33
3	A	808	POV	O21-C21	2.66	1.41	1.33
3	B	809	POV	O21-C21	2.66	1.41	1.33
2	A	802	Y01	CAK-CAI	2.66	1.55	1.50
3	D	811	POV	O21-C21	2.65	1.41	1.33
3	A	813	POV	O31-C31	2.65	1.41	1.33
3	C	801	POV	O21-C21	2.64	1.41	1.34
2	A	812	Y01	CAV-CBC	-2.64	1.45	1.52
3	D	808	POV	O31-C31	2.64	1.41	1.33
3	D	802	POV	O31-C31	2.63	1.41	1.33
3	A	805	POV	O21-C2	-2.56	1.40	1.46
6	A	816	GEN	C8-C7	-2.55	1.33	1.39
2	A	801	Y01	CAK-CAI	2.53	1.55	1.50
3	C	801	POV	O21-C2	-2.51	1.40	1.46
3	B	812	POV	O21-C2	-2.50	1.40	1.46
2	B	804	Y01	CAO-CBB	2.49	1.60	1.54
3	D	808	POV	O21-C2	-2.48	1.40	1.46
2	A	801	Y01	CAR-CBC	-2.46	1.44	1.51
3	B	806	POV	O21-C2	-2.45	1.40	1.46
3	D	801	POV	O21-C2	-2.44	1.40	1.46
2	C	803	Y01	CAK-CAI	2.43	1.55	1.50
3	D	806	POV	O21-C2	-2.43	1.40	1.46
2	B	802	Y01	CAV-CBC	-2.43	1.46	1.52
3	D	802	POV	O21-C2	-2.42	1.40	1.46
2	D	805	Y01	CAK-CAI	2.41	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	806	POV	O21-C2	-2.41	1.40	1.46
3	A	806	POV	O21-C2	-2.40	1.40	1.46
2	A	812	Y01	CAO-CBB	2.40	1.60	1.54
6	D	813	GEN	C8-C7	-2.40	1.34	1.39
3	B	807	POV	O21-C2	-2.37	1.40	1.46
2	B	804	Y01	CAV-CBC	-2.36	1.46	1.52
3	B	813	POV	O21-C2	-2.35	1.40	1.46
3	B	811	POV	O21-C2	-2.34	1.40	1.46
2	D	804	Y01	CAK-CAI	2.33	1.55	1.50
3	A	811	POV	O21-C2	-2.33	1.40	1.46
2	A	802	Y01	CAO-CBB	2.33	1.60	1.54
2	C	802	Y01	CAO-CBB	2.32	1.60	1.54
3	A	813	POV	O21-C2	-2.31	1.40	1.46
2	B	804	Y01	CAR-CBC	-2.31	1.44	1.51
2	B	803	Y01	CAK-CAI	2.29	1.55	1.50
2	B	802	Y01	CAO-CBB	2.29	1.60	1.54
2	C	802	Y01	CAS-CBF	-2.27	1.50	1.53
2	B	802	Y01	CAK-CAI	2.25	1.55	1.50
2	C	802	Y01	CAV-CBC	-2.25	1.46	1.52
2	C	802	Y01	CAR-CBC	-2.23	1.45	1.51
2	A	801	Y01	CAV-CBC	-2.23	1.46	1.52
2	D	805	Y01	CAO-CBB	2.21	1.60	1.54
2	D	804	Y01	CAV-CBC	-2.21	1.46	1.52
2	D	804	Y01	CAR-CBC	-2.19	1.45	1.51
2	C	804	Y01	CAO-CBB	2.18	1.60	1.54
2	C	803	Y01	CAO-CBB	2.17	1.60	1.54
2	A	803	Y01	CAO-CBB	2.15	1.59	1.54
3	C	810	POV	O21-C2	-2.14	1.41	1.46
2	A	801	Y01	CAO-CBB	2.11	1.59	1.54
2	D	805	Y01	CAR-CBC	-2.11	1.45	1.51
2	B	803	Y01	CAO-CBB	2.11	1.59	1.54
2	B	803	Y01	CAV-CBC	-2.10	1.47	1.52
2	C	803	Y01	OAW-CBC	2.09	1.51	1.46
2	B	804	Y01	CAS-CBF	-2.09	1.50	1.53
6	D	813	GEN	O2-C2	2.08	1.41	1.37
2	D	805	Y01	CAV-CBC	-2.07	1.47	1.52
2	B	802	Y01	CAR-CBC	-2.07	1.45	1.51
2	B	804	Y01	CAK-CAI	2.07	1.54	1.50
2	D	804	Y01	CAO-CBB	2.07	1.59	1.54
2	C	803	Y01	CAR-CBC	-2.03	1.45	1.51

All (353) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	804	Y01	CAD-CBH-CBF	-13.42	95.68	111.68
2	C	803	Y01	CAD-CBH-CBF	-13.34	95.77	111.68
2	D	805	Y01	CAD-CBH-CBF	-13.00	96.18	111.68
2	A	803	Y01	CAD-CBH-CBF	-11.68	97.76	111.68
2	C	804	Y01	CAD-CBH-CBF	-11.55	97.91	111.68
2	A	812	Y01	CAD-CBH-CBF	-10.80	98.80	111.68
2	A	801	Y01	CAU-CBI-CBE	-9.73	102.00	116.57
2	B	803	Y01	CAD-CBH-CBF	-9.25	100.65	111.68
2	C	803	Y01	CAU-CBI-CBE	-9.21	102.79	116.57
2	B	803	Y01	CAU-CBI-CBE	-8.66	103.61	116.57
2	C	802	Y01	CAU-CBI-CBE	-8.50	103.85	116.57
2	C	804	Y01	CAU-CBI-CBE	-8.22	104.27	116.57
2	A	802	Y01	CAD-CBH-CBF	-7.95	102.20	111.68
2	A	812	Y01	CAV-CAZ-CAI	-7.77	109.41	120.61
2	A	803	Y01	CAU-CBI-CBE	-7.62	105.16	116.57
2	A	802	Y01	CAU-CBI-CBE	-7.56	105.26	116.57
2	D	805	Y01	CAU-CBI-CBE	-7.52	105.31	116.57
2	A	803	Y01	CAV-CAZ-CAI	-7.50	109.80	120.61
2	C	804	Y01	CAV-CAZ-CAI	-7.46	109.86	120.61
2	C	803	Y01	CBG-CBI-CBE	7.44	108.89	100.07
2	A	801	Y01	CBG-CBI-CBE	7.40	108.84	100.07
2	B	803	Y01	CBG-CBI-CBE	7.02	108.39	100.07
2	A	802	Y01	CBG-CBI-CBE	6.95	108.31	100.07
2	D	805	Y01	CBF-CBH-CAZ	6.83	120.36	109.65
2	C	802	Y01	CBG-CBI-CBE	6.74	108.06	100.07
2	D	804	Y01	CAU-CBI-CBE	-6.69	106.55	116.57
2	B	802	Y01	CBD-CAK-CAI	6.67	122.32	112.73
2	B	803	Y01	CBF-CBH-CAZ	6.66	120.09	109.65
2	B	804	Y01	CBF-CBH-CAZ	6.60	120.00	109.65
2	B	802	Y01	CAU-CBI-CBE	-6.56	106.75	116.57
2	D	804	Y01	CAK-CAI-CAZ	-6.35	113.35	125.06
2	C	804	Y01	CBG-CBI-CBE	6.30	107.54	100.07
2	C	803	Y01	CBF-CBH-CAZ	6.28	119.50	109.65
2	A	812	Y01	CBF-CBH-CAZ	6.28	119.49	109.65
2	A	803	Y01	CBG-CBI-CBE	6.27	107.50	100.07
2	A	801	Y01	CAD-CBH-CBF	-6.26	104.22	111.68
2	D	805	Y01	CAK-CBD-CBF	6.21	117.24	109.71
2	D	805	Y01	CBG-CBI-CBE	6.15	107.36	100.07
2	A	803	Y01	CAK-CAI-CAZ	-6.09	113.82	125.06
2	C	803	Y01	CBD-CAK-CAI	6.06	121.44	112.73
2	D	804	Y01	CBG-CBI-CBE	6.05	107.24	100.07
2	A	803	Y01	CBF-CBH-CAZ	6.02	119.10	109.65
2	C	802	Y01	CAU-CBI-CBG	5.95	116.51	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	804	Y01	CBG-CBI-CBE	5.94	107.11	100.07
2	A	801	Y01	CAU-CBI-CBG	5.94	116.49	107.27
2	A	812	Y01	CAU-CBI-CBE	-5.92	107.71	116.57
2	B	804	Y01	CAK-CAI-CAZ	-5.92	114.14	125.06
2	C	804	Y01	CBF-CBH-CAZ	5.91	118.92	109.65
2	A	801	Y01	CBF-CBH-CAZ	5.86	118.84	109.65
2	B	802	Y01	CBG-CBI-CBE	5.85	107.00	100.07
2	D	804	Y01	CAT-CAR-CBC	5.82	120.24	110.33
2	C	803	Y01	CAK-CAI-CAZ	-5.81	114.34	125.06
2	A	801	Y01	CAK-CAI-CAZ	-5.81	114.35	125.06
2	B	802	Y01	CAK-CAI-CAZ	-5.78	114.39	125.06
2	A	802	Y01	CAK-CAI-CAZ	-5.71	114.52	125.06
2	D	804	Y01	CAU-CBI-CBG	5.70	116.11	107.27
2	A	812	Y01	CAK-CAI-CAZ	-5.64	114.65	125.06
2	C	804	Y01	CAK-CAI-CAZ	-5.62	114.69	125.06
2	D	804	Y01	CBF-CBH-CAZ	5.57	118.39	109.65
2	B	802	Y01	CAD-CBH-CBF	-5.55	105.06	111.68
2	C	802	Y01	CAK-CAI-CAZ	-5.53	114.85	125.06
2	C	803	Y01	CAD-CBH-CAT	5.49	118.09	109.43
2	B	804	Y01	CAS-CAU-CBI	5.48	122.17	112.78
2	C	802	Y01	CBF-CBH-CAZ	5.44	118.18	109.65
2	B	802	Y01	CAK-CBD-CBF	5.38	116.24	109.71
2	C	802	Y01	CBF-CBD-CBG	5.38	116.29	109.09
2	A	812	Y01	OAW-CAY-CAM	5.37	123.08	111.50
2	D	805	Y01	CAS-CBF-CBH	5.36	120.14	113.08
2	B	803	Y01	CAK-CAI-CAZ	-5.35	115.19	125.06
2	D	805	Y01	CBD-CAK-CAI	5.29	120.33	112.73
2	B	802	Y01	CAU-CBI-CBG	5.28	115.46	107.27
2	C	802	Y01	CAT-CBH-CBF	-5.25	101.40	108.73
2	D	805	Y01	CAK-CAI-CAZ	-5.24	115.39	125.06
2	B	803	Y01	CAV-CAZ-CAI	-5.24	113.06	120.61
2	A	802	Y01	CAU-CBI-CBG	5.23	115.39	107.27
2	A	802	Y01	CAT-CAR-CBC	5.21	119.21	110.33
2	A	812	Y01	CAU-CBI-CBG	5.17	115.29	107.27
2	A	802	Y01	CBI-CBG-CBD	5.16	122.03	114.38
2	C	804	Y01	CAS-CAU-CBI	5.14	121.60	112.78
3	A	813	POV	O21-C21-C22	5.13	122.55	111.50
2	B	802	Y01	CAT-CAR-CBC	5.11	119.04	110.33
2	B	802	Y01	CBF-CBH-CAZ	5.09	117.64	109.65
2	C	803	Y01	CAS-CAU-CBI	5.08	121.50	112.78
2	B	804	Y01	CAK-CBD-CBF	5.07	115.86	109.71
2	C	803	Y01	OAW-CBC-CAV	5.03	118.42	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	804	Y01	CAU-CBI-CBG	5.00	115.03	107.27
2	A	803	Y01	OAW-CAY-CAM	4.99	122.25	111.50
2	A	801	Y01	CAT-CBH-CBF	-4.97	101.78	108.73
2	B	803	Y01	CAS-CAU-CBI	4.97	121.30	112.78
2	A	803	Y01	CAS-CAU-CBI	4.95	121.26	112.78
2	B	804	Y01	CBD-CAK-CAI	4.95	119.84	112.73
2	A	803	Y01	CAU-CBI-CBG	4.91	114.89	107.27
2	A	802	Y01	CBF-CBH-CAZ	4.91	117.34	109.65
2	A	801	Y01	CAS-CAU-CBI	4.86	121.11	112.78
2	D	804	Y01	CAS-CAU-CBI	4.84	121.07	112.78
2	C	802	Y01	CBI-CBE-CBB	-4.79	111.98	119.49
2	B	802	Y01	CAS-CAU-CBI	4.78	120.98	112.78
2	A	802	Y01	CAS-CAU-CBI	4.77	120.97	112.78
2	A	812	Y01	CBD-CAK-CAI	4.77	119.58	112.73
2	A	812	Y01	CAS-CAU-CBI	4.76	120.95	112.78
2	D	805	Y01	CBH-CBF-CBD	4.75	119.87	112.73
2	C	802	Y01	CBI-CBG-CBD	4.75	121.42	114.38
2	C	802	Y01	CAS-CAU-CBI	4.74	120.91	112.78
2	B	803	Y01	CBI-CBG-CBD	4.74	121.39	114.38
2	D	804	Y01	CAD-CBH-CBF	-4.73	106.04	111.68
2	B	803	Y01	CAU-CBI-CBG	4.71	114.58	107.27
2	C	803	Y01	CAU-CBI-CBG	4.70	114.57	107.27
2	D	804	Y01	OAW-CAY-CAM	4.67	121.56	111.50
2	B	804	Y01	CAV-CAZ-CAI	-4.65	113.91	120.61
2	B	802	Y01	CBI-CBE-CBB	-4.65	112.21	119.49
2	B	803	Y01	OAW-CAY-CAM	4.64	121.51	111.50
2	D	804	Y01	CBD-CAK-CAI	4.63	119.38	112.73
2	D	805	Y01	CAU-CBI-CBG	4.63	114.45	107.27
2	A	802	Y01	OAW-CAY-CAM	4.58	121.38	111.50
2	A	812	Y01	CBG-CBI-CBE	4.56	105.47	100.07
2	A	812	Y01	CAT-CAR-CBC	4.56	118.09	110.33
2	D	805	Y01	CAS-CAU-CBI	4.55	120.58	112.78
2	C	803	Y01	CAV-CAZ-CAI	-4.46	114.17	120.61
2	B	804	Y01	CBH-CBF-CBD	4.46	119.42	112.73
2	C	803	Y01	CBH-CBF-CBD	4.44	119.40	112.73
2	B	803	Y01	CAT-CAR-CBC	4.44	117.90	110.33
2	D	804	Y01	CBI-CBE-CBB	-4.44	112.54	119.49
2	A	812	Y01	CAK-CBD-CBF	4.41	115.06	109.71
2	A	802	Y01	CBI-CBE-CBB	-4.39	112.61	119.49
2	A	801	Y01	CBI-CBE-CBB	-4.36	112.65	119.49
2	A	802	Y01	CAV-CAZ-CAI	-4.36	114.33	120.61
2	C	803	Y01	CBI-CBG-CBD	4.36	120.84	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	802	Y01	OAW-CAY-CAM	4.31	120.80	111.50
2	B	803	Y01	CBD-CAK-CAI	4.30	118.91	112.73
2	C	802	Y01	CAD-CBH-CBF	-4.29	106.57	111.68
2	D	805	Y01	CBI-CBE-CBB	-4.27	112.80	119.49
2	B	804	Y01	CAC-CBB-CAO	-4.24	103.71	110.36
2	A	801	Y01	CBI-CBG-CBD	4.24	120.67	114.38
2	C	803	Y01	CAT-CBH-CBF	-4.20	102.86	108.73
2	A	802	Y01	CBC-CAV-CAZ	4.17	117.99	111.52
2	A	802	Y01	CBD-CAK-CAI	4.15	118.69	112.73
2	A	801	Y01	OAW-CAY-CAM	4.14	120.42	111.50
3	C	801	POV	O21-C21-C22	4.10	120.34	111.50
2	A	812	Y01	CBI-CBE-CBB	-4.09	113.09	119.49
2	C	803	Y01	CAK-CBD-CBF	4.08	114.66	109.71
2	B	802	Y01	CAR-CBC-CAV	4.06	117.04	110.99
2	B	804	Y01	CAU-CBI-CBG	4.04	113.54	107.27
2	C	802	Y01	OAW-CAY-CAM	4.04	120.21	111.50
2	A	803	Y01	CAK-CBD-CBF	4.02	114.58	109.71
2	B	804	Y01	CAS-CBF-CBH	4.02	118.37	113.08
3	D	806	POV	O21-C21-C22	4.01	120.14	111.50
2	C	804	Y01	CBI-CBG-CBD	4.01	120.31	114.38
3	B	807	POV	O21-C21-C22	3.99	120.10	111.50
2	A	801	Y01	CBD-CAK-CAI	3.97	118.43	112.73
2	C	804	Y01	OAW-CAY-CAM	3.96	120.03	111.50
2	D	805	Y01	CAV-CAZ-CAI	-3.94	114.93	120.61
2	B	804	Y01	OAW-CBC-CAV	3.92	116.15	108.12
3	A	806	POV	O21-C21-C22	3.92	119.95	111.50
3	A	810	POV	O21-C21-C22	3.91	119.92	111.50
2	D	804	Y01	CAV-CAZ-CBH	-3.90	111.24	116.42
3	B	811	POV	O21-C21-C22	3.89	119.88	111.50
2	C	803	Y01	CBI-CBE-CBB	-3.88	113.41	119.49
3	B	813	POV	O21-C21-C22	3.88	119.86	111.50
2	C	804	Y01	CBH-CBF-CBD	3.88	118.55	112.73
2	B	804	Y01	CAU-CBI-CBE	-3.88	110.77	116.57
2	D	804	Y01	CAR-CBC-CAV	3.88	116.77	110.99
3	C	810	POV	O21-C21-C22	3.87	119.85	111.50
3	A	811	POV	O21-C21-C22	3.85	119.80	111.50
2	A	812	Y01	CBH-CBF-CBD	3.83	118.47	112.73
3	D	801	POV	O21-C21-C22	3.82	119.74	111.50
2	D	805	Y01	OAW-CBC-CAV	3.81	115.92	108.12
3	D	808	POV	O21-C21-C22	3.80	119.69	111.50
2	A	802	Y01	CBF-CBD-CBG	3.78	114.16	109.09
2	C	804	Y01	CBD-CAK-CAI	3.78	118.17	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	804	Y01	CAT-CBH-CBF	-3.78	103.45	108.73
2	C	804	Y01	CAS-CBF-CBH	3.77	118.05	113.08
2	A	801	Y01	CBF-CBD-CBG	3.71	114.06	109.09
2	C	804	Y01	CBI-CBE-CBB	-3.69	113.71	119.49
2	D	804	Y01	CAK-CBD-CBF	3.68	114.17	109.71
2	A	803	Y01	CBH-CBF-CBD	3.68	118.25	112.73
2	B	804	Y01	CAE-CBI-CBE	-3.66	104.88	111.71
3	C	806	POV	O21-C21-C22	3.66	119.39	111.50
3	D	802	POV	O21-C21-C22	3.65	119.36	111.50
2	D	804	Y01	CBC-CAV-CAZ	3.63	117.16	111.52
2	C	804	Y01	CAK-CBD-CBF	3.63	114.11	109.71
2	A	803	Y01	CAS-CBF-CBH	3.62	117.85	113.08
2	A	803	Y01	CBI-CBG-CBD	3.60	119.72	114.38
3	D	809	POV	O21-C21-C22	3.60	119.26	111.50
2	A	802	Y01	CBH-CAZ-CAI	-3.57	117.45	122.90
3	B	806	POV	O21-C21-C22	3.56	119.18	111.50
2	B	803	Y01	CBI-CBE-CBB	-3.52	113.98	119.49
2	A	803	Y01	CBD-CAK-CAI	3.51	117.77	112.73
3	B	812	POV	O21-C21-C22	3.50	119.05	111.50
2	C	804	Y01	CAT-CAR-CBC	3.49	116.27	110.33
2	A	803	Y01	CAT-CAR-CBC	3.47	116.25	110.33
2	B	803	Y01	CBC-CAV-CAZ	3.46	116.89	111.52
2	B	802	Y01	CAV-CAZ-CBH	-3.43	111.86	116.42
2	D	804	Y01	CBI-CBG-CBD	3.43	119.46	114.38
2	C	802	Y01	CAT-CAR-CBC	3.41	116.14	110.33
2	C	803	Y01	OAW-CBC-CAR	3.41	116.55	108.33
2	D	805	Y01	OAW-CAY-CAM	3.40	118.83	111.50
2	B	804	Y01	CBI-CBG-CBD	3.40	119.41	114.38
2	C	802	Y01	CBD-CAK-CAI	3.40	117.61	112.73
3	A	805	POV	O21-C21-C22	3.39	118.80	111.50
2	C	804	Y01	CAC-CBB-CBE	-3.38	107.74	112.92
2	C	803	Y01	CAS-CBF-CBH	3.38	117.53	113.08
2	A	812	Y01	CAC-CBB-CBE	-3.36	107.78	112.92
2	A	803	Y01	CBI-CBE-CBB	-3.36	114.23	119.49
2	B	802	Y01	CBH-CBF-CBD	3.35	117.76	112.73
2	A	812	Y01	CAS-CBF-CBH	3.34	117.48	113.08
2	A	802	Y01	CAK-CBD-CBF	3.34	113.75	109.71
2	C	802	Y01	CAR-CBC-CAV	3.33	115.96	110.99
2	C	802	Y01	CAV-CAZ-CBH	-3.33	111.99	116.42
2	A	803	Y01	CAO-CBB-CBE	3.30	117.10	110.28
2	B	803	Y01	CAO-CBB-CBE	3.28	117.06	110.28
2	C	802	Y01	CAQ-CBG-CBD	-3.28	113.68	119.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	804	Y01	CAO-CBB-CBE	3.26	117.01	110.28
2	C	803	Y01	CAP-CBE-CBI	3.23	107.74	103.84
2	B	803	Y01	CAK-CBD-CBF	3.22	113.62	109.71
2	B	803	Y01	CBH-CBF-CBD	3.22	117.56	112.73
2	C	803	Y01	CBH-CAZ-CAI	-3.21	117.99	122.90
2	A	801	Y01	CAV-CAZ-CAI	-3.19	116.01	120.61
2	A	803	Y01	CAC-CBB-CBE	-3.17	108.07	112.92
2	B	803	Y01	CAT-CBH-CBF	-3.16	104.31	108.73
2	B	803	Y01	CAC-CBB-CBE	-3.14	108.11	112.92
2	A	801	Y01	CAC-CBB-CBE	-3.12	108.14	112.92
2	B	803	Y01	CBF-CBD-CBG	3.08	113.22	109.09
2	A	803	Y01	OAW-CBC-CAR	3.08	115.76	108.33
2	B	802	Y01	CBC-CAV-CAZ	3.05	116.26	111.52
2	A	812	Y01	CBI-CBG-CBD	3.04	118.88	114.38
2	B	802	Y01	CAV-CAZ-CAI	-3.04	116.23	120.61
2	A	802	Y01	CAS-CBF-CBH	3.02	117.06	113.08
2	B	802	Y01	CAT-CBH-CBF	-3.00	104.54	108.73
2	D	805	Y01	CAP-CBE-CBI	2.99	107.44	103.84
2	B	804	Y01	OAW-CAY-CAM	2.97	117.91	111.50
2	D	805	Y01	CAT-CBH-CBF	-2.96	104.59	108.73
2	D	805	Y01	CAK-CBD-CBG	2.95	115.18	110.91
2	A	801	Y01	CAO-CBB-CBE	2.93	116.34	110.28
2	A	801	Y01	CAP-CBE-CBI	2.90	107.33	103.84
2	B	804	Y01	CAP-CBE-CBI	-2.89	100.36	103.84
2	A	801	Y01	CBC-OAW-CAY	-2.89	110.69	117.79
2	C	803	Y01	OAW-CAY-CAM	2.87	117.69	111.50
2	B	802	Y01	CAC-CBB-CBE	-2.87	108.52	112.92
2	B	803	Y01	CAR-CBC-CAV	2.86	115.26	110.99
2	D	805	Y01	CAO-CBB-CBE	2.86	116.19	110.28
2	C	803	Y01	CBC-OAW-CAY	2.86	124.83	117.79
2	D	805	Y01	CBI-CBG-CBD	2.85	118.61	114.38
2	B	802	Y01	CBI-CBG-CBD	2.85	118.61	114.38
2	C	802	Y01	CAO-CBB-CBE	2.83	116.13	110.28
2	C	802	Y01	CBC-CAV-CAZ	2.83	115.91	111.52
2	A	802	Y01	CAQ-CBG-CBD	-2.83	114.43	119.08
2	D	805	Y01	CAC-CBB-CBE	-2.82	108.60	112.92
2	D	804	Y01	CBH-CAZ-CAI	-2.78	118.64	122.90
2	D	804	Y01	CAC-CBB-CAO	-2.78	106.00	110.36
2	A	802	Y01	CAO-CBB-CBE	2.76	115.99	110.28
2	C	804	Y01	OAW-CBC-CAR	2.75	114.97	108.33
2	A	801	Y01	CAD-CBH-CAT	2.73	113.74	109.43
2	A	812	Y01	CAO-CBB-CBE	2.73	115.93	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	805	POV	O31-C31-C32	2.71	120.41	111.91
2	B	804	Y01	CAT-CAR-CBC	2.71	114.94	110.33
2	C	804	Y01	CAD-CBH-CAZ	2.71	112.72	108.34
2	C	803	Y01	CAO-CBB-CBE	2.70	115.87	110.28
2	A	801	Y01	CBH-CAZ-CAI	-2.69	118.78	122.90
2	A	801	Y01	CAV-CAZ-CBH	-2.68	112.86	116.42
2	C	802	Y01	CAV-CAZ-CAI	-2.67	116.76	120.61
2	B	802	Y01	CAO-CBB-CBE	2.67	115.79	110.28
2	B	803	Y01	CAP-CBE-CBI	2.64	107.03	103.84
6	D	813	GEN	C1-C10-C5	-2.63	120.13	123.05
2	D	805	Y01	CAT-CAR-CBC	2.63	114.81	110.33
2	A	802	Y01	CAD-CBH-CAT	2.63	113.58	109.43
3	A	810	POV	O31-C31-C32	2.62	120.13	111.91
2	C	802	Y01	CAC-CBB-CBE	-2.61	108.92	112.92
2	C	802	Y01	CAK-CBD-CBF	2.60	112.86	109.71
3	A	806	POV	O31-C31-C32	2.60	120.05	111.91
2	B	803	Y01	CAS-CBF-CBH	2.58	116.48	113.08
3	B	812	POV	O31-C31-C32	2.57	119.97	111.91
2	B	804	Y01	CBH-CAZ-CAI	-2.57	118.97	122.90
3	A	813	POV	O31-C31-C32	2.57	119.96	111.91
2	C	804	Y01	CAP-CBE-CBI	2.55	106.92	103.84
2	C	802	Y01	CBH-CAZ-CAI	-2.55	119.00	122.90
2	D	804	Y01	CAE-CBI-CBE	-2.54	106.97	111.71
3	B	807	POV	O31-C31-C32	2.52	119.82	111.91
2	D	804	Y01	CAO-CBB-CBE	2.51	115.48	110.28
3	B	811	POV	O31-C31-C32	2.51	119.77	111.91
3	C	806	POV	O31-C31-C32	2.50	119.77	111.91
3	C	801	POV	O31-C31-C32	2.49	119.72	111.91
3	D	802	POV	O31-C31-C32	2.49	119.72	111.91
3	B	806	POV	O31-C31-C32	2.48	119.69	111.91
3	D	808	POV	O31-C31-C32	2.48	119.69	111.91
2	A	802	Y01	CAD-CBH-CAZ	2.47	112.34	108.34
2	B	803	Y01	CAQ-CBG-CBD	-2.47	115.01	119.08
3	A	811	POV	O31-C31-C32	2.47	119.66	111.91
3	D	801	POV	O31-C31-C32	2.47	119.66	111.91
2	A	801	Y01	CAK-CBD-CBF	2.46	112.70	109.71
2	A	803	Y01	CAD-CBH-CAZ	2.46	112.32	108.34
2	A	803	Y01	CAP-CBE-CBI	2.46	106.80	103.84
3	B	813	POV	O31-C31-C32	2.45	119.58	111.91
2	D	804	Y01	CAQ-CBG-CBI	-2.44	100.91	103.84
2	B	802	Y01	CBH-CAZ-CAI	-2.41	119.22	122.90
2	A	812	Y01	CAD-CBH-CAZ	2.41	112.24	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	802	Y01	CAC-CBB-CBE	-2.40	109.25	112.92
2	A	801	Y01	CBC-CAV-CAZ	2.40	115.25	111.52
3	C	806	POV	C14-N-C12	2.38	119.67	109.92
2	C	804	Y01	CBF-CBD-CBG	2.38	112.28	109.09
6	D	813	GEN	O9-C10-C1	2.38	118.88	116.07
3	D	806	POV	C14-N-C12	2.37	119.59	109.92
2	D	804	Y01	CAP-CBE-CBI	-2.36	101.00	103.84
3	D	806	POV	O31-C31-C32	2.35	119.29	111.91
6	A	816	GEN	C5-C6-C7	-2.35	116.49	120.60
2	D	804	Y01	CAR-CAT-CBH	2.35	117.82	112.74
3	A	806	POV	C14-N-C12	2.34	119.50	109.92
3	C	810	POV	O31-C31-C32	2.33	119.22	111.91
2	A	802	Y01	CBH-CBF-CBD	2.33	116.23	112.73
2	A	812	Y01	CAE-CBI-CBE	-2.32	107.38	111.71
2	C	803	Y01	CAD-CBH-CAZ	2.32	112.09	108.34
3	D	809	POV	O31-C31-C32	2.31	119.15	111.91
3	A	813	POV	C14-N-C12	2.31	119.36	109.92
3	B	813	POV	C14-N-C12	2.30	119.33	109.92
3	D	809	POV	C14-N-C12	2.29	119.29	109.92
6	D	813	GEN	C5-C6-C7	-2.29	116.60	120.60
6	A	816	GEN	C1-C10-C5	-2.28	120.53	123.05
3	C	801	POV	C14-N-C12	2.23	119.04	109.92
3	B	806	POV	C14-N-C12	2.22	119.01	109.92
2	B	804	Y01	CAO-CBB-CBE	2.21	114.85	110.28
3	B	807	POV	C14-N-C12	2.20	118.94	109.92
2	A	801	Y01	OAH-CAX-CAL	2.20	121.11	114.03
2	D	805	Y01	CBH-CAZ-CAI	-2.20	119.54	122.90
2	A	802	Y01	CAR-CBC-CAV	2.19	114.25	110.99
2	D	804	Y01	CBH-CBF-CBD	2.18	116.01	112.73
2	B	804	Y01	OAW-CBC-CAR	2.18	113.59	108.33
3	D	808	POV	C14-N-C12	2.17	118.78	109.92
2	D	804	Y01	CAV-CAZ-CAI	-2.16	117.50	120.61
3	D	801	POV	C2-O21-C21	-2.16	112.48	117.79
3	A	813	POV	O21-C21-O22	-2.15	118.52	123.70
2	A	802	Y01	CAU-CAS-CBF	-2.14	109.41	113.11
2	C	802	Y01	CAC-CBB-CAO	-2.14	107.02	110.36
2	B	802	Y01	CBC-OAW-CAY	-2.13	112.56	117.79
2	B	803	Y01	CBH-CAZ-CAI	-2.12	119.65	122.90
2	B	804	Y01	CAR-CAT-CBH	2.12	117.33	112.74
2	D	804	Y01	CAE-CBI-CBG	-2.12	107.77	111.71
2	A	802	Y01	CAT-CBH-CBF	-2.12	105.77	108.73
2	B	802	Y01	OAW-CAY-OAG	-2.10	118.62	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	810	POV	C14-N-C12	2.10	118.49	109.92
2	A	802	Y01	CAE-CBI-CBE	-2.09	107.81	111.71
2	A	812	Y01	OAW-CAY-OAG	-2.09	118.65	123.70
2	A	803	Y01	CBC-OAW-CAY	-2.08	112.66	117.79
3	D	802	POV	C14-N-C12	2.08	118.41	109.92
2	A	802	Y01	CAR-CAT-CBH	2.08	117.24	112.74
2	D	805	Y01	OAW-CBC-CAR	2.07	113.32	108.33
2	D	805	Y01	CAE-CBI-CAU	-2.06	107.34	110.59
2	D	805	Y01	CAD-CBH-CAT	2.05	112.67	109.43
2	B	802	Y01	CAE-CBI-CBE	-2.05	107.90	111.71
2	A	802	Y01	CAP-CBE-CBB	2.04	115.31	112.15
2	C	802	Y01	CAP-CBE-CBB	2.04	115.30	112.15
3	A	811	POV	C14-N-C12	2.03	118.24	109.92
2	B	804	Y01	CAD-CBH-CAZ	2.01	111.60	108.34
2	C	803	Y01	CAC-CBB-CBE	-2.01	109.84	112.92
3	D	801	POV	C14-N-C12	2.00	118.10	109.92

All (48) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	801	Y01	CBF
2	A	801	Y01	CBC
2	A	801	Y01	CBD
2	A	801	Y01	CBG
2	A	802	Y01	CBF
2	A	802	Y01	CBC
2	A	802	Y01	CBD
2	A	802	Y01	CBG
2	A	803	Y01	CBF
2	A	803	Y01	CBC
2	A	803	Y01	CBD
2	A	803	Y01	CBG
2	A	812	Y01	CBF
2	A	812	Y01	CBC
2	A	812	Y01	CBD
2	A	812	Y01	CBG
2	B	802	Y01	CBF
2	B	802	Y01	CBC
2	B	802	Y01	CBD
2	B	802	Y01	CBG
2	B	803	Y01	CBF
2	B	803	Y01	CBC

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Mol	Chain	Res	Type	Atom
2	B	803	Y01	CBD
2	B	803	Y01	CBG
2	B	804	Y01	CBF
2	B	804	Y01	CBC
2	B	804	Y01	CBD
2	B	804	Y01	CBG
2	C	802	Y01	CBF
2	C	802	Y01	CBC
2	C	802	Y01	CBD
2	C	802	Y01	CBG
2	C	803	Y01	CBF
2	C	803	Y01	CBC
2	C	803	Y01	CBD
2	C	803	Y01	CBG
2	C	804	Y01	CBF
2	C	804	Y01	CBC
2	C	804	Y01	CBD
2	C	804	Y01	CBG
2	D	804	Y01	CBF
2	D	804	Y01	CBC
2	D	804	Y01	CBD
2	D	804	Y01	CBG
2	D	805	Y01	CBF
2	D	805	Y01	CBC
2	D	805	Y01	CBD
2	D	805	Y01	CBG

All (744) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	Y01	CAO-CBB-CBE-CAP
2	A	801	Y01	CAC-CBB-CBE-CBI
2	A	802	Y01	CAO-CBB-CBE-CAP
2	A	802	Y01	CAO-CBB-CBE-CBI
2	A	802	Y01	CAC-CBB-CBE-CBI
2	A	802	Y01	OAG-CAY-OAW-CBC
2	A	803	Y01	CAO-CBB-CBE-CAP
2	A	803	Y01	CAC-CBB-CBE-CBI
2	A	812	Y01	CAO-CBB-CBE-CAP
2	A	812	Y01	CAO-CBB-CBE-CBI
2	A	812	Y01	CAC-CBB-CBE-CBI
2	A	812	Y01	OAG-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
2	A	812	Y01	CAM-CAY-OAW-CBC
2	B	802	Y01	CAO-CBB-CBE-CAP
2	B	802	Y01	CAC-CBB-CBE-CBI
2	B	802	Y01	CAM-CAY-OAW-CBC
2	B	803	Y01	CAO-CBB-CBE-CAP
2	B	803	Y01	CAC-CBB-CBE-CBI
2	B	803	Y01	OAG-CAY-OAW-CBC
2	B	803	Y01	CAM-CAY-OAW-CBC
2	B	804	Y01	CAV-CBC-OAW-CAY
2	C	802	Y01	CAO-CBB-CBE-CAP
2	C	802	Y01	CAO-CBB-CBE-CBI
2	C	802	Y01	CAC-CBB-CBE-CAP
2	C	802	Y01	CAC-CBB-CBE-CBI
2	C	803	Y01	CAV-CBC-OAW-CAY
2	C	803	Y01	CAM-CAY-OAW-CBC
2	C	804	Y01	CAO-CBB-CBE-CAP
2	C	804	Y01	CAC-CBB-CBE-CBI
2	D	804	Y01	CAC-CBB-CBE-CBI
2	D	804	Y01	CAV-CBC-OAW-CAY
2	D	804	Y01	OAG-CAY-OAW-CBC
2	D	804	Y01	CAM-CAY-OAW-CBC
2	D	805	Y01	CAV-CBC-OAW-CAY
3	A	806	POV	C1-O11-P-O12
3	A	806	POV	C1-O11-P-O13
3	A	806	POV	C1-O11-P-O14
3	A	806	POV	C11-O12-P-O11
3	A	806	POV	O12-C11-C12-N
3	A	810	POV	C11-O12-P-O13
3	A	810	POV	O12-C11-C12-N
3	A	811	POV	O12-C11-C12-N
3	A	811	POV	C22-C21-O21-C2
3	A	811	POV	O22-C21-O21-C2
3	A	813	POV	C11-O12-P-O13
3	A	813	POV	O12-C11-C12-N
3	A	813	POV	C22-C21-O21-C2
3	A	813	POV	O22-C21-O21-C2
3	B	806	POV	C1-O11-P-O13
3	B	806	POV	C1-O11-P-O14
3	B	806	POV	C11-O12-P-O14
3	B	806	POV	C29-C210-C211-C212
3	B	807	POV	C11-O12-P-O11
3	B	807	POV	C11-O12-P-O13

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Mol	Chain	Res	Type	Atoms
3	B	807	POV	C11-O12-P-O14
3	B	807	POV	O11-C1-C2-O21
3	B	807	POV	C22-C21-O21-C2
3	B	807	POV	O22-C21-O21-C2
3	B	811	POV	O11-C1-C2-O21
3	B	812	POV	C11-O12-P-O14
3	B	813	POV	C1-O11-P-O12
3	B	813	POV	C1-O11-P-O13
3	B	813	POV	C1-O11-P-O14
3	C	801	POV	C1-O11-P-O13
3	C	801	POV	C1-O11-P-O14
3	C	801	POV	C11-O12-P-O13
3	C	801	POV	C11-O12-P-O14
3	C	801	POV	C29-C210-C211-C212
3	C	801	POV	O12-C11-C12-N
3	C	801	POV	C22-C21-O21-C2
3	C	806	POV	C11-O12-P-O13
3	C	806	POV	O12-C11-C12-N
3	C	806	POV	O22-C21-O21-C2
3	C	810	POV	O12-C11-C12-N
3	C	810	POV	C22-C21-O21-C2
3	D	801	POV	O12-C11-C12-N
3	D	801	POV	C22-C21-O21-C2
3	D	801	POV	O22-C21-O21-C2
3	D	802	POV	O12-C11-C12-N
3	D	806	POV	O12-C11-C12-N
3	D	808	POV	C11-O12-P-O11
3	D	808	POV	C11-O12-P-O13
3	D	808	POV	C11-O12-P-O14
3	D	808	POV	O12-C11-C12-N
3	D	809	POV	C1-O11-P-O13
3	D	809	POV	C1-O11-P-O14
3	D	809	POV	C11-O12-P-O11
3	D	809	POV	O12-C11-C12-N
3	C	806	POV	O32-C31-O31-C3
2	A	801	Y01	CAC-CBB-CBE-CAP
2	A	802	Y01	CAC-CBB-CBE-CAP
2	A	803	Y01	CAC-CBB-CBE-CAP
2	A	812	Y01	CAC-CBB-CBE-CAP
2	B	802	Y01	CAC-CBB-CBE-CAP
2	B	803	Y01	CAC-CBB-CBE-CAP
2	C	804	Y01	CAC-CBB-CBE-CAP

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Mol	Chain	Res	Type	Atoms
2	D	804	Y01	CAC-CBB-CBE-CAP
2	D	805	Y01	CAC-CBB-CBE-CBI
2	D	804	Y01	CAO-CBB-CBE-CAP
2	A	801	Y01	CAO-CBB-CBE-CBI
2	A	803	Y01	CAO-CBB-CBE-CBI
2	B	802	Y01	CAO-CBB-CBE-CBI
2	B	803	Y01	CAO-CBB-CBE-CBI
2	C	804	Y01	CAO-CBB-CBE-CBI
2	D	804	Y01	CAO-CBB-CBE-CBI
2	D	805	Y01	CAO-CBB-CBE-CBI
2	B	802	Y01	OAG-CAY-OAW-CBC
2	C	803	Y01	OAG-CAY-OAW-CBC
3	B	812	POV	O22-C21-O21-C2
3	C	801	POV	O22-C21-O21-C2
3	C	810	POV	O22-C21-O21-C2
3	D	809	POV	O22-C21-O21-C2
3	C	806	POV	C32-C31-O31-C3
2	A	802	Y01	CAM-CAY-OAW-CBC
3	B	812	POV	C22-C21-O21-C2
3	C	806	POV	C22-C21-O21-C2
2	C	803	Y01	CAC-CBB-CBE-CAP
2	D	805	Y01	CAC-CBB-CBE-CAP
2	C	803	Y01	CAC-CBB-CBE-CBI
2	D	805	Y01	CAO-CBB-CBE-CAP
2	C	803	Y01	CAO-CBB-CBE-CBI
3	D	808	POV	C32-C31-O31-C3
3	A	808	POV	C211-C210-C29-C28
3	B	809	POV	C211-C210-C29-C28
3	A	809	POV	C34-C35-C36-C37
3	A	810	POV	O32-C31-O31-C3
2	C	803	Y01	CAO-CBB-CBE-CAP
3	A	810	POV	C32-C31-O31-C3
3	A	810	POV	C22-C21-O21-C2
3	B	811	POV	C22-C21-O21-C2
3	D	809	POV	C22-C21-O21-C2
2	B	804	Y01	CAC-CBB-CBE-CBI
3	C	810	POV	C21-C22-C23-C24
3	D	809	POV	C36-C37-C38-C39
2	A	801	Y01	CAJ-CAO-CBB-CBE
2	C	803	Y01	CAJ-CAO-CBB-CBE
3	D	809	POV	C2-C1-O11-P
2	C	803	Y01	CAJ-CAO-CBB-CAC

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Mol	Chain	Res	Type	Atoms
3	D	808	POV	O32-C31-O31-C3
3	A	810	POV	O22-C21-O21-C2
3	A	811	POV	C39-C310-C311-C312
3	B	807	POV	C22-C23-C24-C25
3	C	801	POV	C32-C31-O31-C3
3	C	810	POV	C24-C25-C26-C27
3	A	808	POV	C21-C22-C23-C24
2	C	802	Y01	CAJ-CAO-CBB-CBE
3	A	805	POV	C24-C25-C26-C27
2	A	801	Y01	CAJ-CAO-CBB-CAC
3	A	811	POV	O21-C2-C3-O31
3	B	811	POV	O22-C21-O21-C2
3	A	810	POV	C21-C22-C23-C24
3	D	801	POV	C21-C22-C23-C24
3	C	808	POV	C211-C210-C29-C28
3	D	811	POV	C211-C210-C29-C28
2	A	803	Y01	CAN-CAJ-CAO-CBB
2	C	804	Y01	CAN-CAJ-CAO-CBB
2	D	804	Y01	CAO-CAJ-CAN-CBA
3	C	806	POV	C32-C33-C34-C35
3	C	806	POV	C31-C32-C33-C34
2	D	805	Y01	CAX-CAL-CAM-CAY
3	A	813	POV	C32-C31-O31-C3
2	C	802	Y01	CAJ-CAO-CBB-CAC
3	B	807	POV	C31-C32-C33-C34
3	D	802	POV	C31-C32-C33-C34
3	D	809	POV	C21-C22-C23-C24
3	D	809	POV	C31-C32-C33-C34
2	B	804	Y01	CAN-CAJ-CAO-CBB
3	C	801	POV	O32-C31-O31-C3
2	C	802	Y01	CAN-CAJ-CAO-CBB
3	D	806	POV	C31-C32-C33-C34
2	B	802	Y01	CAO-CAJ-CAN-CBA
3	A	807	POV	C311-C310-C39-C38
2	B	804	Y01	CAO-CBB-CBE-CBI
3	B	807	POV	C26-C27-C28-C29
2	D	804	Y01	CAX-CAL-CAM-CAY
2	A	802	Y01	CAN-CAJ-CAO-CBB
3	D	801	POV	C39-C310-C311-C312
3	A	810	POV	C11-O12-P-O11
3	A	813	POV	C11-O12-P-O11
3	B	806	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
3	B	806	POV	C11-O12-P-O11
3	B	811	POV	C1-O11-P-O12
3	B	812	POV	C1-O11-P-O12
3	B	812	POV	C11-O12-P-O11
3	C	801	POV	C1-O11-P-O12
3	C	801	POV	C11-O12-P-O11
3	D	806	POV	C1-O11-P-O12
3	D	806	POV	C11-O12-P-O11
3	D	809	POV	C1-O11-P-O12
3	D	801	POV	C23-C24-C25-C26
3	A	810	POV	C36-C37-C38-C39
3	A	806	POV	C32-C31-O31-C3
3	B	813	POV	C32-C31-O31-C3
3	B	806	POV	C24-C25-C26-C27
3	C	801	POV	C21-C22-C23-C24
3	C	806	POV	C213-C214-C215-C216
3	C	809	POV	C311-C310-C39-C38
3	D	802	POV	C22-C23-C24-C25
3	B	813	POV	C22-C21-O21-C2
3	D	802	POV	C22-C21-O21-C2
3	A	805	POV	C213-C214-C215-C216
3	A	806	POV	C36-C37-C38-C39
3	A	810	POV	C34-C35-C36-C37
3	A	811	POV	C211-C212-C213-C214
3	B	801	POV	C311-C310-C39-C38
3	B	811	POV	C211-C212-C213-C214
3	C	801	POV	C23-C24-C25-C26
3	C	810	POV	C25-C26-C27-C28
3	D	802	POV	C24-C25-C26-C27
3	D	803	POV	C36-C37-C38-C39
3	D	806	POV	C310-C311-C312-C313
3	D	811	POV	C24-C25-C26-C27
3	A	813	POV	O32-C31-O31-C3
3	A	806	POV	C211-C212-C213-C214
3	A	806	POV	C25-C26-C27-C28
3	A	809	POV	C35-C36-C37-C38
3	A	811	POV	C213-C214-C215-C216
3	A	813	POV	C22-C23-C24-C25
3	B	810	POV	C37-C38-C39-C310
3	D	806	POV	C311-C312-C313-C314
3	D	806	POV	C32-C33-C34-C35
3	D	807	POV	C311-C310-C39-C38

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Mol	Chain	Res	Type	Atoms
3	B	813	POV	O22-C21-O21-C2
3	D	802	POV	O22-C21-O21-C2
3	D	808	POV	C21-C22-C23-C24
3	A	813	POV	C24-C25-C26-C27
3	B	807	POV	C23-C24-C25-C26
3	B	812	POV	C22-C23-C24-C25
3	D	809	POV	C311-C310-C39-C38
3	C	806	POV	O11-C1-C2-O21
3	B	808	POV	C37-C38-C39-C310
3	C	801	POV	C22-C23-C24-C25
3	C	806	POV	C211-C212-C213-C214
3	C	810	POV	C23-C24-C25-C26
3	A	806	POV	C32-C33-C34-C35
3	D	808	POV	C36-C37-C38-C39
3	A	810	POV	C33-C34-C35-C36
3	B	811	POV	C212-C213-C214-C215
3	A	805	POV	C214-C215-C216-C217
3	A	805	POV	C35-C36-C37-C38
3	A	810	POV	C22-C23-C24-C25
3	D	801	POV	C32-C33-C34-C35
3	D	810	POV	C35-C36-C37-C38
2	D	804	Y01	CAR-CBC-OAW-CAY
3	B	807	POV	C21-C22-C23-C24
3	A	805	POV	C37-C38-C39-C310
3	A	807	POV	C39-C310-C311-C312
3	A	809	POV	C39-C310-C311-C312
3	A	810	POV	C311-C312-C313-C314
3	D	802	POV	C311-C310-C39-C38
3	D	802	POV	C32-C33-C34-C35
3	D	808	POV	C32-C33-C34-C35
3	D	809	POV	C213-C214-C215-C216
3	D	810	POV	C311-C310-C39-C38
3	A	806	POV	O32-C31-O31-C3
3	A	805	POV	C22-C23-C24-C25
3	A	808	POV	C23-C24-C25-C26
3	B	805	POV	C39-C310-C311-C312
3	B	811	POV	C39-C310-C311-C312
3	B	812	POV	C24-C25-C26-C27
3	B	813	POV	C23-C24-C25-C26
3	C	808	POV	C25-C26-C27-C28
3	D	802	POV	C36-C37-C38-C39
3	D	808	POV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
3	D	810	POV	C39-C310-C311-C312
3	B	806	POV	O22-C21-O21-C2
3	B	806	POV	C22-C21-O21-C2
3	A	806	POV	C311-C312-C313-C314
3	A	810	POV	C211-C212-C213-C214
3	D	808	POV	C33-C34-C35-C36
3	D	809	POV	C24-C25-C26-C27
3	A	805	POV	C31-C32-C33-C34
3	B	812	POV	C31-C32-C33-C34
3	A	805	POV	C32-C33-C34-C35
3	A	805	POV	C34-C35-C36-C37
3	B	806	POV	C22-C23-C24-C25
3	B	806	POV	C36-C37-C38-C39
3	B	812	POV	C32-C33-C34-C35
3	C	806	POV	C36-C37-C38-C39
3	C	810	POV	C213-C214-C215-C216
3	C	810	POV	C22-C23-C24-C25
3	B	813	POV	O32-C31-O31-C3
2	A	802	Y01	CAX-CAL-CAM-CAY
3	A	806	POV	C37-C38-C39-C310
3	D	806	POV	C35-C36-C37-C38
3	B	801	POV	C37-C38-C39-C310
3	B	808	POV	C32-C33-C34-C35
3	C	810	POV	C311-C310-C39-C38
3	D	809	POV	C22-C23-C24-C25
3	A	809	POV	C33-C34-C35-C36
3	D	806	POV	C21-C22-C23-C24
3	A	811	POV	C24-C25-C26-C27
3	B	812	POV	C35-C36-C37-C38
3	D	808	POV	C311-C312-C313-C314
2	B	804	Y01	OAG-CAY-OAW-CBC
3	A	813	POV	C35-C36-C37-C38
3	D	806	POV	C34-C35-C36-C37
3	D	808	POV	C312-C313-C314-C315
3	B	809	POV	C22-C23-C24-C25
2	B	804	Y01	CAM-CAY-OAW-CBC
2	D	805	Y01	CAM-CAY-OAW-CBC
3	A	806	POV	C22-C21-O21-C2
3	C	801	POV	C311-C310-C39-C38
3	A	806	POV	C34-C35-C36-C37
3	A	807	POV	C36-C37-C38-C39
3	B	807	POV	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
3	B	811	POV	C22-C23-C24-C25
3	D	809	POV	C34-C35-C36-C37
3	A	805	POV	C36-C37-C38-C39
3	B	812	POV	C37-C38-C39-C310
3	A	808	POV	C211-C212-C213-C214
3	D	801	POV	C211-C212-C213-C214
3	B	812	POV	C214-C215-C216-C217
2	D	805	Y01	OAG-CAY-OAW-CBC
3	A	806	POV	O22-C21-O21-C2
3	C	806	POV	C22-C23-C24-C25
3	D	809	POV	C312-C313-C314-C315
3	A	806	POV	C31-C32-C33-C34
3	B	807	POV	C312-C313-C314-C315
3	B	813	POV	C311-C312-C313-C314
3	D	806	POV	C33-C34-C35-C36
3	D	808	POV	C211-C212-C213-C214
3	A	806	POV	C22-C23-C24-C25
3	D	803	POV	C37-C38-C39-C310
3	D	808	POV	C213-C214-C215-C216
3	D	809	POV	C214-C215-C216-C217
3	A	813	POV	C23-C24-C25-C26
3	C	805	POV	C34-C35-C36-C37
3	A	806	POV	C27-C28-C29-C210
3	A	804	POV	C36-C37-C38-C39
3	D	808	POV	C212-C213-C214-C215
3	D	812	POV	C36-C37-C38-C39
3	B	809	POV	C210-C211-C212-C213
3	D	806	POV	C210-C211-C212-C213
3	D	808	POV	C210-C211-C212-C213
3	B	805	POV	C311-C310-C39-C38
3	D	803	POV	C31-C32-C33-C34
2	D	805	Y01	CAN-CAJ-CAO-CBB
3	D	808	POV	C22-C23-C24-C25
3	B	809	POV	C24-C25-C26-C27
3	C	801	POV	C311-C312-C313-C314
3	C	806	POV	C35-C36-C37-C38
3	D	807	POV	C37-C38-C39-C310
3	B	807	POV	C211-C212-C213-C214
3	D	812	POV	C35-C36-C37-C38
3	B	813	POV	C32-C33-C34-C35
3	C	805	POV	C32-C33-C34-C35
3	D	808	POV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
2	A	812	Y01	CAO-CAJ-CAN-CBA
3	B	801	POV	C33-C34-C35-C36
2	C	802	Y01	CAM-CAY-OAW-CBC
3	D	806	POV	C22-C21-O21-C2
3	D	808	POV	C22-C21-O21-C2
3	A	806	POV	O11-C1-C2-O21
3	D	809	POV	O11-C1-C2-O21
3	B	806	POV	C39-C310-C311-C312
3	D	806	POV	C24-C25-C26-C27
3	A	810	POV	C24-C25-C26-C27
3	C	810	POV	C33-C34-C35-C36
3	D	806	POV	O22-C21-O21-C2
3	D	808	POV	O22-C21-O21-C2
3	C	808	POV	C21-C22-C23-C24
3	A	811	POV	C311-C312-C313-C314
3	C	806	POV	C311-C310-C39-C38
3	A	804	POV	C32-C33-C34-C35
3	A	813	POV	C36-C37-C38-C39
3	B	813	POV	C311-C310-C39-C38
3	D	801	POV	C212-C213-C214-C215
3	B	811	POV	C25-C26-C27-C28
3	A	805	POV	C311-C310-C39-C38
3	B	807	POV	C311-C312-C313-C314
3	D	801	POV	C34-C35-C36-C37
3	D	808	POV	C39-C310-C311-C312
2	C	802	Y01	OAG-CAY-OAW-CBC
2	A	801	Y01	CAM-CAY-OAW-CBC
3	A	809	POV	C37-C38-C39-C310
3	B	809	POV	C25-C26-C27-C28
3	B	811	POV	C311-C310-C39-C38
3	D	811	POV	C29-C210-C211-C212
3	C	806	POV	C11-O12-P-O11
3	D	809	POV	C311-C312-C313-C314
3	D	809	POV	C35-C36-C37-C38
3	C	806	POV	C34-C35-C36-C37
3	A	806	POV	O11-C1-C2-C3
3	B	807	POV	O11-C1-C2-C3
3	C	806	POV	O11-C1-C2-C3
3	C	809	POV	C36-C37-C38-C39
3	D	801	POV	C36-C37-C38-C39
3	B	813	POV	C31-C32-C33-C34
3	C	801	POV	C310-C311-C312-C313

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Mol	Chain	Res	Type	Atoms
3	D	806	POV	C37-C38-C39-C310
3	B	807	POV	C210-C211-C212-C213
3	C	801	POV	C26-C27-C28-C29
3	C	801	POV	C33-C34-C35-C36
3	A	811	POV	C1-C2-C3-O31
3	A	813	POV	C1-C2-C3-O31
3	B	809	POV	C213-C214-C215-C216
3	D	801	POV	C37-C38-C39-C310
3	D	806	POV	C313-C314-C315-C316
3	A	809	POV	C31-C32-C33-C34
3	C	809	POV	C39-C310-C311-C312
3	A	809	POV	C311-C310-C39-C38
3	A	811	POV	C311-C310-C39-C38
3	A	810	POV	C39-C310-C311-C312
3	A	807	POV	C310-C311-C312-C313
3	A	804	POV	C31-C32-C33-C34
3	A	810	POV	C1-C2-O21-C21
3	D	809	POV	C3-C2-O21-C21
3	A	810	POV	C35-C36-C37-C38
3	C	809	POV	C31-C32-C33-C34
3	D	806	POV	C22-C23-C24-C25
2	A	802	Y01	CAV-CBC-OAW-CAY
3	B	806	POV	C313-C314-C315-C316
3	D	801	POV	C311-C310-C39-C38
2	B	804	Y01	CAC-CBB-CBE-CAP
3	D	802	POV	C213-C214-C215-C216
3	A	811	POV	C32-C33-C34-C35
3	D	802	POV	C311-C312-C313-C314
3	D	803	POV	C35-C36-C37-C38
3	A	805	POV	C310-C311-C312-C313
3	B	807	POV	O21-C2-C3-O31
3	B	805	POV	C32-C33-C34-C35
3	D	806	POV	C23-C24-C25-C26
3	B	806	POV	C32-C33-C34-C35
3	D	801	POV	C311-C312-C313-C314
3	B	807	POV	C36-C37-C38-C39
3	B	808	POV	C311-C310-C39-C38
3	D	811	POV	C22-C23-C24-C25
3	C	810	POV	C32-C33-C34-C35
3	B	807	POV	C313-C314-C315-C316
3	D	812	POV	C34-C35-C36-C37
3	A	811	POV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
3	A	805	POV	C311-C312-C313-C314
3	D	802	POV	C210-C211-C212-C213
3	B	813	POV	C25-C26-C27-C28
3	D	809	POV	O11-C1-C2-C3
3	C	801	POV	C24-C25-C26-C27
3	A	813	POV	C21-C22-C23-C24
2	A	812	Y01	CAN-CAJ-CAO-CBB
3	B	806	POV	C311-C310-C39-C38
3	B	810	POV	C311-C310-C39-C38
3	A	806	POV	C35-C36-C37-C38
3	A	805	POV	C312-C313-C314-C315
3	A	806	POV	C215-C216-C217-C218
3	A	808	POV	C24-C25-C26-C27
3	A	811	POV	C215-C216-C217-C218
3	A	808	POV	C213-C214-C215-C216
3	B	813	POV	C24-C25-C26-C27
3	C	805	POV	C36-C37-C38-C39
3	C	806	POV	C23-C24-C25-C26
3	A	806	POV	C1-C2-C3-O31
2	B	804	Y01	CAJ-CAO-CBB-CBE
3	A	806	POV	C21-C22-C23-C24
3	C	801	POV	C32-C33-C34-C35
3	D	801	POV	C35-C36-C37-C38
3	D	807	POV	C310-C311-C312-C313
3	B	812	POV	C311-C310-C39-C38
3	A	805	POV	C11-O12-P-O11
3	B	807	POV	C1-O11-P-O12
3	A	805	POV	C33-C34-C35-C36
3	B	806	POV	O11-C1-C2-O21
3	D	802	POV	O11-C1-C2-O21
3	B	812	POV	C215-C216-C217-C218
3	D	808	POV	C313-C314-C315-C316
3	A	806	POV	O21-C2-C3-O31
3	B	806	POV	O21-C2-C3-O31
3	D	801	POV	O21-C2-C3-O31
3	D	806	POV	O21-C2-C3-O31
3	D	808	POV	O21-C2-C3-O31
3	A	804	POV	C34-C35-C36-C37
3	A	806	POV	C24-C25-C26-C27
3	B	805	POV	C34-C35-C36-C37
2	A	801	Y01	OAG-CAY-OAW-CBC
3	D	812	POV	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
3	A	806	POV	C311-C310-C39-C38
3	B	812	POV	C39-C310-C311-C312
3	D	807	POV	C32-C33-C34-C35
3	D	809	POV	C211-C212-C213-C214
3	A	808	POV	C26-C27-C28-C29
3	A	807	POV	C31-C32-C33-C34
3	D	806	POV	C25-C26-C27-C28
3	D	807	POV	C36-C37-C38-C39
3	A	805	POV	C11-C12-N-C15
3	A	806	POV	C214-C215-C216-C217
3	B	801	POV	C39-C310-C311-C312
3	D	809	POV	C25-C26-C27-C28
3	B	806	POV	C311-C312-C313-C314
3	B	813	POV	C39-C310-C311-C312
3	D	808	POV	C215-C216-C217-C218
3	B	812	POV	C33-C34-C35-C36
3	C	801	POV	C36-C37-C38-C39
3	A	813	POV	C29-C210-C211-C212
3	B	807	POV	C311-C310-C39-C38
3	C	809	POV	C35-C36-C37-C38
3	A	813	POV	O11-C1-C2-C3
3	B	806	POV	O11-C1-C2-C3
3	B	812	POV	O11-C1-C2-C3
3	D	802	POV	O11-C1-C2-C3
3	D	808	POV	C37-C38-C39-C310
3	D	801	POV	C210-C211-C212-C213
3	C	809	POV	C310-C311-C312-C313
3	D	809	POV	C37-C38-C39-C310
3	D	810	POV	C310-C311-C312-C313
2	A	802	Y01	CAO-CAJ-CAN-CBA
3	D	802	POV	C34-C35-C36-C37
3	D	801	POV	C310-C311-C312-C313
3	A	810	POV	C25-C26-C27-C28
3	B	810	POV	C36-C37-C38-C39
3	C	808	POV	C23-C24-C25-C26
3	D	810	POV	C36-C37-C38-C39
3	C	805	POV	C31-C32-C33-C34
3	A	806	POV	C312-C313-C314-C315
3	D	806	POV	C213-C214-C215-C216
3	B	810	POV	C31-C32-C33-C34
3	C	806	POV	C2-C1-O11-P
3	D	806	POV	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	C	804	Y01	CAM-CAY-OAW-CBC
3	C	808	POV	C24-C25-C26-C27
3	B	812	POV	O11-C1-C2-O21
3	D	801	POV	O11-C1-C2-O21
3	C	806	POV	C214-C215-C216-C217
2	C	804	Y01	CAX-CAL-CAM-CAY
3	B	811	POV	C36-C37-C38-C39
3	A	810	POV	C311-C310-C39-C38
3	B	813	POV	O21-C2-C3-O31
3	C	801	POV	C34-C35-C36-C37
3	D	806	POV	C39-C310-C311-C312
3	C	808	POV	C26-C27-C28-C29
3	A	811	POV	C312-C313-C314-C315
3	B	810	POV	C33-C34-C35-C36
3	C	809	POV	C34-C35-C36-C37
2	C	804	Y01	OAG-CAY-OAW-CBC
3	C	810	POV	C39-C310-C311-C312
3	A	807	POV	C33-C34-C35-C36
3	A	807	POV	C35-C36-C37-C38
3	A	813	POV	C310-C311-C312-C313
3	B	807	POV	C25-C26-C27-C28
3	B	813	POV	C312-C313-C314-C315
3	C	810	POV	C210-C211-C212-C213
3	D	809	POV	C26-C27-C28-C29
3	A	811	POV	C1-O11-P-O12
3	C	810	POV	C36-C37-C38-C39
3	D	801	POV	C214-C215-C216-C217
3	A	805	POV	C1-O11-P-O13
3	A	806	POV	C11-O12-P-O13
3	A	810	POV	C11-O12-P-O14
3	A	813	POV	C11-O12-P-O14
3	B	811	POV	C1-O11-P-O14
3	B	812	POV	C1-O11-P-O13
3	B	812	POV	C1-O11-P-O14
3	B	812	POV	C11-O12-P-O13
3	C	806	POV	C11-O12-P-O14
3	D	806	POV	C1-O11-P-O13
3	D	806	POV	C11-O12-P-O13
3	D	806	POV	C11-O12-P-O14
3	B	811	POV	O11-C1-C2-C3
3	C	810	POV	O11-C1-C2-C3
3	D	801	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	813	POV	C34-C35-C36-C37
3	A	810	POV	C23-C24-C25-C26
3	B	807	POV	C39-C310-C311-C312
3	A	813	POV	O11-C1-C2-O21
3	C	810	POV	O11-C1-C2-O21
2	B	804	Y01	CAO-CBB-CBE-CAP
3	B	806	POV	C34-C35-C36-C37
3	A	810	POV	C1-C2-C3-O31
3	B	806	POV	O12-C11-C12-N
3	B	807	POV	C1-C2-C3-O31
3	B	807	POV	O12-C11-C12-N
3	B	811	POV	O12-C11-C12-N
3	B	813	POV	O12-C11-C12-N
3	A	813	POV	O21-C2-C3-O31
3	A	808	POV	C22-C23-C24-C25
3	D	809	POV	C23-C24-C25-C26
3	D	806	POV	C211-C212-C213-C214
3	C	807	POV	C31-C32-C33-C34
3	A	810	POV	C313-C314-C315-C316
3	A	805	POV	C11-C12-N-C14
3	D	802	POV	C23-C24-C25-C26
3	B	810	POV	C39-C310-C311-C312
3	B	808	POV	C36-C37-C38-C39
3	D	802	POV	C3-C2-O21-C21
3	A	808	POV	C29-C210-C211-C212
3	D	806	POV	C2-C1-O11-P
3	C	810	POV	C214-C215-C216-C217
3	B	810	POV	C34-C35-C36-C37
3	C	806	POV	C215-C216-C217-C218
3	B	813	POV	C213-C214-C215-C216
3	A	810	POV	C1-O11-P-O12
3	A	813	POV	C1-O11-P-O12
3	B	811	POV	C11-O12-P-O11
3	C	810	POV	C1-O11-P-O12
3	D	801	POV	C11-O12-P-O11
3	D	802	POV	C11-O12-P-O11
3	D	810	POV	C33-C34-C35-C36
3	C	808	POV	C211-C212-C213-C214
3	D	801	POV	C31-C32-C33-C34
3	D	806	POV	O21-C21-C22-C23
3	A	813	POV	C34-C35-C36-C37
3	B	807	POV	C310-C311-C312-C313

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Mol	Chain	Res	Type	Atoms
3	C	806	POV	C24-C25-C26-C27
3	D	807	POV	C31-C32-C33-C34
3	A	805	POV	C21-C22-C23-C24
3	C	807	POV	C310-C311-C312-C313
3	B	807	POV	C213-C214-C215-C216
3	D	803	POV	C33-C34-C35-C36
3	B	805	POV	C36-C37-C38-C39
2	A	802	Y01	CAJ-CAN-CBA-CAB
2	A	812	Y01	CAJ-CAO-CBB-CAC
3	A	808	POV	C25-C26-C27-C28
3	B	807	POV	C215-C216-C217-C218
3	D	809	POV	C310-C311-C312-C313
3	D	808	POV	C25-C26-C27-C28
3	D	811	POV	C211-C212-C213-C214
3	D	806	POV	C26-C27-C28-C29
3	D	801	POV	C22-C23-C24-C25
2	A	802	Y01	CAJ-CAN-CBA-CAA
3	B	812	POV	C213-C214-C215-C216
3	B	813	POV	C1-C2-C3-O31
3	D	801	POV	C1-C2-C3-O31
3	C	807	POV	C37-C38-C39-C310
2	A	812	Y01	CAM-CAL-CAX-OAF
3	D	806	POV	C214-C215-C216-C217
3	B	806	POV	C37-C38-C39-C310
3	A	805	POV	C11-C12-N-C13
2	A	801	Y01	CAN-CAJ-CAO-CBB
3	A	810	POV	C27-C28-C29-C210
3	C	801	POV	C25-C26-C27-C28
3	B	811	POV	O32-C31-O31-C3
3	C	806	POV	C21-C22-C23-C24
2	D	805	Y01	CAM-CAL-CAX-OAH
3	B	811	POV	C32-C31-O31-C3
3	B	810	POV	C310-C311-C312-C313
3	B	812	POV	C212-C213-C214-C215
3	C	810	POV	C310-C311-C312-C313
3	A	810	POV	C310-C311-C312-C313
3	A	811	POV	C313-C314-C315-C316
3	B	810	POV	C32-C33-C34-C35
3	A	810	POV	O31-C31-C32-C33
3	C	810	POV	C212-C213-C214-C215
3	B	808	POV	C39-C310-C311-C312
3	D	806	POV	C29-C210-C211-C212

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Mol	Chain	Res	Type	Atoms
2	D	805	Y01	CAM-CAL-CAX-OAF
3	B	812	POV	C11-C12-N-C15
3	D	811	POV	C27-C28-C29-C210
3	B	812	POV	C2-C1-O11-P
3	D	802	POV	O21-C2-C3-O31
3	D	809	POV	C33-C34-C35-C36
2	A	801	Y01	CAL-CAM-CAY-OAW
3	D	808	POV	C310-C311-C312-C313
3	A	810	POV	C215-C216-C217-C218
3	A	813	POV	C311-C312-C313-C314
3	A	804	POV	C310-C311-C312-C313
3	D	810	POV	C37-C38-C39-C310
2	A	802	Y01	CAM-CAL-CAX-OAH
2	A	812	Y01	CAM-CAL-CAX-OAH
3	B	811	POV	O21-C21-C22-C23
3	A	805	POV	C27-C28-C29-C210
3	B	807	POV	C29-C210-C211-C212
3	D	802	POV	C29-C210-C211-C212
3	B	813	POV	C1-C2-O21-C21
3	D	802	POV	C1-C2-O21-C21
3	B	813	POV	C22-C23-C24-C25
2	B	804	Y01	CAM-CAL-CAX-OAH
3	C	810	POV	C211-C212-C213-C214
3	B	808	POV	C33-C34-C35-C36
3	D	803	POV	C311-C310-C39-C38
3	D	802	POV	C313-C314-C315-C316
3	C	807	POV	C33-C34-C35-C36
3	A	806	POV	C26-C27-C28-C29
3	B	806	POV	C1-C2-C3-O31
3	D	808	POV	C1-C2-C3-O31
3	B	813	POV	C212-C213-C214-C215
3	D	806	POV	O11-C1-C2-O21
3	D	808	POV	O21-C21-C22-C23
2	A	802	Y01	CAM-CAL-CAX-OAF
2	C	804	Y01	CAM-CAL-CAX-OAH
3	C	809	POV	C32-C33-C34-C35
3	A	805	POV	C29-C210-C211-C212
3	B	809	POV	C27-C28-C29-C210
2	C	804	Y01	CAM-CAL-CAX-OAF
3	B	812	POV	C26-C27-C28-C29
3	D	809	POV	C212-C213-C214-C215
3	D	806	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	B	804	Y01	CAM-CAL-CAX-OAF
2	D	804	Y01	CAL-CAM-CAY-OAW
3	C	810	POV	O21-C2-C3-O31
3	D	806	POV	C27-C28-C29-C210
3	A	805	POV	O22-C21-O21-C2
2	C	802	Y01	CAL-CAM-CAY-OAW
3	D	810	POV	C34-C35-C36-C37
3	A	808	POV	C212-C213-C214-C215
2	B	804	Y01	CAL-CAM-CAY-OAW
3	A	811	POV	O21-C21-C22-C23
3	B	811	POV	O31-C31-C32-C33
3	B	807	POV	C214-C215-C216-C217
3	D	810	POV	C31-C32-C33-C34
3	D	811	POV	C213-C214-C215-C216
3	B	812	POV	C29-C210-C211-C212
3	C	801	POV	C27-C28-C29-C210
3	A	805	POV	C39-C310-C311-C312
3	B	801	POV	C32-C33-C34-C35
3	C	810	POV	O21-C21-C22-C23
2	A	801	Y01	CAL-CAM-CAY-OAG
3	D	812	POV	C32-C33-C34-C35
3	B	811	POV	O32-C31-C32-C33
3	D	808	POV	O22-C21-C22-C23
3	B	811	POV	O22-C21-C22-C23
3	A	807	POV	C32-C33-C34-C35
3	A	805	POV	C11-O12-P-O13
3	A	811	POV	C1-O11-P-O14
3	A	813	POV	C1-O11-P-O14
3	B	811	POV	C11-O12-P-O14
3	C	810	POV	C1-O11-P-O14
3	D	809	POV	C11-O12-P-O13
3	A	811	POV	O22-C21-C22-C23
2	A	802	Y01	CAL-CAM-CAY-OAW
2	C	802	Y01	CAL-CAM-CAY-OAG
3	B	811	POV	C23-C24-C25-C26
3	A	808	POV	C210-C211-C212-C213
3	C	801	POV	C312-C313-C314-C315
3	B	813	POV	C3-C2-O21-C21
3	D	801	POV	C12-C11-O12-P
3	D	806	POV	C12-C11-O12-P
2	D	804	Y01	CAL-CAM-CAY-OAG
3	D	806	POV	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
3	C	806	POV	C310-C311-C312-C313
2	A	812	Y01	CAL-CAM-CAY-OAW
3	B	813	POV	C215-C216-C217-C218
2	D	805	Y01	CAL-CAM-CAY-OAW
2	D	804	Y01	CAN-CAJ-CAO-CBB
3	D	803	POV	C34-C35-C36-C37
2	A	812	Y01	CAL-CAM-CAY-OAG
3	B	806	POV	O21-C21-C22-C23
3	C	806	POV	O31-C31-C32-C33
3	D	801	POV	O21-C21-C22-C23
3	D	806	POV	O31-C31-C32-C33
2	A	802	Y01	CAL-CAM-CAY-OAG
3	D	802	POV	C312-C313-C314-C315
3	C	810	POV	O22-C21-C22-C23
3	C	806	POV	O32-C31-C32-C33
3	B	812	POV	C11-C12-N-C13
2	B	802	Y01	CAM-CAL-CAX-OAH
2	C	803	Y01	CAM-CAL-CAX-OAH

There are no ring outliers.

38 monomers are involved in 194 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	807	POV	1	0
3	B	809	POV	1	0
2	A	803	Y01	10	0
3	B	801	POV	1	0
3	D	807	POV	1	0
3	C	801	POV	1	0
2	A	812	Y01	16	0
2	C	804	Y01	10	0
3	A	810	POV	2	0
3	A	806	POV	1	0
3	D	808	POV	3	0
3	D	812	POV	1	0
3	B	807	POV	1	0
2	C	803	Y01	11	0
3	D	801	POV	3	0
3	B	806	POV	1	0
3	C	806	POV	6	0
2	B	804	Y01	12	0
3	B	811	POV	4	0

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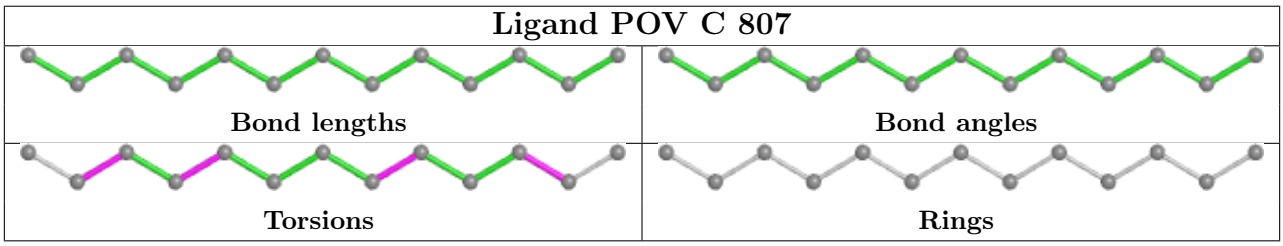
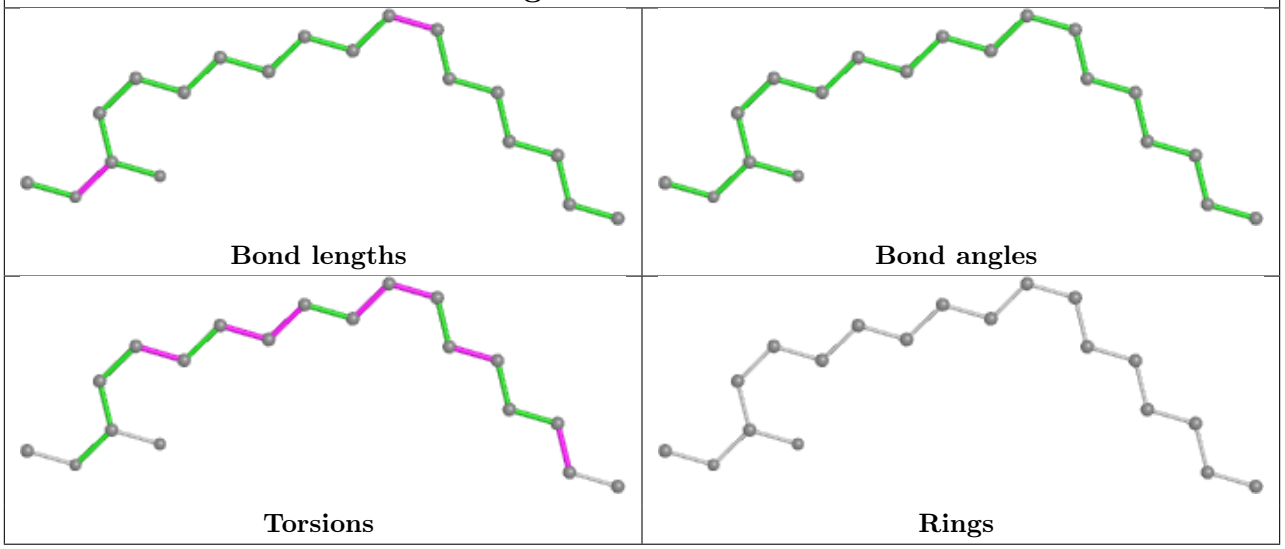
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	813	POV	4	0
3	A	811	POV	3	0
2	D	805	Y01	11	0
2	B	802	Y01	12	0
6	A	816	GEN	1	0
2	C	802	Y01	13	0
2	A	801	Y01	10	0
2	A	802	Y01	12	0
3	C	809	POV	1	0
2	B	803	Y01	14	0
3	A	808	POV	1	0
3	C	810	POV	4	0
3	D	811	POV	3	0
3	A	813	POV	4	0
3	A	809	POV	1	0
3	B	812	POV	3	0
3	D	809	POV	4	0
3	D	806	POV	2	0
2	D	804	Y01	12	0

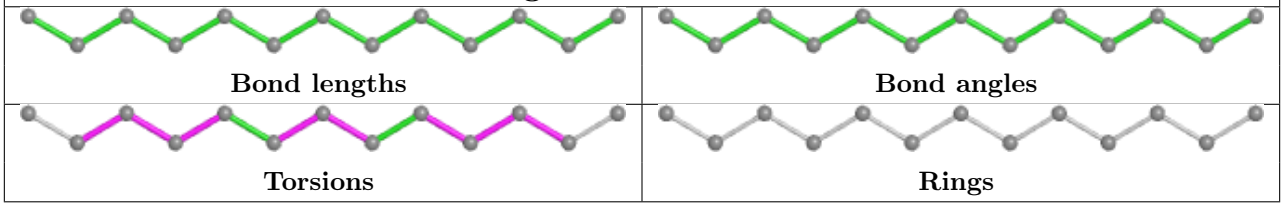
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



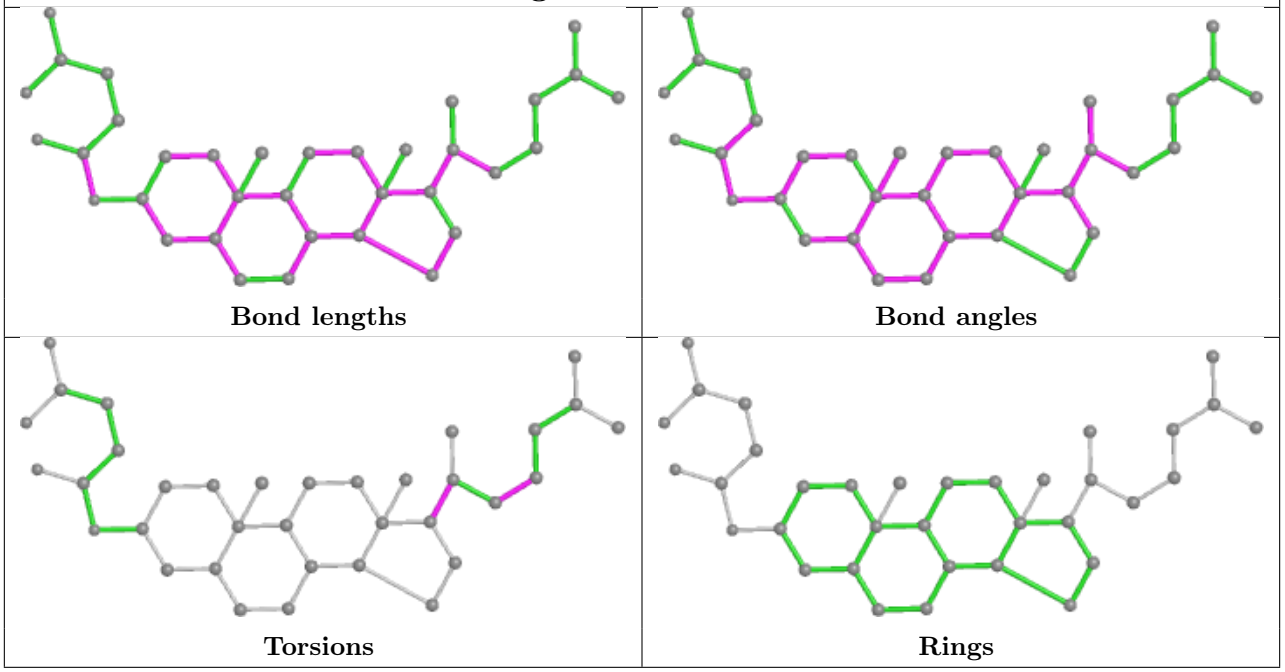
Ligand POV B 809



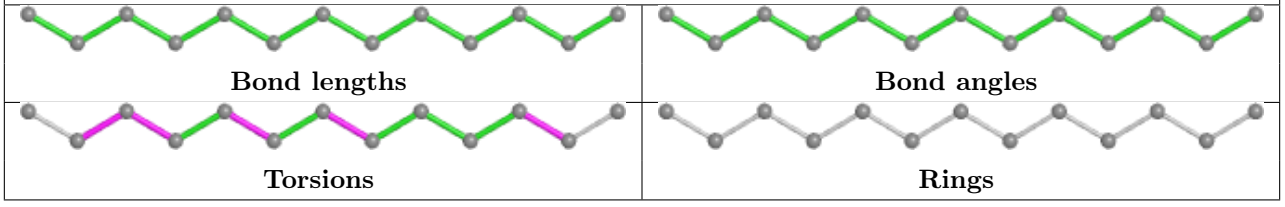
Ligand POV A 807



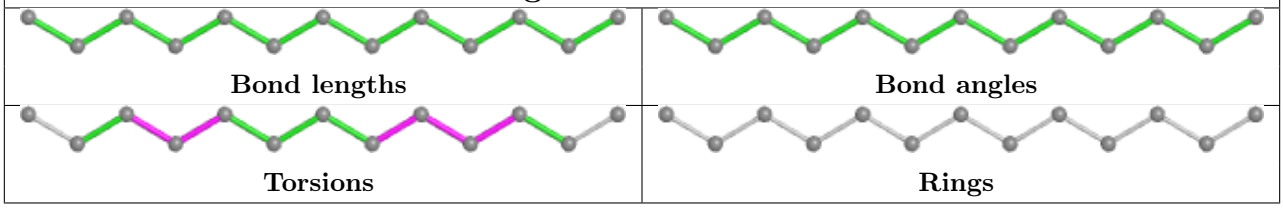
Ligand Y01 A 803



Ligand POV A 804



Ligand POV B 801



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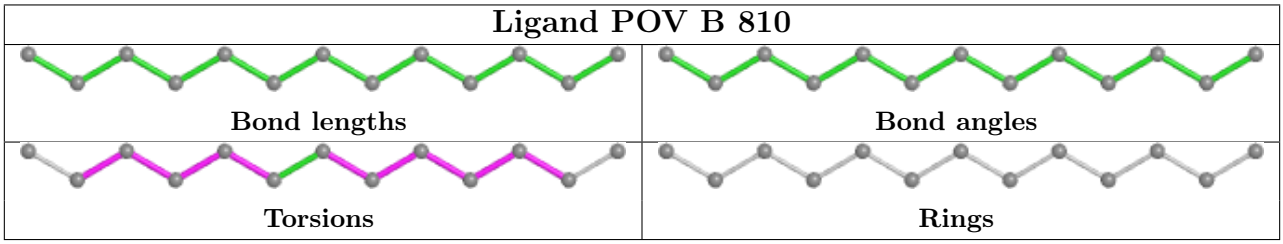
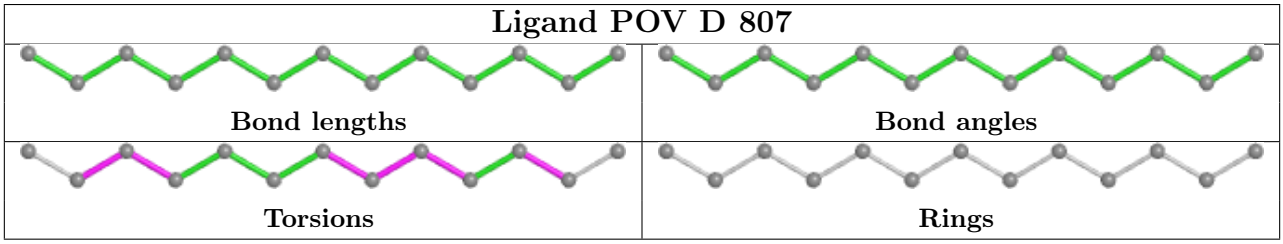
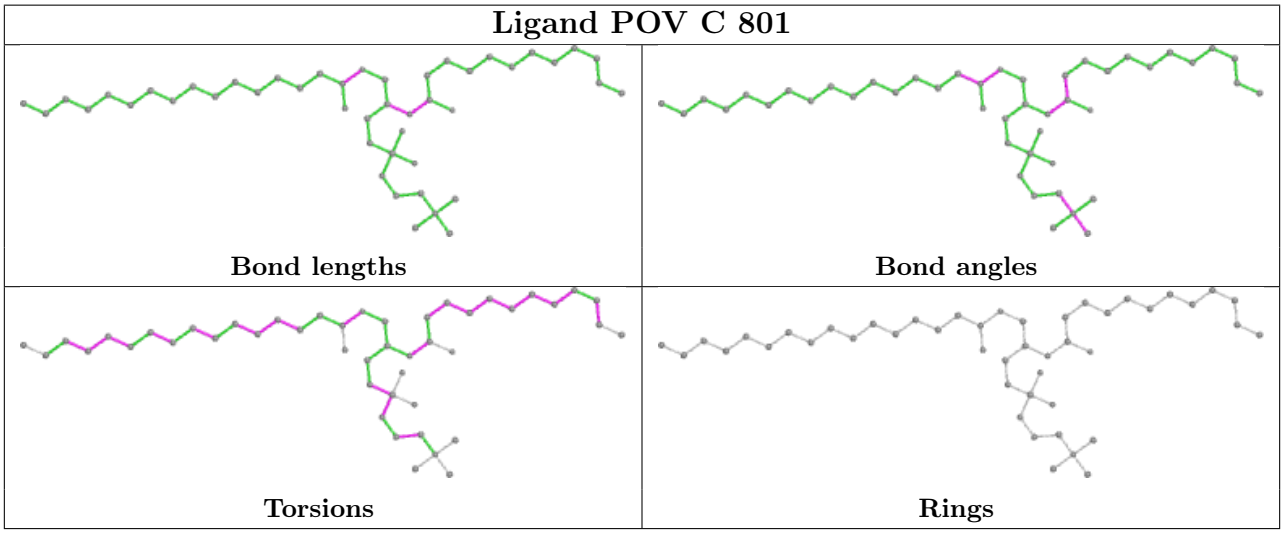


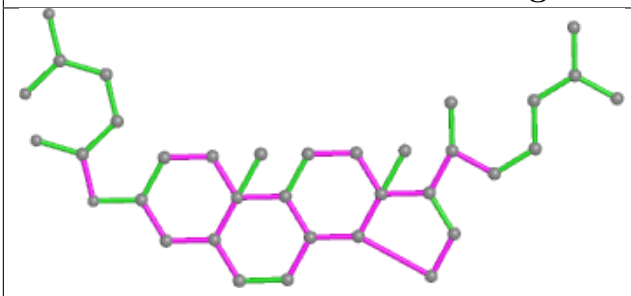
Ligand POV D 807



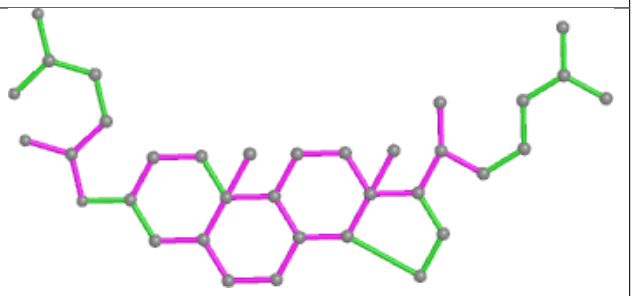
Ligand POV C 801



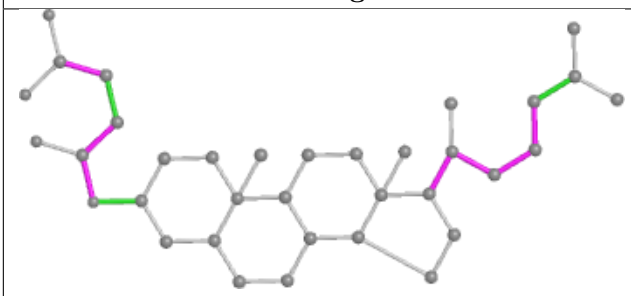
Ligand Y01 A 812



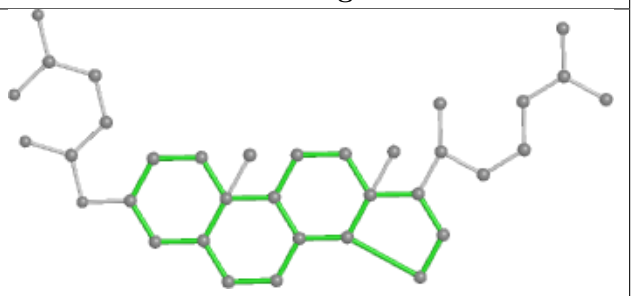
Bond lengths



Bond angles

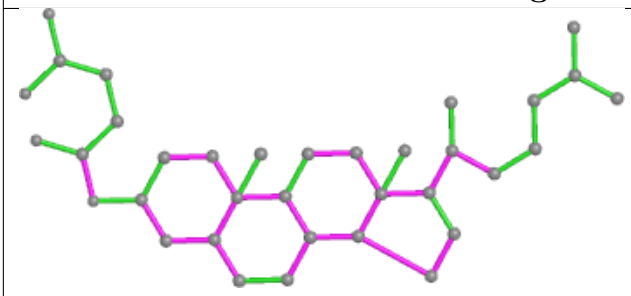


Torsions

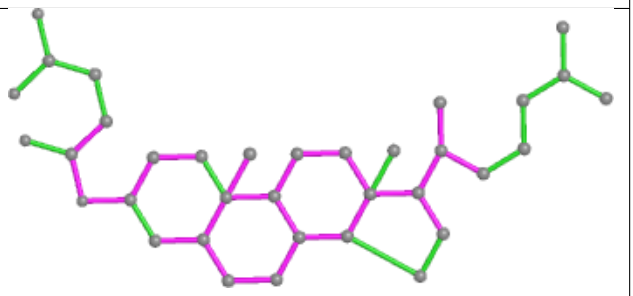


Rings

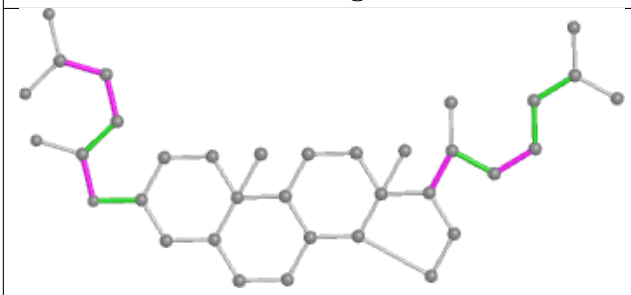
Ligand Y01 C 804



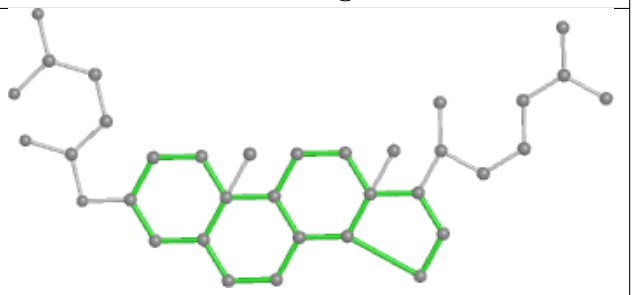
Bond lengths



Bond angles

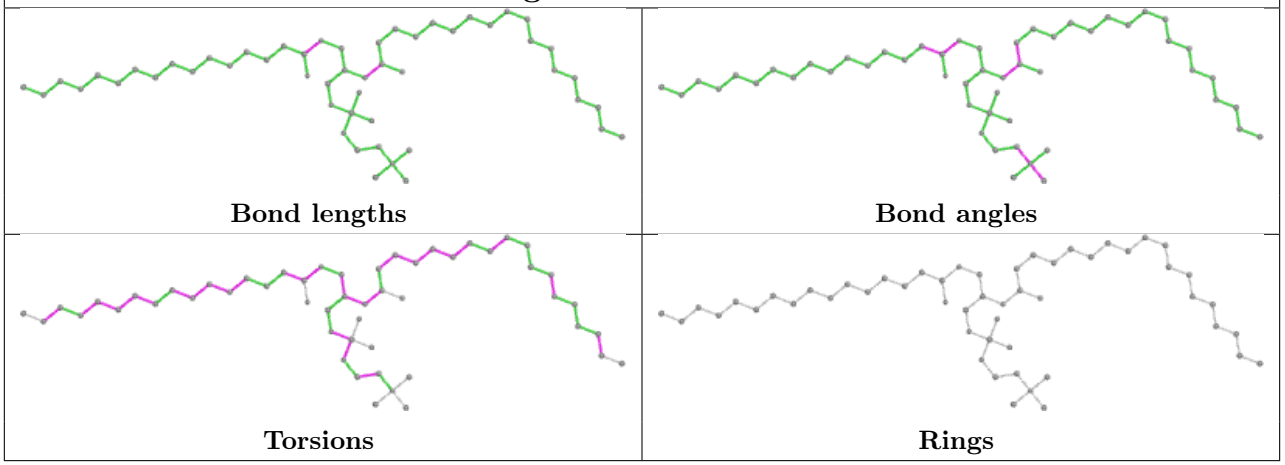


Torsions

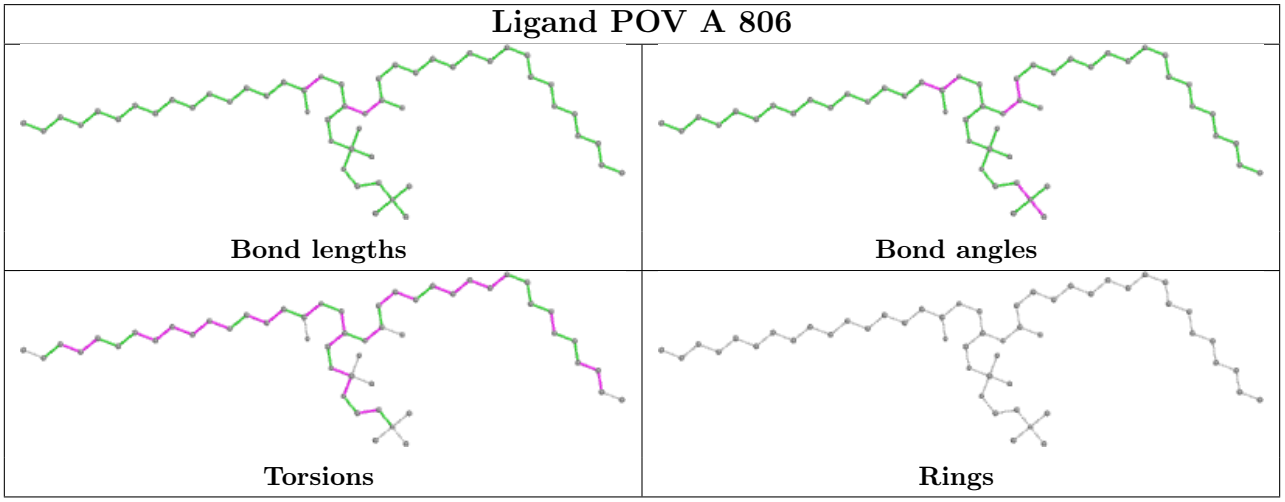


Rings

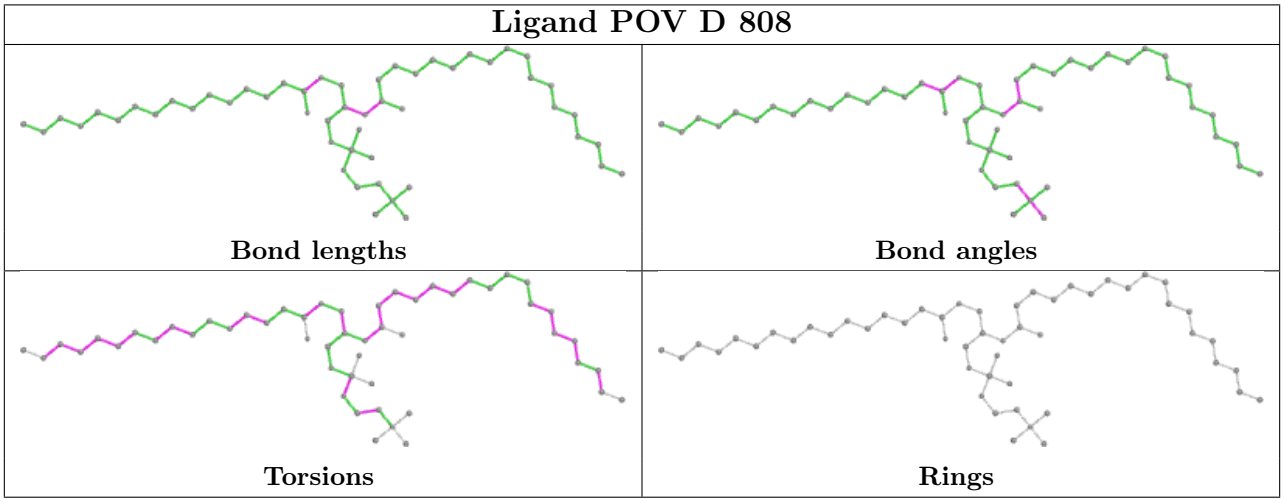
Ligand POV A 810



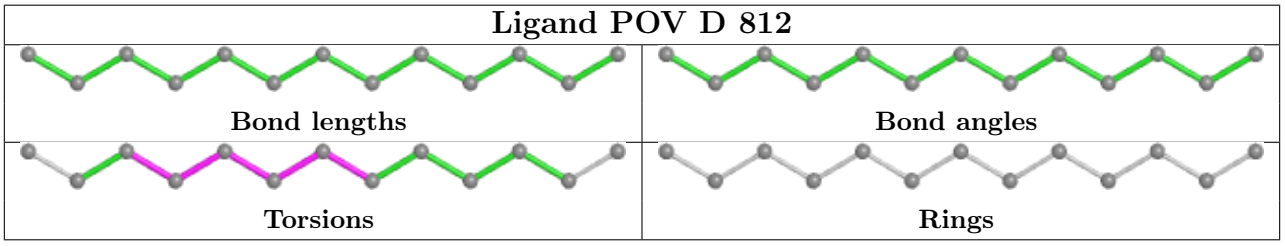
Ligand POV A 806



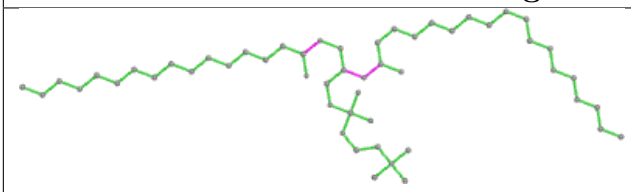
Ligand POV D 808



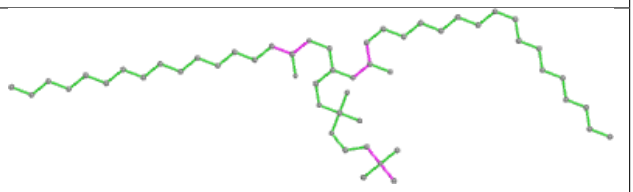
Ligand POV D 812



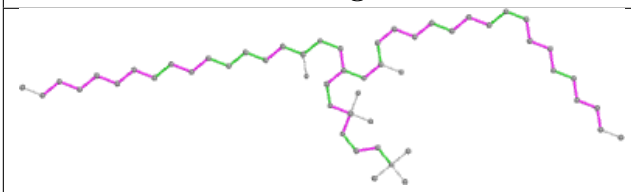
Ligand POV B 807



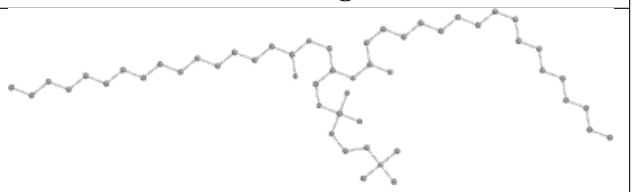
Bond lengths



Bond angles

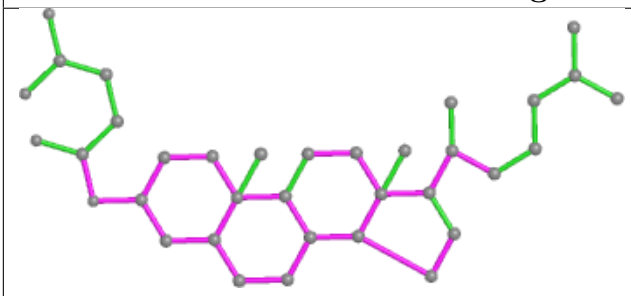


Torsions

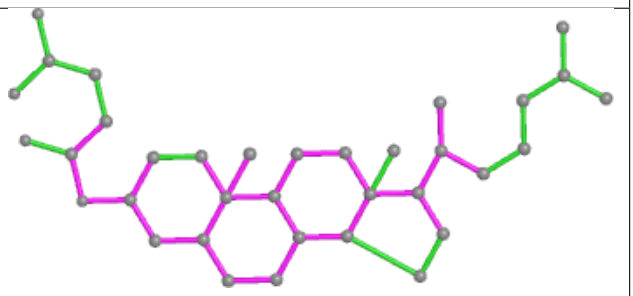


Rings

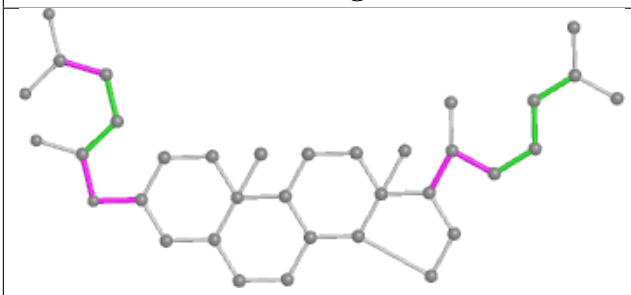
Ligand Y01 C 803



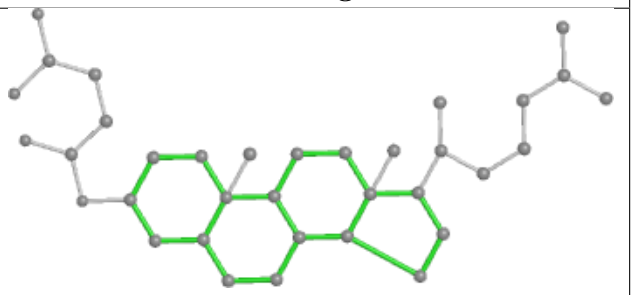
Bond lengths



Bond angles

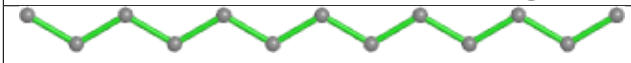


Torsions

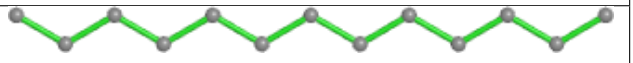


Rings

Ligand POV C 805



Bond lengths

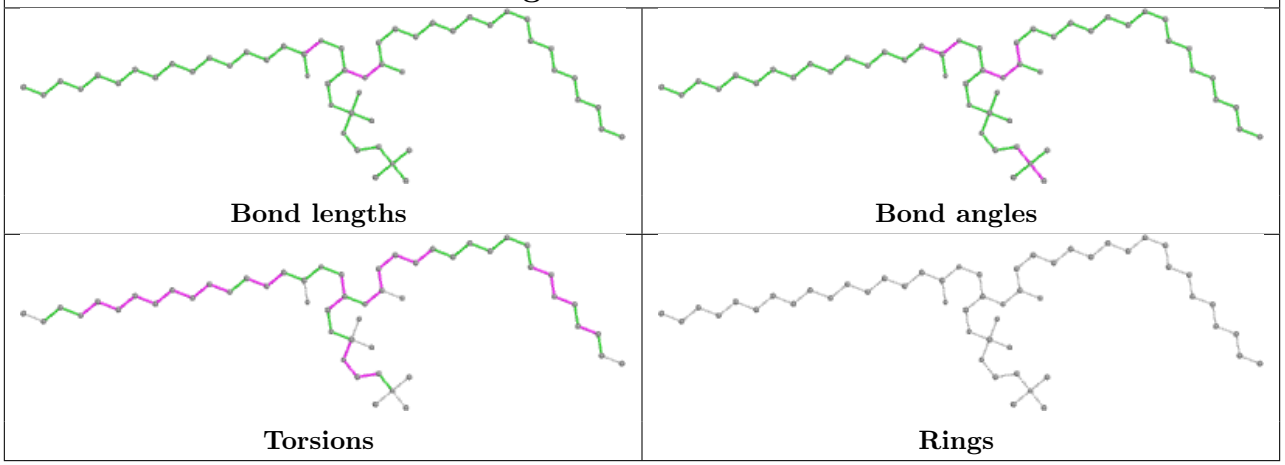


Bond angles

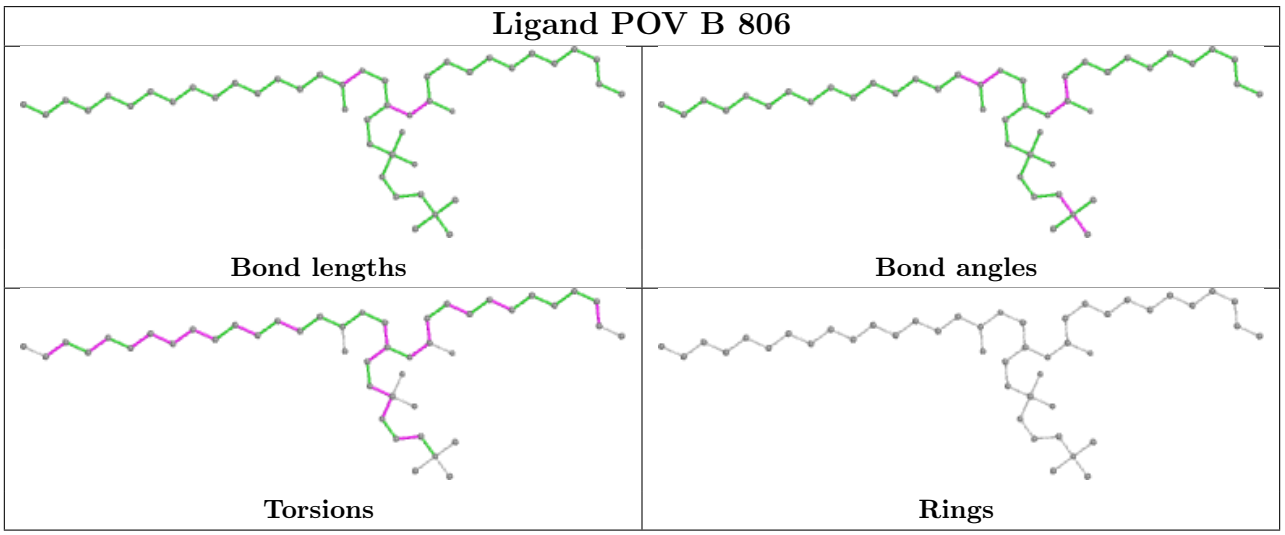
Torsions

Rings

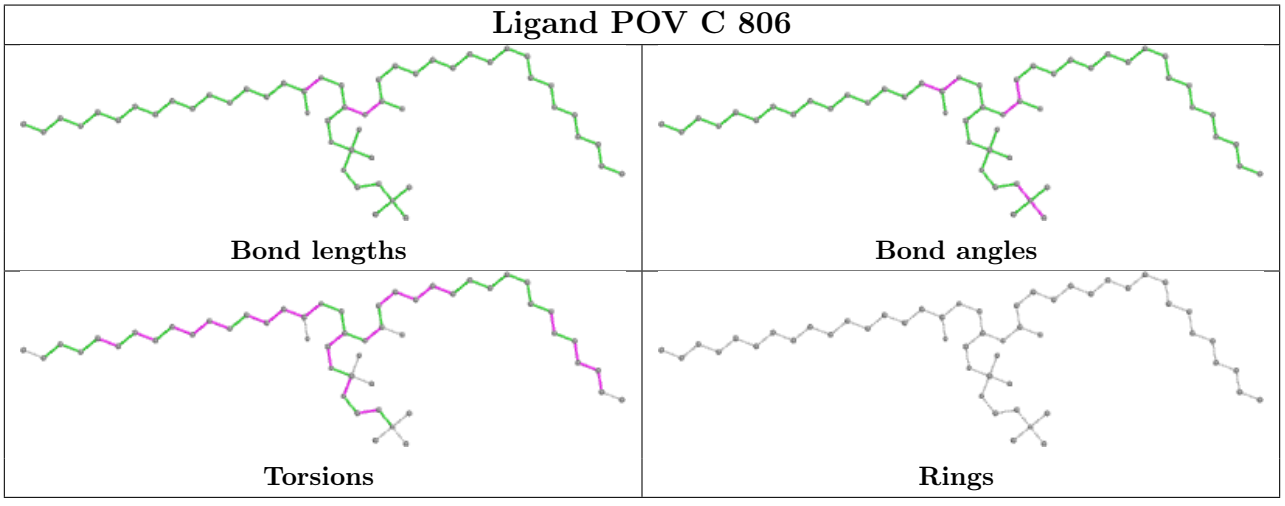
Ligand POV D 801



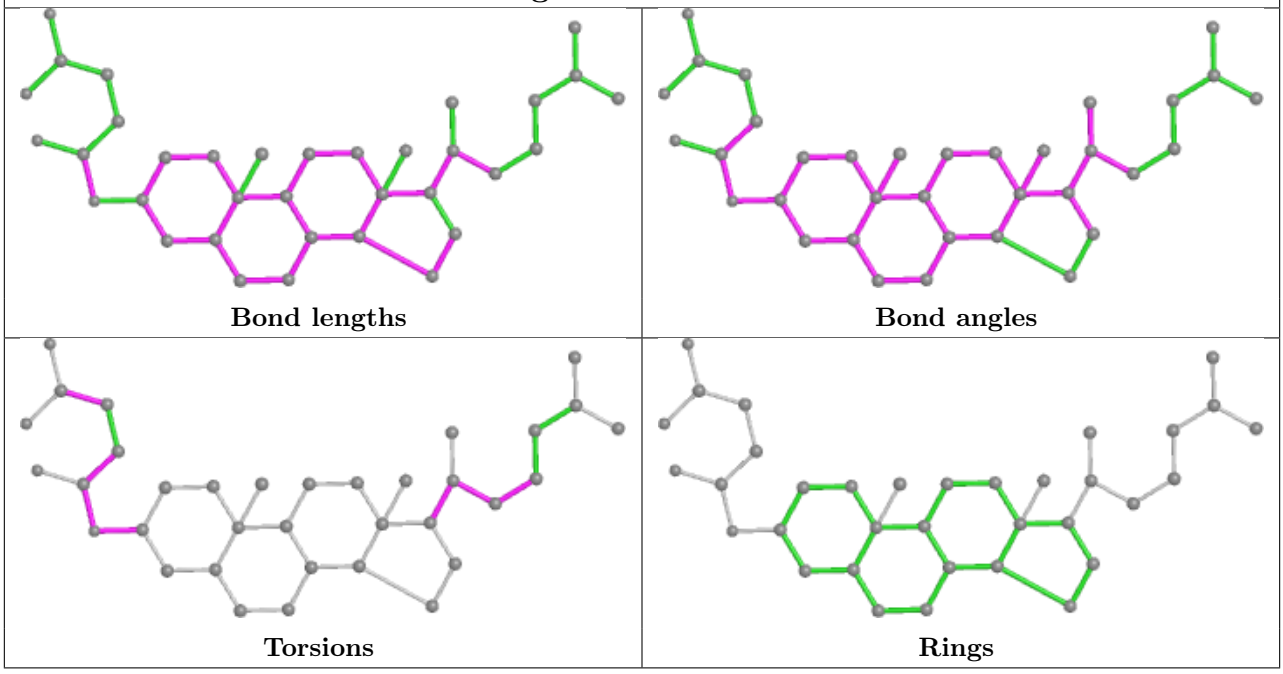
Ligand POV B 806



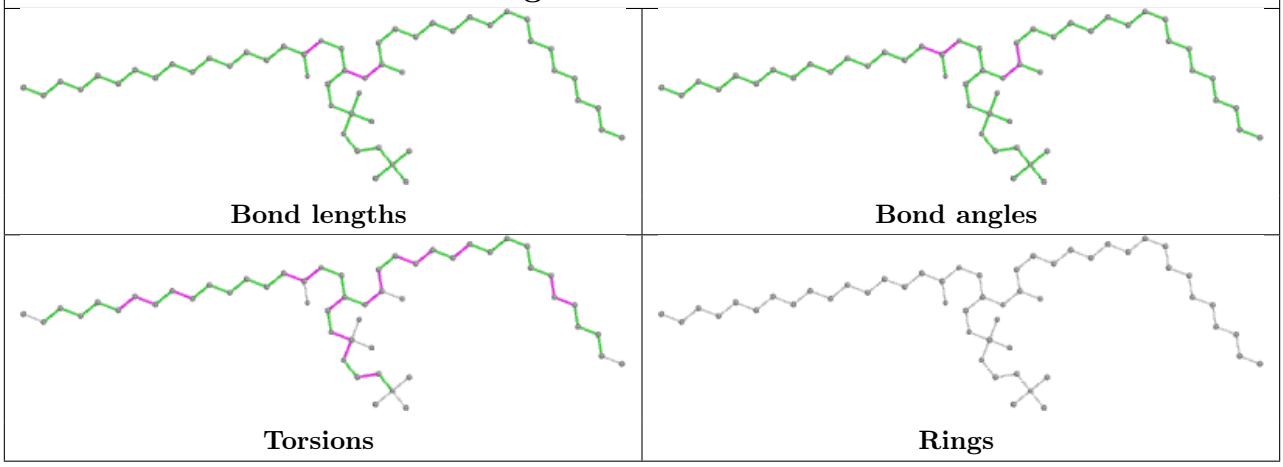
Ligand POV C 806



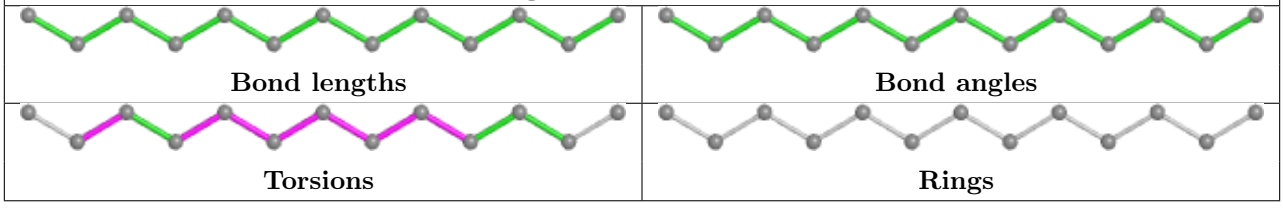
Ligand Y01 B 804



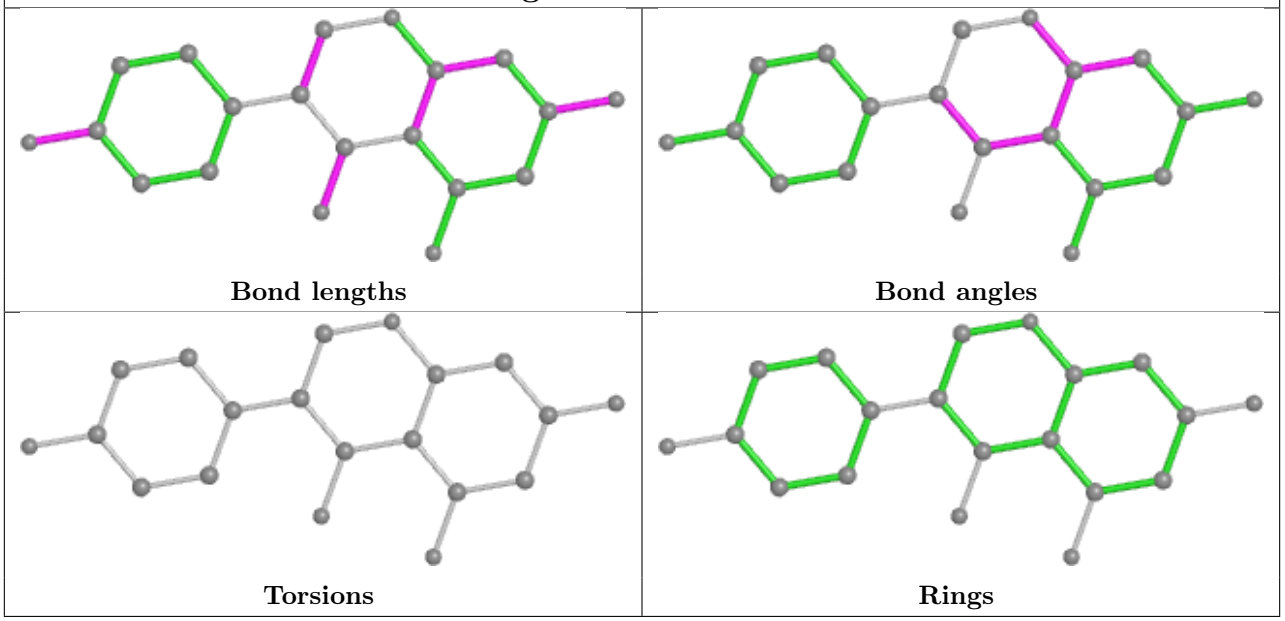
Ligand POV B 811



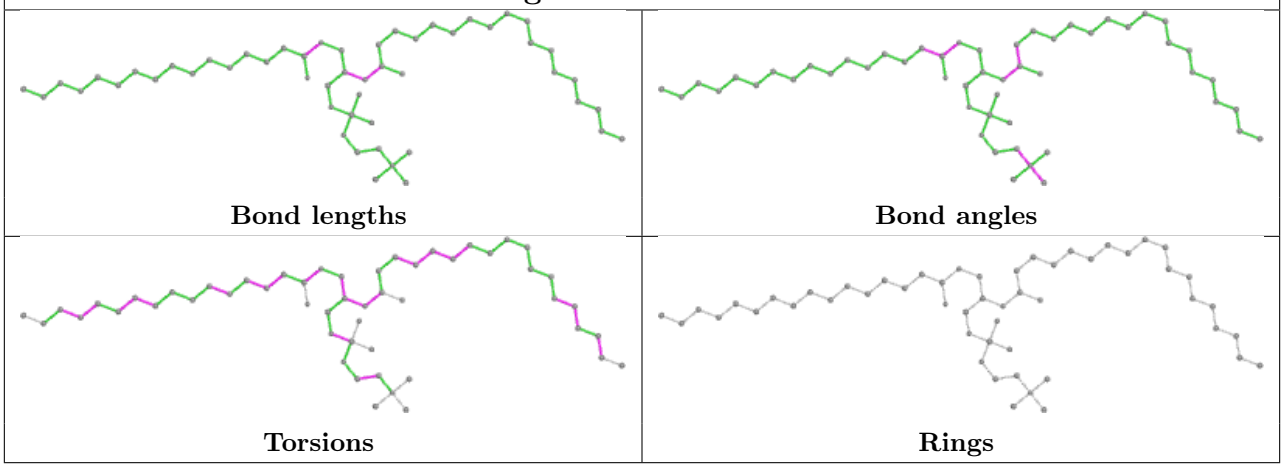
Ligand POV D 803



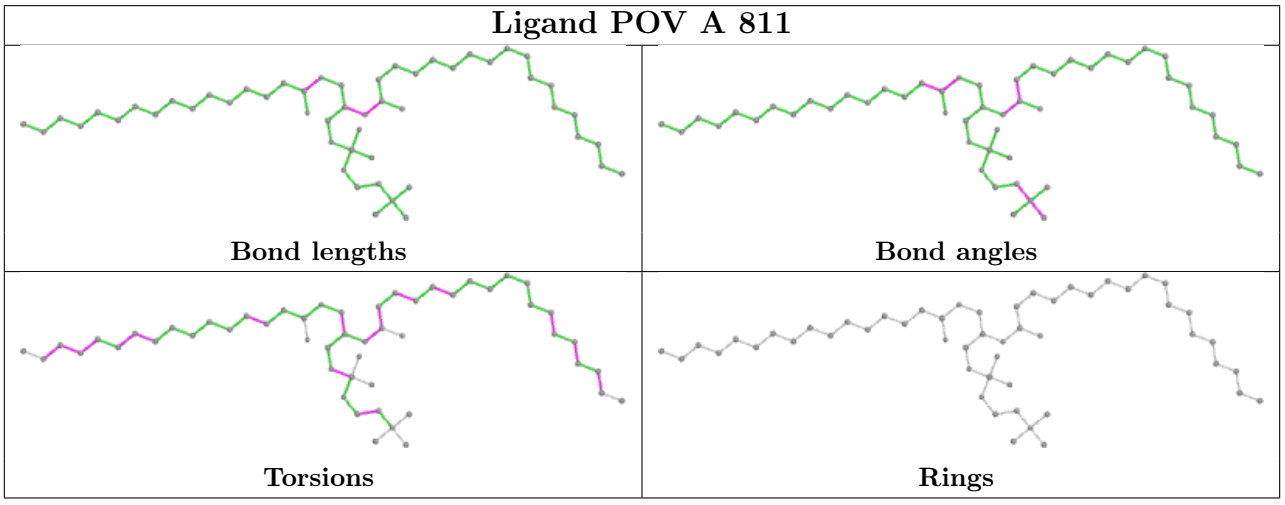
Ligand GEN D 813



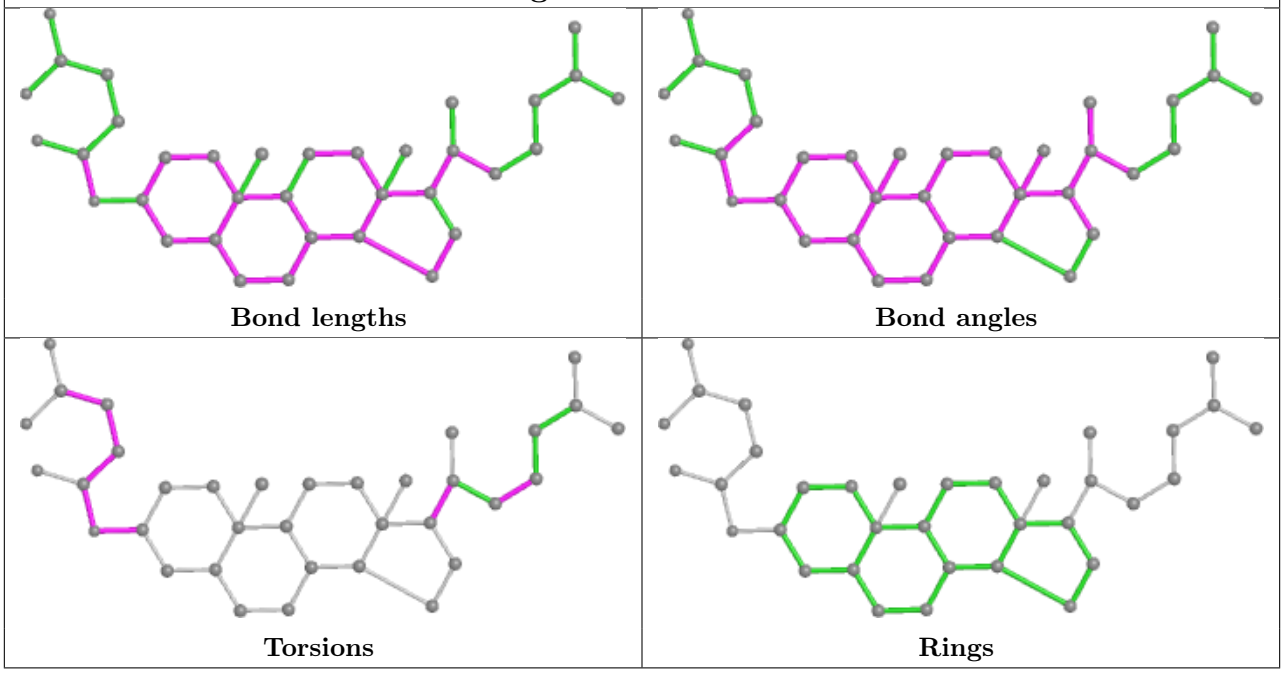
Ligand POV B 813



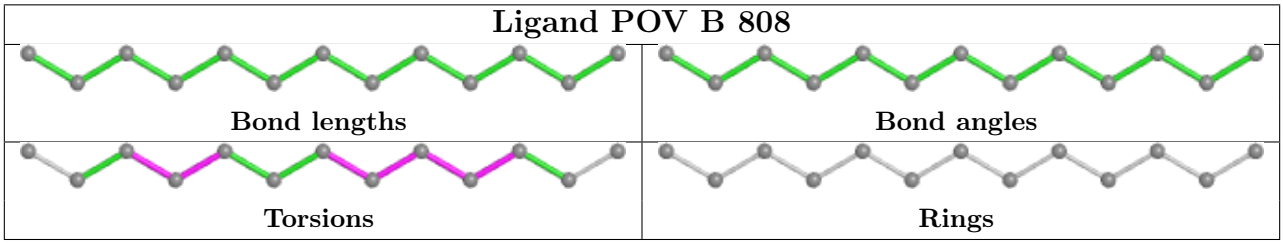
Ligand POV A 811



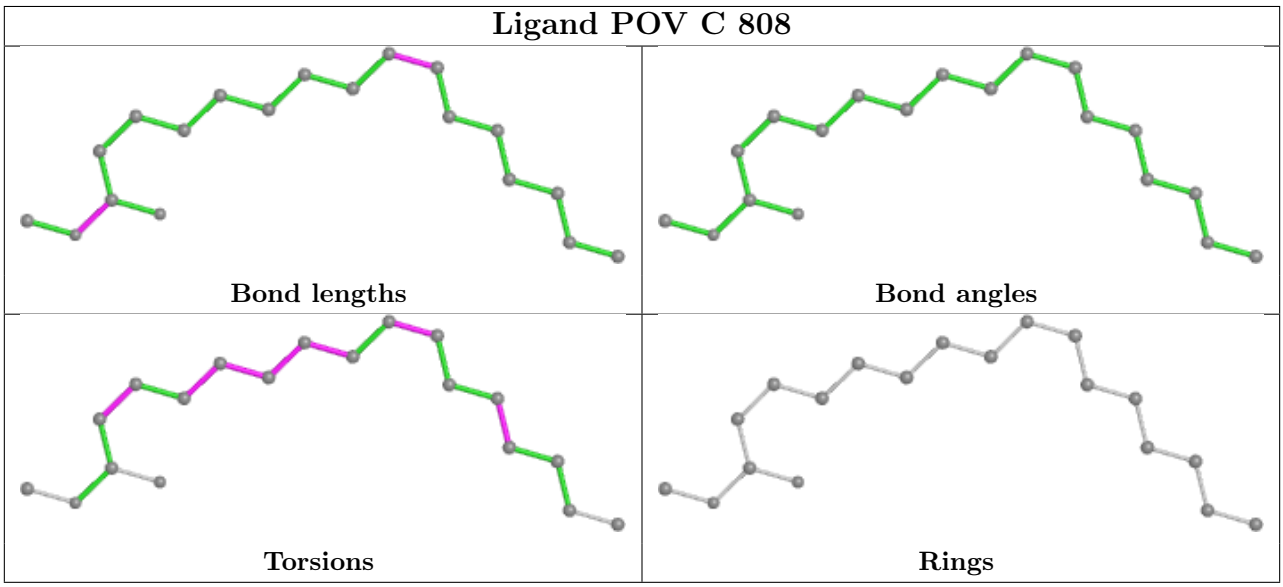
Ligand Y01 D 805



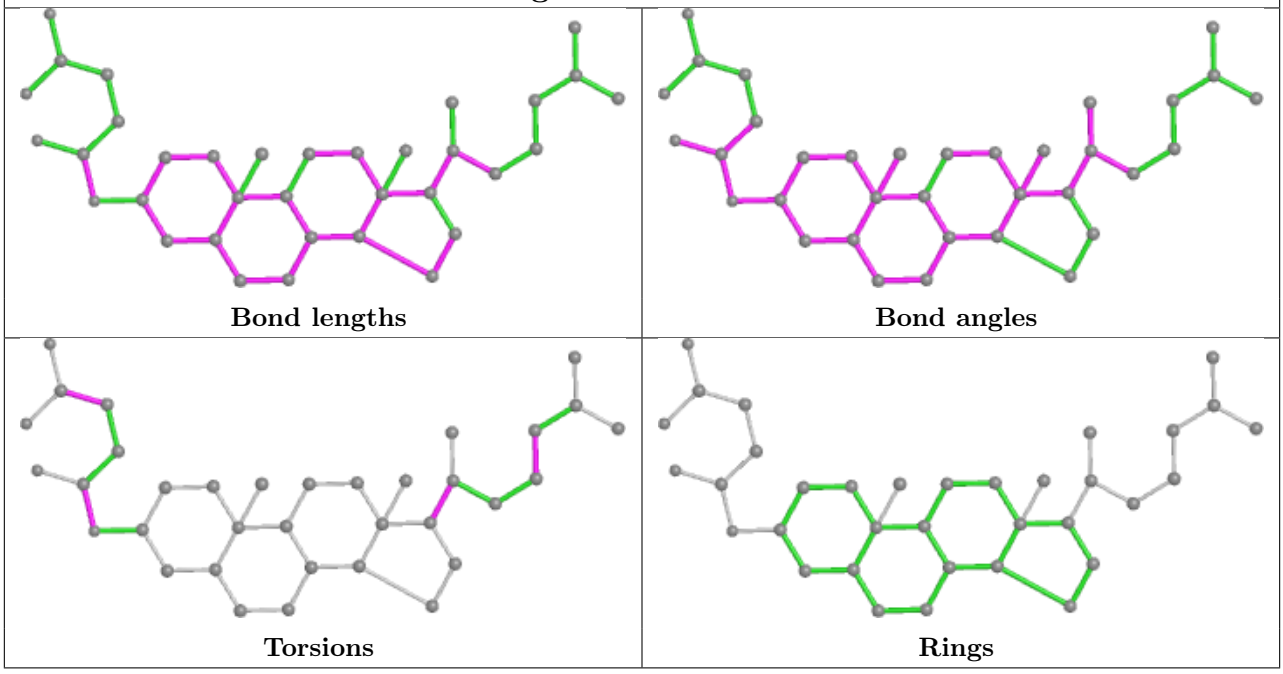
Ligand POV B 808



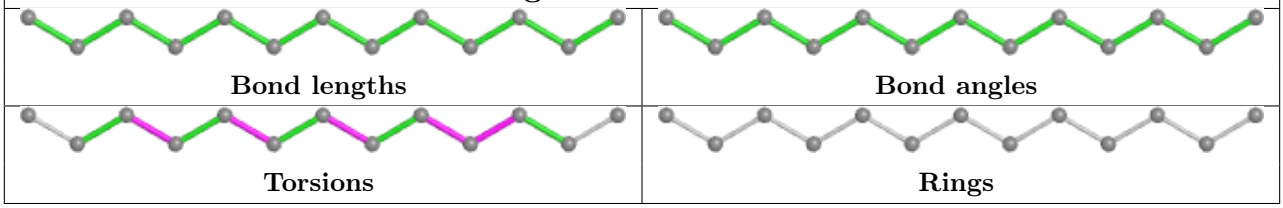
Ligand POV C 808



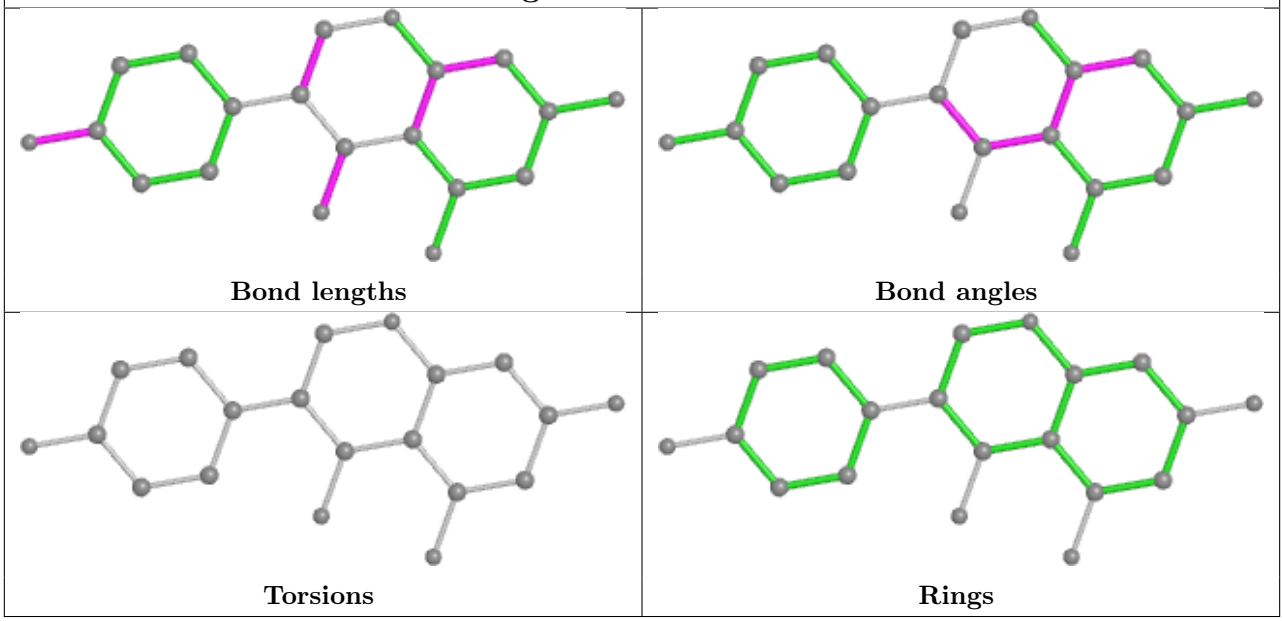
Ligand Y01 B 802



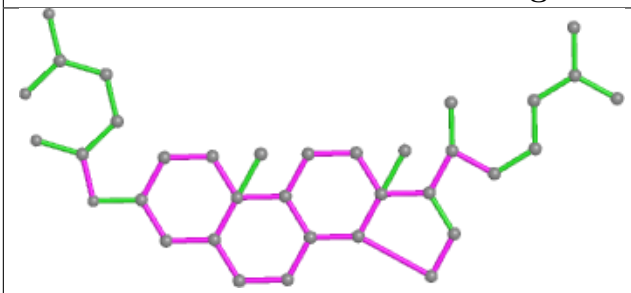
Ligand POV B 805



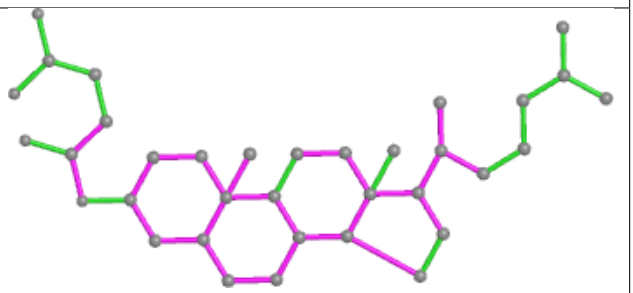
Ligand GEN A 816



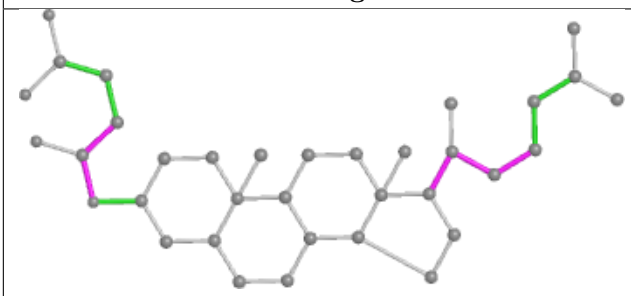
Ligand Y01 C 802



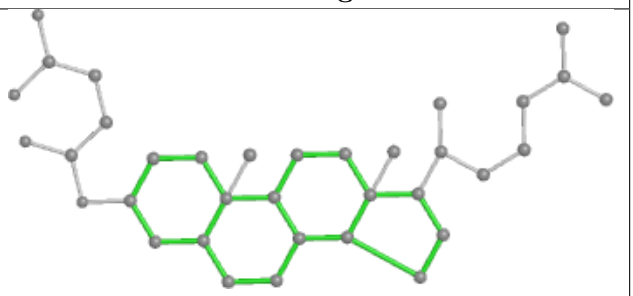
Bond lengths



Bond angles

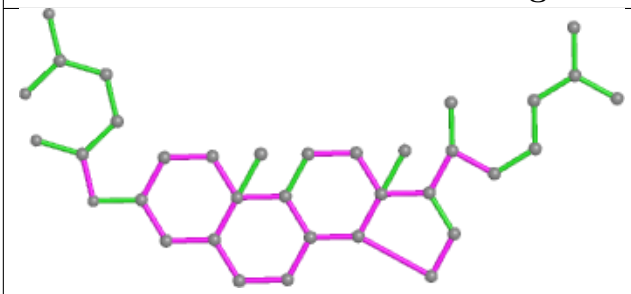


Torsions

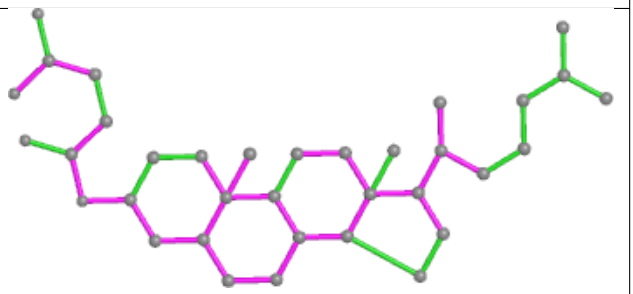


Rings

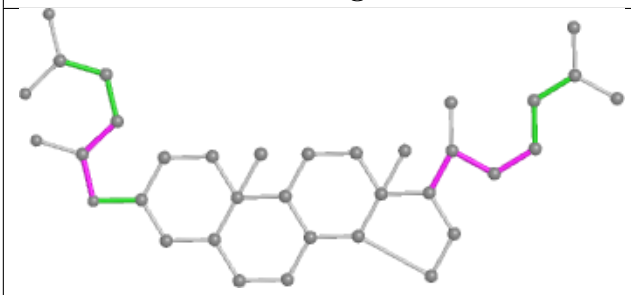
Ligand Y01 A 801



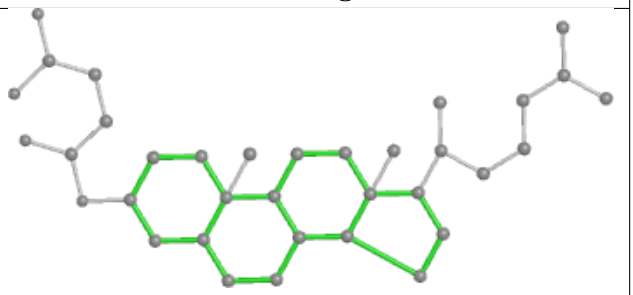
Bond lengths



Bond angles

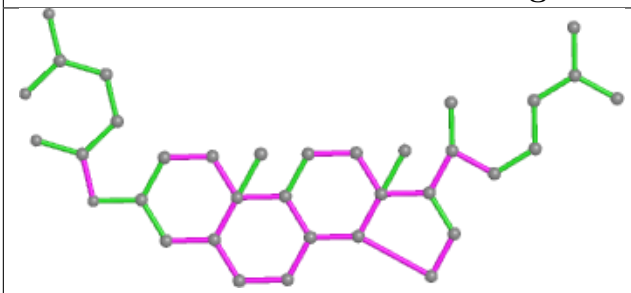


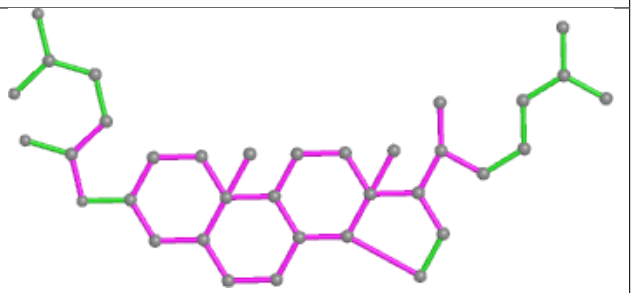
Torsions

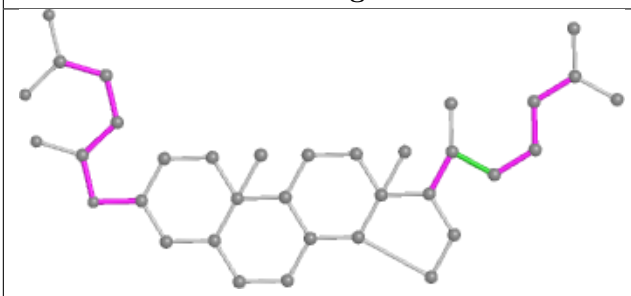


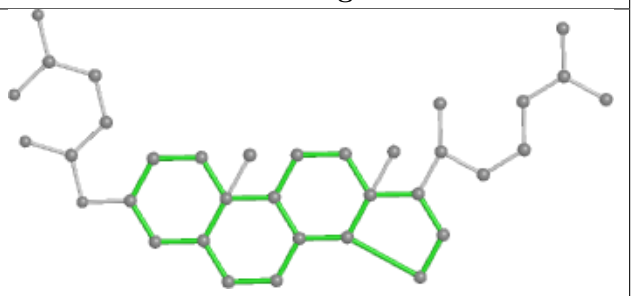
Rings

Ligand Y01 A 802


Bond lengths


Bond angles

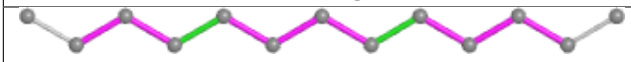

Torsions

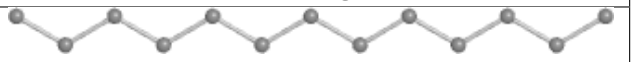

Rings

Ligand POV C 809

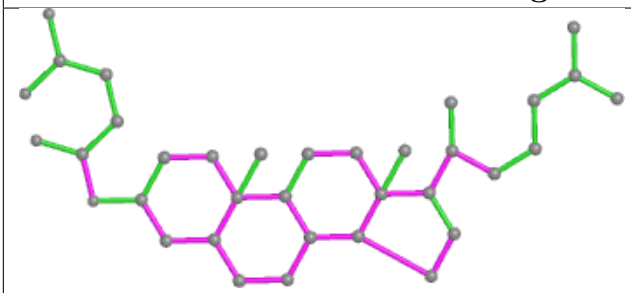

Bond lengths

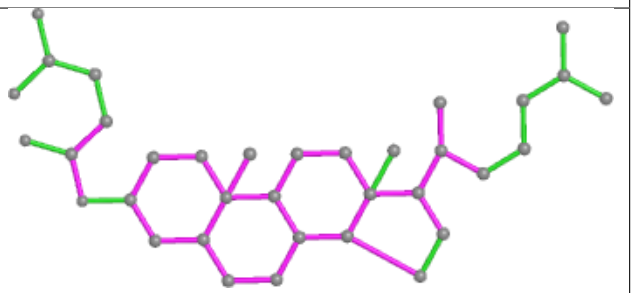

Bond angles

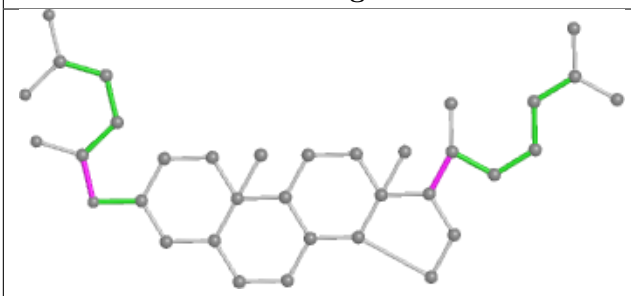

Torsions

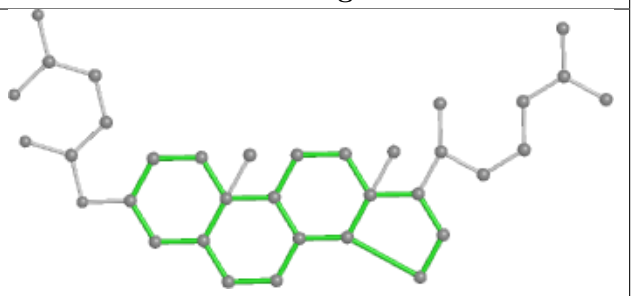

Rings

Ligand Y01 B 803

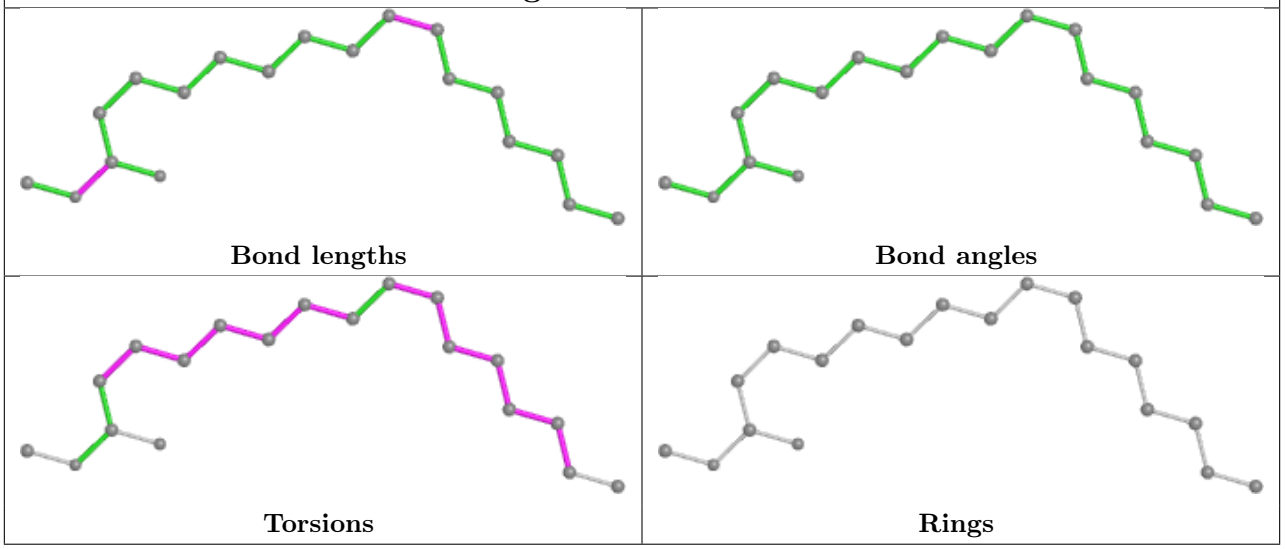

Bond lengths


Bond angles

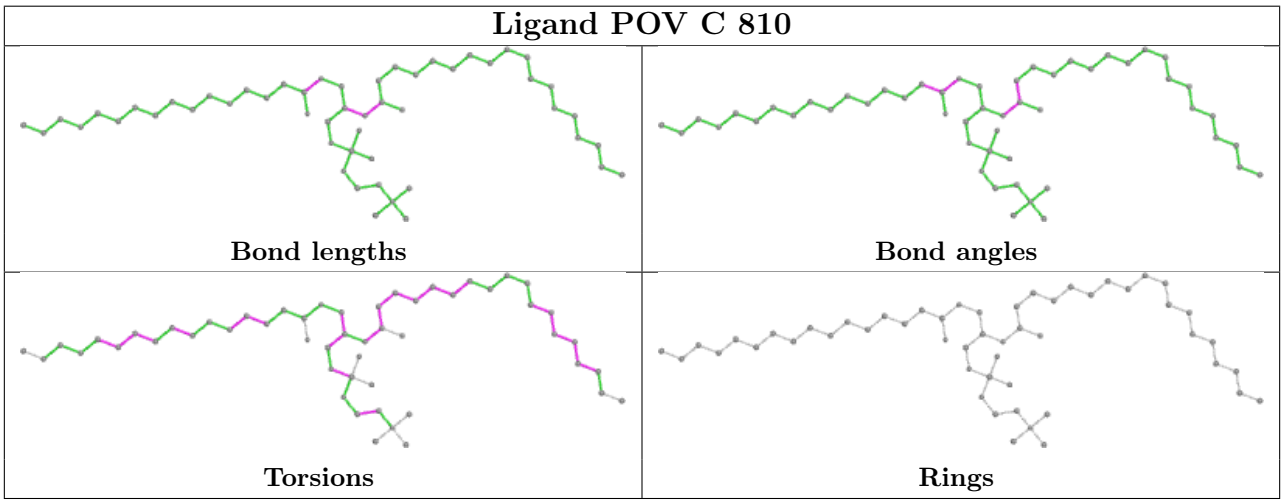

Torsions


Rings

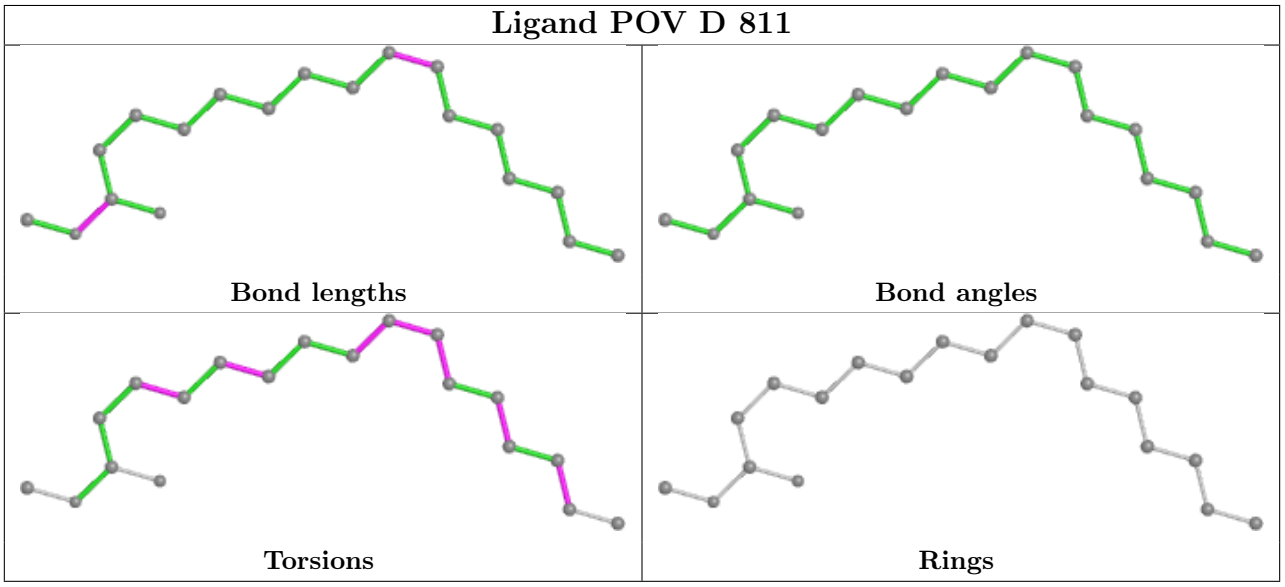
Ligand POV A 808



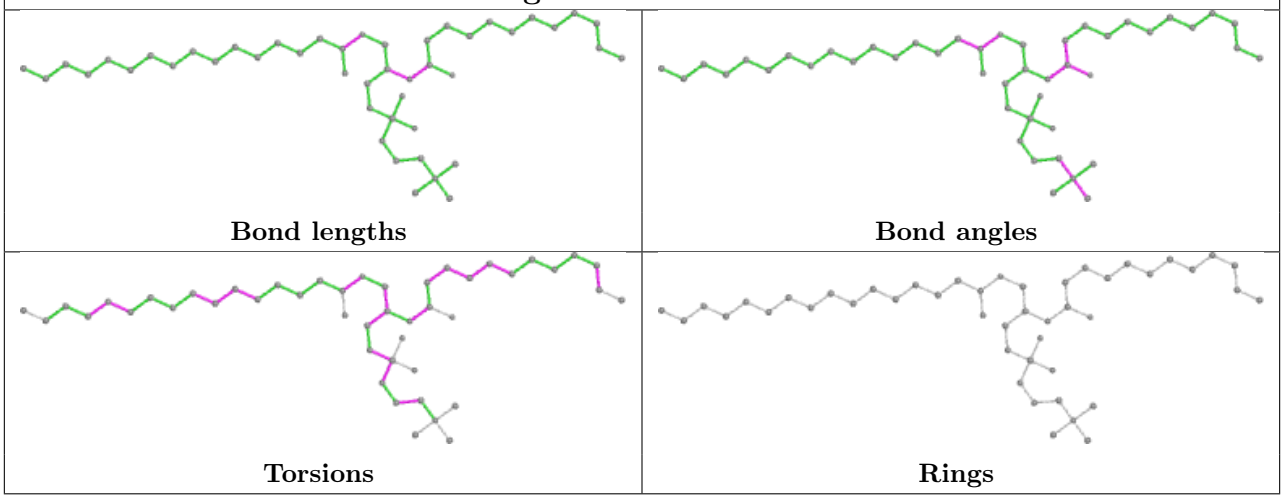
Ligand POV C 810



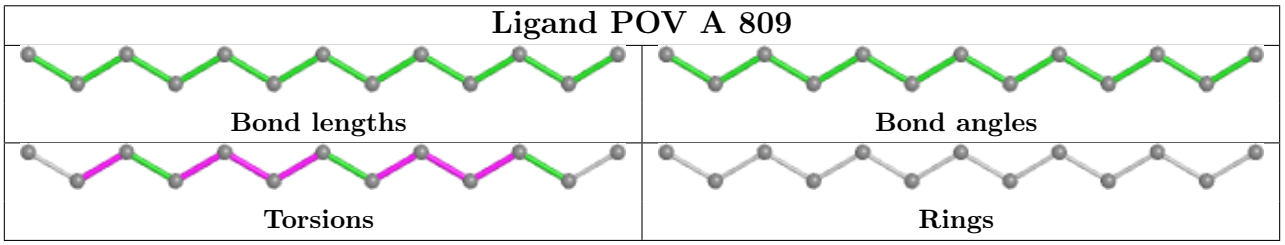
Ligand POV D 811



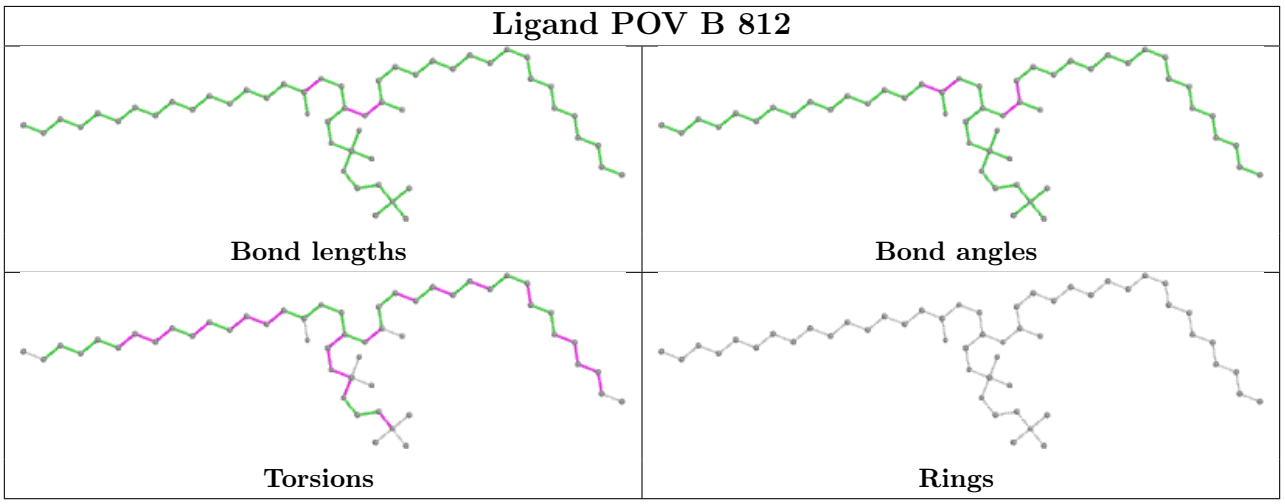
Ligand POV A 813



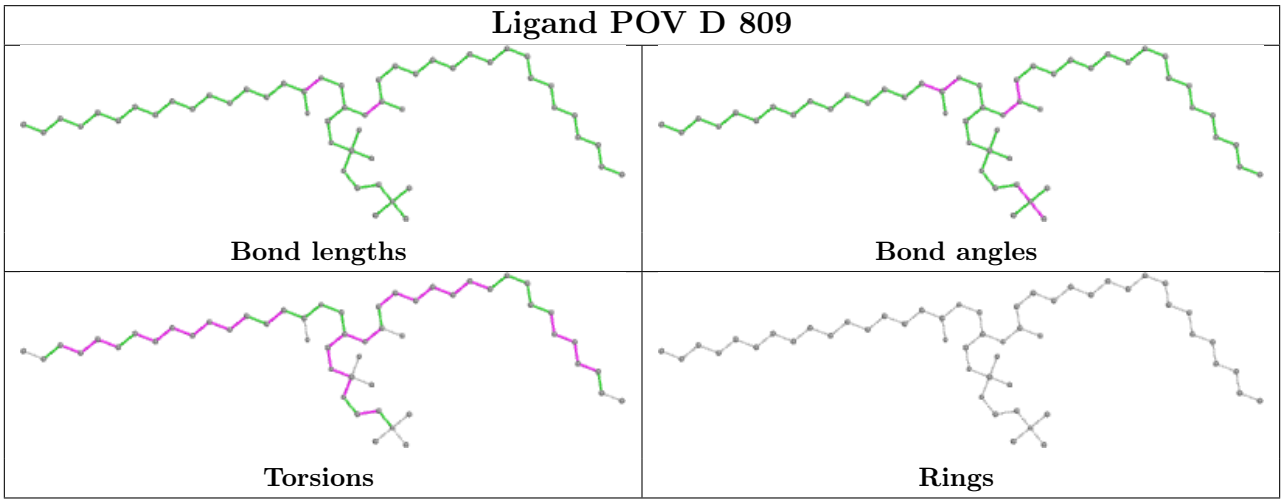
Ligand POV A 809



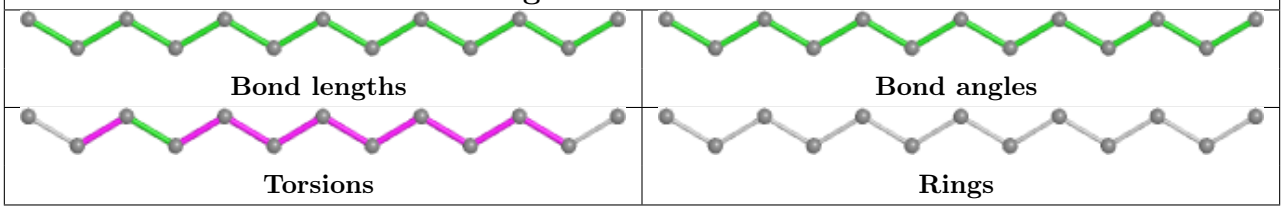
Ligand POV B 812



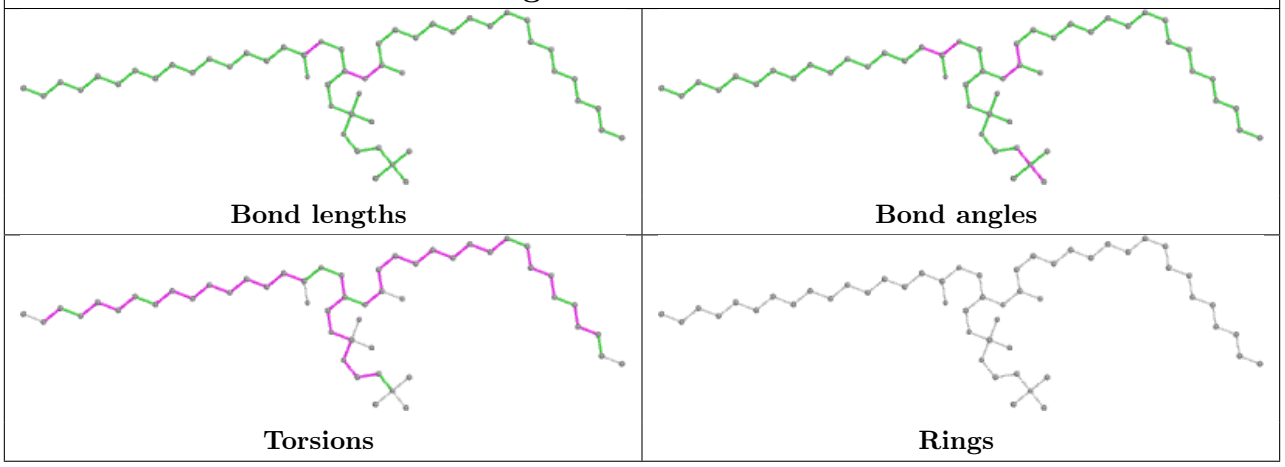
Ligand POV D 809



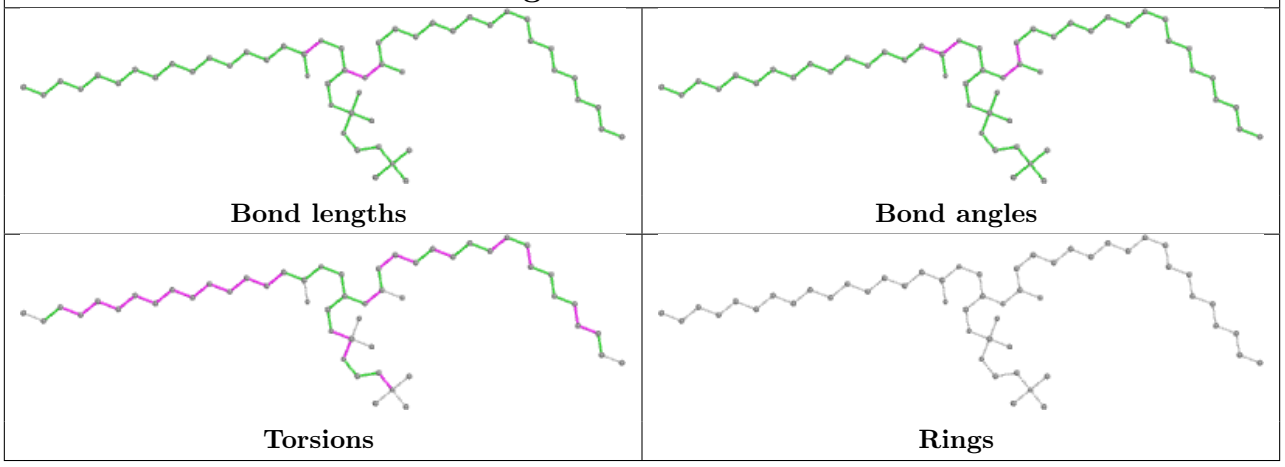
Ligand POV D 810

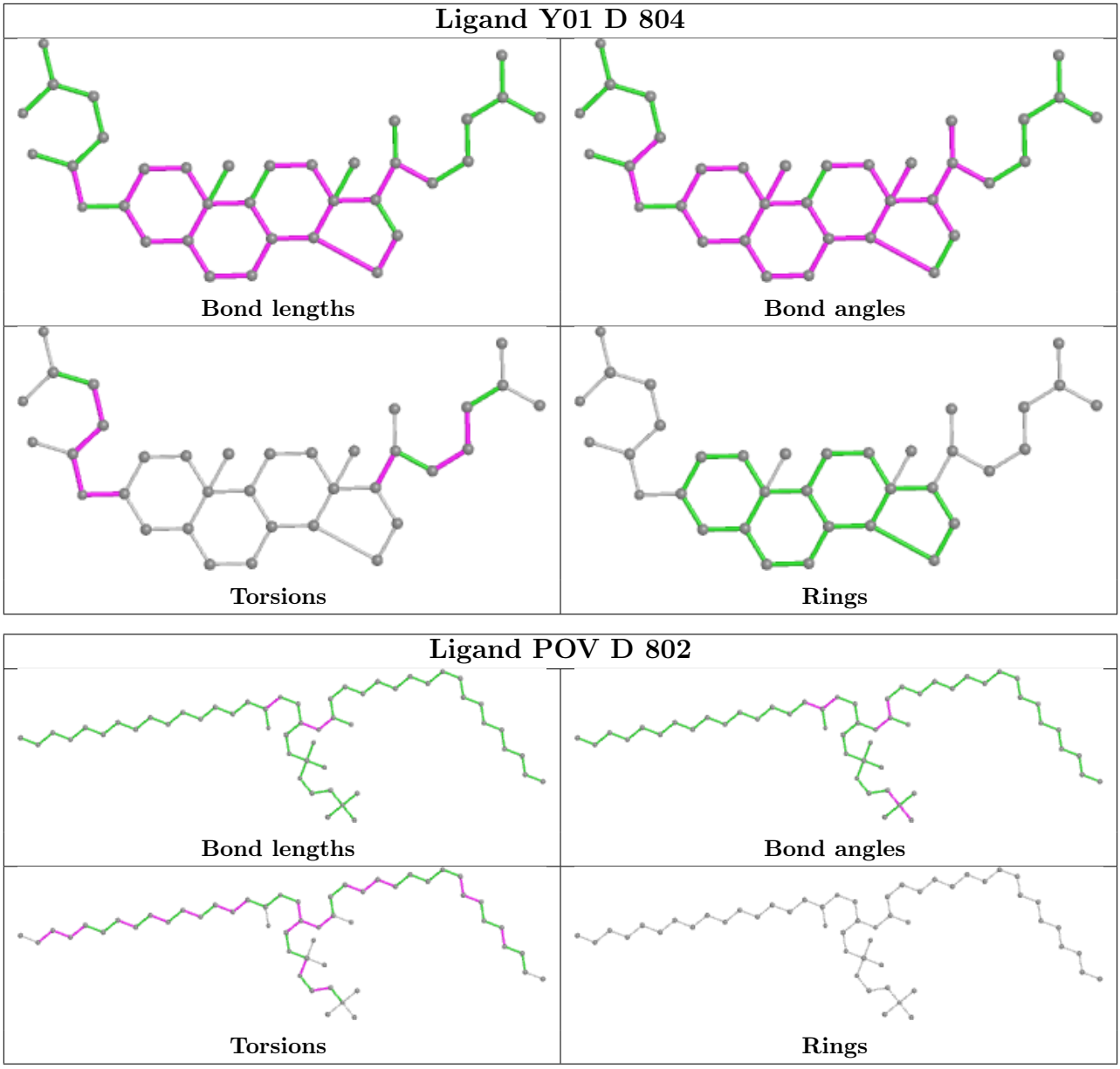


Ligand POV D 806



Ligand POV A 805





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

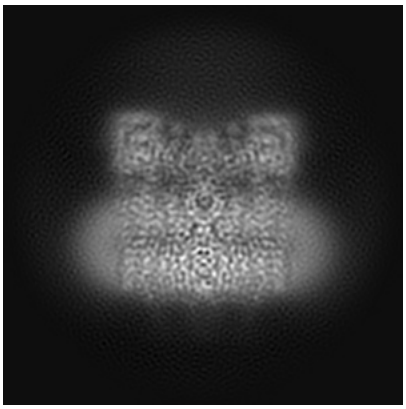
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29343. These allow visual inspection of the internal detail of the map and identification of artifacts.

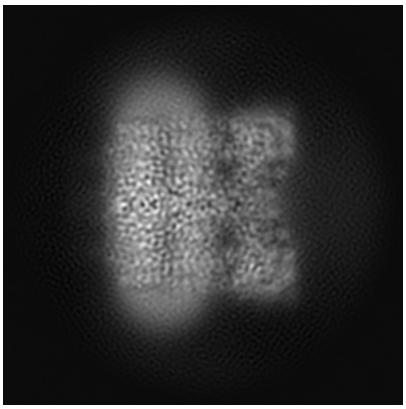
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

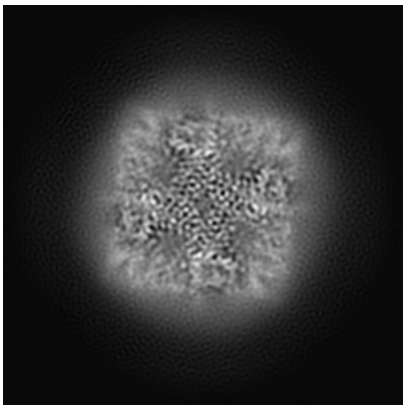
6.1.1 Primary map



X

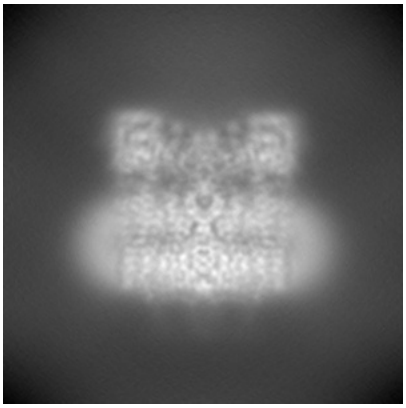


Y

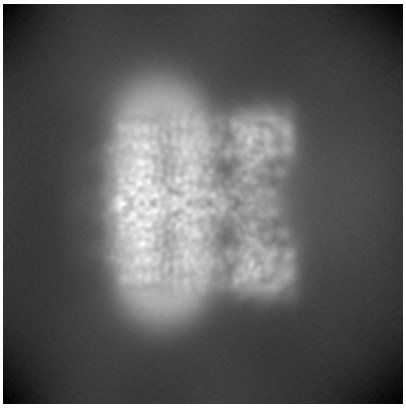


Z

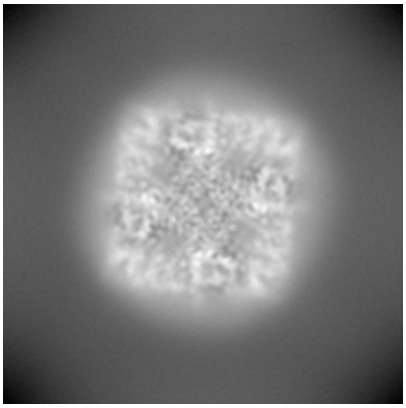
6.1.2 Raw map



X



Y

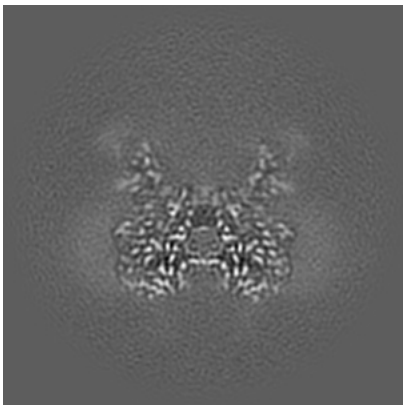


Z

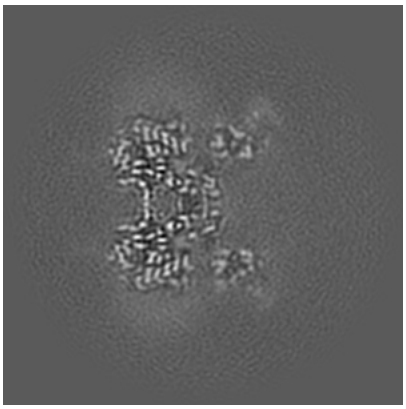
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

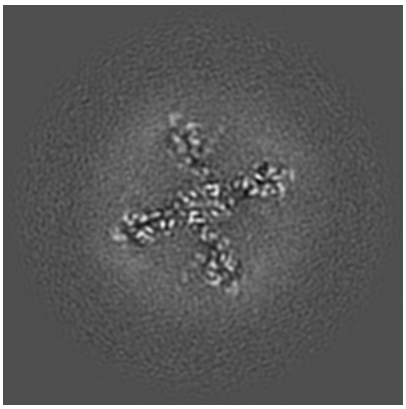
6.2.1 Primary map



X Index: 128

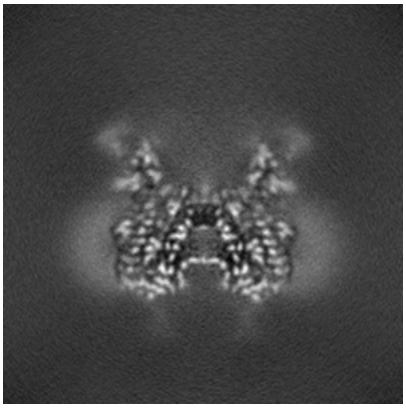


Y Index: 128

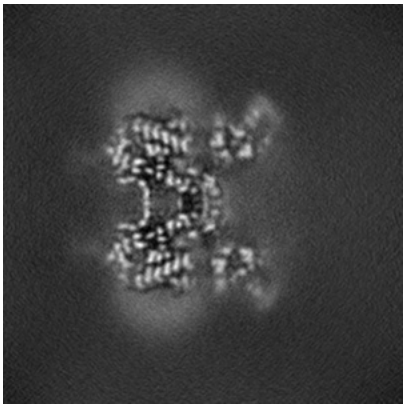


Z Index: 128

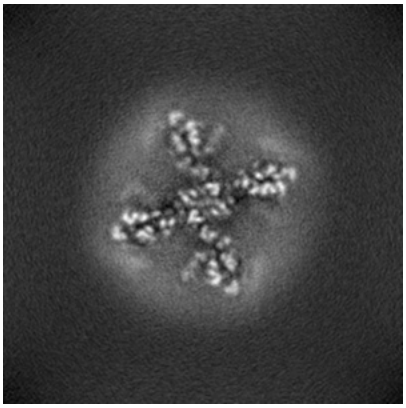
6.2.2 Raw map



X Index: 128



Y Index: 128

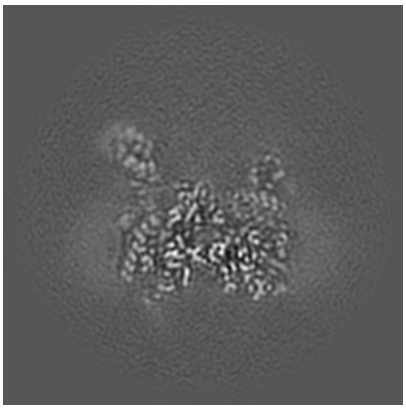


Z Index: 128

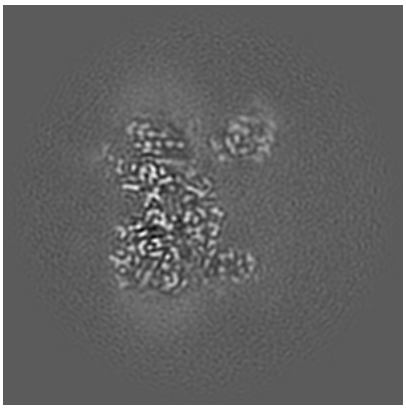
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

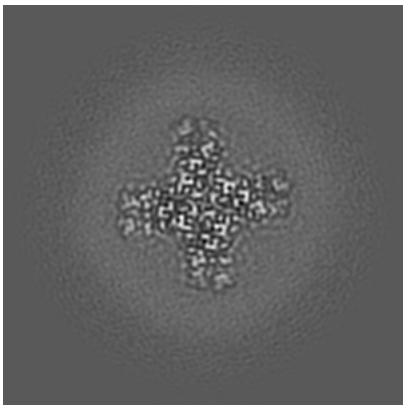
6.3.1 Primary map



X Index: 123

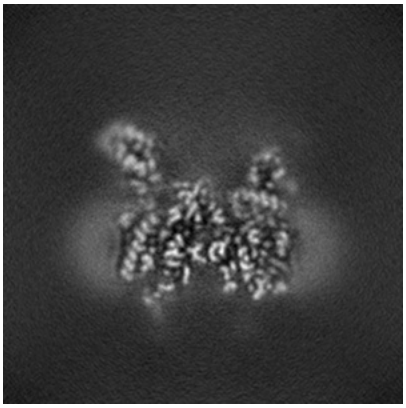


Y Index: 123

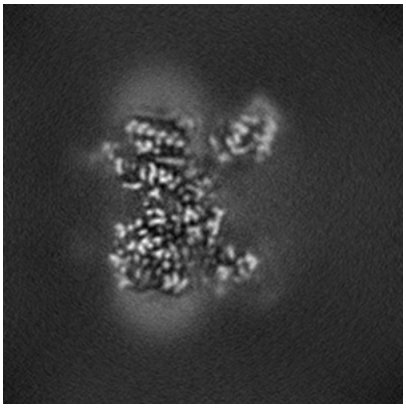


Z Index: 93

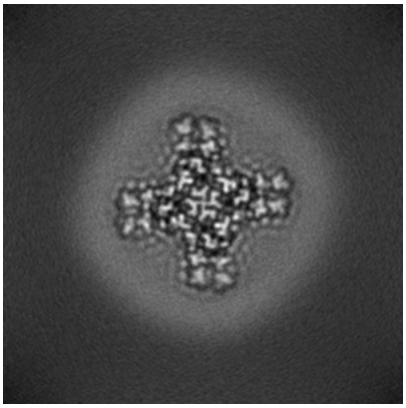
6.3.2 Raw map



X Index: 123



Y Index: 124

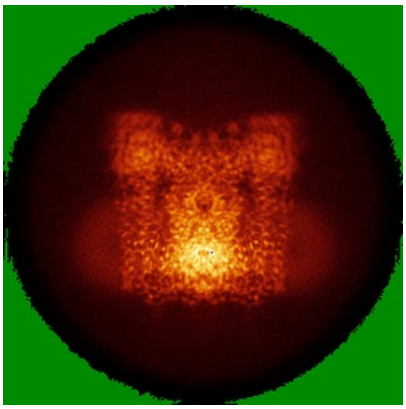


Z Index: 92

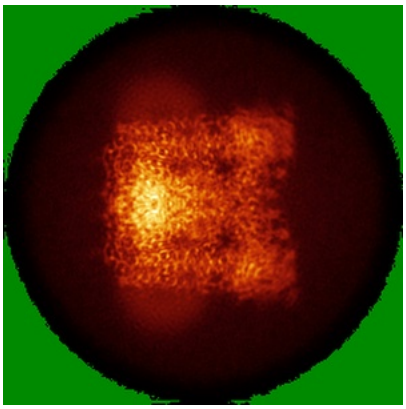
The images above show the largest variance slices of the map in three orthogonal directions.

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

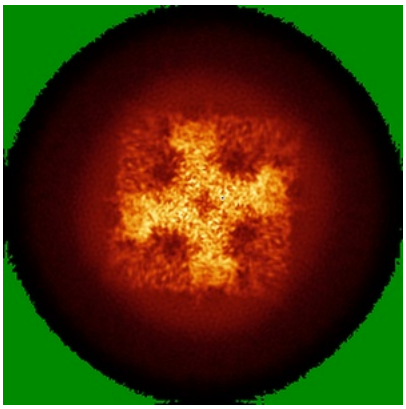
6.4.1 Primary map



X

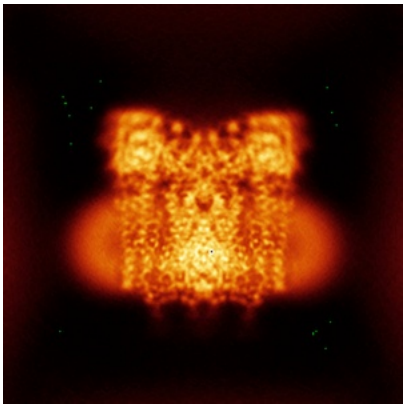


Y

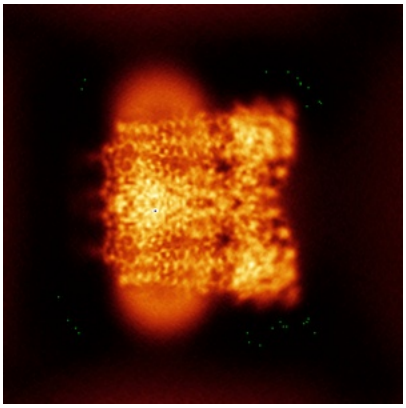


Z

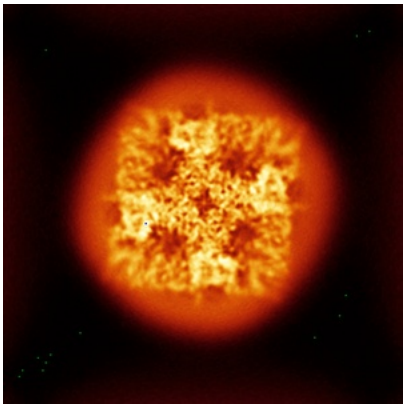
6.4.2 Raw map



X



Y

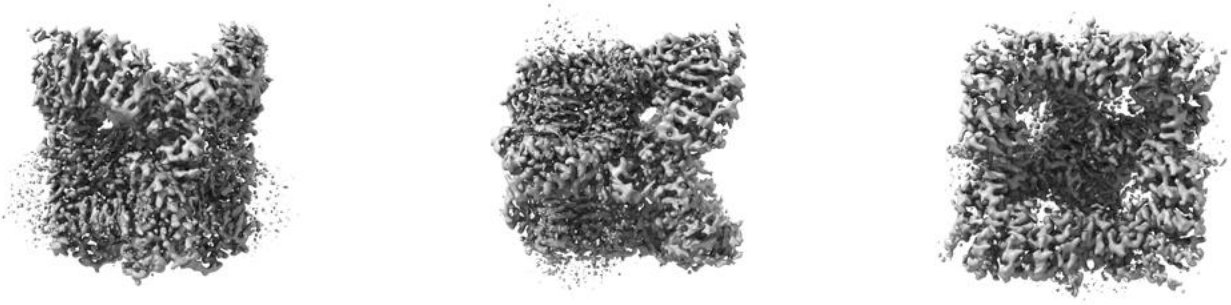


Z

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)

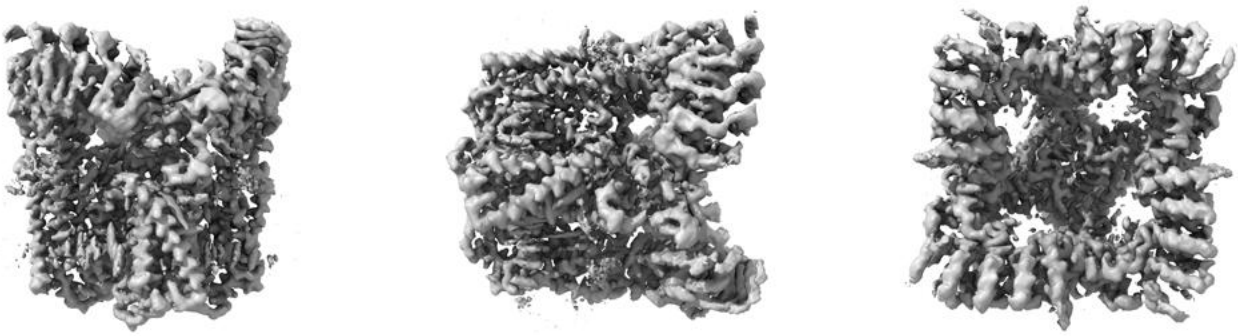
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.537. 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.

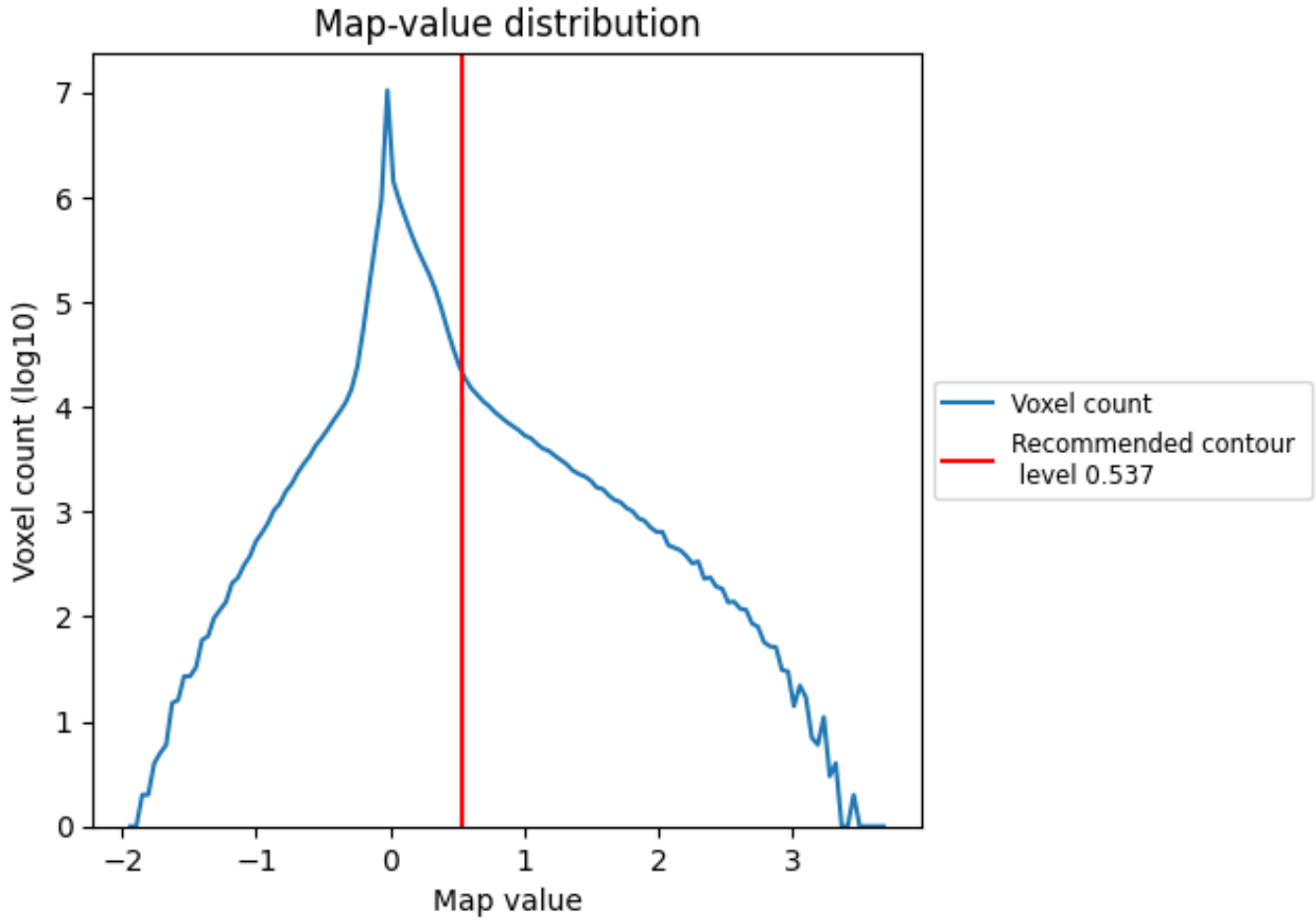
6.6 Mask visualisation (i)

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

7 Map analysis

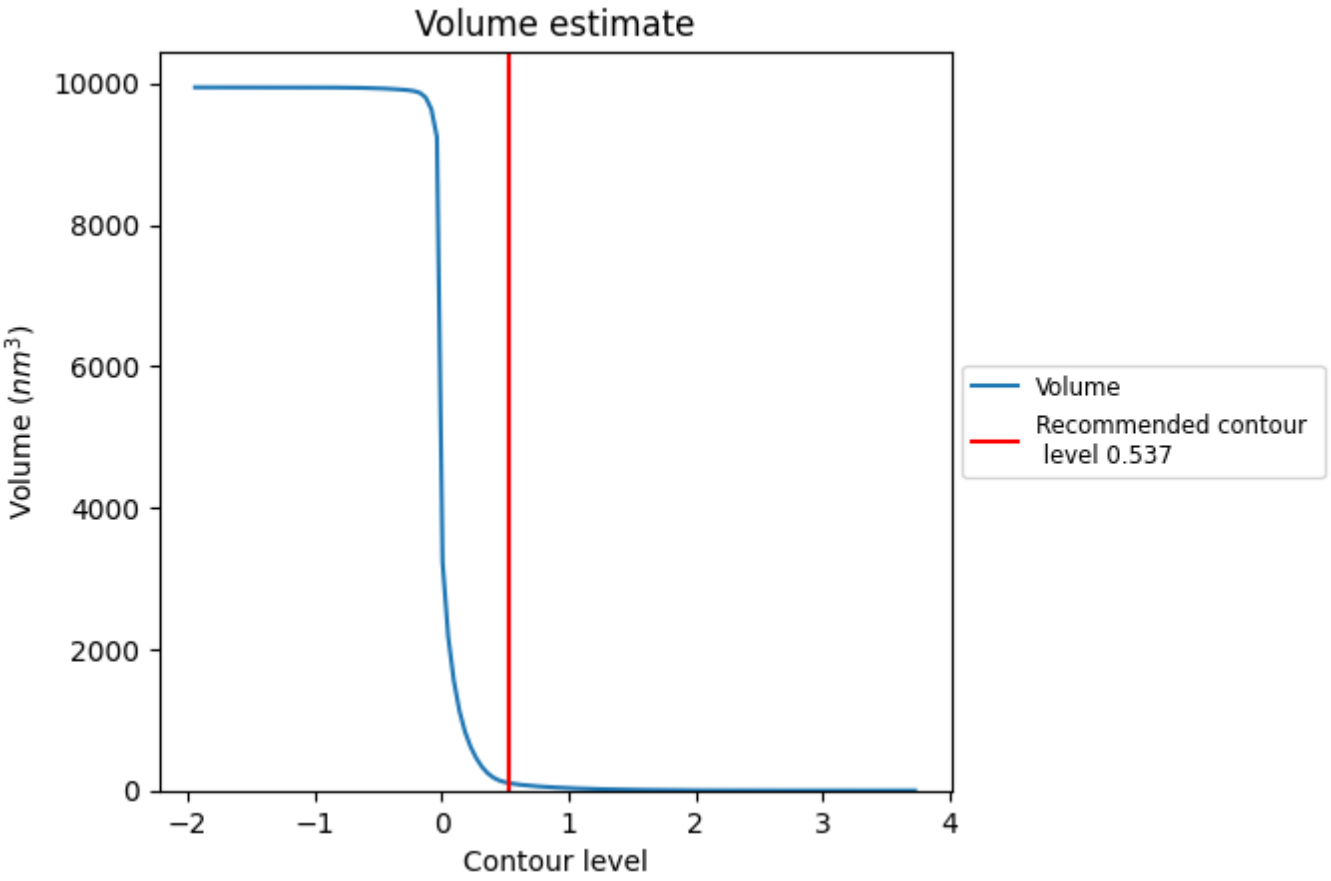
This section contains the results of statistical analysis of the map.

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.

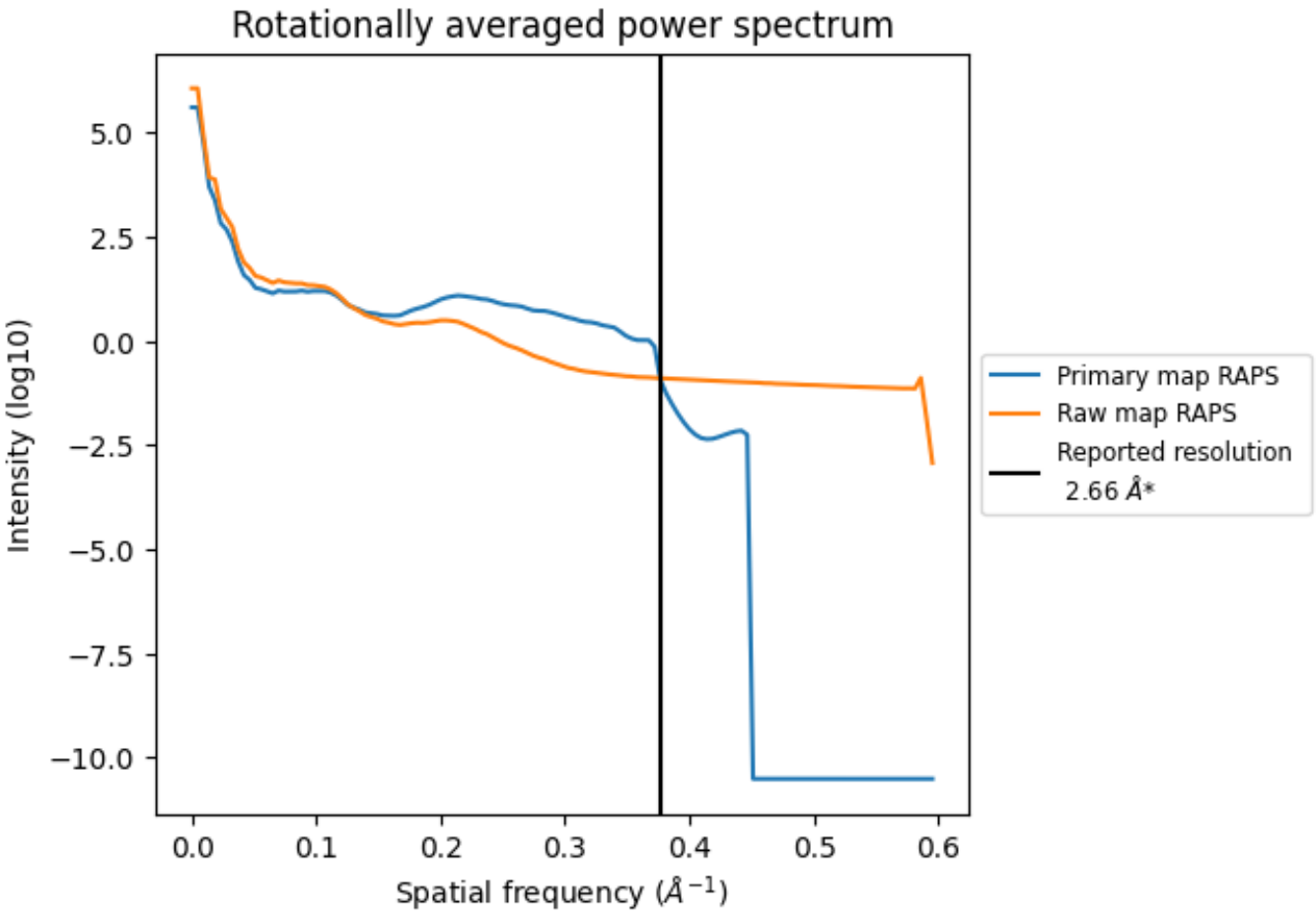
7.2 Volume estimate



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

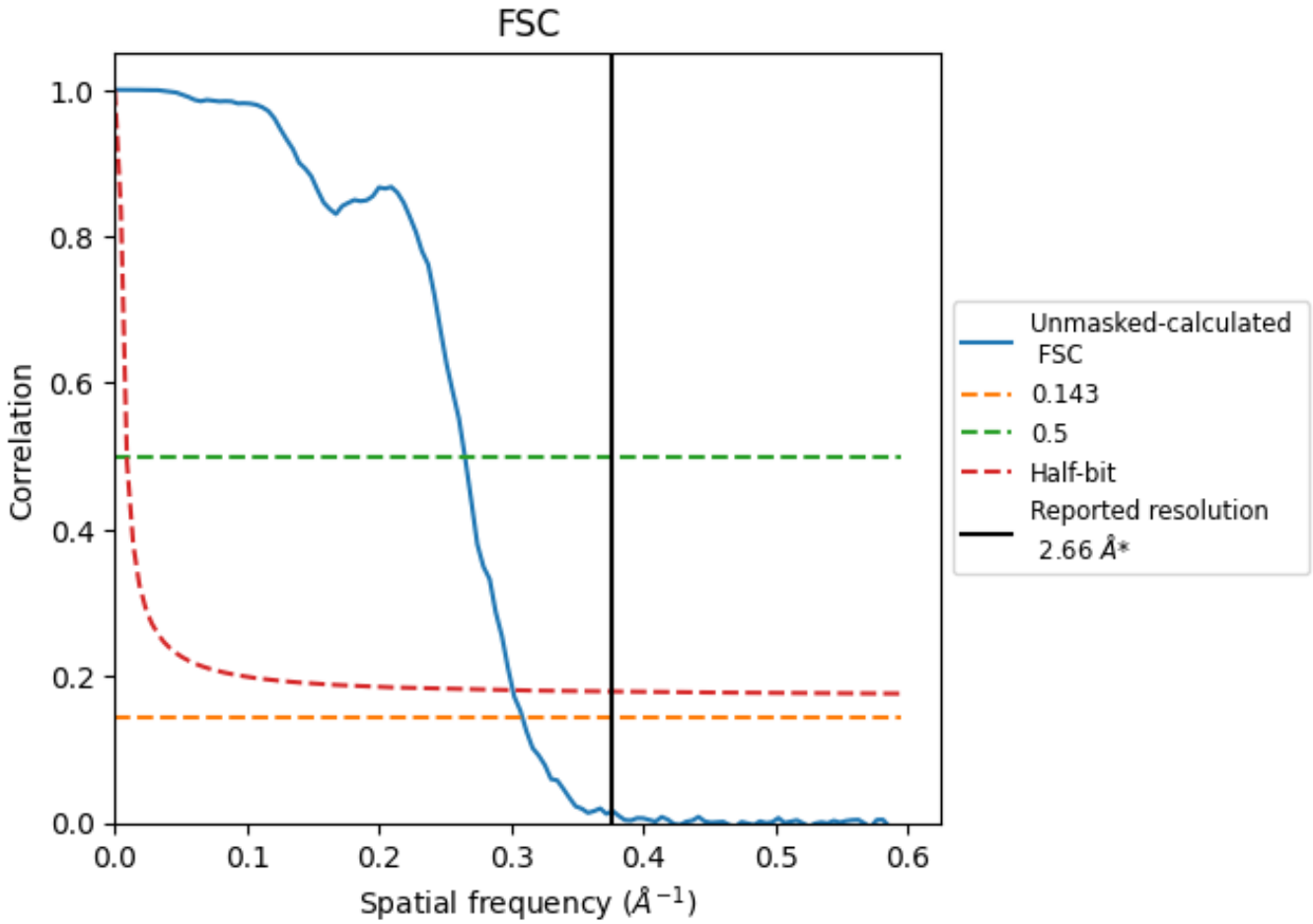


*Reported resolution corresponds to spatial frequency of 0.376 $Å^{-1}$

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 0.376 Å^{-1}

8.2 Resolution estimates (i)

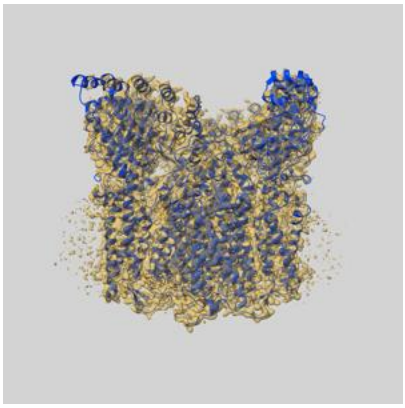
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.24	3.78	3.32

*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 3.24 differs from the reported value 2.66 by more than 10 %

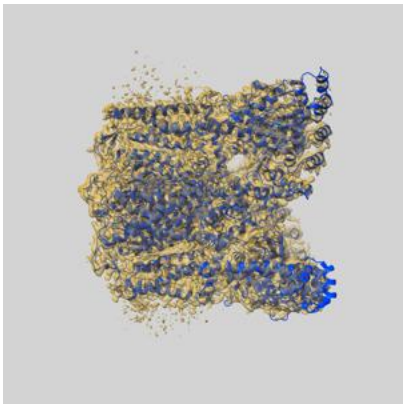
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29343 and PDB model 8FOA. Per-residue inclusion information can be found in section 3 on page 9.

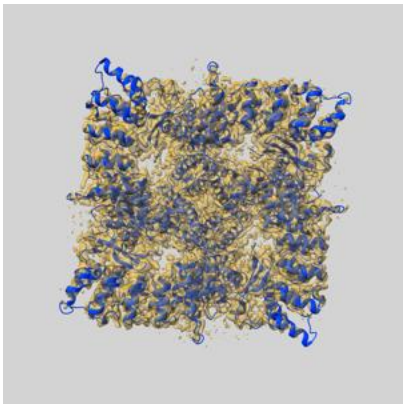
9.1 Map-model overlay



X



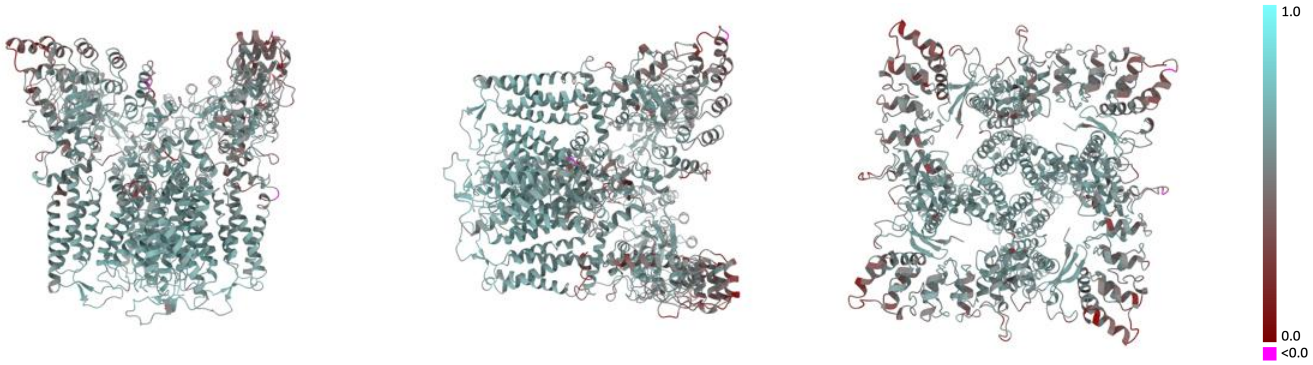
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.537 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.

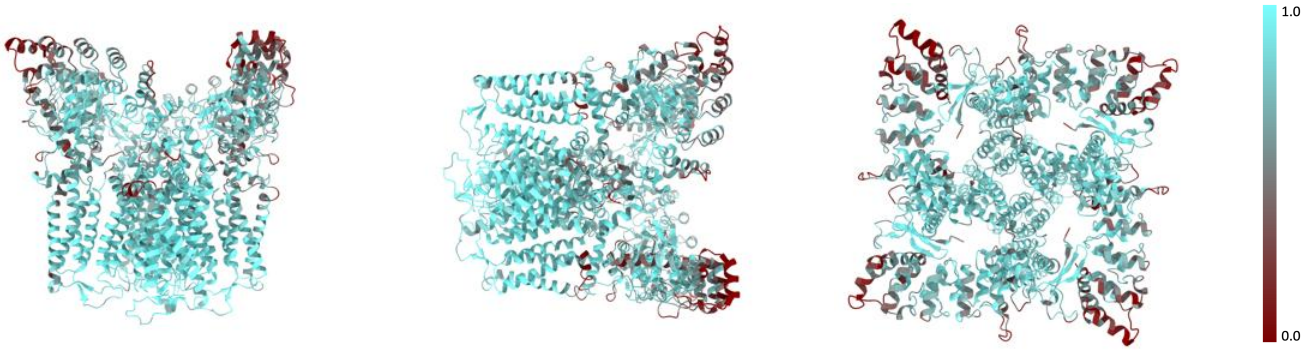
9.2 Q-score mapped to coordinate model (i)



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.

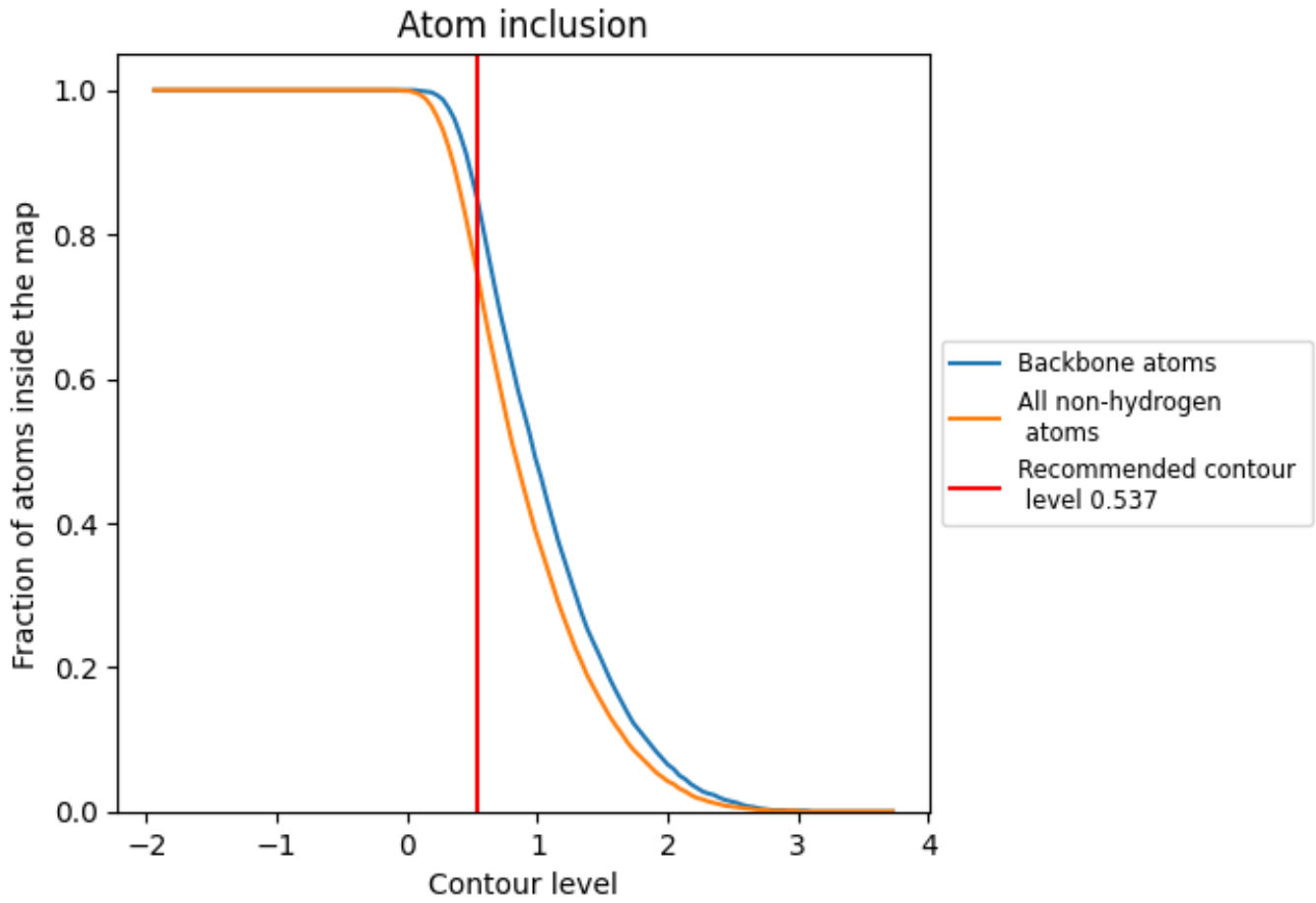
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.537).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 75% 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 (0.537) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7470	0.5460
A	0.7660	0.5540
B	0.7590	0.5520
C	0.7210	0.5330
D	0.7420	0.5440