Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 02:17 PM EST

PDB ID	:	7MIN
EMDB ID	:	EMD-23857
Title	:	Mouse TRPV3 in cNW11 nanodiscs, closed state at 42 degrees Celsius
Authors	:	Nadezhdin, K.D.; Neuberger, A.; Sobolevsky, A.I.
Deposited on	:	2021-04-17
Resolution	:	3.09 Å(reported)

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

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

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

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

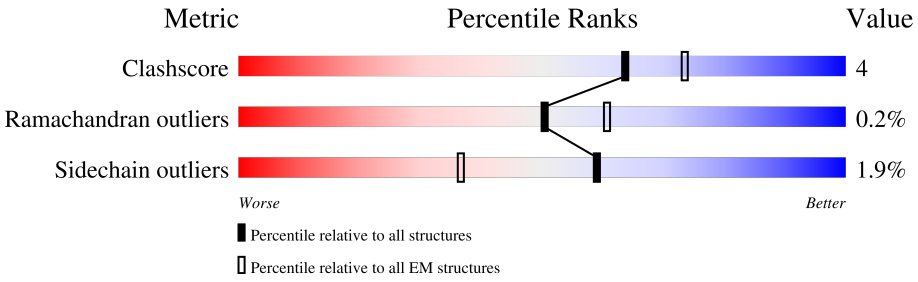
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.09 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	808	10% 73% 6% 21%
1	B	808	11% 73% 6% 21%
1	C	808	11% 72% 7% 21%
1	D	808	11% 72% 7% 21%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22728 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 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	640	Total	C	N	O	S	0	0
			5213	3388	860	934	31		
1	B	640	Total	C	N	O	S	0	0
			5213	3388	860	934	31		
1	C	640	Total	C	N	O	S	0	0
			5213	3388	860	934	31		
1	D	640	Total	C	N	O	S	0	0
			5213	3388	860	934	31		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	792	LEU	-	expression tag	UNP Q8K424
A	793	VAL	-	expression tag	UNP Q8K424
A	794	PRO	-	expression tag	UNP Q8K424
A	795	ARG	-	expression tag	UNP Q8K424
A	796	GLY	-	expression tag	UNP Q8K424
A	797	SER	-	expression tag	UNP Q8K424
A	798	ALA	-	expression tag	UNP Q8K424
A	799	ALA	-	expression tag	UNP Q8K424
A	800	ALA	-	expression tag	UNP Q8K424
A	801	TRP	-	expression tag	UNP Q8K424
A	802	SER	-	expression tag	UNP Q8K424
A	803	HIS	-	expression tag	UNP Q8K424
A	804	PRO	-	expression tag	UNP Q8K424
A	805	GLN	-	expression tag	UNP Q8K424
A	806	PHE	-	expression tag	UNP Q8K424
A	807	GLU	-	expression tag	UNP Q8K424
A	808	LYS	-	expression tag	UNP Q8K424
B	792	LEU	-	expression tag	UNP Q8K424
B	793	VAL	-	expression tag	UNP Q8K424
B	794	PRO	-	expression tag	UNP Q8K424
B	795	ARG	-	expression tag	UNP Q8K424

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Chain	Residue	Modelled	Actual	Comment	Reference
B	796	GLY	-	expression tag	UNP Q8K424
B	797	SER	-	expression tag	UNP Q8K424
B	798	ALA	-	expression tag	UNP Q8K424
B	799	ALA	-	expression tag	UNP Q8K424
B	800	ALA	-	expression tag	UNP Q8K424
B	801	TRP	-	expression tag	UNP Q8K424
B	802	SER	-	expression tag	UNP Q8K424
B	803	HIS	-	expression tag	UNP Q8K424
B	804	PRO	-	expression tag	UNP Q8K424
B	805	GLN	-	expression tag	UNP Q8K424
B	806	PHE	-	expression tag	UNP Q8K424
B	807	GLU	-	expression tag	UNP Q8K424
B	808	LYS	-	expression tag	UNP Q8K424
C	792	LEU	-	expression tag	UNP Q8K424
C	793	VAL	-	expression tag	UNP Q8K424
C	794	PRO	-	expression tag	UNP Q8K424
C	795	ARG	-	expression tag	UNP Q8K424
C	796	GLY	-	expression tag	UNP Q8K424
C	797	SER	-	expression tag	UNP Q8K424
C	798	ALA	-	expression tag	UNP Q8K424
C	799	ALA	-	expression tag	UNP Q8K424
C	800	ALA	-	expression tag	UNP Q8K424
C	801	TRP	-	expression tag	UNP Q8K424
C	802	SER	-	expression tag	UNP Q8K424
C	803	HIS	-	expression tag	UNP Q8K424
C	804	PRO	-	expression tag	UNP Q8K424
C	805	GLN	-	expression tag	UNP Q8K424
C	806	PHE	-	expression tag	UNP Q8K424
C	807	GLU	-	expression tag	UNP Q8K424
C	808	LYS	-	expression tag	UNP Q8K424
D	792	LEU	-	expression tag	UNP Q8K424
D	793	VAL	-	expression tag	UNP Q8K424
D	794	PRO	-	expression tag	UNP Q8K424
D	795	ARG	-	expression tag	UNP Q8K424
D	796	GLY	-	expression tag	UNP Q8K424
D	797	SER	-	expression tag	UNP Q8K424
D	798	ALA	-	expression tag	UNP Q8K424
D	799	ALA	-	expression tag	UNP Q8K424
D	800	ALA	-	expression tag	UNP Q8K424
D	801	TRP	-	expression tag	UNP Q8K424
D	802	SER	-	expression tag	UNP Q8K424
D	803	HIS	-	expression tag	UNP Q8K424

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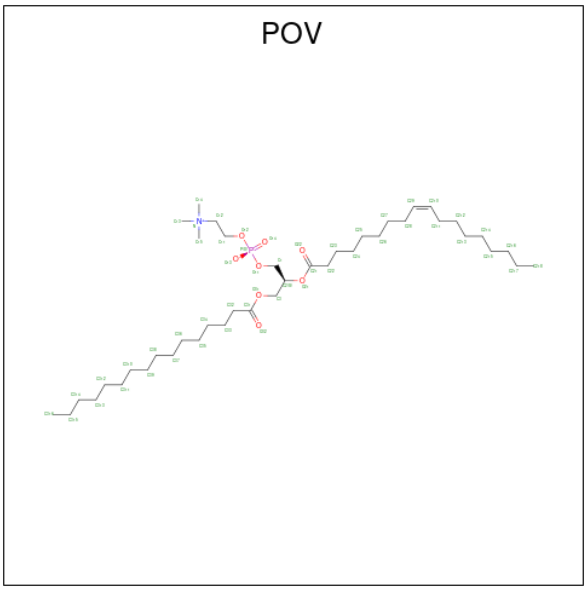
Chain	Residue	Modelled	Actual	Comment	Reference
D	804	PRO	-	expression tag	UNP Q8K424
D	805	GLN	-	expression tag	UNP Q8K424
D	806	PHE	-	expression tag	UNP Q8K424
D	807	GLU	-	expression tag	UNP Q8K424
D	808	LYS	-	expression tag	UNP Q8K424

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



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	A	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	A	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	A	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	A	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	A	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	A	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	A	1	Total	C	N	O	P	0
			468	378	9	72	9	

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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	B	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	B	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	B	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	B	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	B	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	B	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	B	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	B	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	B	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	B	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	C	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	C	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	C	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	C	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	C	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	C	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	C	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	C	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	C	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	D	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	D	1	Total	C	N	O	P	0
			468	378	9	72	9	

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Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	D	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	D	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	D	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	D	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	D	1	Total	C	N	O	P	0
			468	378	9	72	9	
2	D	1	Total	C	N	O	P	0
			468	378	9	72	9	

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

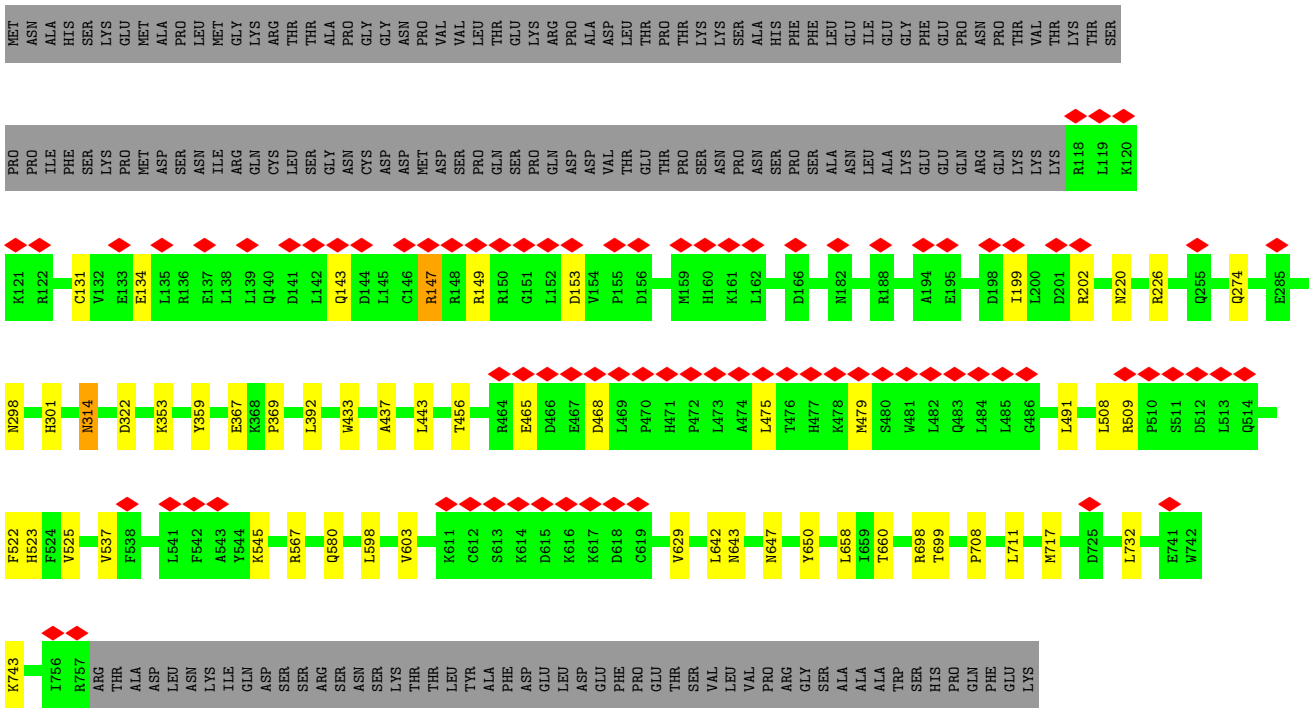
Mol	Chain	Residues	Atoms		AltConf
3	A	4	Total	Na	0
			4	4	

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.

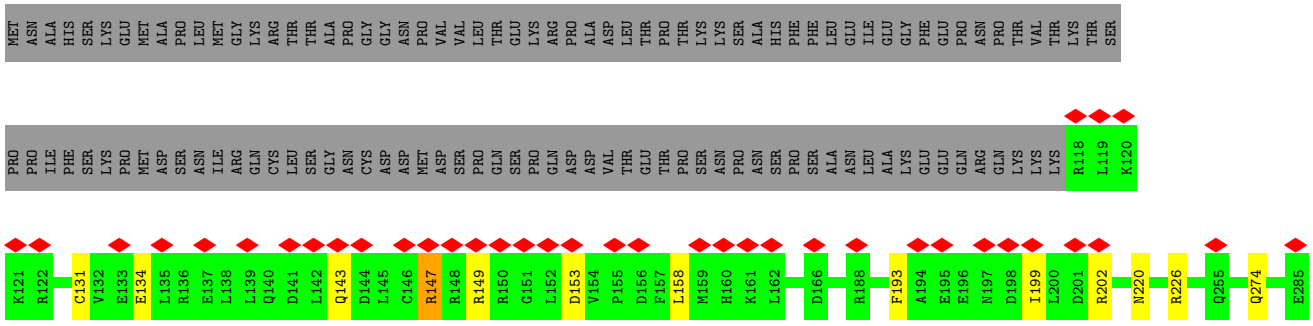
• Molecule 1: Transient receptor potential cation channel subfamily V member 3

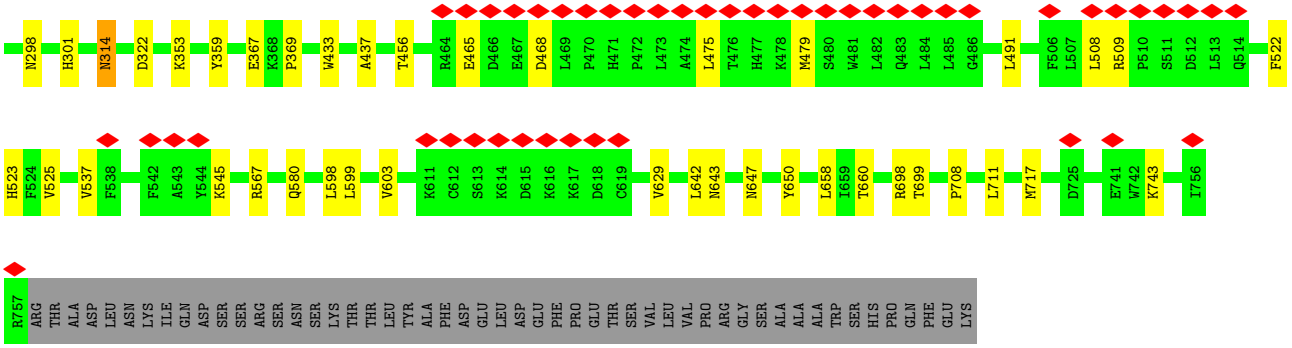
Chain A:



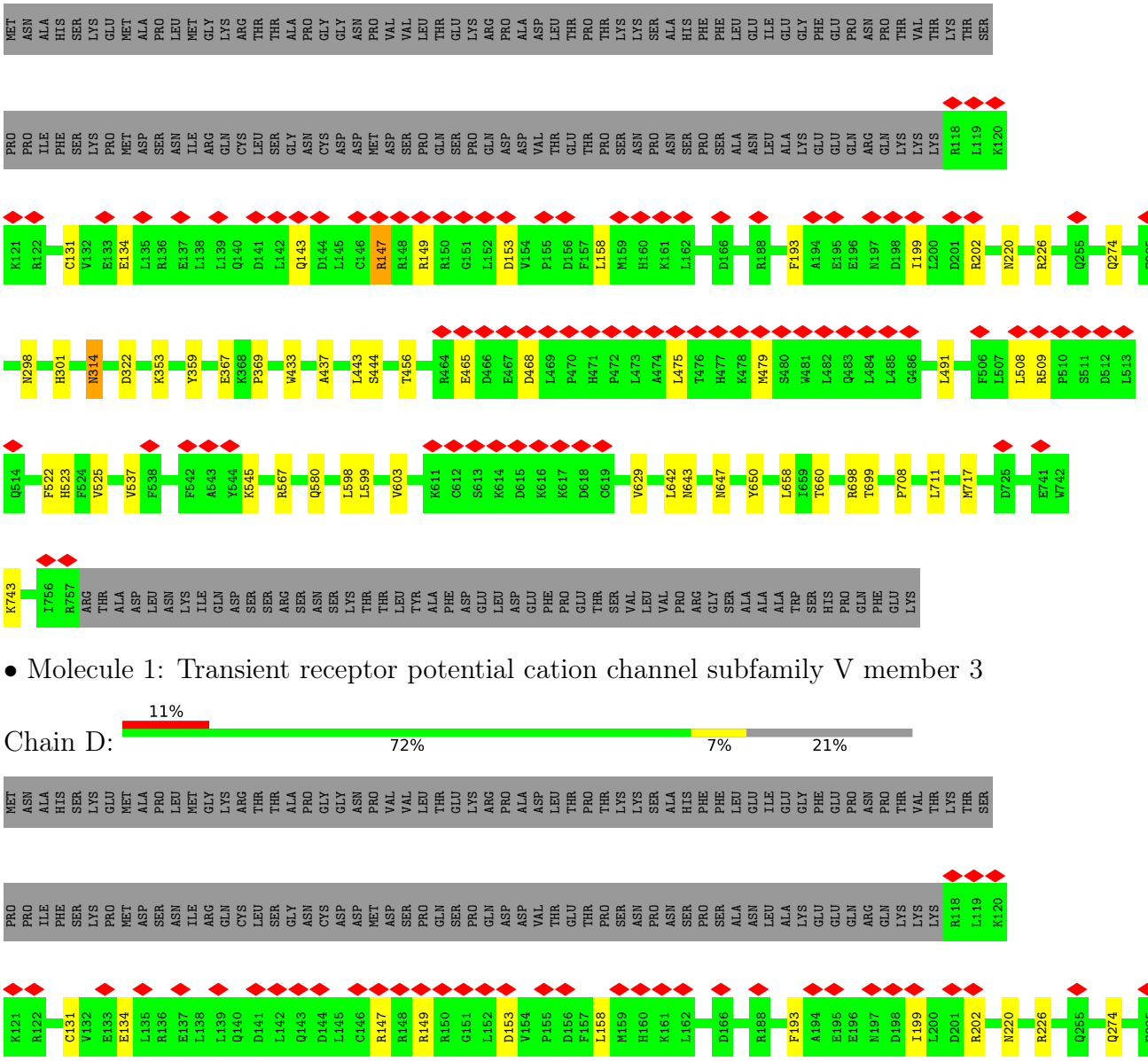
• Molecule 1: Transient receptor potential cation channel subfamily V member 3

Chain B:

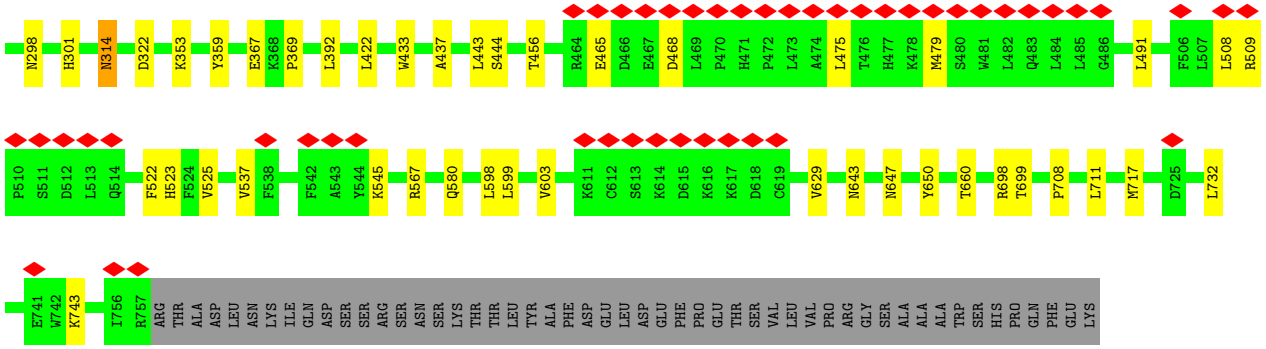




• Molecule 1: Transient receptor potential cation channel subfamily V member 3



• Molecule 1: Transient receptor potential cation channel subfamily V member 3


N298 H301 N314 D322 K353 Y359 E367 K368 P369 L392 L422 W433 A437 L443 S444 T456 R464 E465 D466 E467 D468 L469 P470 H471 P472 L473 A474 L475 T476 H477 K478 M479 S480 W481 L482 Q483 L484 L485 G486 L491 F506 L507 L508 R509
P510 S511 D512 L513 Q514 F522 H523 F524 V525 V537 F538 F542 A543 Y544 K545 R567 Q580 L598 L599 V603 K611 G612 S613 K614 D615 K616 K617 D618 G619 V629 N643 N647 Y650 T660 R698 T699 P708 L711 M717 D725 L732
E741 W742 K743 I756 R757 ARG THR ALA ASP LEU ASN LYS ILE GLN ASP SER SER ARG SER ASN SER LYS THR THR LEU TYR ALA PHE ASP GLU LEU ASP GLU PHE PRO GLU THR SER VAL LEU VAL PRO ARG GLY SER ALA ALA ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39182	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 ($e^-/Å^2$)	59	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0173	Depositor
Map size (Å)	222.92992, 222.92992, 222.92992	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87082, 0.87082, 0.87082	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.39	0/5327	0.56	0/7211
1	B	0.39	0/5327	0.56	0/7211
1	C	0.39	0/5327	0.56	0/7211
1	D	0.39	0/5327	0.56	0/7211
All	All	0.39	0/21308	0.56	0/28844

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5213	0	5280	29	0
1	B	5213	0	5280	28	0
1	C	5213	0	5280	31	0
1	D	5213	0	5280	31	0
2	A	468	0	738	30	0
2	B	468	0	738	30	0
2	C	468	0	738	34	0
2	D	468	0	738	30	0
3	A	4	0	0	0	0
All	All	22728	0	24072	202	0

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

All (202) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:ARG:HH11	2:D:909:POV:H13	1.49	0.77
1:A:567:ARG:HH11	2:A:904:POV:H13	1.54	0.73
1:B:567:ARG:HH11	2:B:907:POV:H13	1.54	0.73
1:C:567:ARG:HH11	2:C:907:POV:H13	1.54	0.72
1:C:367:GLU:HG2	1:C:369:PRO:HD2	1.83	0.61
1:D:367:GLU:HG2	1:D:369:PRO:HD2	1.83	0.61
1:B:367:GLU:HG2	1:B:369:PRO:HD2	1.83	0.60
1:A:367:GLU:HG2	1:A:369:PRO:HD2	1.83	0.60
1:C:567:ARG:NH2	1:C:699:THR:OG1	2.36	0.59
1:D:567:ARG:NH2	1:D:699:THR:OG1	2.36	0.59
1:B:567:ARG:NH2	1:B:699:THR:OG1	2.36	0.58
1:A:567:ARG:NH2	1:A:699:THR:OG1	2.36	0.58
1:A:660:THR:HG23	2:A:906:POV:H31D	1.85	0.57
1:C:660:THR:HG23	2:C:909:POV:H31D	1.87	0.57
2:B:905:POV:H34A	2:B:905:POV:H28A	1.86	0.57
2:A:901:POV:H21E	2:A:903:POV:H312	1.87	0.56
2:D:906:POV:H21E	2:D:908:POV:H312	1.87	0.56
2:A:905:POV:H29	2:B:907:POV:H31F	1.87	0.56
2:B:904:POV:H21E	2:B:906:POV:H312	1.88	0.56
1:D:131:CYS:HB3	1:D:134:GLU:HB2	1.87	0.56
1:A:131:CYS:HB3	1:A:134:GLU:HB2	1.87	0.56
2:C:904:POV:H21E	2:C:906:POV:H312	1.87	0.56
2:B:908:POV:H29	2:C:907:POV:H31F	1.87	0.56
1:A:199:ILE:HG22	1:A:202:ARG:HB2	1.88	0.56
1:B:131:CYS:HB3	1:B:134:GLU:HB2	1.87	0.56
1:B:199:ILE:HG22	1:B:202:ARG:HB2	1.88	0.56
1:C:131:CYS:HB3	1:C:134:GLU:HB2	1.87	0.55
1:C:199:ILE:HG22	1:C:202:ARG:HB2	1.88	0.55
1:B:660:THR:HG23	2:B:909:POV:H31D	1.89	0.55
2:C:906:POV:H22	2:C:906:POV:H15B	1.89	0.55
2:B:902:POV:H3A	2:B:902:POV:H15B	1.89	0.54
1:D:298:ASN:OD1	1:D:301:HIS:ND1	2.36	0.54
2:A:904:POV:H31F	2:D:901:POV:H29	1.88	0.54
1:D:199:ILE:HG22	1:D:202:ARG:HB2	1.88	0.54
2:D:904:POV:H3A	2:D:904:POV:H15B	1.89	0.54
1:D:660:THR:HG23	2:D:902:POV:H31D	1.87	0.54
2:C:908:POV:H29	2:D:909:POV:H31F	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:TRP:HA	1:B:437:ALA:HB3	1.90	0.54
1:C:433:TRP:HA	1:C:437:ALA:HB3	1.90	0.54
2:D:908:POV:H22	2:D:908:POV:H15B	1.90	0.54
2:A:908:POV:H3A	2:A:908:POV:H15B	1.89	0.53
2:A:903:POV:H38A	2:A:903:POV:H214	1.90	0.53
2:B:906:POV:H22	2:B:906:POV:H15B	1.89	0.53
2:A:903:POV:H22	2:A:903:POV:H15B	1.89	0.53
2:D:908:POV:H214	2:D:908:POV:H38A	1.90	0.53
2:B:906:POV:H214	2:B:906:POV:H38A	1.90	0.52
2:C:902:POV:H15B	2:C:902:POV:H3A	1.89	0.52
1:D:433:TRP:HA	1:D:437:ALA:HB3	1.90	0.52
1:A:433:TRP:HA	1:A:437:ALA:HB3	1.90	0.52
1:A:298:ASN:OD1	1:A:301:HIS:ND1	2.36	0.52
1:A:465:GLU:HB2	1:A:468:ASP:HB2	1.92	0.52
1:C:603:VAL:HG11	1:D:456:THR:HG23	1.91	0.52
1:A:456:THR:HG23	1:D:603:VAL:HG11	1.92	0.52
2:C:906:POV:H38A	2:C:906:POV:H214	1.90	0.52
1:B:465:GLU:HB2	1:B:468:ASP:HB2	1.92	0.51
1:A:523:HIS:HD2	2:A:902:POV:H15	1.76	0.51
1:C:465:GLU:HB2	1:C:468:ASP:HB2	1.92	0.51
2:C:905:POV:H34A	2:C:905:POV:H28A	1.92	0.51
1:A:603:VAL:HG11	1:B:456:THR:HG23	1.92	0.51
1:C:522:PHE:HA	1:C:525:VAL:HG12	1.93	0.51
1:D:465:GLU:HB2	1:D:468:ASP:HB2	1.92	0.51
2:A:907:POV:H213	2:D:906:POV:H314	1.93	0.51
2:B:901:POV:H21G	2:B:903:POV:H35A	1.93	0.50
2:B:906:POV:H316	2:C:903:POV:H35	1.94	0.50
1:D:522:PHE:HA	1:D:525:VAL:HG12	1.93	0.50
2:A:901:POV:H314	2:B:901:POV:H213	1.94	0.50
2:C:904:POV:H314	2:D:903:POV:H213	1.93	0.50
2:A:909:POV:H31C	2:A:909:POV:H29	1.92	0.50
1:B:523:HIS:HD2	2:B:905:POV:H15	1.76	0.50
1:B:603:VAL:HG11	1:C:456:THR:HG23	1.92	0.50
1:C:523:HIS:HD2	2:C:905:POV:H15	1.76	0.50
1:D:523:HIS:HD2	2:D:907:POV:H15	1.76	0.50
1:A:522:PHE:HA	1:A:525:VAL:HG12	1.93	0.50
1:B:298:ASN:OD1	1:B:301:HIS:ND1	2.36	0.50
2:C:903:POV:H29	2:C:903:POV:H31C	1.94	0.50
2:A:903:POV:H316	2:B:903:POV:H35	1.94	0.49
2:C:901:POV:H21G	2:C:903:POV:H35A	1.93	0.49
1:B:522:PHE:HA	1:B:525:VAL:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:MET:SD	1:B:717:MET:N	2.86	0.49
2:B:903:POV:H29	2:B:903:POV:H31C	1.94	0.49
1:A:717:MET:SD	1:A:717:MET:N	2.86	0.49
2:B:904:POV:H314	2:C:901:POV:H213	1.94	0.49
1:C:298:ASN:OD1	1:C:301:HIS:ND1	2.36	0.49
2:D:905:POV:H31C	2:D:905:POV:H29	1.94	0.49
1:D:717:MET:SD	1:D:717:MET:N	2.86	0.49
2:A:907:POV:H21G	2:A:909:POV:H35A	1.94	0.49
2:D:903:POV:H21G	2:D:905:POV:H35A	1.93	0.49
2:A:909:POV:H35	2:D:908:POV:H316	1.95	0.48
1:C:717:MET:SD	1:C:717:MET:N	2.86	0.48
1:B:508:LEU:HD13	1:B:698:ARG:HH22	1.79	0.48
2:C:901:POV:H211	2:C:901:POV:H21D	1.75	0.48
1:A:508:LEU:HD13	1:A:698:ARG:HH22	1.79	0.48
1:C:149:ARG:NH2	1:C:153:ASP:OD1	2.47	0.48
1:A:149:ARG:NH2	1:A:153:ASP:OD1	2.47	0.48
2:C:903:POV:H13B	2:C:903:POV:H11	1.75	0.47
1:B:149:ARG:NH2	1:B:153:ASP:OD1	2.47	0.47
1:C:508:LEU:HD13	1:C:698:ARG:HH22	1.79	0.47
1:D:508:LEU:HD13	1:D:698:ARG:HH22	1.79	0.47
1:D:149:ARG:NH2	1:D:153:ASP:OD1	2.47	0.47
1:C:708:PRO:HD2	1:C:711:LEU:HD23	1.97	0.47
1:A:545:LYS:O	1:D:650:TYR:OH	2.33	0.46
1:A:708:PRO:HD2	1:A:711:LEU:HD23	1.98	0.46
1:D:708:PRO:HD2	1:D:711:LEU:HD23	1.98	0.46
1:B:708:PRO:HD2	1:B:711:LEU:HD23	1.97	0.46
2:C:906:POV:H316	2:D:905:POV:H35	1.96	0.46
1:A:598:LEU:HD21	1:A:629:VAL:HG13	1.97	0.46
1:C:598:LEU:HD21	1:C:629:VAL:HG13	1.97	0.46
1:B:598:LEU:HD21	1:B:629:VAL:HG13	1.97	0.45
2:C:901:POV:H21D	2:C:901:POV:H217	1.78	0.45
1:D:491:LEU:HD21	1:D:537:VAL:HG21	1.98	0.45
1:D:598:LEU:HD21	1:D:629:VAL:HG13	1.97	0.45
2:A:907:POV:H211	2:A:907:POV:H21D	1.75	0.45
2:A:909:POV:H13B	2:A:909:POV:H11	1.75	0.45
1:D:443:LEU:HD13	2:D:907:POV:H34	1.99	0.45
1:B:491:LEU:HD21	1:B:537:VAL:HG21	1.98	0.45
2:B:904:POV:H36A	2:B:904:POV:H33	1.78	0.45
1:C:491:LEU:HD21	1:C:537:VAL:HG21	1.98	0.45
1:C:143:GLN:O	1:C:147:ARG:NE	2.45	0.44
1:D:443:LEU:HD11	2:D:903:POV:H31E	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LEU:HD13	2:A:902:POV:H34A	1.99	0.44
1:A:491:LEU:HD21	1:A:537:VAL:HG21	1.98	0.44
2:C:904:POV:H36A	2:C:904:POV:H33	1.78	0.43
1:C:650:TYR:OH	1:D:545:LYS:O	2.36	0.43
2:B:901:POV:H21D	2:B:901:POV:H211	1.75	0.43
2:C:902:POV:H2	2:C:902:POV:H12A	2.00	0.43
2:A:907:POV:H25	2:A:907:POV:H22	1.86	0.43
2:A:908:POV:H312	2:A:908:POV:H39	1.84	0.43
2:B:908:POV:H39	2:B:908:POV:H31C	1.83	0.43
1:D:322:ASP:OD1	1:D:359:TYR:OH	2.37	0.43
2:D:902:POV:H11A	2:D:902:POV:H13A	1.79	0.43
2:A:902:POV:H37A	2:A:902:POV:H34	1.71	0.43
1:B:143:GLN:O	1:B:147:ARG:NE	2.45	0.43
2:C:904:POV:H11	2:C:904:POV:H15B	1.86	0.43
2:D:903:POV:H217	2:D:903:POV:H21D	1.78	0.43
1:B:650:TYR:OH	1:C:545:LYS:O	2.36	0.43
2:B:902:POV:H12A	2:B:902:POV:H2	2.01	0.43
2:B:903:POV:H28A	2:B:903:POV:H21A	1.86	0.43
1:C:322:ASP:OD1	1:C:359:TYR:OH	2.37	0.43
2:C:902:POV:H39	2:C:902:POV:H312	1.83	0.43
2:D:903:POV:H25	2:D:903:POV:H22	1.86	0.43
2:A:907:POV:H21D	2:A:907:POV:H217	1.78	0.42
1:C:443:LEU:HD11	2:C:901:POV:H31E	2.01	0.42
2:A:908:POV:H21F	2:A:908:POV:H213	1.83	0.42
2:B:901:POV:H21D	2:B:901:POV:H217	1.78	0.42
1:D:444:SER:OG	2:D:907:POV:O14	2.33	0.42
1:A:322:ASP:OD1	1:A:359:TYR:OH	2.37	0.42
2:B:903:POV:H13B	2:B:903:POV:H11	1.75	0.42
2:D:904:POV:H12A	2:D:904:POV:H2	2.01	0.42
2:C:903:POV:H25A	2:C:903:POV:H28	1.83	0.42
2:A:909:POV:H25A	2:A:909:POV:H28	1.81	0.42
1:A:650:TYR:OH	1:B:545:LYS:O	2.38	0.42
1:B:322:ASP:OD1	1:B:359:TYR:OH	2.37	0.42
1:A:226:ARG:HG2	1:A:274:GLN:NE2	2.35	0.42
1:B:226:ARG:HG2	1:B:274:GLN:NE2	2.35	0.42
2:C:901:POV:H33A	2:C:901:POV:H36	1.87	0.42
2:C:903:POV:H28A	2:C:903:POV:H21A	1.86	0.42
1:B:599:LEU:HD21	2:B:904:POV:H29	2.02	0.41
2:C:907:POV:H13B	2:C:907:POV:H11A	1.74	0.41
1:D:599:LEU:HD21	2:D:906:POV:H29	2.02	0.41
2:A:904:POV:H11A	2:A:904:POV:H13B	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:908:POV:H12A	2:A:908:POV:H2	2.00	0.41
1:B:642:LEU:HD11	1:B:658:LEU:HD21	2.03	0.41
2:C:902:POV:H28A	2:C:902:POV:H21C	2.02	0.41
2:A:905:POV:H35	2:A:905:POV:H32A	1.83	0.41
2:D:904:POV:H312	2:D:904:POV:H39	1.84	0.41
2:A:908:POV:H28A	2:A:908:POV:H21C	2.02	0.41
1:B:226:ARG:HG2	1:B:274:GLN:HE21	1.86	0.41
1:D:226:ARG:HG2	1:D:274:GLN:NE2	2.35	0.41
1:D:422:LEU:HD13	1:D:422:LEU:HA	1.95	0.41
2:D:901:POV:H32A	2:D:901:POV:H35	1.83	0.41
2:D:903:POV:H36	2:D:903:POV:H33A	1.87	0.41
2:D:908:POV:H38	2:D:908:POV:H31B	1.83	0.41
1:A:642:LEU:HD11	1:A:658:LEU:HD21	2.03	0.41
1:B:158:LEU:HD21	1:B:193:PHE:HE2	1.86	0.41
1:C:226:ARG:HG2	1:C:274:GLN:HE21	1.86	0.41
1:C:226:ARG:HG2	1:C:274:GLN:NE2	2.35	0.41
1:A:143:GLN:O	1:A:147:ARG:NE	2.45	0.41
2:A:906:POV:H11A	2:A:906:POV:H13A	1.79	0.41
1:C:642:LEU:HD11	1:C:658:LEU:HD21	2.03	0.41
2:C:902:POV:H213	2:C:902:POV:H21F	1.84	0.41
2:D:906:POV:H15B	2:D:906:POV:H11	1.86	0.41
2:B:903:POV:H25A	2:B:903:POV:H28	1.83	0.40
1:C:158:LEU:HD21	1:C:193:PHE:HE2	1.86	0.40
1:C:599:LEU:HD21	2:C:904:POV:H29	2.03	0.40
2:D:905:POV:H25A	2:D:905:POV:H28	1.83	0.40
1:A:567:ARG:HH21	1:A:699:THR:HG1	1.69	0.40
2:B:901:POV:H25	2:B:901:POV:H22	1.86	0.40
2:B:901:POV:H31H	2:B:901:POV:H31D	1.96	0.40
2:B:909:POV:H13A	2:B:909:POV:H11A	1.79	0.40
1:D:158:LEU:HD21	1:D:193:PHE:HE2	1.86	0.40
1:A:392:LEU:HD11	1:A:732:LEU:HB2	2.03	0.40
2:B:901:POV:H36	2:B:901:POV:H33A	1.87	0.40
2:C:908:POV:H32A	2:C:908:POV:H35	1.83	0.40
1:D:392:LEU:HD11	1:D:732:LEU:HB2	2.03	0.40
2:B:908:POV:H32A	2:B:908:POV:H35	1.83	0.40
1:C:444:SER:OG	2:C:905:POV:O14	2.33	0.40
1:C:567:ARG:HH21	1:C:699:THR:HG1	1.66	0.40
2:D:904:POV:H21C	2:D:904:POV:H28A	2.03	0.40
1:A:226:ARG:HG2	1:A:274:GLN:HE21	1.86	0.40
2:A:901:POV:H21G	2:A:901:POV:H214	1.98	0.40
2:C:906:POV:H25	2:C:906:POV:H28A	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:ARG:HG2	1:D:274:GLN:HE21	1.86	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	638/808 (79%)	608 (95%)	29 (4%)	1 (0%)	47	79
1	B	638/808 (79%)	607 (95%)	30 (5%)	1 (0%)	47	79
1	C	638/808 (79%)	608 (95%)	29 (4%)	1 (0%)	47	79
1	D	638/808 (79%)	608 (95%)	29 (4%)	1 (0%)	47	79
All	All	2552/3232 (79%)	2431 (95%)	117 (5%)	4 (0%)	50	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	ASN
1	B	314	ASN
1	C	314	ASN
1	D	314	ASN

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	571/721 (79%)	560 (98%)	11 (2%)	57	81
1	B	571/721 (79%)	560 (98%)	11 (2%)	57	81
1	C	571/721 (79%)	560 (98%)	11 (2%)	57	81
1	D	571/721 (79%)	560 (98%)	11 (2%)	57	81
All	All	2284/2884 (79%)	2240 (98%)	44 (2%)	59	81

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	ARG
1	A	220	ASN
1	A	314	ASN
1	A	353	LYS
1	A	475	LEU
1	A	479	MET
1	A	509	ARG
1	A	580	GLN
1	A	643	ASN
1	A	647	ASN
1	A	743	LYS
1	B	147	ARG
1	B	220	ASN
1	B	314	ASN
1	B	353	LYS
1	B	475	LEU
1	B	479	MET
1	B	509	ARG
1	B	580	GLN
1	B	643	ASN
1	B	647	ASN
1	B	743	LYS
1	C	147	ARG
1	C	220	ASN
1	C	314	ASN
1	C	353	LYS
1	C	475	LEU
1	C	479	MET
1	C	509	ARG
1	C	580	GLN
1	C	643	ASN
1	C	647	ASN
1	C	743	LYS

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Mol	Chain	Res	Type
1	D	147	ARG
1	D	220	ASN
1	D	314	ASN
1	D	353	LYS
1	D	475	LEU
1	D	479	MET
1	D	509	ARG
1	D	580	GLN
1	D	643	ASN
1	D	647	ASN
1	D	743	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	A	227	GLN
1	A	314	ASN
1	A	477	HIS
1	A	523	HIS
1	A	643	ASN
1	B	178	ASN
1	B	220	ASN
1	B	227	GLN
1	B	314	ASN
1	B	477	HIS
1	B	523	HIS
1	B	643	ASN
1	C	178	ASN
1	C	220	ASN
1	C	227	GLN
1	C	314	ASN
1	C	477	HIS
1	C	523	HIS
1	C	643	ASN
1	D	178	ASN
1	D	220	ASN
1	D	227	GLN
1	D	314	ASN
1	D	477	HIS
1	D	523	HIS
1	D	643	ASN

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 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	$\#\|Z\| > 2$
2	POV	A	902	-	51,51,51	1.07	3 (5%)	57,59,59	0.98	4 (7%)
2	POV	C	902	-	51,51,51	1.05	2 (3%)	57,59,59	0.85	2 (3%)
2	POV	D	902	-	51,51,51	1.03	3 (5%)	57,59,59	0.92	3 (5%)
2	POV	A	905	-	51,51,51	1.06	3 (5%)	57,59,59	0.95	4 (7%)
2	POV	A	903	-	51,51,51	1.04	3 (5%)	57,59,59	0.96	3 (5%)
2	POV	D	905	-	51,51,51	1.05	3 (5%)	57,59,59	0.89	3 (5%)
2	POV	C	904	-	51,51,51	1.02	3 (5%)	57,59,59	0.96	3 (5%)
2	POV	C	905	-	51,51,51	1.08	3 (5%)	57,59,59	0.97	4 (7%)
2	POV	D	907	-	51,51,51	1.08	3 (5%)	57,59,59	0.99	4 (7%)
2	POV	C	901	-	51,51,51	1.05	3 (5%)	57,59,59	0.90	3 (5%)
2	POV	D	908	-	51,51,51	1.04	3 (5%)	57,59,59	0.96	3 (5%)
2	POV	B	905	-	51,51,51	1.07	3 (5%)	57,59,59	0.98	4 (7%)
2	POV	C	908	-	51,51,51	1.06	3 (5%)	57,59,59	0.94	4 (7%)
2	POV	D	901	-	51,51,51	1.07	3 (5%)	57,59,59	0.94	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	POV	C	909	-	51,51,51	1.02	3 (5%)	57,59,59	0.92	3 (5%)
2	POV	B	907	-	51,51,51	1.04	3 (5%)	57,59,59	0.97	3 (5%)
2	POV	C	903	-	51,51,51	1.06	3 (5%)	57,59,59	0.89	3 (5%)
2	POV	D	906	-	51,51,51	1.03	3 (5%)	57,59,59	0.96	3 (5%)
2	POV	D	909	-	51,51,51	1.04	3 (5%)	57,59,59	0.95	3 (5%)
2	POV	C	906	-	51,51,51	1.04	3 (5%)	57,59,59	0.95	3 (5%)
2	POV	A	904	-	51,51,51	1.04	3 (5%)	57,59,59	0.98	3 (5%)
2	POV	A	909	-	51,51,51	1.05	3 (5%)	57,59,59	0.89	3 (5%)
2	POV	B	908	-	51,51,51	1.06	3 (5%)	57,59,59	0.94	4 (7%)
2	POV	A	906	-	51,51,51	1.03	3 (5%)	57,59,59	0.92	2 (3%)
2	POV	B	906	-	51,51,51	1.04	3 (5%)	57,59,59	0.95	3 (5%)
2	POV	B	909	-	51,51,51	1.03	3 (5%)	57,59,59	0.92	3 (5%)
2	POV	A	908	-	51,51,51	1.05	2 (3%)	57,59,59	0.85	2 (3%)
2	POV	D	903	-	51,51,51	1.05	3 (5%)	57,59,59	0.90	3 (5%)
2	POV	B	904	-	51,51,51	1.02	3 (5%)	57,59,59	0.96	3 (5%)
2	POV	A	907	-	51,51,51	1.05	3 (5%)	57,59,59	0.90	3 (5%)
2	POV	D	904	-	51,51,51	1.05	2 (3%)	57,59,59	0.85	2 (3%)
2	POV	A	901	-	51,51,51	1.03	3 (5%)	57,59,59	0.96	3 (5%)
2	POV	B	901	-	51,51,51	1.04	3 (5%)	57,59,59	0.90	3 (5%)
2	POV	C	907	-	51,51,51	1.04	3 (5%)	57,59,59	0.97	3 (5%)
2	POV	B	903	-	51,51,51	1.05	3 (5%)	57,59,59	0.89	3 (5%)
2	POV	B	902	-	51,51,51	1.05	2 (3%)	57,59,59	0.85	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	A	902	-	-	37/55/55/55	-
2	POV	C	902	-	-	32/55/55/55	-
2	POV	D	902	-	-	24/55/55/55	-
2	POV	A	905	-	-	22/55/55/55	-
2	POV	A	903	-	-	29/55/55/55	-
2	POV	D	905	-	-	28/55/55/55	-
2	POV	C	904	-	-	21/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	C	905	-	-	35/55/55/55	-
2	POV	D	907	-	-	35/55/55/55	-
2	POV	C	901	-	-	29/55/55/55	-
2	POV	D	908	-	-	29/55/55/55	-
2	POV	B	905	-	-	35/55/55/55	-
2	POV	C	908	-	-	23/55/55/55	-
2	POV	D	901	-	-	23/55/55/55	-
2	POV	C	909	-	-	25/55/55/55	-
2	POV	B	907	-	-	26/55/55/55	-
2	POV	C	903	-	-	28/55/55/55	-
2	POV	D	906	-	-	19/55/55/55	-
2	POV	D	909	-	-	26/55/55/55	-
2	POV	C	906	-	-	29/55/55/55	-
2	POV	A	904	-	-	27/55/55/55	-
2	POV	A	909	-	-	29/55/55/55	-
2	POV	B	908	-	-	22/55/55/55	-
2	POV	A	906	-	-	25/55/55/55	-
2	POV	B	906	-	-	29/55/55/55	-
2	POV	B	909	-	-	25/55/55/55	-
2	POV	A	908	-	-	31/55/55/55	-
2	POV	D	903	-	-	29/55/55/55	-
2	POV	B	904	-	-	20/55/55/55	-
2	POV	A	907	-	-	29/55/55/55	-
2	POV	D	904	-	-	31/55/55/55	-
2	POV	A	901	-	-	21/55/55/55	-
2	POV	B	901	-	-	29/55/55/55	-
2	POV	C	907	-	-	27/55/55/55	-
2	POV	B	903	-	-	28/55/55/55	-
2	POV	B	902	-	-	33/55/55/55	-

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	906	POV	O21-C21	2.95	1.42	1.34
2	D	908	POV	O21-C21	2.94	1.42	1.34
2	C	906	POV	O21-C21	2.93	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	POV	O21-C21	2.92	1.42	1.34
2	A	903	POV	O21-C21	2.91	1.42	1.34
2	A	908	POV	O21-C21	2.89	1.42	1.34
2	D	904	POV	O21-C21	2.89	1.42	1.34
2	C	902	POV	O21-C21	2.89	1.42	1.34
2	B	909	POV	O21-C21	2.88	1.42	1.34
2	A	906	POV	O21-C21	2.88	1.42	1.34
2	D	902	POV	O21-C21	2.88	1.42	1.34
2	C	909	POV	O21-C21	2.87	1.42	1.34
2	D	907	POV	O21-C21	2.79	1.42	1.34
2	B	905	POV	O21-C21	2.78	1.42	1.34
2	A	901	POV	O21-C21	2.78	1.42	1.34
2	C	905	POV	O21-C21	2.78	1.42	1.34
2	C	904	POV	O21-C21	2.78	1.42	1.34
2	D	903	POV	O21-C2	-2.77	1.39	1.46
2	A	907	POV	O21-C2	-2.77	1.39	1.46
2	B	902	POV	O31-C31	2.76	1.41	1.33
2	C	902	POV	O31-C31	2.76	1.41	1.33
2	A	902	POV	O21-C21	2.76	1.42	1.34
2	A	907	POV	O31-C31	2.75	1.41	1.33
2	D	901	POV	O21-C21	2.74	1.42	1.34
2	D	906	POV	O21-C21	2.74	1.42	1.34
2	D	904	POV	O31-C31	2.74	1.41	1.33
2	B	908	POV	O21-C21	2.74	1.42	1.34
2	C	908	POV	O31-C31	2.74	1.41	1.33
2	D	901	POV	O31-C31	2.74	1.41	1.33
2	A	908	POV	O31-C31	2.74	1.41	1.33
2	A	905	POV	O31-C31	2.74	1.41	1.33
2	B	908	POV	O31-C31	2.74	1.41	1.33
2	C	901	POV	O21-C2	-2.73	1.39	1.46
2	B	904	POV	O21-C21	2.73	1.42	1.34
2	B	901	POV	O21-C2	-2.73	1.39	1.46
2	A	905	POV	O21-C21	2.73	1.42	1.34
2	C	909	POV	O31-C31	2.73	1.41	1.33
2	A	906	POV	O31-C31	2.72	1.41	1.33
2	C	903	POV	O21-C2	-2.72	1.39	1.46
2	B	909	POV	O31-C31	2.72	1.41	1.33
2	B	901	POV	O31-C31	2.71	1.41	1.33
2	A	909	POV	O21-C2	-2.71	1.39	1.46
2	C	901	POV	O31-C31	2.71	1.41	1.33
2	C	908	POV	O21-C21	2.71	1.41	1.34
2	D	907	POV	O31-C31	2.71	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	903	POV	O31-C31	2.71	1.41	1.33
2	D	902	POV	O31-C31	2.70	1.41	1.33
2	D	905	POV	O21-C2	-2.69	1.39	1.46
2	B	903	POV	O21-C2	-2.69	1.39	1.46
2	B	907	POV	O21-C2	-2.64	1.40	1.46
2	A	904	POV	O21-C2	-2.64	1.40	1.46
2	B	907	POV	O31-C31	2.64	1.41	1.33
2	D	909	POV	O21-C2	-2.63	1.40	1.46
2	A	907	POV	O21-C21	2.63	1.41	1.34
2	C	903	POV	O21-C21	2.63	1.41	1.34
2	A	902	POV	O31-C31	2.63	1.41	1.33
2	C	905	POV	O31-C31	2.62	1.41	1.33
2	B	907	POV	O21-C21	2.62	1.41	1.34
2	D	909	POV	O31-C31	2.62	1.41	1.33
2	C	907	POV	O21-C2	-2.62	1.40	1.46
2	B	905	POV	O31-C31	2.61	1.41	1.33
2	D	905	POV	O21-C21	2.61	1.41	1.34
2	C	907	POV	O31-C31	2.61	1.41	1.33
2	C	901	POV	O21-C21	2.61	1.41	1.34
2	A	909	POV	O21-C21	2.61	1.41	1.34
2	B	903	POV	O21-C21	2.60	1.41	1.34
2	A	904	POV	O21-C21	2.60	1.41	1.34
2	D	903	POV	O21-C21	2.60	1.41	1.34
2	C	907	POV	O21-C21	2.59	1.41	1.34
2	A	904	POV	O31-C31	2.59	1.40	1.33
2	D	909	POV	O21-C21	2.58	1.41	1.34
2	B	901	POV	O21-C21	2.58	1.41	1.34
2	D	906	POV	O21-C2	-2.57	1.40	1.46
2	B	904	POV	O21-C2	-2.56	1.40	1.46
2	C	904	POV	O21-C2	-2.55	1.40	1.46
2	D	905	POV	O31-C31	2.55	1.40	1.33
2	B	903	POV	O31-C31	2.54	1.40	1.33
2	C	903	POV	O31-C31	2.54	1.40	1.33
2	A	909	POV	O31-C31	2.54	1.40	1.33
2	A	901	POV	O21-C2	-2.54	1.40	1.46
2	D	906	POV	O31-C31	2.52	1.40	1.33
2	A	901	POV	O31-C31	2.50	1.40	1.33
2	D	908	POV	O21-C2	-2.50	1.40	1.46
2	B	904	POV	O31-C31	2.49	1.40	1.33
2	B	905	POV	O21-C2	-2.49	1.40	1.46
2	A	902	POV	O21-C2	-2.49	1.40	1.46
2	C	905	POV	O21-C2	-2.49	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	904	POV	O31-C31	2.47	1.40	1.33
2	A	903	POV	O21-C2	-2.47	1.40	1.46
2	B	908	POV	O21-C2	-2.47	1.40	1.46
2	D	901	POV	O21-C2	-2.47	1.40	1.46
2	B	906	POV	O21-C2	-2.46	1.40	1.46
2	C	908	POV	O21-C2	-2.45	1.40	1.46
2	C	906	POV	O21-C2	-2.44	1.40	1.46
2	B	906	POV	O31-C31	2.43	1.40	1.33
2	D	907	POV	O21-C2	-2.43	1.40	1.46
2	D	908	POV	O31-C31	2.43	1.40	1.33
2	C	906	POV	O31-C31	2.43	1.40	1.33
2	A	905	POV	O21-C2	-2.43	1.40	1.46
2	A	903	POV	O31-C31	2.41	1.40	1.33
2	A	906	POV	O21-C2	-2.30	1.40	1.46
2	D	902	POV	O21-C2	-2.28	1.40	1.46
2	B	909	POV	O21-C2	-2.28	1.40	1.46
2	C	909	POV	O21-C2	-2.28	1.40	1.46

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	905	POV	O21-C21-C22	4.20	120.55	111.50
2	C	908	POV	O21-C21-C22	4.19	120.53	111.50
2	B	908	POV	O21-C21-C22	4.18	120.51	111.50
2	A	901	POV	O21-C21-C22	4.17	120.49	111.50
2	D	901	POV	O21-C21-C22	4.16	120.47	111.50
2	C	904	POV	O21-C21-C22	4.16	120.46	111.50
2	B	904	POV	O21-C21-C22	4.13	120.40	111.50
2	D	906	POV	O21-C21-C22	4.12	120.38	111.50
2	B	906	POV	O21-C21-C22	3.99	120.11	111.50
2	D	908	POV	O21-C21-C22	3.99	120.09	111.50
2	A	903	POV	O21-C21-C22	3.98	120.09	111.50
2	C	906	POV	O21-C21-C22	3.98	120.07	111.50
2	D	907	POV	O21-C21-C22	3.93	119.98	111.50
2	B	905	POV	O21-C21-C22	3.91	119.92	111.50
2	C	905	POV	O21-C21-C22	3.90	119.92	111.50
2	A	902	POV	O21-C21-C22	3.88	119.86	111.50
2	A	904	POV	O21-C21-C22	3.79	119.68	111.50
2	D	909	POV	O21-C21-C22	3.79	119.68	111.50
2	B	907	POV	O21-C21-C22	3.78	119.64	111.50
2	C	907	POV	O21-C21-C22	3.77	119.62	111.50
2	C	909	POV	O21-C21-C22	3.76	119.61	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	902	POV	O21-C21-C22	3.73	119.53	111.50
2	A	906	POV	O21-C21-C22	3.72	119.52	111.50
2	B	909	POV	O21-C21-C22	3.71	119.49	111.50
2	D	903	POV	O21-C21-C22	3.60	119.25	111.50
2	B	901	POV	O21-C21-C22	3.58	119.22	111.50
2	A	907	POV	O21-C21-C22	3.56	119.17	111.50
2	C	901	POV	O21-C21-C22	3.55	119.15	111.50
2	B	902	POV	O21-C21-C22	3.45	118.94	111.50
2	A	908	POV	O21-C21-C22	3.45	118.93	111.50
2	D	904	POV	O21-C21-C22	3.45	118.93	111.50
2	C	902	POV	O21-C21-C22	3.44	118.92	111.50
2	C	903	POV	O21-C21-C22	3.13	118.25	111.50
2	A	909	POV	O21-C21-C22	3.13	118.24	111.50
2	D	905	POV	O21-C21-C22	3.12	118.22	111.50
2	B	903	POV	O21-C21-C22	3.11	118.21	111.50
2	B	905	POV	C15-N-C14	-2.81	101.75	108.97
2	D	907	POV	C15-N-C14	-2.78	101.82	108.97
2	C	905	POV	C15-N-C14	-2.77	101.86	108.97
2	A	902	POV	C15-N-C14	-2.75	101.90	108.97
2	D	907	POV	O31-C31-C32	2.67	120.27	111.91
2	D	909	POV	C14-N-C12	2.65	120.76	109.92
2	B	909	POV	O31-C31-C32	2.58	119.99	111.91
2	A	909	POV	O31-C31-C32	2.57	119.99	111.91
2	C	909	POV	O31-C31-C32	2.57	119.99	111.91
2	D	902	POV	O31-C31-C32	2.57	119.97	111.91
2	A	906	POV	O31-C31-C32	2.56	119.96	111.91
2	B	903	POV	O31-C31-C32	2.56	119.95	111.91
2	D	905	POV	O31-C31-C32	2.56	119.94	111.91
2	C	903	POV	O31-C31-C32	2.55	119.92	111.91
2	A	902	POV	O31-C31-C32	2.55	119.90	111.91
2	D	909	POV	O31-C31-C32	2.53	119.84	111.91
2	D	903	POV	O31-C31-C32	2.52	119.80	111.91
2	A	904	POV	C14-N-C12	2.51	120.20	109.92
2	D	908	POV	O31-C31-C32	2.51	119.79	111.91
2	C	905	POV	O31-C31-C32	2.51	119.78	111.91
2	C	901	POV	O31-C31-C32	2.51	119.78	111.91
2	A	904	POV	O31-C31-C32	2.51	119.78	111.91
2	C	904	POV	O31-C31-C32	2.51	119.77	111.91
2	B	901	POV	O31-C31-C32	2.50	119.77	111.91
2	A	903	POV	O31-C31-C32	2.50	119.75	111.91
2	A	901	POV	O31-C31-C32	2.50	119.75	111.91
2	B	905	POV	O31-C31-C32	2.50	119.74	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	907	POV	C14-N-C12	2.49	120.11	109.92
2	C	906	POV	O31-C31-C32	2.48	119.71	111.91
2	A	907	POV	O31-C31-C32	2.48	119.70	111.91
2	D	901	POV	O31-C31-C32	2.48	119.70	111.91
2	C	907	POV	O31-C31-C32	2.48	119.68	111.91
2	B	906	POV	O31-C31-C32	2.48	119.68	111.91
2	B	907	POV	C14-N-C12	2.47	120.03	109.92
2	B	908	POV	O31-C31-C32	2.47	119.66	111.91
2	B	904	POV	O31-C31-C32	2.47	119.66	111.91
2	A	905	POV	O31-C31-C32	2.47	119.65	111.91
2	C	908	POV	O31-C31-C32	2.46	119.64	111.91
2	B	907	POV	O31-C31-C32	2.46	119.64	111.91
2	D	906	POV	O31-C31-C32	2.46	119.62	111.91
2	C	902	POV	O31-C31-C32	2.36	119.33	111.91
2	A	908	POV	O31-C31-C32	2.36	119.32	111.91
2	D	904	POV	O31-C31-C32	2.36	119.31	111.91
2	B	902	POV	O31-C31-C32	2.35	119.29	111.91
2	A	903	POV	C14-N-C12	2.33	119.44	109.92
2	D	908	POV	C14-N-C12	2.32	119.43	109.92
2	B	906	POV	C14-N-C12	2.32	119.39	109.92
2	C	906	POV	C14-N-C12	2.31	119.37	109.92
2	D	901	POV	C14-N-C12	2.30	119.32	109.92
2	C	908	POV	C14-N-C12	2.29	119.31	109.92
2	A	905	POV	C14-N-C12	2.29	119.29	109.92
2	D	906	POV	C14-N-C12	2.28	119.26	109.92
2	B	908	POV	C14-N-C12	2.28	119.26	109.92
2	A	901	POV	C14-N-C12	2.27	119.22	109.92
2	D	903	POV	C14-N-C12	2.27	119.22	109.92
2	A	907	POV	C14-N-C12	2.27	119.22	109.92
2	B	904	POV	C14-N-C12	2.27	119.20	109.92
2	C	904	POV	C14-N-C12	2.27	119.20	109.92
2	C	901	POV	C14-N-C12	2.26	119.17	109.92
2	B	901	POV	C14-N-C12	2.25	119.13	109.92
2	D	907	POV	C14-N-C12	2.24	119.09	109.92
2	B	905	POV	C14-N-C12	2.22	119.00	109.92
2	C	905	POV	C14-N-C12	2.21	118.94	109.92
2	A	902	POV	C14-N-C12	2.20	118.92	109.92
2	A	905	POV	C2-O21-C21	-2.16	112.46	117.79
2	D	901	POV	C2-O21-C21	-2.15	112.50	117.79
2	B	908	POV	C2-O21-C21	-2.14	112.53	117.79
2	C	908	POV	C2-O21-C21	-2.12	112.58	117.79
2	A	909	POV	C14-N-C12	2.05	118.30	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	903	POV	C14-N-C12	2.04	118.27	109.92
2	C	903	POV	C14-N-C12	2.04	118.25	109.92
2	D	905	POV	C14-N-C12	2.03	118.23	109.92
2	B	909	POV	C14-N-C12	2.00	118.12	109.92
2	C	909	POV	C14-N-C12	2.00	118.11	109.92
2	D	902	POV	C14-N-C12	2.00	118.11	109.92

There are no chirality outliers.

All (990) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	POV	C1-O11-P-O12
2	A	901	POV	C11-O12-P-O13
2	A	901	POV	C11-O12-P-O14
2	A	901	POV	C22-C21-O21-C2
2	A	902	POV	C1-O11-P-O13
2	A	902	POV	C11-O12-P-O13
2	A	902	POV	C11-O12-P-O14
2	A	902	POV	C22-C21-O21-C2
2	A	902	POV	O22-C21-O21-C2
2	A	903	POV	C11-O12-P-O13
2	A	903	POV	C11-O12-P-O14
2	A	904	POV	C1-O11-P-O12
2	A	904	POV	C1-O11-P-O13
2	A	904	POV	C1-O11-P-O14
2	A	904	POV	O12-C11-C12-N
2	A	905	POV	C1-O11-P-O13
2	A	905	POV	C11-O12-P-O14
2	A	905	POV	O11-C1-C2-O21
2	A	905	POV	C22-C21-O21-C2
2	A	906	POV	C1-O11-P-O13
2	A	906	POV	C1-O11-P-O14
2	A	906	POV	C11-O12-P-O13
2	A	908	POV	C1-O11-P-O13
2	A	908	POV	O22-C21-O21-C2
2	A	909	POV	C11-O12-P-O14
2	A	909	POV	O21-C2-C3-O31
2	B	901	POV	C1-O11-P-O13
2	B	902	POV	C1-O11-P-O13
2	B	902	POV	O22-C21-O21-C2
2	B	903	POV	C11-O12-P-O14
2	B	903	POV	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	B	904	POV	C1-O11-P-O12
2	B	904	POV	C11-O12-P-O13
2	B	904	POV	C11-O12-P-O14
2	B	904	POV	C22-C21-O21-C2
2	B	905	POV	C11-O12-P-O13
2	B	905	POV	C11-O12-P-O14
2	B	905	POV	O11-C1-C2-O21
2	B	905	POV	C22-C21-O21-C2
2	B	905	POV	O22-C21-O21-C2
2	B	906	POV	C11-O12-P-O13
2	B	906	POV	C11-O12-P-O14
2	B	907	POV	C1-O11-P-O12
2	B	907	POV	C1-O11-P-O13
2	B	907	POV	C1-O11-P-O14
2	B	907	POV	O12-C11-C12-N
2	B	908	POV	C1-O11-P-O13
2	B	908	POV	C11-O12-P-O14
2	B	908	POV	O11-C1-C2-O21
2	B	908	POV	C22-C21-O21-C2
2	B	909	POV	C1-O11-P-O13
2	B	909	POV	C1-O11-P-O14
2	B	909	POV	C11-O12-P-O13
2	B	909	POV	C11-O12-P-O14
2	C	901	POV	C1-O11-P-O13
2	C	902	POV	C1-O11-P-O13
2	C	902	POV	O22-C21-O21-C2
2	C	903	POV	C11-O12-P-O14
2	C	903	POV	O21-C2-C3-O31
2	C	904	POV	C1-O11-P-O12
2	C	904	POV	C11-O12-P-O13
2	C	904	POV	C11-O12-P-O14
2	C	904	POV	C22-C21-O21-C2
2	C	905	POV	C11-O12-P-O13
2	C	905	POV	C11-O12-P-O14
2	C	905	POV	O11-C1-C2-O21
2	C	905	POV	C22-C21-O21-C2
2	C	905	POV	O22-C21-O21-C2
2	C	906	POV	C11-O12-P-O13
2	C	906	POV	C11-O12-P-O14
2	C	907	POV	C1-O11-P-O12
2	C	907	POV	C1-O11-P-O13
2	C	907	POV	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
2	C	907	POV	O12-C11-C12-N
2	C	908	POV	C1-O11-P-O13
2	C	908	POV	C11-O12-P-O14
2	C	908	POV	O11-C1-C2-O21
2	C	908	POV	C22-C21-O21-C2
2	C	909	POV	C1-O11-P-O13
2	C	909	POV	C1-O11-P-O14
2	C	909	POV	C11-O12-P-O13
2	D	901	POV	C1-O11-P-O13
2	D	901	POV	C11-O12-P-O14
2	D	901	POV	O11-C1-C2-O21
2	D	901	POV	C22-C21-O21-C2
2	D	902	POV	C1-O11-P-O13
2	D	902	POV	C1-O11-P-O14
2	D	902	POV	C11-O12-P-O13
2	D	903	POV	C1-O11-P-O13
2	D	904	POV	C1-O11-P-O13
2	D	904	POV	O22-C21-O21-C2
2	D	905	POV	C11-O12-P-O14
2	D	905	POV	O21-C2-C3-O31
2	D	906	POV	C1-O11-P-O12
2	D	906	POV	C11-O12-P-O13
2	D	906	POV	C11-O12-P-O14
2	D	906	POV	C22-C21-O21-C2
2	D	907	POV	C1-O11-P-O14
2	D	907	POV	C11-O12-P-O11
2	D	907	POV	C11-O12-P-O13
2	D	907	POV	C11-O12-P-O14
2	D	907	POV	O11-C1-C2-O21
2	D	907	POV	C22-C21-O21-C2
2	D	907	POV	O22-C21-O21-C2
2	D	908	POV	C11-O12-P-O13
2	D	908	POV	C11-O12-P-O14
2	D	909	POV	C1-O11-P-O13
2	D	909	POV	C1-O11-P-O14
2	A	904	POV	O32-C31-O31-C3
2	B	907	POV	O32-C31-O31-C3
2	C	907	POV	O32-C31-O31-C3
2	D	909	POV	O32-C31-O31-C3
2	A	903	POV	O32-C31-O31-C3
2	B	906	POV	O32-C31-O31-C3
2	C	906	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
2	D	908	POV	O32-C31-O31-C3
2	A	901	POV	O22-C21-O21-C2
2	A	905	POV	O22-C21-O21-C2
2	B	904	POV	O22-C21-O21-C2
2	B	908	POV	O22-C21-O21-C2
2	C	904	POV	O22-C21-O21-C2
2	C	908	POV	O22-C21-O21-C2
2	D	901	POV	O22-C21-O21-C2
2	D	906	POV	O22-C21-O21-C2
2	A	904	POV	C32-C31-O31-C3
2	B	905	POV	C32-C31-O31-C3
2	B	907	POV	C32-C31-O31-C3
2	C	907	POV	C32-C31-O31-C3
2	D	907	POV	C32-C31-O31-C3
2	D	909	POV	C32-C31-O31-C3
2	A	908	POV	C22-C21-O21-C2
2	B	902	POV	C22-C21-O21-C2
2	C	902	POV	C22-C21-O21-C2
2	D	904	POV	C22-C21-O21-C2
2	B	903	POV	O32-C31-O31-C3
2	A	903	POV	C32-C31-O31-C3
2	A	908	POV	C32-C31-O31-C3
2	A	909	POV	C32-C31-O31-C3
2	B	902	POV	C32-C31-O31-C3
2	B	903	POV	C32-C31-O31-C3
2	B	906	POV	C32-C31-O31-C3
2	C	902	POV	C32-C31-O31-C3
2	C	903	POV	C32-C31-O31-C3
2	C	905	POV	C32-C31-O31-C3
2	C	906	POV	C32-C31-O31-C3
2	D	904	POV	C32-C31-O31-C3
2	D	905	POV	C32-C31-O31-C3
2	D	908	POV	C32-C31-O31-C3
2	A	902	POV	O32-C31-O31-C3
2	A	908	POV	O32-C31-O31-C3
2	A	909	POV	O32-C31-O31-C3
2	B	902	POV	O32-C31-O31-C3
2	C	902	POV	O32-C31-O31-C3
2	C	903	POV	O32-C31-O31-C3
2	C	905	POV	O32-C31-O31-C3
2	D	904	POV	O32-C31-O31-C3
2	D	905	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
2	D	907	POV	O32-C31-O31-C3
2	B	905	POV	O32-C31-O31-C3
2	A	902	POV	C32-C31-O31-C3
2	A	907	POV	C22-C23-C24-C25
2	B	901	POV	C22-C23-C24-C25
2	D	903	POV	C22-C23-C24-C25
2	C	901	POV	C22-C23-C24-C25
2	A	902	POV	O11-C1-C2-O21
2	A	904	POV	O11-C1-C2-O21
2	B	907	POV	O11-C1-C2-O21
2	C	907	POV	O11-C1-C2-O21
2	D	909	POV	O11-C1-C2-O21
2	D	906	POV	C24-C25-C26-C27
2	A	902	POV	C31-C32-C33-C34
2	A	908	POV	C31-C32-C33-C34
2	B	902	POV	C31-C32-C33-C34
2	C	902	POV	C31-C32-C33-C34
2	D	904	POV	C31-C32-C33-C34
2	A	902	POV	C21-C22-C23-C24
2	A	905	POV	C21-C22-C23-C24
2	B	905	POV	C21-C22-C23-C24
2	B	908	POV	C21-C22-C23-C24
2	D	901	POV	C21-C22-C23-C24
2	D	907	POV	C31-C32-C33-C34
2	B	904	POV	C24-C25-C26-C27
2	A	901	POV	C24-C25-C26-C27
2	C	904	POV	C24-C25-C26-C27
2	A	902	POV	C11-C12-N-C14
2	B	905	POV	C11-C12-N-C14
2	C	905	POV	C21-C22-C23-C24
2	C	908	POV	C21-C22-C23-C24
2	D	907	POV	C21-C22-C23-C24
2	D	907	POV	C213-C214-C215-C216
2	B	902	POV	C21-C22-C23-C24
2	C	902	POV	C21-C22-C23-C24
2	D	904	POV	C21-C22-C23-C24
2	A	908	POV	C21-C22-C23-C24
2	C	905	POV	C35-C36-C37-C38
2	A	901	POV	C11-O12-P-O11
2	A	902	POV	C1-O11-P-O12
2	A	902	POV	C11-O12-P-O11
2	A	903	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
2	A	903	POV	C11-O12-P-O11
2	A	905	POV	C1-O11-P-O12
2	A	905	POV	C11-O12-P-O11
2	A	906	POV	C1-O11-P-O12
2	A	906	POV	C11-O12-P-O11
2	A	907	POV	C1-O11-P-O12
2	A	908	POV	C1-O11-P-O12
2	A	909	POV	C11-O12-P-O11
2	B	901	POV	C1-O11-P-O12
2	B	902	POV	C1-O11-P-O12
2	B	903	POV	C11-O12-P-O11
2	B	904	POV	C11-O12-P-O11
2	B	905	POV	C1-O11-P-O12
2	B	905	POV	C11-O12-P-O11
2	B	906	POV	C1-O11-P-O12
2	B	906	POV	C11-O12-P-O11
2	B	908	POV	C1-O11-P-O12
2	B	908	POV	C11-O12-P-O11
2	B	909	POV	C1-O11-P-O12
2	B	909	POV	C11-O12-P-O11
2	C	901	POV	C1-O11-P-O12
2	C	902	POV	C1-O11-P-O12
2	C	903	POV	C11-O12-P-O11
2	C	904	POV	C11-O12-P-O11
2	C	905	POV	C1-O11-P-O12
2	C	905	POV	C11-O12-P-O11
2	C	906	POV	C1-O11-P-O12
2	C	906	POV	C11-O12-P-O11
2	C	908	POV	C1-O11-P-O12
2	C	908	POV	C11-O12-P-O11
2	C	909	POV	C1-O11-P-O12
2	C	909	POV	C11-O12-P-O11
2	D	901	POV	C1-O11-P-O12
2	D	901	POV	C11-O12-P-O11
2	D	902	POV	C1-O11-P-O12
2	D	902	POV	C11-O12-P-O11
2	D	903	POV	C1-O11-P-O12
2	D	904	POV	C1-O11-P-O12
2	D	905	POV	C11-O12-P-O11
2	D	906	POV	C11-O12-P-O11
2	D	907	POV	C1-O11-P-O12
2	D	908	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
2	D	908	POV	C11-O12-P-O11
2	D	909	POV	C1-O11-P-O12
2	A	902	POV	C11-C12-N-C15
2	B	905	POV	C11-C12-N-C15
2	C	905	POV	C11-C12-N-C14
2	C	905	POV	C11-C12-N-C15
2	D	907	POV	C11-C12-N-C14
2	D	907	POV	C11-C12-N-C15
2	A	908	POV	C210-C211-C212-C213
2	B	904	POV	C210-C211-C212-C213
2	D	902	POV	C26-C27-C28-C29
2	D	904	POV	C210-C211-C212-C213
2	A	909	POV	C311-C312-C313-C314
2	C	902	POV	C25-C26-C27-C28
2	D	903	POV	C311-C310-C39-C38
2	D	904	POV	C25-C26-C27-C28
2	D	909	POV	C212-C213-C214-C215
2	A	902	POV	C36-C37-C38-C39
2	A	903	POV	C312-C313-C314-C315
2	A	904	POV	C212-C213-C214-C215
2	A	908	POV	C25-C26-C27-C28
2	B	902	POV	C25-C26-C27-C28
2	B	903	POV	C311-C312-C313-C314
2	B	906	POV	C312-C313-C314-C315
2	B	907	POV	C212-C213-C214-C215
2	C	903	POV	C311-C312-C313-C314
2	C	905	POV	C39-C310-C311-C312
2	C	906	POV	C312-C313-C314-C315
2	C	907	POV	C212-C213-C214-C215
2	D	905	POV	C311-C312-C313-C314
2	D	907	POV	C34-C35-C36-C37
2	D	908	POV	C312-C313-C314-C315
2	A	907	POV	C310-C311-C312-C313
2	A	909	POV	C37-C38-C39-C310
2	B	901	POV	C310-C311-C312-C313
2	B	903	POV	C37-C38-C39-C310
2	C	901	POV	C310-C311-C312-C313
2	C	903	POV	C37-C38-C39-C310
2	D	908	POV	C21-C22-C23-C24
2	A	901	POV	C36-C37-C38-C39
2	B	904	POV	C36-C37-C38-C39
2	B	905	POV	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
2	C	904	POV	C36-C37-C38-C39
2	D	905	POV	C37-C38-C39-C310
2	A	904	POV	C35-C36-C37-C38
2	B	907	POV	C35-C36-C37-C38
2	D	906	POV	C36-C37-C38-C39
2	A	903	POV	C211-C212-C213-C214
2	A	904	POV	C213-C214-C215-C216
2	A	908	POV	C32-C33-C34-C35
2	B	902	POV	C32-C33-C34-C35
2	B	903	POV	C36-C37-C38-C39
2	B	906	POV	C211-C212-C213-C214
2	B	907	POV	C213-C214-C215-C216
2	C	902	POV	C32-C33-C34-C35
2	C	907	POV	C213-C214-C215-C216
2	C	907	POV	C35-C36-C37-C38
2	D	905	POV	C36-C37-C38-C39
2	D	908	POV	C211-C212-C213-C214
2	A	903	POV	C21-C22-C23-C24
2	B	906	POV	C21-C22-C23-C24
2	C	906	POV	C21-C22-C23-C24
2	A	907	POV	C32-C31-O31-C3
2	B	901	POV	C32-C31-O31-C3
2	C	901	POV	C32-C31-O31-C3
2	D	903	POV	C32-C31-O31-C3
2	A	907	POV	C312-C313-C314-C315
2	A	909	POV	C36-C37-C38-C39
2	C	903	POV	C36-C37-C38-C39
2	C	906	POV	C211-C212-C213-C214
2	D	903	POV	C310-C311-C312-C313
2	D	904	POV	C32-C33-C34-C35
2	D	907	POV	C311-C310-C39-C38
2	D	909	POV	C213-C214-C215-C216
2	D	909	POV	C35-C36-C37-C38
2	A	907	POV	C311-C310-C39-C38
2	B	905	POV	C32-C33-C34-C35
2	C	905	POV	C32-C33-C34-C35
2	B	901	POV	C21-C22-C23-C24
2	A	902	POV	C37-C38-C39-C310
2	A	908	POV	C22-C23-C24-C25
2	B	901	POV	C311-C310-C39-C38
2	B	909	POV	C35-C36-C37-C38
2	C	901	POV	C311-C310-C39-C38

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Mol	Chain	Res	Type	Atoms
2	C	902	POV	C22-C23-C24-C25
2	A	903	POV	C212-C213-C214-C215
2	A	906	POV	C35-C36-C37-C38
2	A	909	POV	C311-C310-C39-C38
2	B	902	POV	C22-C23-C24-C25
2	C	909	POV	C35-C36-C37-C38
2	D	903	POV	C312-C313-C314-C315
2	D	904	POV	C22-C23-C24-C25
2	D	905	POV	C311-C310-C39-C38
2	D	908	POV	C212-C213-C214-C215
2	D	909	POV	C24-C25-C26-C27
2	B	903	POV	C311-C310-C39-C38
2	B	906	POV	C212-C213-C214-C215
2	C	903	POV	C311-C310-C39-C38
2	C	903	POV	C212-C213-C214-C215
2	C	906	POV	C212-C213-C214-C215
2	D	902	POV	C35-C36-C37-C38
2	A	901	POV	C210-C211-C212-C213
2	A	906	POV	C26-C27-C28-C29
2	A	908	POV	C26-C27-C28-C29
2	B	902	POV	C210-C211-C212-C213
2	B	902	POV	C26-C27-C28-C29
2	B	909	POV	C26-C27-C28-C29
2	C	902	POV	C210-C211-C212-C213
2	C	902	POV	C26-C27-C28-C29
2	C	904	POV	C210-C211-C212-C213
2	C	909	POV	C26-C27-C28-C29
2	D	904	POV	C26-C27-C28-C29
2	D	906	POV	C210-C211-C212-C213
2	A	907	POV	C21-C22-C23-C24
2	A	901	POV	C34-C35-C36-C37
2	A	902	POV	C24-C25-C26-C27
2	B	901	POV	C312-C313-C314-C315
2	B	904	POV	C34-C35-C36-C37
2	C	901	POV	C312-C313-C314-C315
2	C	904	POV	C34-C35-C36-C37
2	C	908	POV	C213-C214-C215-C216
2	C	908	POV	C22-C23-C24-C25
2	D	901	POV	C311-C310-C39-C38
2	D	905	POV	C310-C311-C312-C313
2	D	906	POV	C34-C35-C36-C37
2	D	907	POV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
2	A	902	POV	C11-C12-N-C13
2	B	905	POV	C11-C12-N-C13
2	C	905	POV	C11-C12-N-C13
2	D	907	POV	C11-C12-N-C13
2	B	901	POV	C211-C212-C213-C214
2	B	903	POV	C310-C311-C312-C313
2	B	903	POV	C212-C213-C214-C215
2	C	903	POV	C310-C311-C312-C313
2	D	901	POV	C22-C23-C24-C25
2	D	905	POV	C212-C213-C214-C215
2	A	904	POV	C24-C25-C26-C27
2	A	909	POV	C310-C311-C312-C313
2	A	909	POV	C212-C213-C214-C215
2	B	907	POV	C24-C25-C26-C27
2	B	908	POV	C213-C214-C215-C216
2	B	908	POV	C22-C23-C24-C25
2	C	901	POV	C211-C212-C213-C214
2	C	907	POV	C24-C25-C26-C27
2	C	908	POV	C311-C310-C39-C38
2	D	901	POV	C213-C214-C215-C216
2	C	901	POV	C21-C22-C23-C24
2	D	903	POV	C21-C22-C23-C24
2	A	905	POV	C311-C310-C39-C38
2	A	905	POV	C213-C214-C215-C216
2	A	905	POV	C22-C23-C24-C25
2	A	906	POV	C23-C24-C25-C26
2	B	908	POV	C311-C310-C39-C38
2	B	909	POV	C23-C24-C25-C26
2	A	901	POV	C213-C214-C215-C216
2	A	905	POV	C37-C38-C39-C310
2	B	908	POV	C37-C38-C39-C310
2	B	909	POV	C312-C313-C314-C315
2	D	907	POV	C39-C310-C311-C312
2	A	906	POV	C312-C313-C314-C315
2	B	903	POV	C34-C35-C36-C37
2	B	905	POV	C35-C36-C37-C38
2	C	903	POV	C34-C35-C36-C37
2	C	908	POV	C37-C38-C39-C310
2	C	909	POV	C312-C313-C314-C315
2	A	901	POV	C310-C311-C312-C313
2	A	903	POV	C311-C312-C313-C314
2	A	909	POV	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
2	B	904	POV	C310-C311-C312-C313
2	B	904	POV	C213-C214-C215-C216
2	B	905	POV	C24-C25-C26-C27
2	B	906	POV	C311-C312-C313-C314
2	C	902	POV	C214-C215-C216-C217
2	C	904	POV	C213-C214-C215-C216
2	D	901	POV	C37-C38-C39-C310
2	D	905	POV	C34-C35-C36-C37
2	D	908	POV	C311-C312-C313-C314
2	A	901	POV	C22-C23-C24-C25
2	B	902	POV	C214-C215-C216-C217
2	C	904	POV	C310-C311-C312-C313
2	C	905	POV	C24-C25-C26-C27
2	C	905	POV	C36-C37-C38-C39
2	D	902	POV	C312-C313-C314-C315
2	C	904	POV	C22-C23-C24-C25
2	D	909	POV	C22-C21-O21-C2
2	C	905	POV	C22-C23-C24-C25
2	C	906	POV	C311-C312-C313-C314
2	D	906	POV	C213-C214-C215-C216
2	A	902	POV	C310-C311-C312-C313
2	A	902	POV	C22-C23-C24-C25
2	A	907	POV	C211-C212-C213-C214
2	D	902	POV	C23-C24-C25-C26
2	D	906	POV	C310-C311-C312-C313
2	D	907	POV	C33-C34-C35-C36
2	A	908	POV	C214-C215-C216-C217
2	D	904	POV	C214-C215-C216-C217
2	D	903	POV	C211-C212-C213-C214
2	A	906	POV	C27-C28-C29-C210
2	B	909	POV	C27-C28-C29-C210
2	C	909	POV	C27-C28-C29-C210
2	D	902	POV	C27-C28-C29-C210
2	B	905	POV	C22-C23-C24-C25
2	C	905	POV	C311-C310-C39-C38
2	C	909	POV	C23-C24-C25-C26
2	C	907	POV	O22-C21-O21-C2
2	D	909	POV	O22-C21-O21-C2
2	A	902	POV	C33-C34-C35-C36
2	D	908	POV	C214-C215-C216-C217
2	A	907	POV	O32-C31-O31-C3
2	B	901	POV	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
2	C	901	POV	O32-C31-O31-C3
2	D	903	POV	O32-C31-O31-C3
2	A	903	POV	C214-C215-C216-C217
2	B	902	POV	C36-C37-C38-C39
2	C	902	POV	C36-C37-C38-C39
2	C	906	POV	C214-C215-C216-C217
2	B	906	POV	C214-C215-C216-C217
2	A	904	POV	C22-C21-O21-C2
2	B	907	POV	C22-C21-O21-C2
2	C	905	POV	C213-C214-C215-C216
2	D	904	POV	C36-C37-C38-C39
2	B	904	POV	C22-C23-C24-C25
2	D	907	POV	C26-C27-C28-C29
2	A	904	POV	O22-C21-O21-C2
2	A	909	POV	O22-C21-O21-C2
2	B	903	POV	O22-C21-O21-C2
2	B	907	POV	O22-C21-O21-C2
2	D	905	POV	O22-C21-O21-C2
2	A	908	POV	C36-C37-C38-C39
2	B	905	POV	C23-C24-C25-C26
2	A	909	POV	C22-C21-O21-C2
2	B	903	POV	C22-C21-O21-C2
2	C	903	POV	C22-C21-O21-C2
2	C	907	POV	C22-C21-O21-C2
2	D	905	POV	C22-C21-O21-C2
2	D	903	POV	C24-C25-C26-C27
2	C	903	POV	O22-C21-O21-C2
2	A	905	POV	C211-C212-C213-C214
2	B	908	POV	C211-C212-C213-C214
2	D	907	POV	O21-C2-C3-O31
2	C	908	POV	C211-C212-C213-C214
2	D	901	POV	C211-C212-C213-C214
2	A	904	POV	C31-C32-C33-C34
2	B	907	POV	C31-C32-C33-C34
2	C	907	POV	C31-C32-C33-C34
2	D	909	POV	C31-C32-C33-C34
2	A	903	POV	C37-C38-C39-C310
2	B	906	POV	C37-C38-C39-C310
2	C	906	POV	C37-C38-C39-C310
2	D	908	POV	C37-C38-C39-C310
2	A	901	POV	C33-C34-C35-C36
2	D	906	POV	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
2	B	905	POV	C212-C213-C214-C215
2	C	901	POV	C24-C25-C26-C27
2	B	901	POV	C24-C25-C26-C27
2	B	904	POV	C33-C34-C35-C36
2	D	902	POV	C39-C310-C311-C312
2	A	907	POV	C11-O12-P-O11
2	B	901	POV	C11-O12-P-O11
2	C	901	POV	C11-O12-P-O11
2	D	903	POV	C11-O12-P-O11
2	C	904	POV	C33-C34-C35-C36
2	A	902	POV	O11-C1-C2-C3
2	A	908	POV	O11-C1-C2-C3
2	B	902	POV	O11-C1-C2-C3
2	B	905	POV	O11-C1-C2-C3
2	C	902	POV	O11-C1-C2-C3
2	C	905	POV	O11-C1-C2-C3
2	D	904	POV	O11-C1-C2-C3
2	D	907	POV	O11-C1-C2-C3
2	A	906	POV	C39-C310-C311-C312
2	A	907	POV	C24-C25-C26-C27
2	B	909	POV	C39-C310-C311-C312
2	D	909	POV	C22-C23-C24-C25
2	A	902	POV	C23-C24-C25-C26
2	C	909	POV	C39-C310-C311-C312
2	D	909	POV	C210-C211-C212-C213
2	A	903	POV	C39-C310-C311-C312
2	B	906	POV	C39-C310-C311-C312
2	C	906	POV	C39-C310-C311-C312
2	D	908	POV	C39-C310-C311-C312
2	D	906	POV	C35-C36-C37-C38
2	A	904	POV	C1-C2-C3-O31
2	B	907	POV	C1-C2-C3-O31
2	C	907	POV	C1-C2-C3-O31
2	D	906	POV	C22-C23-C24-C25
2	D	909	POV	C1-C2-C3-O31
2	A	902	POV	C311-C310-C39-C38
2	A	902	POV	C212-C213-C214-C215
2	C	905	POV	C212-C213-C214-C215
2	D	905	POV	C33-C34-C35-C36
2	C	905	POV	C23-C24-C25-C26
2	A	904	POV	C210-C211-C212-C213
2	B	907	POV	C210-C211-C212-C213

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Mol	Chain	Res	Type	Atoms
2	C	907	POV	C210-C211-C212-C213
2	A	909	POV	C33-C34-C35-C36
2	B	903	POV	C33-C34-C35-C36
2	A	907	POV	C37-C38-C39-C310
2	C	903	POV	C33-C34-C35-C36
2	A	902	POV	C213-C214-C215-C216
2	B	901	POV	C37-C38-C39-C310
2	A	908	POV	C3-C2-O21-C21
2	B	902	POV	C3-C2-O21-C21
2	C	902	POV	C3-C2-O21-C21
2	D	904	POV	C3-C2-O21-C21
2	C	907	POV	C37-C38-C39-C310
2	D	904	POV	C313-C314-C315-C316
2	D	906	POV	C211-C212-C213-C214
2	A	908	POV	C313-C314-C315-C316
2	B	902	POV	C313-C314-C315-C316
2	C	902	POV	C313-C314-C315-C316
2	B	907	POV	C22-C23-C24-C25
2	D	901	POV	C39-C310-C311-C312
2	D	903	POV	C37-C38-C39-C310
2	D	909	POV	C25-C26-C27-C28
2	C	907	POV	C22-C23-C24-C25
2	A	904	POV	C22-C23-C24-C25
2	A	901	POV	C211-C212-C213-C214
2	A	902	POV	C35-C36-C37-C38
2	B	907	POV	C25-C26-C27-C28
2	B	907	POV	C37-C38-C39-C310
2	C	901	POV	C212-C213-C214-C215
2	C	907	POV	C25-C26-C27-C28
2	D	908	POV	C213-C214-C215-C216
2	C	904	POV	C35-C36-C37-C38
2	C	906	POV	C213-C214-C215-C216
2	A	903	POV	C213-C214-C215-C216
2	B	906	POV	C213-C214-C215-C216
2	A	902	POV	C34-C35-C36-C37
2	A	904	POV	C25-C26-C27-C28
2	B	901	POV	C212-C213-C214-C215
2	B	904	POV	C211-C212-C213-C214
2	C	904	POV	C211-C212-C213-C214
2	B	905	POV	C213-C214-C215-C216
2	C	909	POV	C24-C25-C26-C27
2	A	907	POV	C212-C213-C214-C215

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Mol	Chain	Res	Type	Atoms
2	B	904	POV	C35-C36-C37-C38
2	C	901	POV	C37-C38-C39-C310
2	A	909	POV	C213-C214-C215-C216
2	A	904	POV	O11-C1-C2-C3
2	B	907	POV	O11-C1-C2-C3
2	C	907	POV	O11-C1-C2-C3
2	D	909	POV	O11-C1-C2-C3
2	A	901	POV	C35-C36-C37-C38
2	B	905	POV	C211-C212-C213-C214
2	B	907	POV	C36-C37-C38-C39
2	D	902	POV	C24-C25-C26-C27
2	A	906	POV	C24-C25-C26-C27
2	C	907	POV	C36-C37-C38-C39
2	B	909	POV	C24-C25-C26-C27
2	C	905	POV	C31-C32-C33-C34
2	C	907	POV	C311-C310-C39-C38
2	B	907	POV	C311-C310-C39-C38
2	D	909	POV	C37-C38-C39-C310
2	D	901	POV	C23-C24-C25-C26
2	D	903	POV	C212-C213-C214-C215
2	D	909	POV	C36-C37-C38-C39
2	B	902	POV	C37-C38-C39-C310
2	D	907	POV	C212-C213-C214-C215
2	D	905	POV	C1-C2-C3-O31
2	A	909	POV	C32-C33-C34-C35
2	B	903	POV	C32-C33-C34-C35
2	C	902	POV	C37-C38-C39-C310
2	C	903	POV	C32-C33-C34-C35
2	D	905	POV	C32-C33-C34-C35
2	D	907	POV	C24-C25-C26-C27
2	B	908	POV	C23-C24-C25-C26
2	D	903	POV	C36-C37-C38-C39
2	A	904	POV	C36-C37-C38-C39
2	A	908	POV	C311-C310-C39-C38
2	D	909	POV	C311-C310-C39-C38
2	D	901	POV	C27-C28-C29-C210
2	C	908	POV	C39-C310-C311-C312
2	A	905	POV	C23-C24-C25-C26
2	B	903	POV	C213-C214-C215-C216
2	A	906	POV	O11-C1-C2-O21
2	A	908	POV	O11-C1-C2-O21
2	B	902	POV	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
2	C	902	POV	O11-C1-C2-O21
2	C	909	POV	O11-C1-C2-O21
2	D	902	POV	O11-C1-C2-O21
2	D	904	POV	O11-C1-C2-O21
2	C	908	POV	C23-C24-C25-C26
2	D	904	POV	C311-C310-C39-C38
2	D	904	POV	C37-C38-C39-C310
2	A	908	POV	C37-C38-C39-C310
2	A	905	POV	C39-C310-C311-C312
2	A	904	POV	O21-C2-C3-O31
2	A	907	POV	O21-C2-C3-O31
2	B	901	POV	O21-C2-C3-O31
2	B	907	POV	O21-C2-C3-O31
2	C	901	POV	O21-C2-C3-O31
2	C	907	POV	O21-C2-C3-O31
2	D	903	POV	O21-C2-C3-O31
2	D	909	POV	O21-C2-C3-O31
2	C	908	POV	C27-C28-C29-C210
2	B	908	POV	C39-C310-C311-C312
2	D	905	POV	C213-C214-C215-C216
2	A	904	POV	C311-C310-C39-C38
2	A	908	POV	C2-C1-O11-P
2	B	902	POV	C2-C1-O11-P
2	C	902	POV	C2-C1-O11-P
2	D	904	POV	C2-C1-O11-P
2	B	905	POV	C210-C211-C212-C213
2	B	902	POV	C311-C310-C39-C38
2	C	902	POV	C311-C310-C39-C38
2	C	903	POV	C213-C214-C215-C216
2	A	905	POV	O11-C1-C2-C3
2	B	908	POV	O11-C1-C2-C3
2	C	908	POV	O11-C1-C2-C3
2	D	901	POV	O11-C1-C2-C3
2	A	907	POV	C36-C37-C38-C39
2	B	901	POV	C36-C37-C38-C39
2	C	901	POV	C311-C312-C313-C314
2	A	904	POV	C37-C38-C39-C310
2	C	909	POV	C34-C35-C36-C37
2	A	903	POV	C210-C211-C212-C213
2	B	906	POV	C210-C211-C212-C213
2	C	906	POV	C210-C211-C212-C213
2	D	908	POV	C210-C211-C212-C213

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Mol	Chain	Res	Type	Atoms
2	A	908	POV	C1-C2-C3-O31
2	A	909	POV	C1-C2-C3-O31
2	B	902	POV	C1-C2-C3-O31
2	B	903	POV	C1-C2-C3-O31
2	C	902	POV	C1-C2-C3-O31
2	C	903	POV	C1-C2-C3-O31
2	D	904	POV	C1-C2-C3-O31
2	D	903	POV	C214-C215-C216-C217
2	B	909	POV	O11-C1-C2-O21
2	C	901	POV	C36-C37-C38-C39
2	A	905	POV	C27-C28-C29-C210
2	B	908	POV	C27-C28-C29-C210
2	A	902	POV	O21-C2-C3-O31
2	B	905	POV	O21-C2-C3-O31
2	C	905	POV	O21-C2-C3-O31
2	A	906	POV	C34-C35-C36-C37
2	A	907	POV	C214-C215-C216-C217
2	D	902	POV	C34-C35-C36-C37
2	D	902	POV	C36-C37-C38-C39
2	B	909	POV	C34-C35-C36-C37
2	B	901	POV	C214-C215-C216-C217
2	C	901	POV	C214-C215-C216-C217
2	C	909	POV	C36-C37-C38-C39
2	D	909	POV	C11-O12-P-O11
2	A	909	POV	C312-C313-C314-C315
2	C	903	POV	C2-C1-O11-P
2	D	905	POV	C2-C1-O11-P
2	A	902	POV	C1-O11-P-O14
2	A	903	POV	C1-O11-P-O13
2	A	903	POV	C1-O11-P-O14
2	A	904	POV	C11-O12-P-O14
2	A	905	POV	C11-O12-P-O13
2	A	906	POV	C11-O12-P-O14
2	A	907	POV	C1-O11-P-O13
2	A	907	POV	C1-O11-P-O14
2	A	908	POV	C1-O11-P-O14
2	A	908	POV	C11-O12-P-O14
2	A	909	POV	C1-O11-P-O13
2	A	909	POV	C11-O12-P-O13
2	B	901	POV	C1-O11-P-O14
2	B	902	POV	C1-O11-P-O14
2	B	902	POV	C11-O12-P-O14

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Mol	Chain	Res	Type	Atoms
2	B	903	POV	C1-O11-P-O13
2	B	903	POV	C11-O12-P-O13
2	B	905	POV	C1-O11-P-O14
2	B	906	POV	C1-O11-P-O13
2	B	906	POV	C1-O11-P-O14
2	B	907	POV	C11-O12-P-O14
2	B	908	POV	C11-O12-P-O13
2	C	901	POV	C1-O11-P-O14
2	C	902	POV	C1-O11-P-O14
2	C	902	POV	C11-O12-P-O14
2	C	903	POV	C1-O11-P-O13
2	C	903	POV	C11-O12-P-O13
2	C	905	POV	C1-O11-P-O14
2	C	906	POV	C1-O11-P-O13
2	C	906	POV	C1-O11-P-O14
2	C	907	POV	C11-O12-P-O14
2	C	908	POV	C11-O12-P-O13
2	C	909	POV	C11-O12-P-O14
2	D	901	POV	C11-O12-P-O13
2	D	902	POV	C11-O12-P-O14
2	D	903	POV	C1-O11-P-O14
2	D	904	POV	C1-O11-P-O14
2	D	904	POV	C11-O12-P-O14
2	D	905	POV	C1-O11-P-O13
2	D	905	POV	C11-O12-P-O13
2	D	908	POV	C1-O11-P-O13
2	D	908	POV	C1-O11-P-O14
2	A	906	POV	O11-C1-C2-C3
2	B	909	POV	O11-C1-C2-C3
2	C	909	POV	O11-C1-C2-C3
2	D	902	POV	O11-C1-C2-C3
2	B	905	POV	C311-C310-C39-C38
2	B	903	POV	C312-C313-C314-C315
2	C	903	POV	C312-C313-C314-C315
2	D	905	POV	C312-C313-C314-C315
2	A	906	POV	C36-C37-C38-C39
2	A	902	POV	C210-C211-C212-C213
2	C	905	POV	C210-C211-C212-C213
2	B	909	POV	C36-C37-C38-C39
2	B	905	POV	C312-C313-C314-C315
2	C	909	POV	C311-C310-C39-C38
2	D	905	POV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
2	A	906	POV	C21-C22-C23-C24
2	B	909	POV	C21-C22-C23-C24
2	A	907	POV	C35-C36-C37-C38
2	B	903	POV	C24-C25-C26-C27
2	B	901	POV	C35-C36-C37-C38
2	C	903	POV	C24-C25-C26-C27
2	A	902	POV	C1-C2-C3-O31
2	A	905	POV	O12-C11-C12-N
2	A	906	POV	O12-C11-C12-N
2	A	907	POV	O12-C11-C12-N
2	A	908	POV	O12-C11-C12-N
2	B	901	POV	O12-C11-C12-N
2	B	902	POV	O12-C11-C12-N
2	B	905	POV	C1-C2-C3-O31
2	B	908	POV	O12-C11-C12-N
2	B	909	POV	O12-C11-C12-N
2	C	901	POV	O12-C11-C12-N
2	C	902	POV	O12-C11-C12-N
2	C	905	POV	C1-C2-C3-O31
2	C	908	POV	O12-C11-C12-N
2	C	909	POV	O12-C11-C12-N
2	D	901	POV	O12-C11-C12-N
2	D	902	POV	C311-C310-C39-C38
2	D	903	POV	O12-C11-C12-N
2	D	904	POV	O12-C11-C12-N
2	D	907	POV	C1-C2-C3-O31
2	D	909	POV	O12-C11-C12-N
2	A	908	POV	O21-C2-C3-O31
2	B	902	POV	O21-C2-C3-O31
2	C	902	POV	O21-C2-C3-O31
2	D	904	POV	O21-C2-C3-O31
2	A	902	POV	C211-C212-C213-C214
2	A	909	POV	C24-C25-C26-C27
2	C	901	POV	C35-C36-C37-C38
2	A	909	POV	C2-C1-O11-P
2	B	903	POV	C2-C1-O11-P
2	C	902	POV	C212-C213-C214-C215
2	D	903	POV	C35-C36-C37-C38
2	B	902	POV	C212-C213-C214-C215
2	B	903	POV	C214-C215-C216-C217
2	A	905	POV	C214-C215-C216-C217
2	B	908	POV	C214-C215-C216-C217

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Mol	Chain	Res	Type	Atoms
2	C	903	POV	C214-C215-C216-C217
2	D	905	POV	C214-C215-C216-C217
2	D	906	POV	C214-C215-C216-C217
2	B	906	POV	C32-C33-C34-C35
2	D	901	POV	C214-C215-C216-C217
2	A	906	POV	C311-C310-C39-C38
2	A	907	POV	C311-C312-C313-C314
2	C	906	POV	C32-C33-C34-C35
2	B	904	POV	C214-C215-C216-C217
2	A	908	POV	C212-C213-C214-C215
2	A	901	POV	C214-C215-C216-C217
2	A	903	POV	C32-C33-C34-C35
2	D	908	POV	C32-C33-C34-C35
2	C	904	POV	C214-C215-C216-C217
2	C	908	POV	C214-C215-C216-C217
2	B	909	POV	C311-C310-C39-C38
2	D	904	POV	C212-C213-C214-C215
2	C	909	POV	C21-C22-C23-C24
2	D	902	POV	C21-C22-C23-C24
2	B	901	POV	C311-C312-C313-C314
2	D	902	POV	C311-C312-C313-C314
2	A	906	POV	C310-C311-C312-C313
2	D	902	POV	C310-C311-C312-C313
2	D	903	POV	C311-C312-C313-C314
2	A	906	POV	C311-C312-C313-C314
2	C	906	POV	C35-C36-C37-C38
2	A	903	POV	C35-C36-C37-C38
2	B	909	POV	C311-C312-C313-C314
2	B	906	POV	C35-C36-C37-C38
2	D	908	POV	C35-C36-C37-C38
2	B	909	POV	C310-C311-C312-C313
2	A	906	POV	C210-C211-C212-C213
2	B	909	POV	C210-C211-C212-C213
2	C	909	POV	C210-C211-C212-C213
2	D	902	POV	C210-C211-C212-C213
2	D	903	POV	C25-C26-C27-C28
2	C	909	POV	C310-C311-C312-C313
2	B	901	POV	C25-C26-C27-C28
2	C	901	POV	C25-C26-C27-C28
2	A	907	POV	C25-C26-C27-C28
2	C	909	POV	C311-C312-C313-C314
2	A	905	POV	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	B	908	POV	C1-C2-C3-O31
2	C	908	POV	C1-C2-C3-O31
2	D	901	POV	C1-C2-C3-O31
2	A	907	POV	C26-C27-C28-C29
2	C	901	POV	C26-C27-C28-C29
2	D	904	POV	C215-C216-C217-C218
2	C	909	POV	C215-C216-C217-C218
2	D	907	POV	C25-C26-C27-C28
2	D	907	POV	C35-C36-C37-C38
2	A	909	POV	C214-C215-C216-C217
2	B	901	POV	C26-C27-C28-C29
2	A	901	POV	C23-C24-C25-C26
2	B	902	POV	C215-C216-C217-C218
2	C	904	POV	C23-C24-C25-C26
2	A	906	POV	C215-C216-C217-C218
2	A	903	POV	C311-C310-C39-C38
2	B	906	POV	C311-C310-C39-C38
2	D	908	POV	C311-C310-C39-C38
2	B	905	POV	C214-C215-C216-C217
2	A	908	POV	C215-C216-C217-C218
2	C	906	POV	C311-C310-C39-C38
2	B	909	POV	C215-C216-C217-C218
2	C	902	POV	C215-C216-C217-C218
2	D	907	POV	C32-C33-C34-C35
2	A	909	POV	O21-C21-C22-C23
2	C	903	POV	O21-C21-C22-C23
2	D	908	POV	O21-C21-C22-C23
2	B	906	POV	O21-C21-C22-C23
2	C	905	POV	C211-C212-C213-C214
2	D	902	POV	C215-C216-C217-C218
2	A	903	POV	O21-C21-C22-C23
2	B	903	POV	O21-C21-C22-C23
2	C	906	POV	O21-C21-C22-C23
2	D	905	POV	O21-C21-C22-C23
2	C	909	POV	C29-C210-C211-C212
2	A	902	POV	C27-C28-C29-C210
2	D	906	POV	C23-C24-C25-C26
2	D	907	POV	C27-C28-C29-C210
2	D	901	POV	C310-C311-C312-C313
2	B	909	POV	C29-C210-C211-C212
2	D	902	POV	C29-C210-C211-C212
2	A	907	POV	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	B	901	POV	C1-C2-C3-O31
2	C	901	POV	C1-C2-C3-O31
2	D	903	POV	C1-C2-C3-O31
2	A	903	POV	C11-C12-N-C14
2	B	906	POV	C11-C12-N-C14
2	C	906	POV	C11-C12-N-C14
2	D	908	POV	C11-C12-N-C14
2	A	902	POV	C214-C215-C216-C217
2	B	903	POV	C211-C212-C213-C214
2	C	903	POV	C211-C212-C213-C214
2	A	906	POV	C29-C210-C211-C212
2	D	905	POV	C211-C212-C213-C214
2	D	908	POV	C215-C216-C217-C218
2	A	907	POV	O31-C31-C32-C33
2	B	905	POV	C29-C210-C211-C212
2	B	906	POV	C215-C216-C217-C218
2	B	901	POV	O31-C31-C32-C33
2	C	901	POV	O31-C31-C32-C33
2	D	903	POV	O31-C31-C32-C33
2	D	908	POV	C24-C25-C26-C27
2	C	901	POV	C32-C33-C34-C35
2	D	905	POV	C22-C23-C24-C25
2	D	903	POV	C26-C27-C28-C29
2	A	901	POV	C25-C26-C27-C28
2	A	907	POV	C32-C33-C34-C35
2	B	903	POV	C22-C23-C24-C25
2	C	903	POV	C22-C23-C24-C25
2	C	905	POV	C27-C28-C29-C210
2	B	901	POV	C32-C33-C34-C35
2	C	906	POV	C215-C216-C217-C218
2	D	903	POV	C32-C33-C34-C35
2	C	904	POV	C25-C26-C27-C28
2	D	903	POV	C215-C216-C217-C218
2	D	907	POV	C312-C313-C314-C315
2	B	904	POV	C25-C26-C27-C28
2	C	905	POV	C312-C313-C314-C315
2	A	903	POV	C215-C216-C217-C218
2	A	907	POV	C29-C210-C211-C212
2	C	901	POV	C29-C210-C211-C212
2	C	908	POV	C29-C210-C211-C212
2	D	903	POV	C29-C210-C211-C212
2	D	908	POV	C29-C210-C211-C212

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Mol	Chain	Res	Type	Atoms
2	A	903	POV	C24-C25-C26-C27
2	C	907	POV	C33-C34-C35-C36
2	A	908	POV	C23-C24-C25-C26
2	B	901	POV	C215-C216-C217-C218
2	A	903	POV	C29-C210-C211-C212
2	B	901	POV	C29-C210-C211-C212
2	B	905	POV	C27-C28-C29-C210
2	B	906	POV	C29-C210-C211-C212
2	C	906	POV	C29-C210-C211-C212
2	B	906	POV	C24-C25-C26-C27
2	B	907	POV	C33-C34-C35-C36
2	C	902	POV	C23-C24-C25-C26
2	C	906	POV	C24-C25-C26-C27
2	D	907	POV	C23-C24-C25-C26
2	A	909	POV	C22-C23-C24-C25
2	A	904	POV	C11-O12-P-O11
2	C	907	POV	C11-O12-P-O11
2	A	907	POV	O32-C31-C32-C33
2	B	901	POV	O32-C31-C32-C33
2	A	909	POV	C211-C212-C213-C214
2	A	909	POV	C25-C26-C27-C28
2	C	901	POV	C215-C216-C217-C218
2	A	903	POV	C11-C12-N-C13
2	A	903	POV	C11-C12-N-C15
2	B	906	POV	C11-C12-N-C13
2	B	906	POV	C11-C12-N-C15
2	C	904	POV	C1-O11-P-O13
2	C	906	POV	C11-C12-N-C13
2	C	906	POV	C11-C12-N-C15
2	D	908	POV	C11-C12-N-C13
2	D	908	POV	C11-C12-N-C15
2	C	901	POV	O32-C31-C32-C33
2	D	903	POV	O32-C31-C32-C33
2	B	904	POV	C23-C24-C25-C26
2	B	904	POV	C311-C312-C313-C314
2	A	907	POV	C215-C216-C217-C218
2	B	902	POV	C23-C24-C25-C26
2	A	901	POV	C311-C312-C313-C314
2	D	904	POV	C23-C24-C25-C26
2	A	903	POV	C12-C11-O12-P
2	A	908	POV	C12-C11-O12-P
2	A	909	POV	C12-C11-O12-P

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Mol	Chain	Res	Type	Atoms
2	B	902	POV	C12-C11-O12-P
2	B	903	POV	C12-C11-O12-P
2	B	906	POV	C12-C11-O12-P
2	C	902	POV	C12-C11-O12-P
2	C	903	POV	C12-C11-O12-P
2	C	906	POV	C12-C11-O12-P
2	D	904	POV	C12-C11-O12-P
2	D	905	POV	C12-C11-O12-P
2	D	908	POV	C12-C11-O12-P
2	C	904	POV	C313-C314-C315-C316
2	B	905	POV	C33-C34-C35-C36
2	C	908	POV	C34-C35-C36-C37
2	A	905	POV	C29-C210-C211-C212
2	B	908	POV	C29-C210-C211-C212
2	B	905	POV	O21-C21-C22-C23
2	B	907	POV	O21-C21-C22-C23
2	D	909	POV	C33-C34-C35-C36
2	A	902	POV	O21-C21-C22-C23
2	A	904	POV	O21-C21-C22-C23
2	C	905	POV	O21-C21-C22-C23
2	C	907	POV	O21-C21-C22-C23
2	D	906	POV	C313-C314-C315-C316
2	D	907	POV	O21-C21-C22-C23
2	D	901	POV	C29-C210-C211-C212
2	A	904	POV	C33-C34-C35-C36
2	B	902	POV	C39-C310-C311-C312
2	D	909	POV	O21-C21-C22-C23
2	A	901	POV	C313-C314-C315-C316
2	B	905	POV	O22-C21-C22-C23
2	C	902	POV	C39-C310-C311-C312
2	C	905	POV	C29-C210-C211-C212
2	B	902	POV	C34-C35-C36-C37
2	A	902	POV	O22-C21-C22-C23
2	C	905	POV	O22-C21-C22-C23
2	D	907	POV	O22-C21-C22-C23

There are no ring outliers.

36 monomers are involved in 112 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	POV	3	0
2	C	902	POV	5	0

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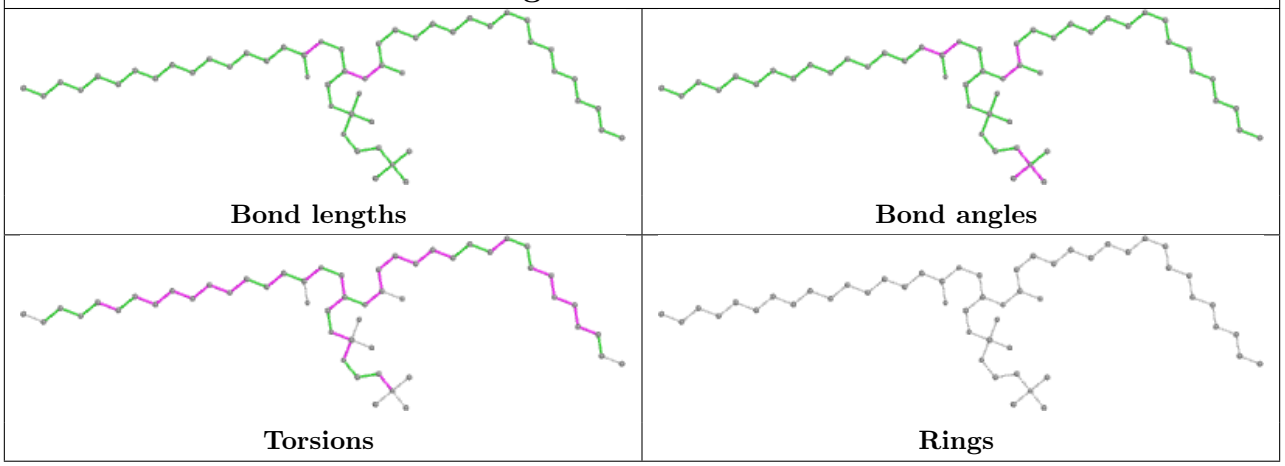
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	902	POV	2	0
2	A	905	POV	2	0
2	A	903	POV	4	0
2	D	905	POV	4	0
2	C	904	POV	5	0
2	C	905	POV	3	0
2	D	907	POV	3	0
2	C	901	POV	6	0
2	D	908	POV	5	0
2	B	905	POV	2	0
2	C	908	POV	2	0
2	D	901	POV	2	0
2	C	909	POV	1	0
2	B	907	POV	2	0
2	C	903	POV	6	0
2	D	906	POV	4	0
2	D	909	POV	2	0
2	C	906	POV	5	0
2	A	904	POV	3	0
2	A	909	POV	5	0
2	B	908	POV	3	0
2	A	906	POV	2	0
2	B	906	POV	4	0
2	B	909	POV	2	0
2	A	908	POV	5	0
2	D	903	POV	6	0
2	B	904	POV	4	0
2	A	907	POV	5	0
2	D	904	POV	4	0
2	A	901	POV	3	0
2	B	901	POV	7	0
2	C	907	POV	3	0
2	B	903	POV	6	0
2	B	902	POV	2	0

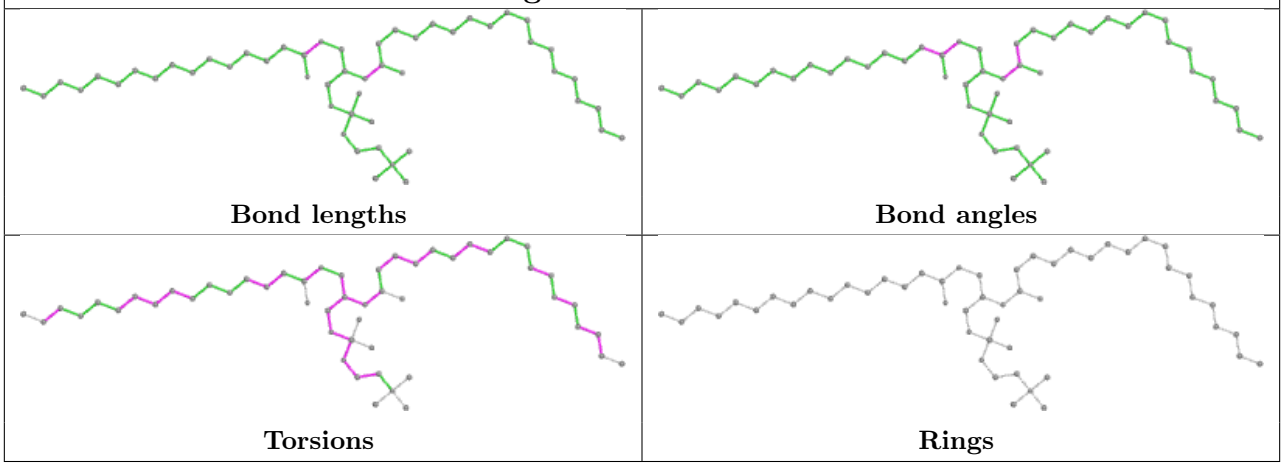
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

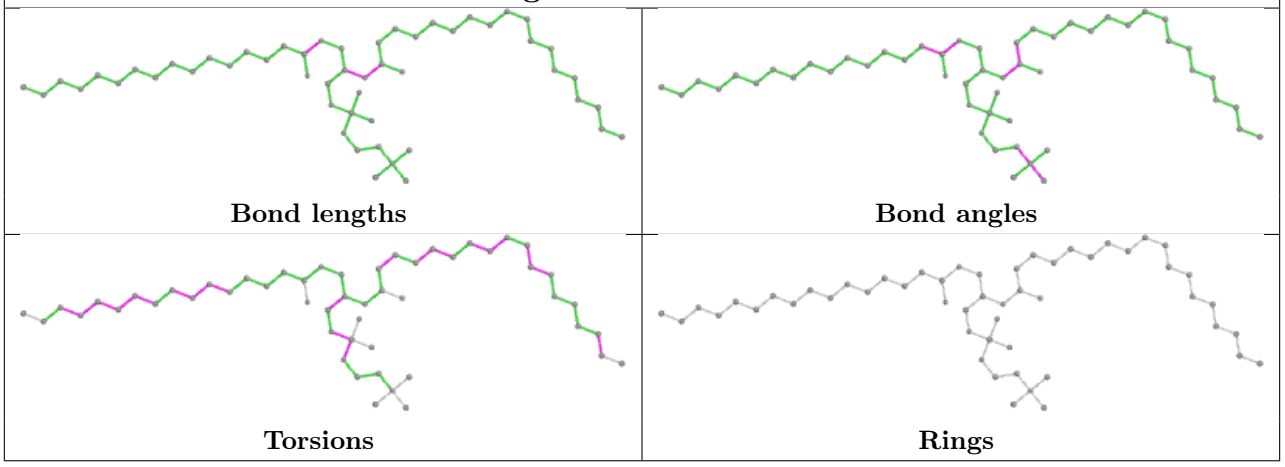
Ligand POV A 902



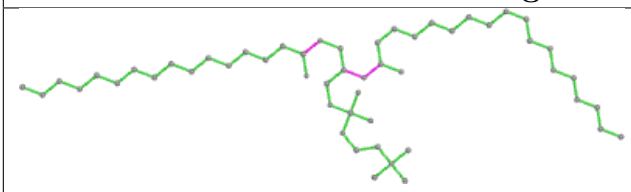
Ligand POV C 902



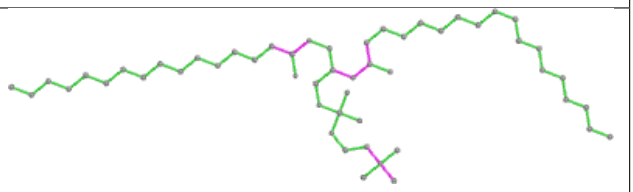
Ligand POV D 902



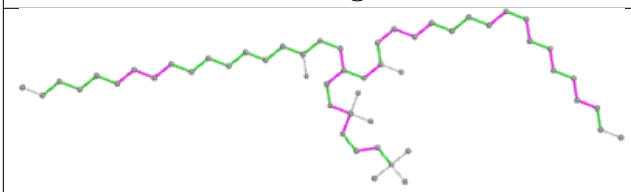
Ligand POV A 905



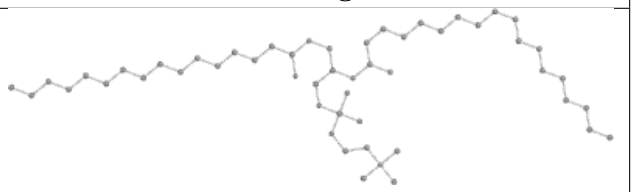
Bond lengths



Bond angles

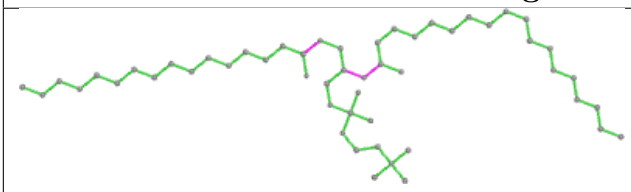


Torsions

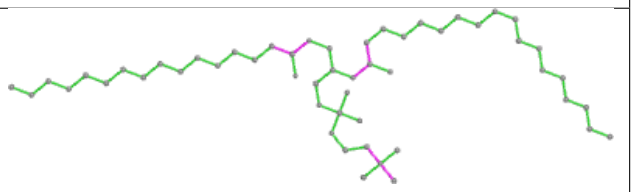


Rings

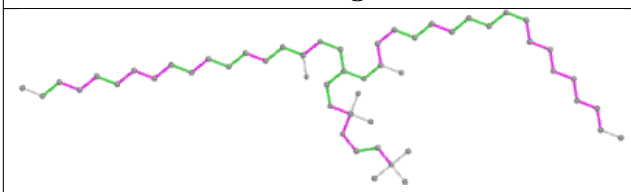
Ligand POV A 903



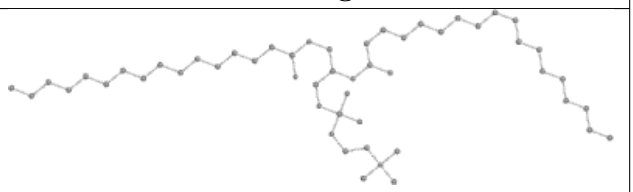
Bond lengths



Bond angles

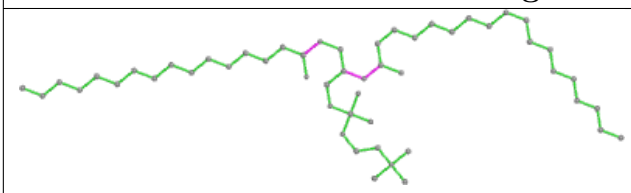


Torsions



Rings

Ligand POV D 905



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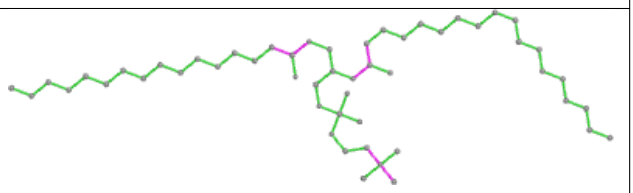
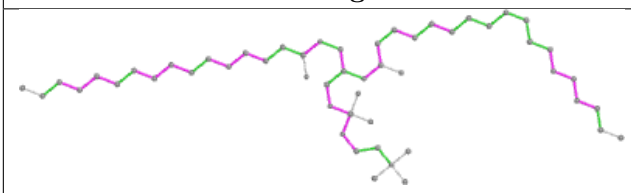


Bond angles



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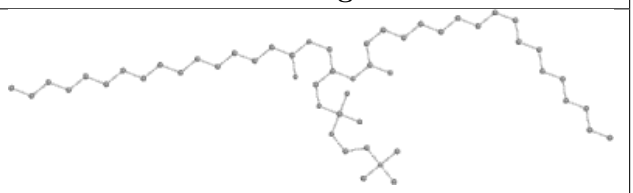
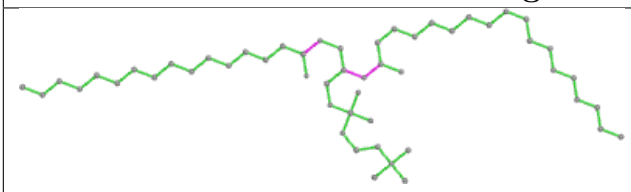


Rings

Ligand POV C 904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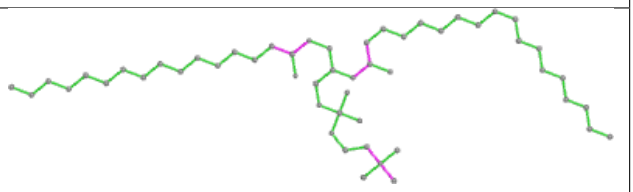
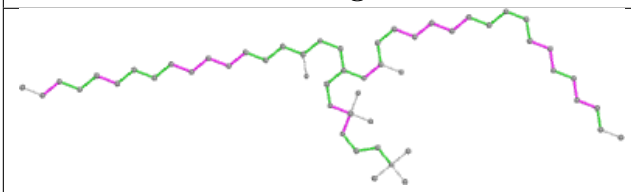

Bond angles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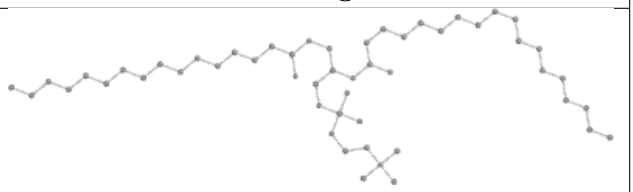
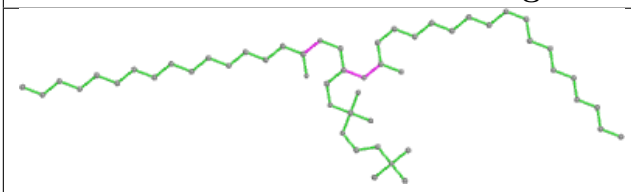

Rings

Ligand POV C 905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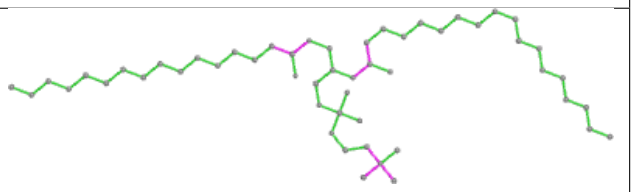
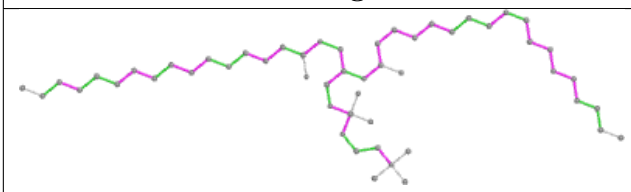

Bond angles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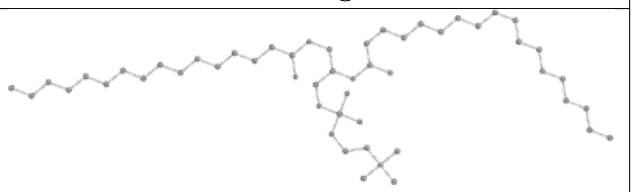
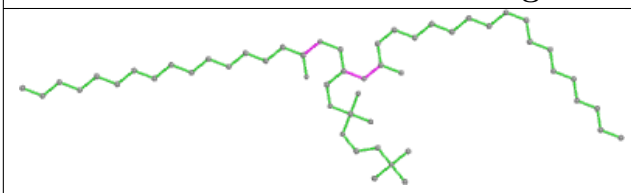

Rings

Ligand POV D 907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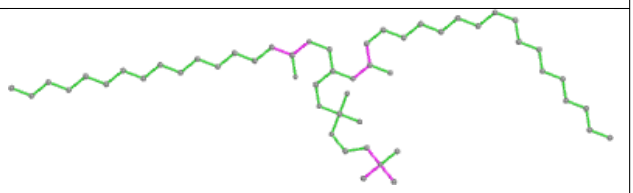
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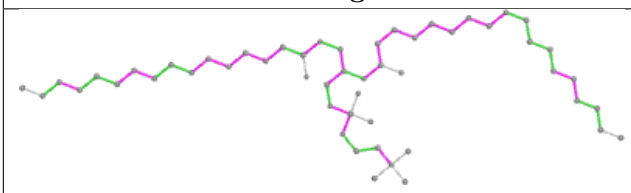
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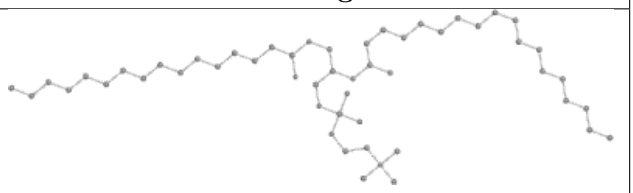
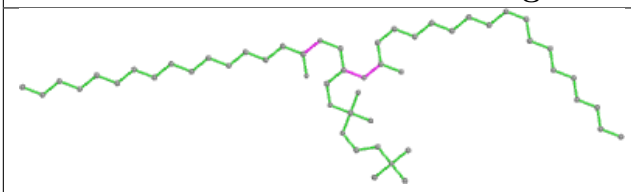

Rings

Ligand POV C 901



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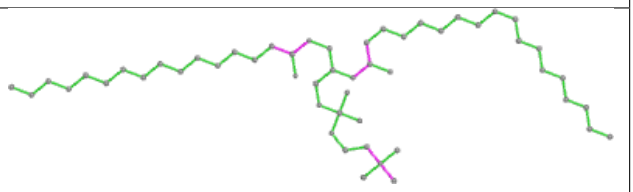
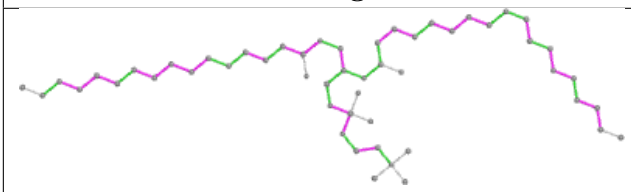


Bond angles



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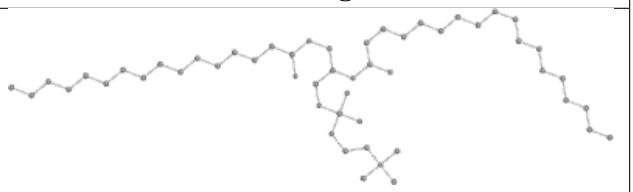
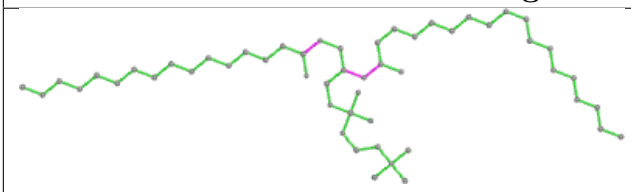


Rings

Ligand POV D 908



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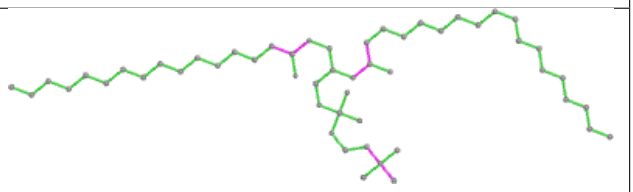

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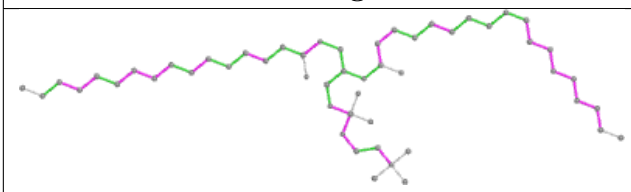

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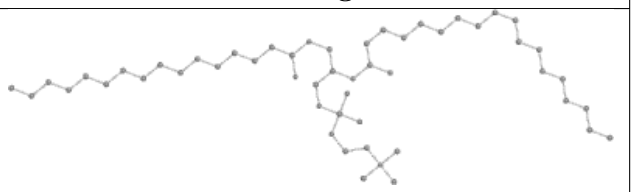
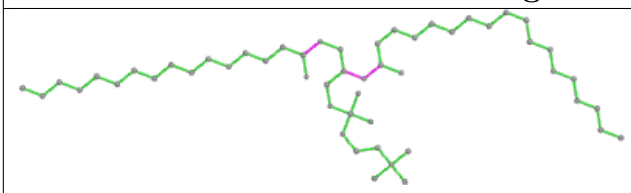


Rings

Ligand POV B 905



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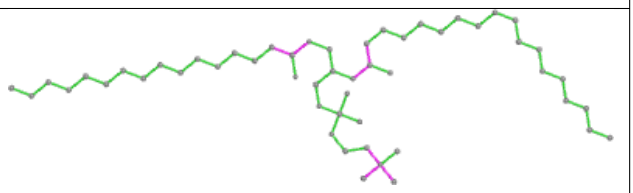
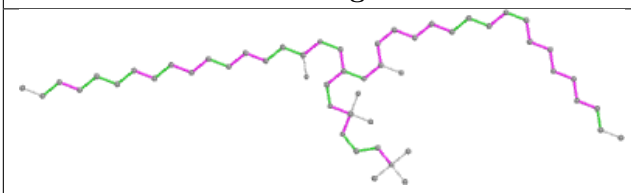


Bond angles



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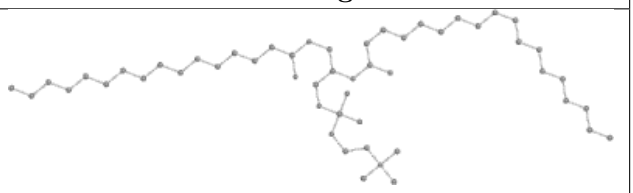
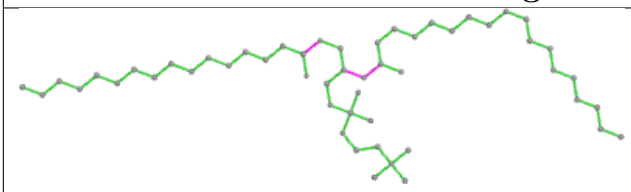


Rings

Ligand POV C 908



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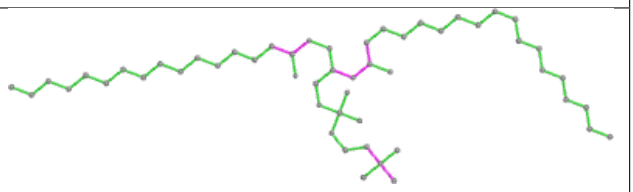
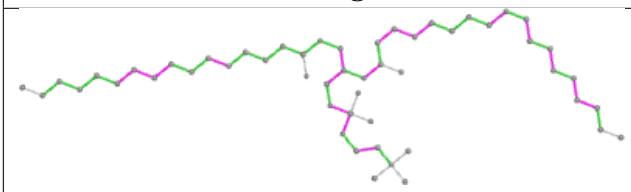


Bond angles



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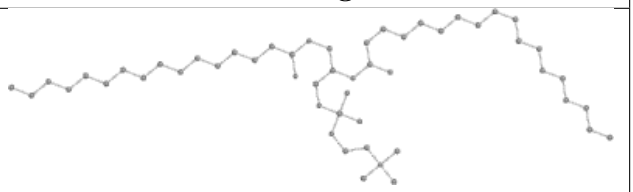
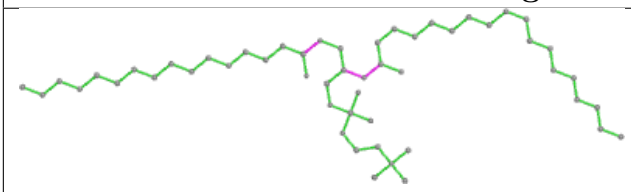


Rings

Ligand POV D 901



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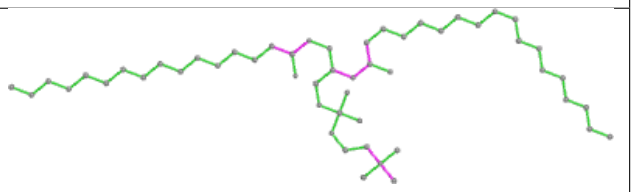
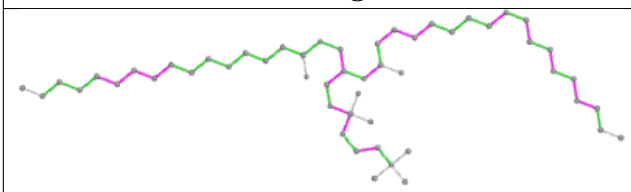


Bond angles



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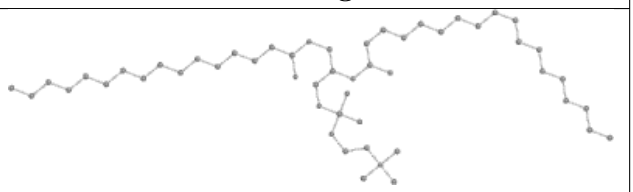
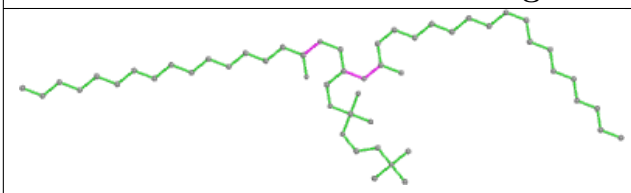


Rings

Ligand POV C 909



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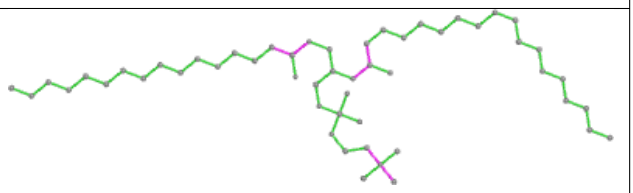

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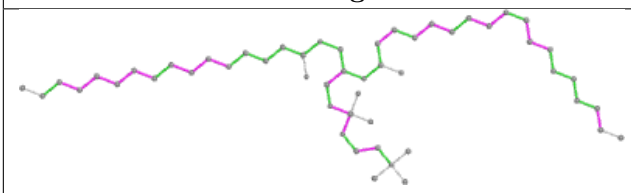

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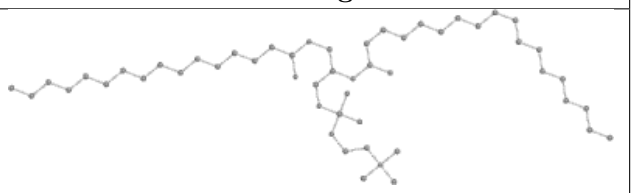
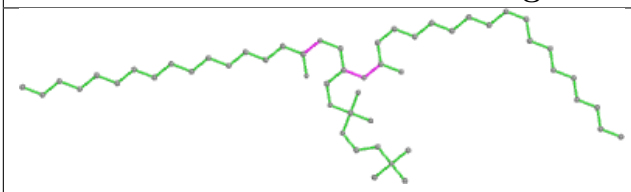
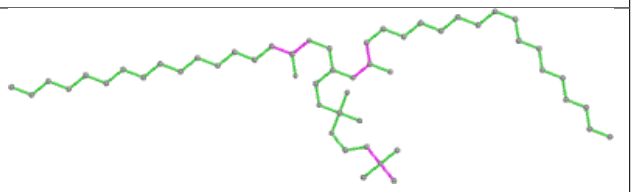


Rings

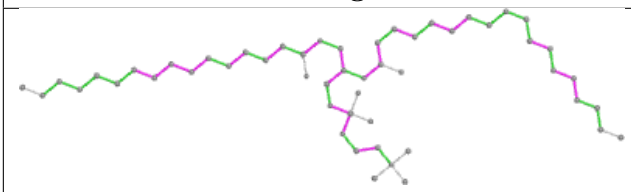
Ligand POV B 907



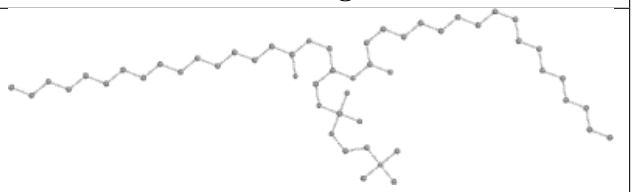
Bond lengths



Bond angles

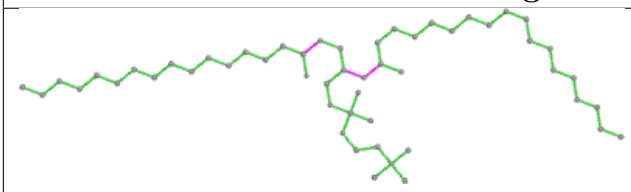


Torsions



Rings

Ligand POV C 903



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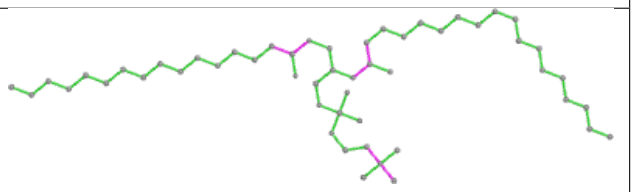
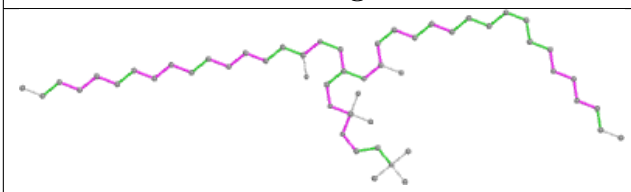


Bond angles



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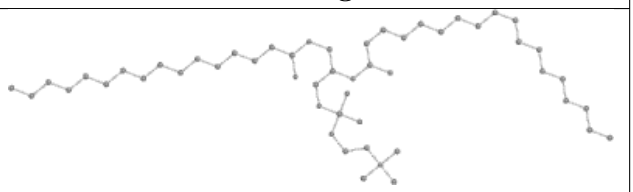
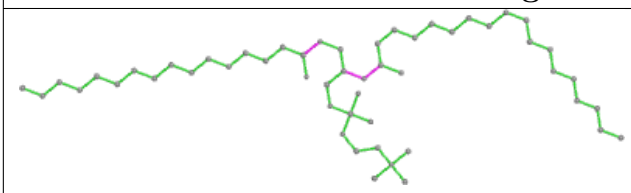
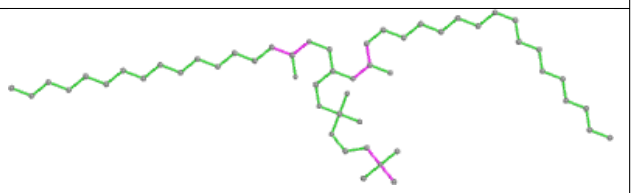


Rings

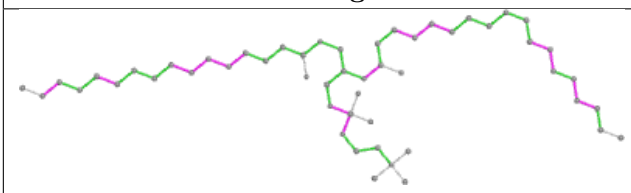
Ligand POV D 906



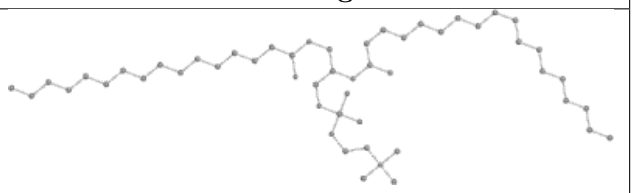
Bond lengths



Bond angles

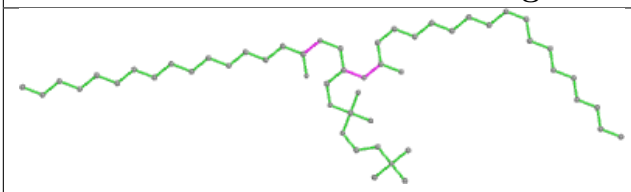


Torsions

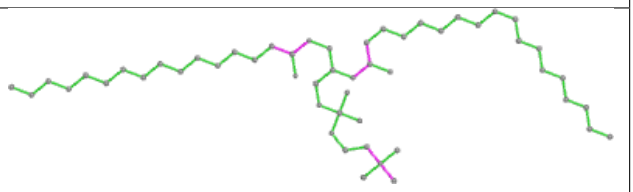


Rings

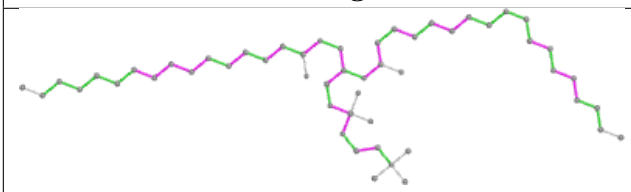
Ligand POV D 909



Bond lengths



Bond angles



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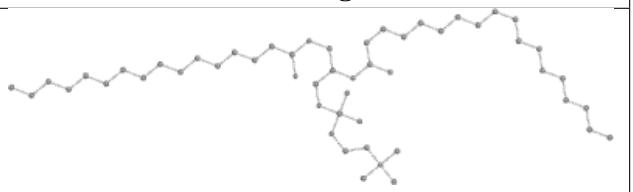
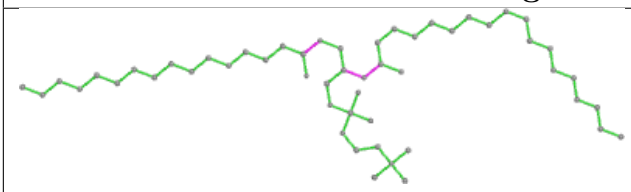


Rings

Ligand POV C 906



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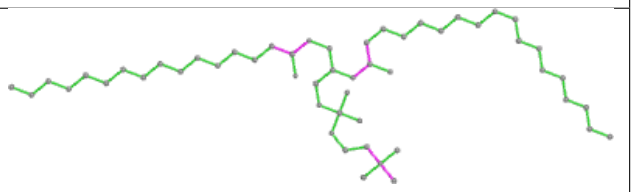

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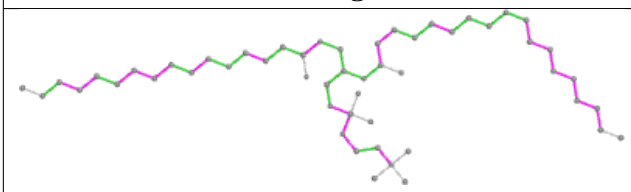

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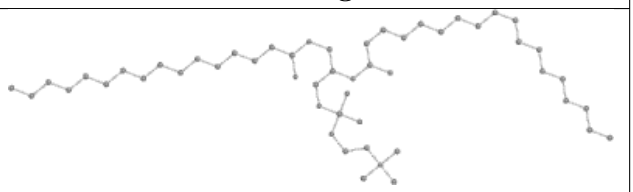
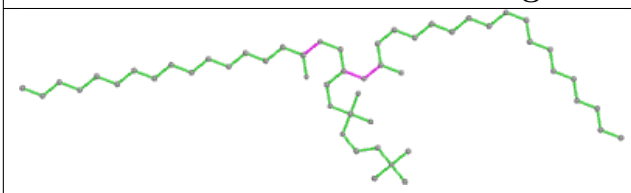


Rings

Ligand POV A 904



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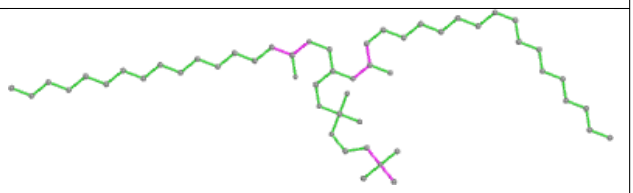
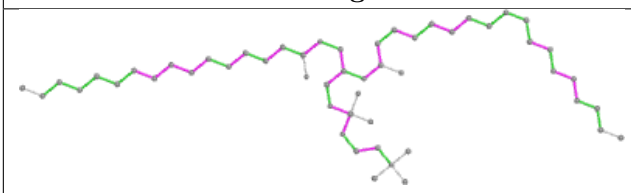


Bond angles



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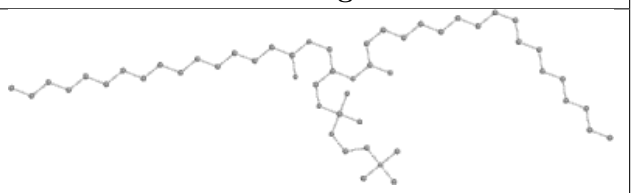
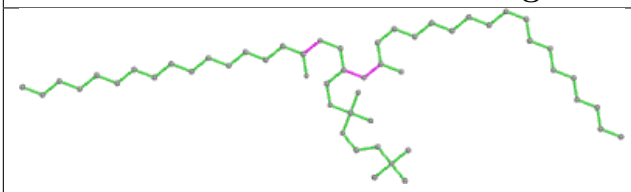


Rings

Ligand POV A 909



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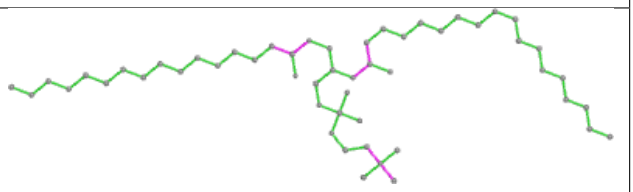

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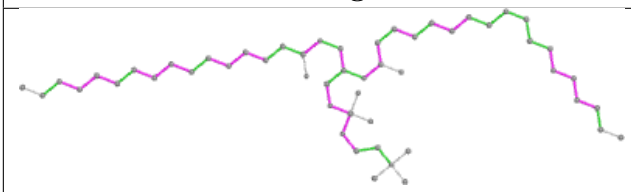

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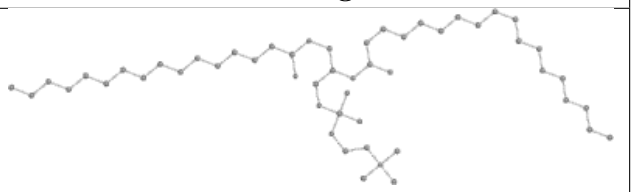
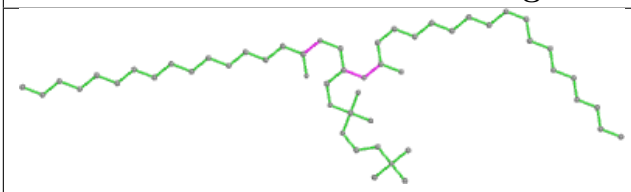


Rings

Ligand POV B 908



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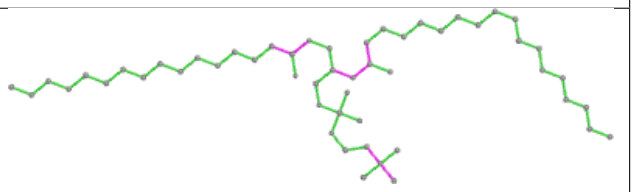

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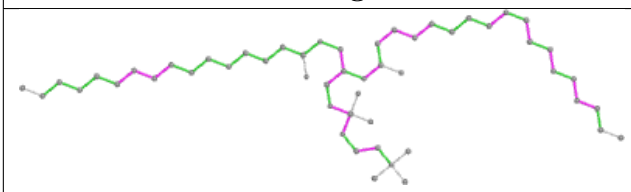

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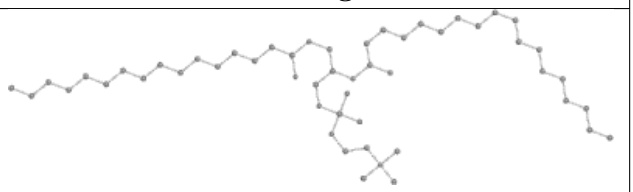
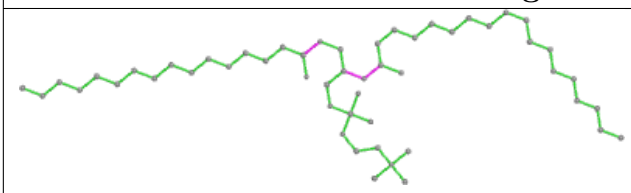


Rings

Ligand POV A 906



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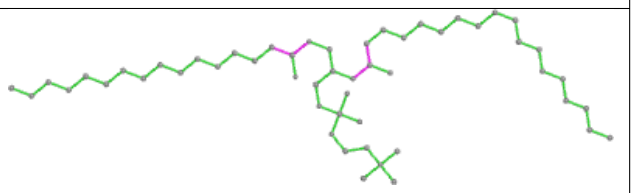

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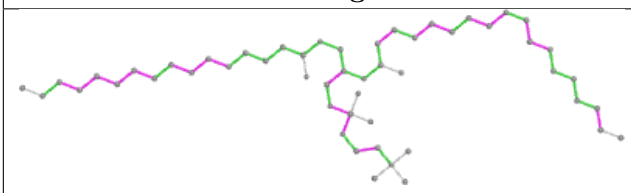

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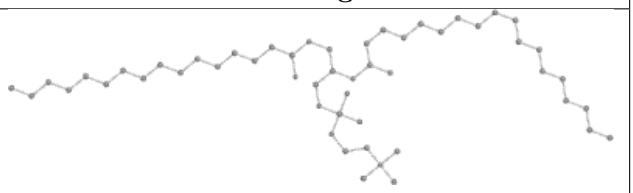
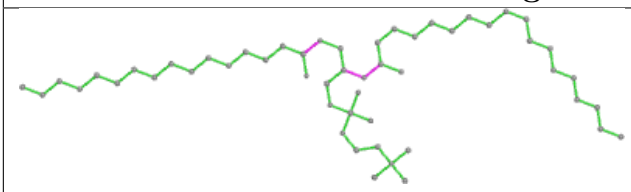


Rings

Ligand POV B 906



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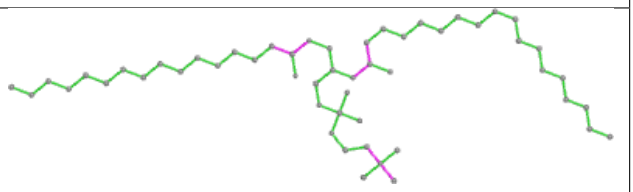

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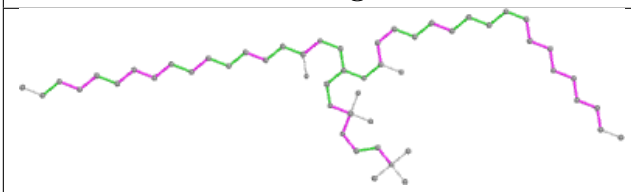

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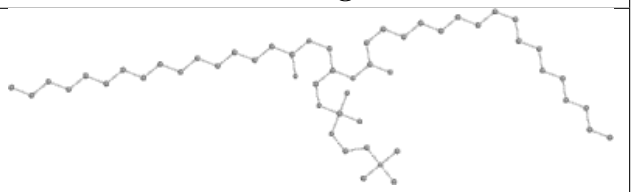
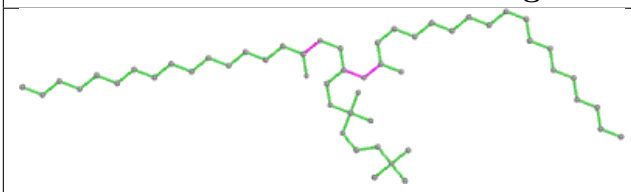


Rings

Ligand POV B 909



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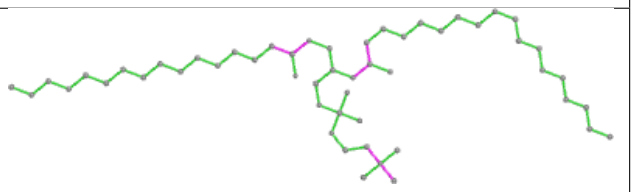
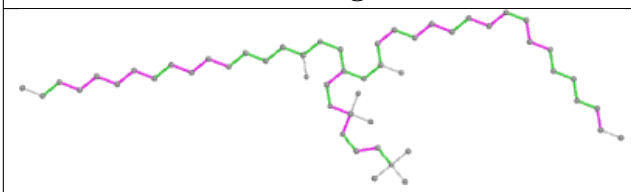


Bond angles



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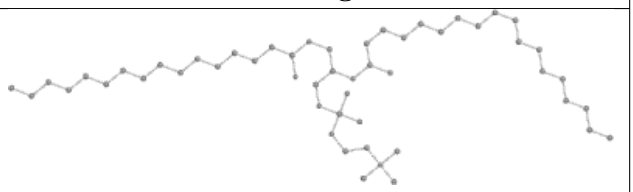
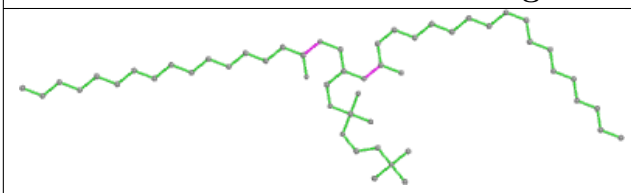


Rings

Ligand POV A 908



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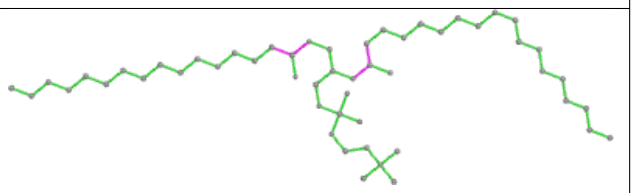
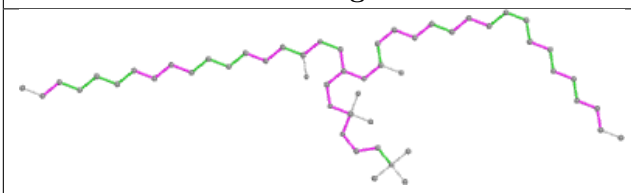


Bond angles



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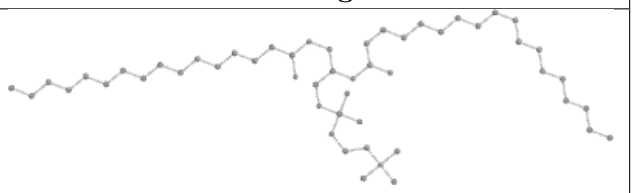
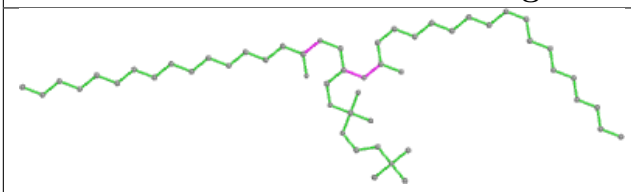


Rings

Ligand POV D 903



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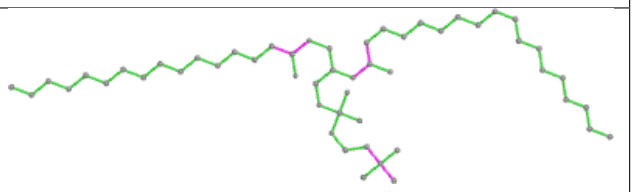
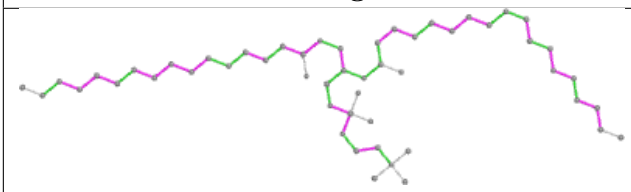


Bond angles



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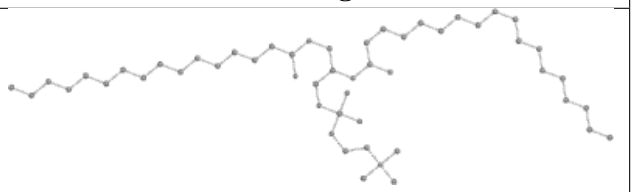
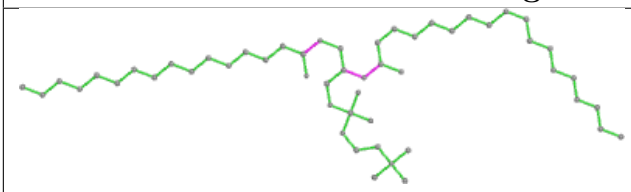


Rings

Ligand POV B 904



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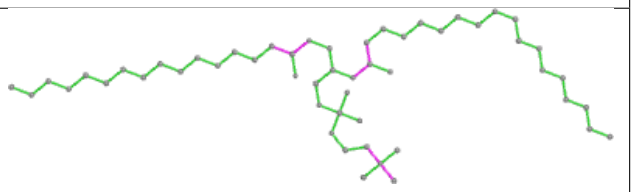
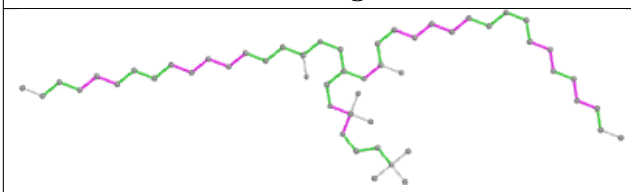


Bond angles



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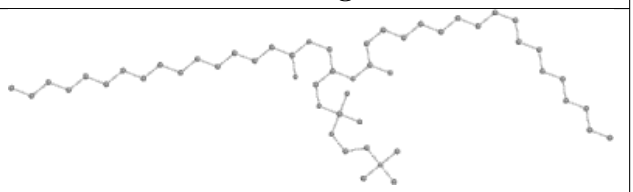
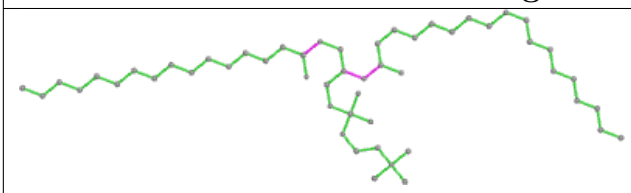


Rings

Ligand POV A 907



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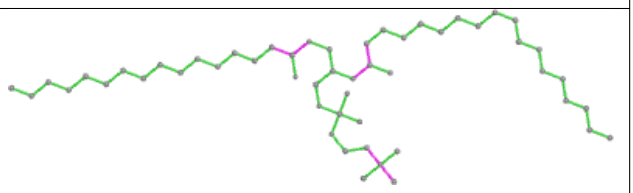
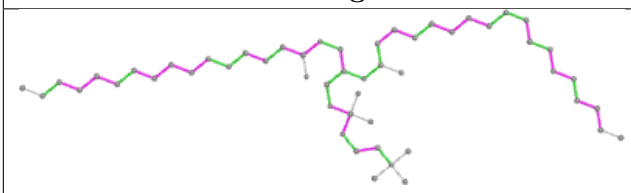


Bond angles



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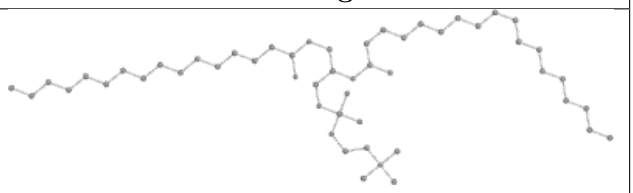
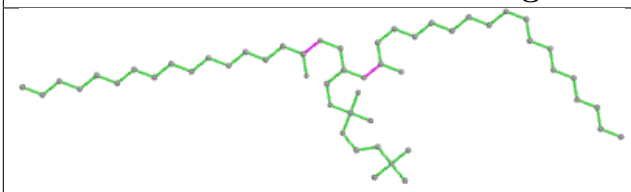


Rings

Ligand POV D 904



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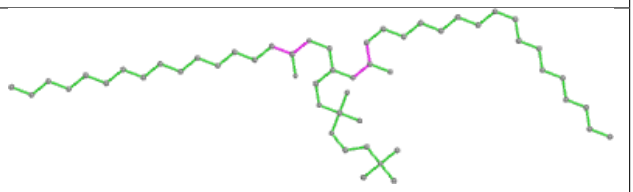
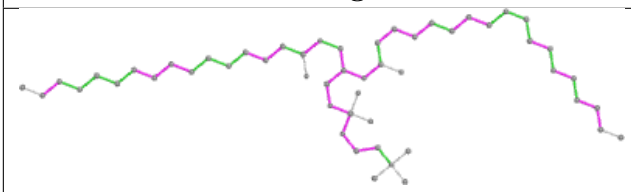


Bond angles



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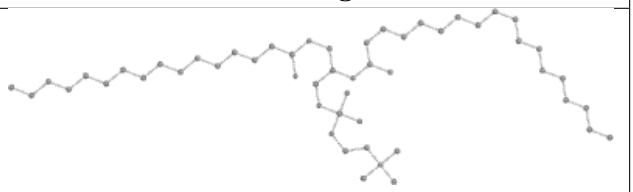
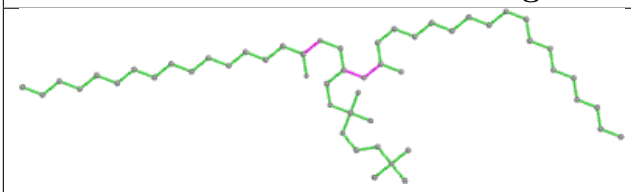
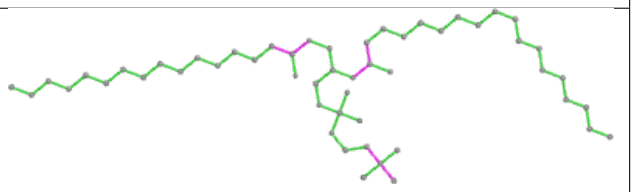


Rings

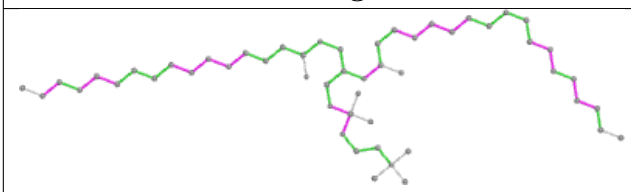
Ligand POV A 901



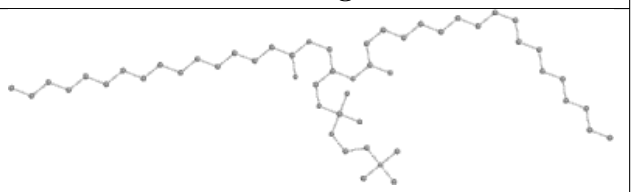
Bond lengths



Bond angles

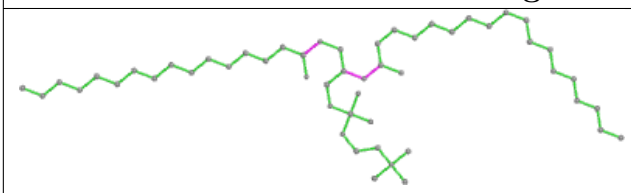


Torsions

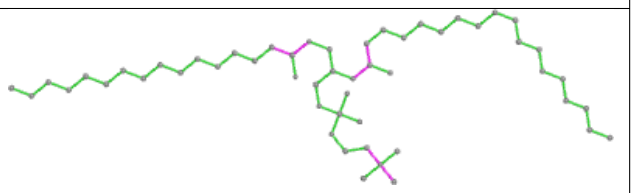


Rings

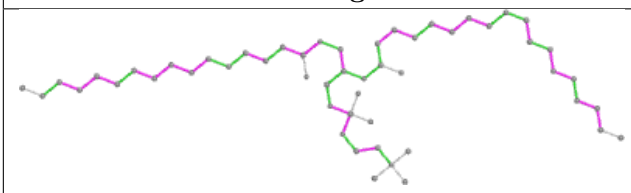
Ligand POV B 901



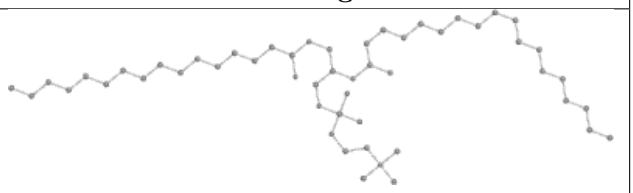
Bond lengths



Bond angles

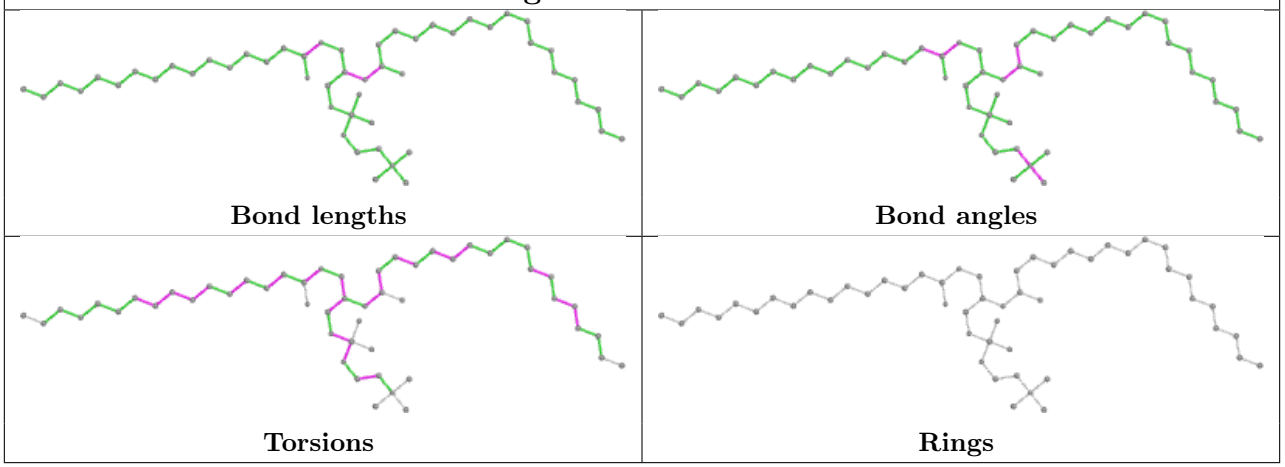


Torsions

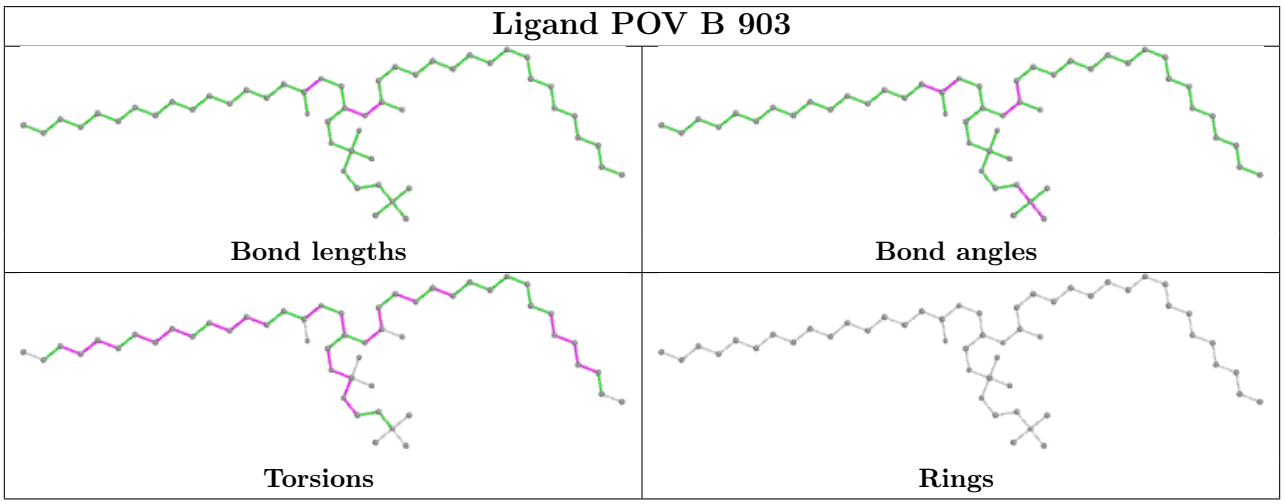


Rings

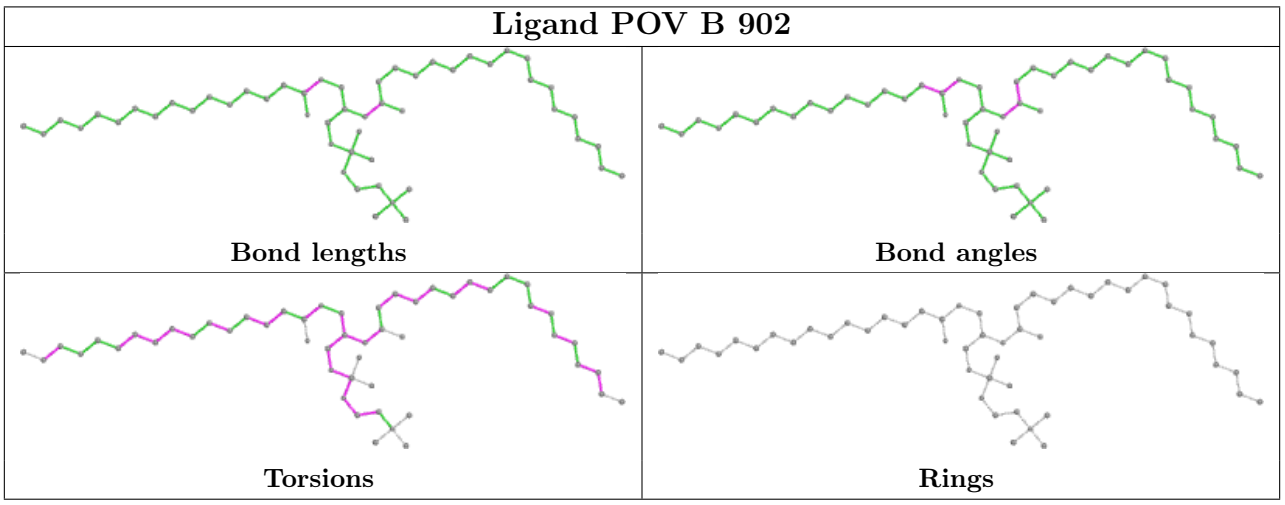
Ligand POV C 907



Ligand POV B 903



Ligand POV B 902



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

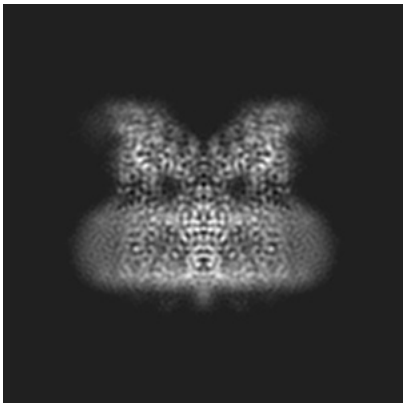
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23857. These allow visual inspection of the internal detail of the map and identification of artifacts.

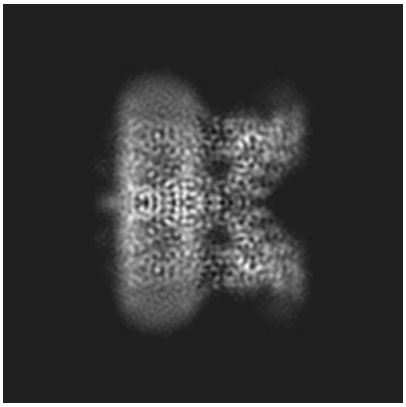
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

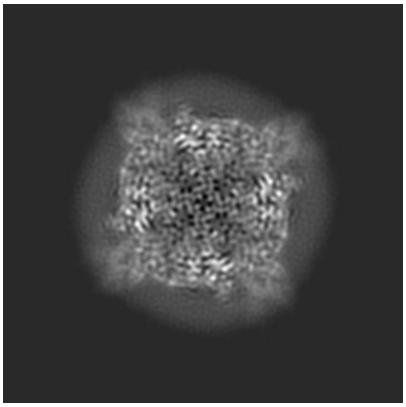
6.1.1 Primary map



X



Y



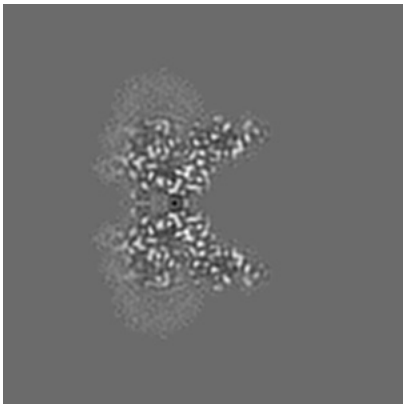
Z

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

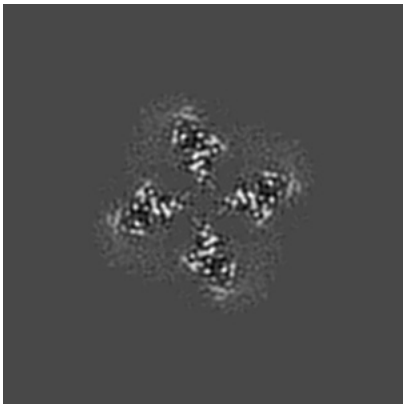
6.2 Central slices

6.2.1 Primary map

X Index: 128



Y Index: 128

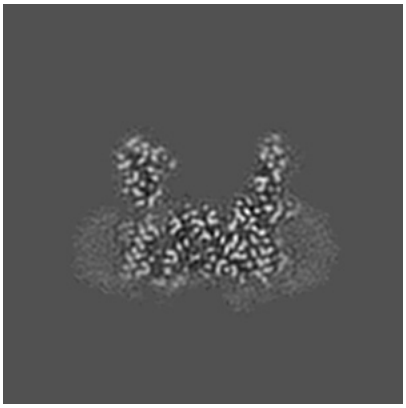


Z Index: 128

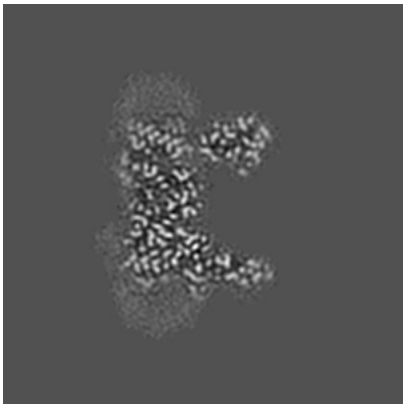
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 121



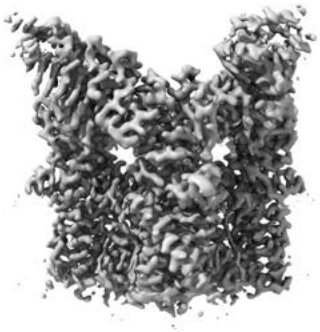
Y Index: 121

Z Index: 156

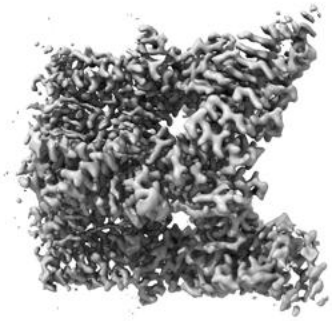
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

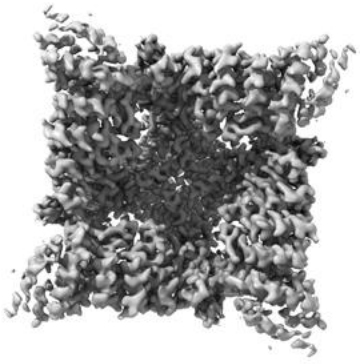
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0173. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

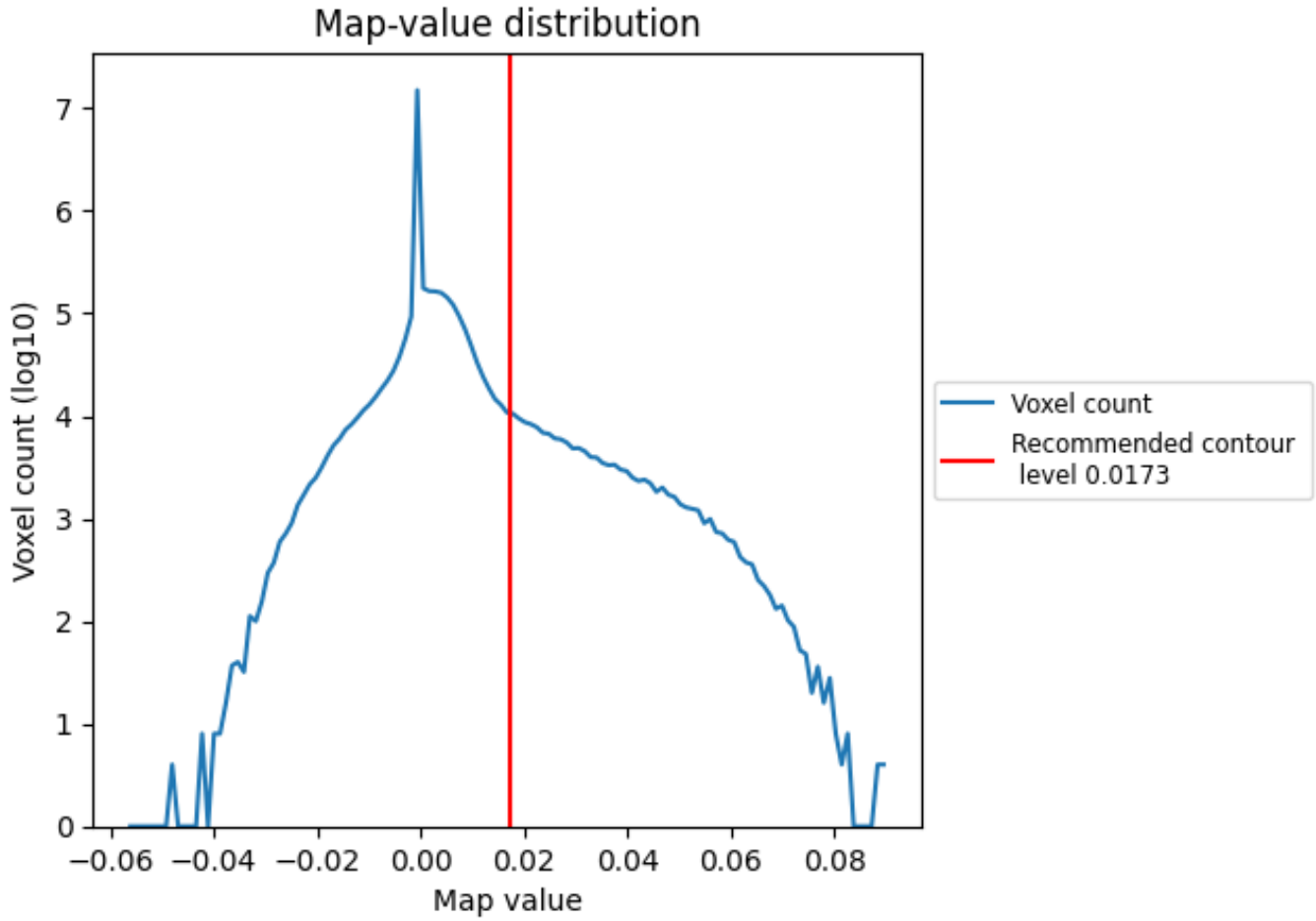
6.5 Mask visualisation (i)

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

7 Map analysis

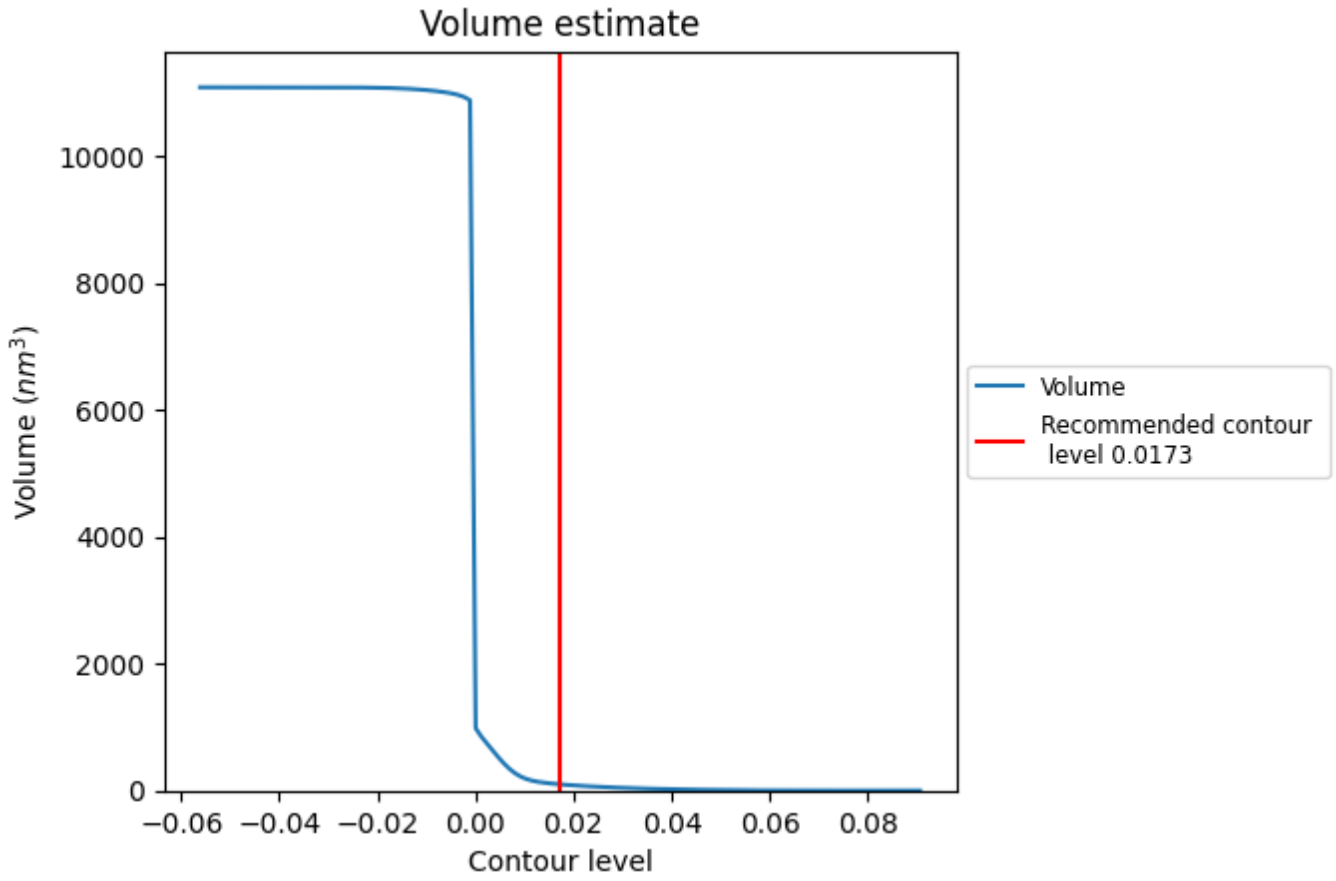
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

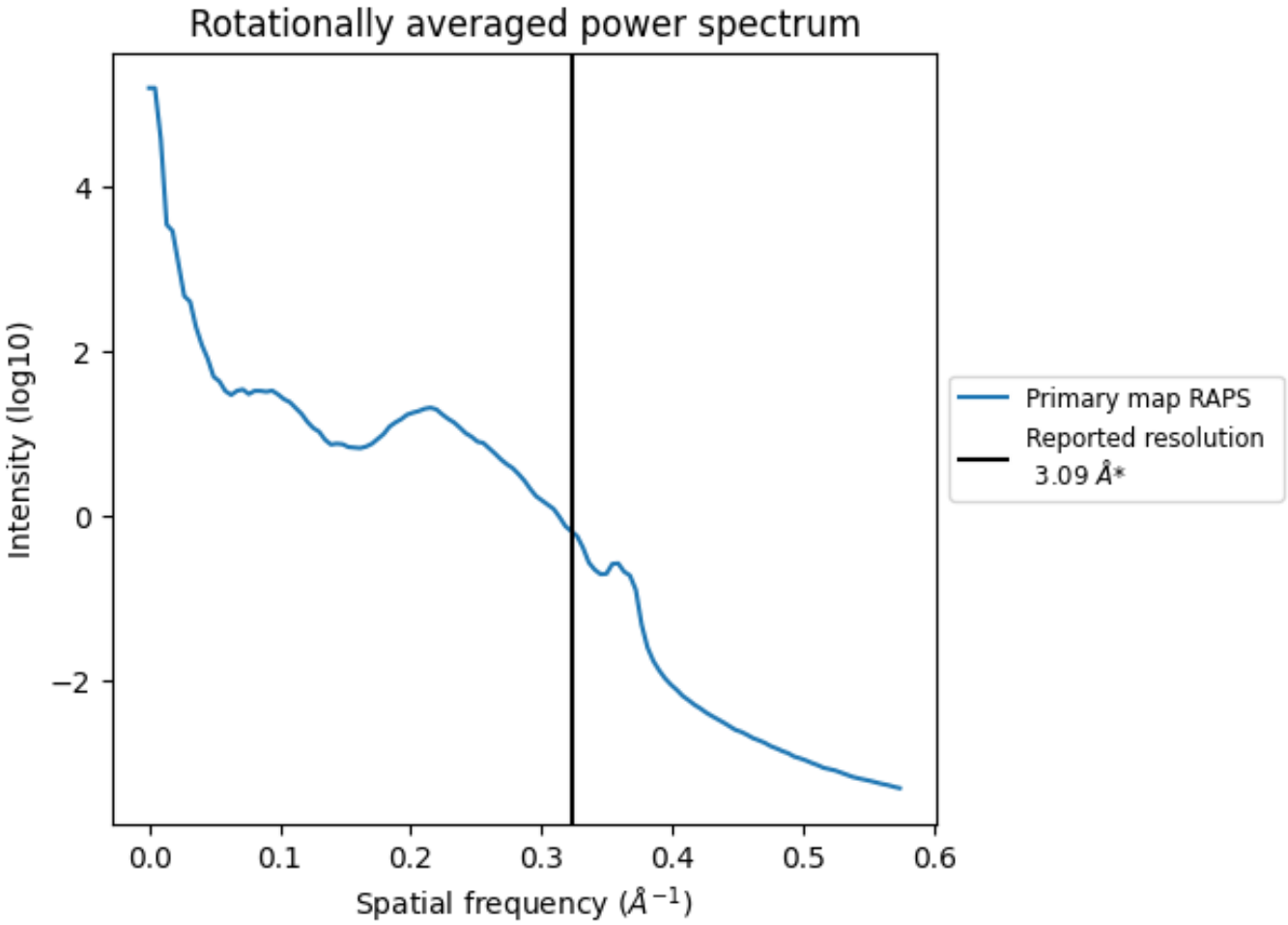
7.2 Volume estimate (i)



The volume at the recommended contour level is 98 nm^3; this corresponds to an approximate mass of 88 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 0.324 Å^{-1}

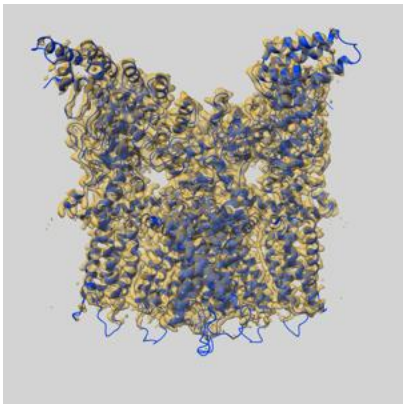
8 Fourier-Shell correlation

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

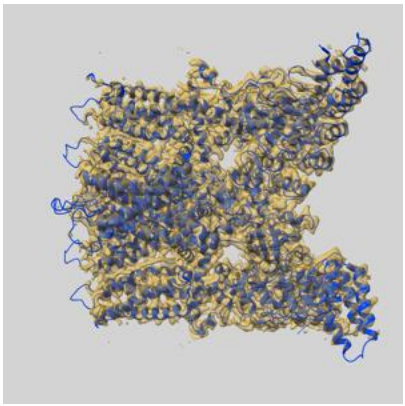
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23857 and PDB model 7MIN. Per-residue inclusion information can be found in section 3 on page 8.

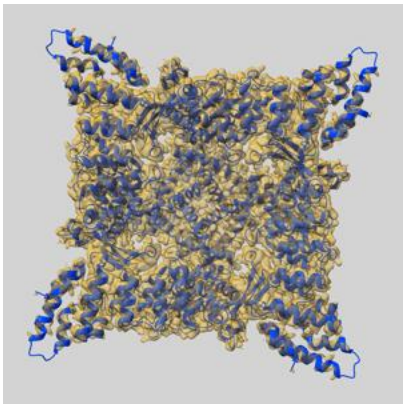
9.1 Map-model overlay



X



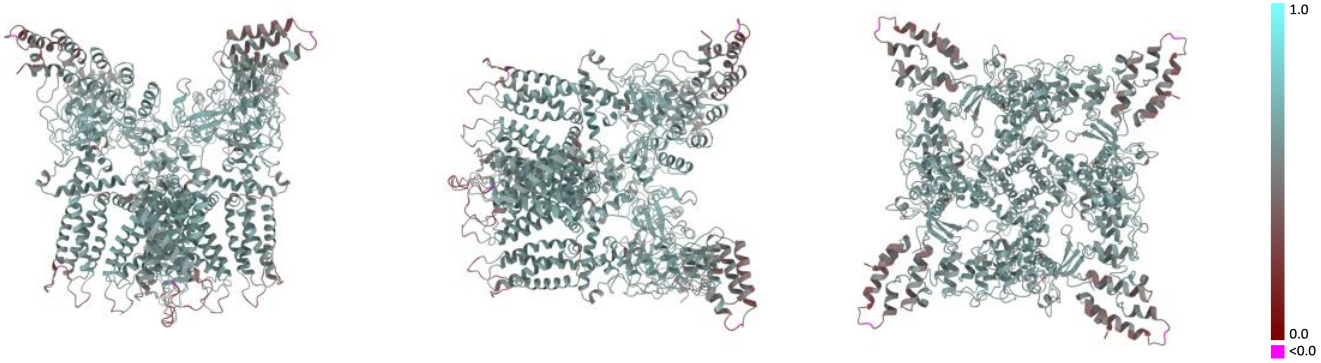
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0173 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.

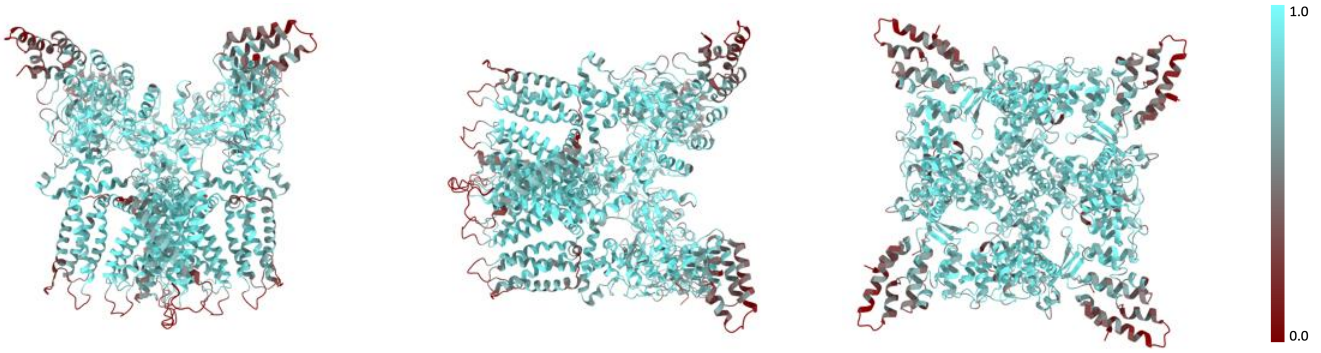
9.2 Q-score mapped to coordinate model (i)



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.

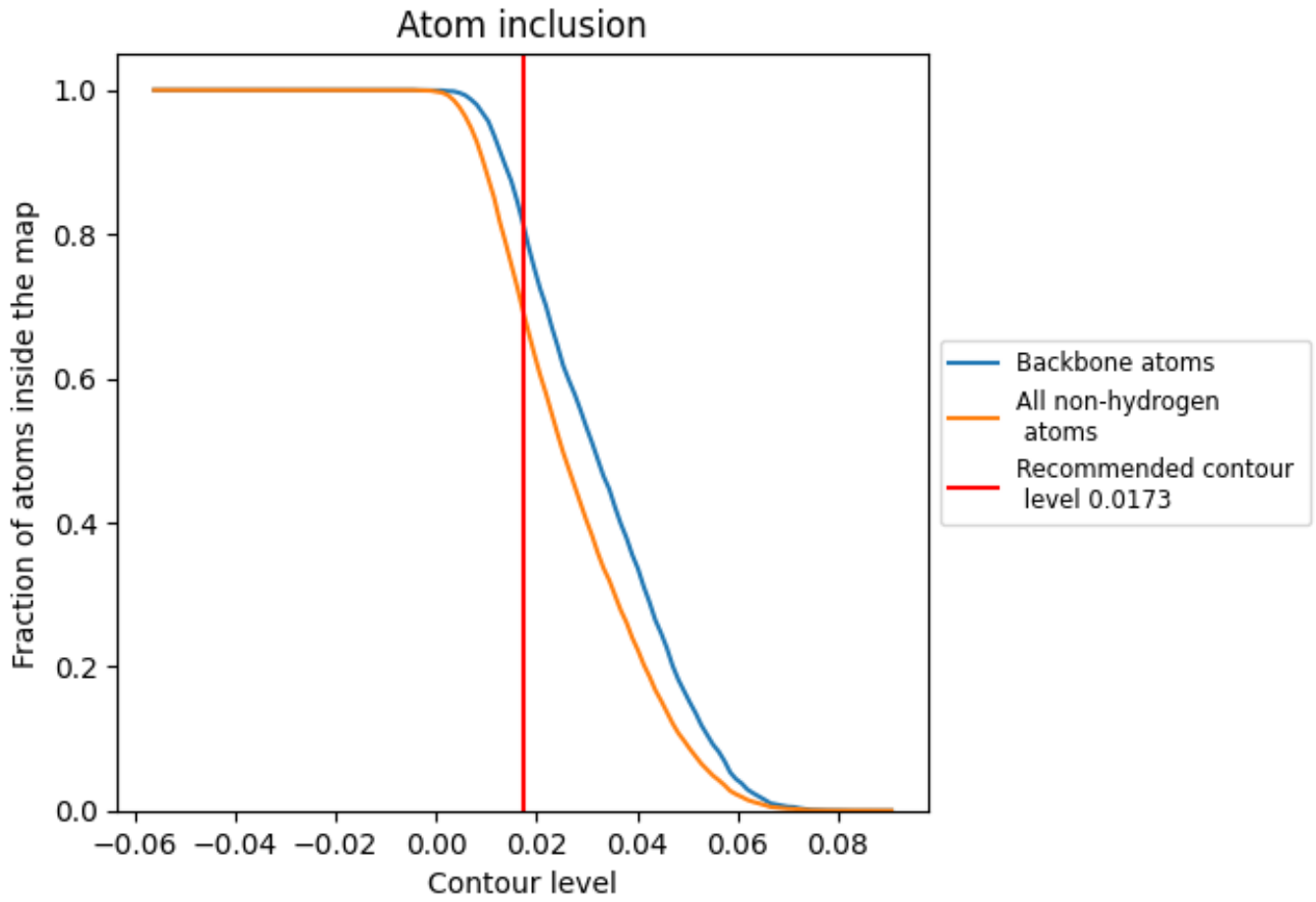
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0173).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 69% 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 (0.0173) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6934	0.5480
A	0.6938	0.5480
B	0.6931	0.5490
C	0.6931	0.5480
D	0.6938	0.5470