



Full wwPDB EM Validation Report ⓘ

Jun 2, 2026 – 12:20 AM JST

PDB ID : 9UED / pdb_00009ued
EMDB ID : EMD-64082
Title : Cryo-EM structure of human TRPV3 in complex with sevoflurane determined in MSP2N2 nanodisc
Authors : Lu, X.; Yao, J.
Deposited on : 2025-04-08
Resolution : 3.29 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

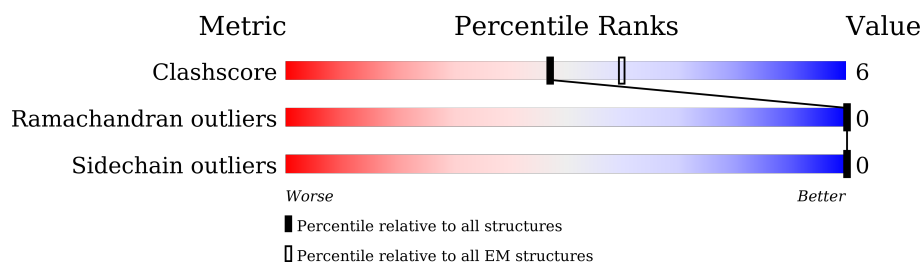
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.29 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	802	
1	B	802	
1	C	802	
1	D	802	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20020 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	602	Total	C	N	O	S	0	0
			4889	3194	797	869	29		
1	B	602	Total	C	N	O	S	0	0
			4889	3194	797	869	29		
1	C	602	Total	C	N	O	S	0	0
			4889	3194	797	869	29		
1	D	602	Total	C	N	O	S	0	0
			4889	3194	797	869	29		

There are 52 discrepancies between the modelled and reference sequences:

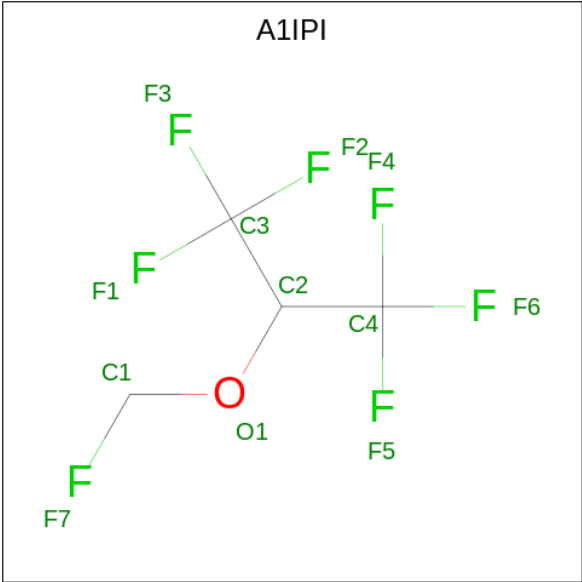
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	VAL	ILE	variant	UNP Q8NET8
A	791	ALA	-	expression tag	UNP Q8NET8
A	792	ALA	-	expression tag	UNP Q8NET8
A	793	ALA	-	expression tag	UNP Q8NET8
A	794	SER	-	expression tag	UNP Q8NET8
A	795	ASN	-	expression tag	UNP Q8NET8
A	796	SER	-	expression tag	UNP Q8NET8
A	797	LEU	-	expression tag	UNP Q8NET8
A	798	GLU	-	expression tag	UNP Q8NET8
A	799	VAL	-	expression tag	UNP Q8NET8
A	800	LEU	-	expression tag	UNP Q8NET8
A	801	PHE	-	expression tag	UNP Q8NET8
A	802	GLN	-	expression tag	UNP Q8NET8
B	25	VAL	ILE	variant	UNP Q8NET8
B	791	ALA	-	expression tag	UNP Q8NET8
B	792	ALA	-	expression tag	UNP Q8NET8
B	793	ALA	-	expression tag	UNP Q8NET8
B	794	SER	-	expression tag	UNP Q8NET8
B	795	ASN	-	expression tag	UNP Q8NET8
B	796	SER	-	expression tag	UNP Q8NET8
B	797	LEU	-	expression tag	UNP Q8NET8

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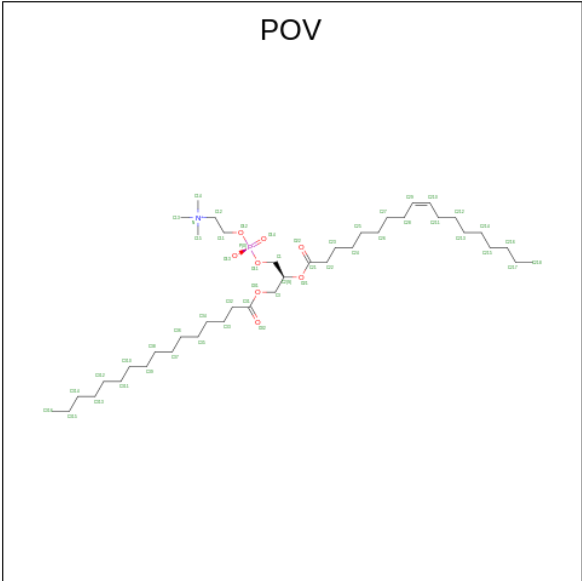
Chain	Residue	Modelled	Actual	Comment	Reference
B	798	GLU	-	expression tag	UNP Q8NET8
B	799	VAL	-	expression tag	UNP Q8NET8
B	800	LEU	-	expression tag	UNP Q8NET8
B	801	PHE	-	expression tag	UNP Q8NET8
B	802	GLN	-	expression tag	UNP Q8NET8
C	25	VAL	ILE	variant	UNP Q8NET8
C	791	ALA	-	expression tag	UNP Q8NET8
C	792	ALA	-	expression tag	UNP Q8NET8
C	793	ALA	-	expression tag	UNP Q8NET8
C	794	SER	-	expression tag	UNP Q8NET8
C	795	ASN	-	expression tag	UNP Q8NET8
C	796	SER	-	expression tag	UNP Q8NET8
C	797	LEU	-	expression tag	UNP Q8NET8
C	798	GLU	-	expression tag	UNP Q8NET8
C	799	VAL	-	expression tag	UNP Q8NET8
C	800	LEU	-	expression tag	UNP Q8NET8
C	801	PHE	-	expression tag	UNP Q8NET8
C	802	GLN	-	expression tag	UNP Q8NET8
D	25	VAL	ILE	variant	UNP Q8NET8
D	791	ALA	-	expression tag	UNP Q8NET8
D	792	ALA	-	expression tag	UNP Q8NET8
D	793	ALA	-	expression tag	UNP Q8NET8
D	794	SER	-	expression tag	UNP Q8NET8
D	795	ASN	-	expression tag	UNP Q8NET8
D	796	SER	-	expression tag	UNP Q8NET8
D	797	LEU	-	expression tag	UNP Q8NET8
D	798	GLU	-	expression tag	UNP Q8NET8
D	799	VAL	-	expression tag	UNP Q8NET8
D	800	LEU	-	expression tag	UNP Q8NET8
D	801	PHE	-	expression tag	UNP Q8NET8
D	802	GLN	-	expression tag	UNP Q8NET8

- Molecule 2 is sevoflurane (CCD ID: A1IPI) (formula: $C_4H_3F_7O$) (labeled as "Ligand of Interest" by depositor).

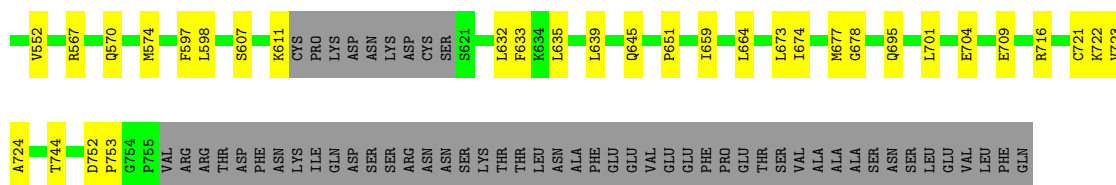


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	F	O	0
			12	4	7	1	
2	A	1	Total	C	F	O	0
			12	4	7	1	
2	B	1	Total	C	F	O	0
			12	4	7	1	
2	C	1	Total	C	F	O	0
			12	4	7	1	

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).

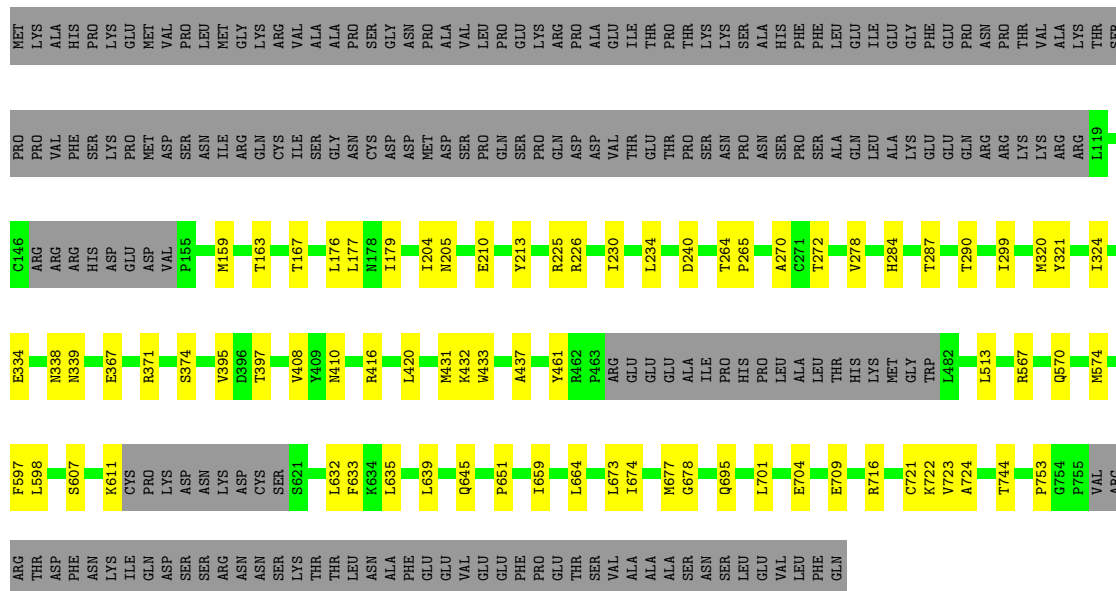


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	D	1	Total	C	N	O	P	0
			52	42	1	8	1	



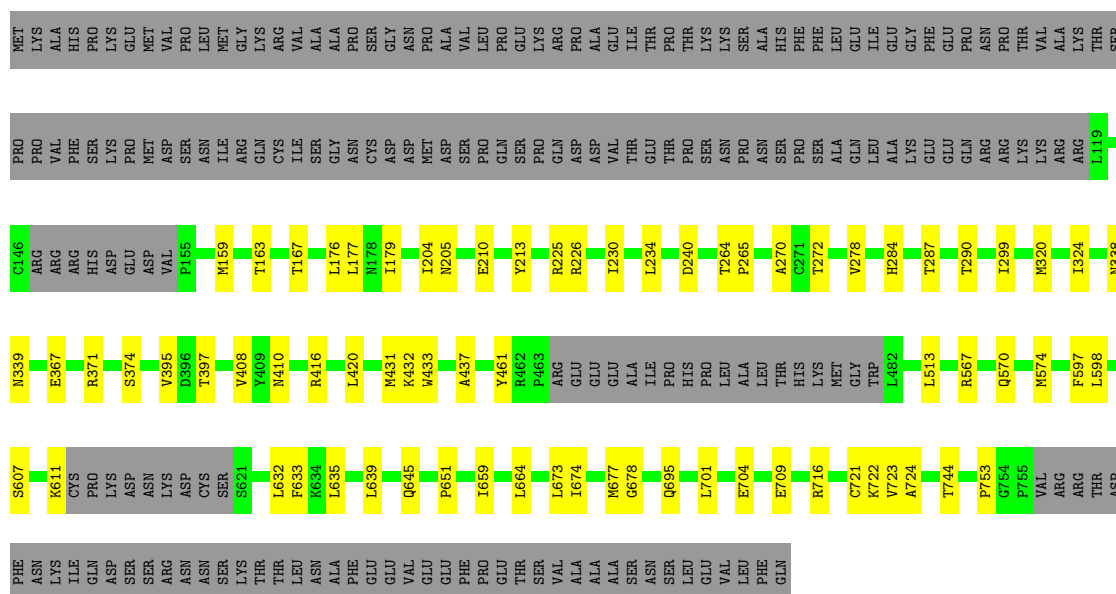
- Molecule 1: Transient receptor potential cation channel subfamily V member 3

Chain C: 66% 9% 25%



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

Chain D: 66% 9% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38843	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	-1300	Depositor
Maximum defocus (nm)	-1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: POV, A1IPI

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	0.13	0/4994	0.28	0/6754
1	B	0.13	0/4994	0.28	0/6754
1	C	0.13	0/4994	0.28	0/6754
1	D	0.13	0/4994	0.28	0/6754
All	All	0.13	0/19976	0.28	0/27016

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4889	0	4964	67	0
1	B	4889	0	4964	69	0
1	C	4889	0	4964	61	0
1	D	4889	0	4964	64	0
2	A	24	0	0	2	0
2	B	12	0	0	1	0
2	C	12	0	0	1	0
3	A	104	0	164	2	0
3	B	104	0	164	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	104	0	164	1	0
3	D	104	0	164	2	0
All	All	20020	0	20512	242	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 6.

All (242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:673:LEU:CD1	1:B:677:MET:HE2	1.70	1.21
1:D:673:LEU:CD1	1:D:677:MET:HE2	1.69	1.21
1:C:673:LEU:CD1	1:C:677:MET:HE2	1.71	1.18
1:A:673:LEU:CD1	1:A:677:MET:HE2	1.73	1.17
1:A:673:LEU:HD11	1:A:677:MET:HE2	1.22	1.13
1:D:673:LEU:HD11	1:D:677:MET:HE2	1.19	1.10
1:B:673:LEU:HD11	1:B:677:MET:HE2	1.19	1.09
1:C:673:LEU:HD11	1:C:677:MET:HE2	1.22	1.07
1:B:673:LEU:HD11	1:B:677:MET:CE	2.04	0.86
1:D:673:LEU:HD11	1:D:677:MET:CE	2.04	0.86
1:A:673:LEU:HD11	1:A:677:MET:CE	2.09	0.82
1:C:673:LEU:HD11	1:C:677:MET:CE	2.07	0.82
1:C:213:TYR:OH	1:D:753:PRO:O	2.02	0.78
1:A:213:TYR:OH	1:B:753:PRO:O	2.02	0.78
1:A:753:PRO:O	1:D:213:TYR:OH	2.02	0.78
1:B:213:TYR:OH	1:C:753:PRO:O	2.02	0.77
1:C:397:THR:OG1	1:C:704:GLU:OE2	2.03	0.76
1:D:570:GLN:NE2	1:D:574:MET:SD	2.59	0.76
1:B:570:GLN:NE2	1:B:574:MET:SD	2.59	0.75
1:A:570:GLN:NE2	1:A:574:MET:SD	2.59	0.75
1:C:570:GLN:NE2	1:C:574:MET:SD	2.59	0.75
1:B:397:THR:OG1	1:B:704:GLU:OE2	2.03	0.74
1:D:567:ARG:NH1	1:D:695:GLN:OE1	2.22	0.73
1:C:567:ARG:NH1	1:C:695:GLN:OE1	2.22	0.73
1:A:397:THR:OG1	1:A:704:GLU:OE2	2.03	0.72
1:A:567:ARG:NH1	1:A:695:GLN:OE1	2.22	0.72
1:B:567:ARG:NH1	1:B:695:GLN:OE1	2.22	0.71
1:B:433:TRP:HA	1:B:437:ALA:HB3	1.77	0.67
1:A:461:TYR:C	3:A:904:POV:H13	2.20	0.67
1:A:167:THR:OG1	1:A:210:GLU:OE2	2.12	0.66
1:D:159:MET:O	1:D:163:THR:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:ASN:OD1	1:D:339:ASN:N	2.29	0.66
1:D:461:TYR:C	3:D:901:POV:H13	2.20	0.66
1:C:461:TYR:C	3:C:901:POV:H13	2.20	0.66
1:A:338:ASN:OD1	1:A:339:ASN:N	2.28	0.66
1:B:461:TYR:C	3:B:901:POV:H13	2.20	0.66
1:B:159:MET:O	1:B:163:THR:N	2.28	0.66
1:C:159:MET:O	1:C:163:THR:N	2.28	0.66
1:D:433:TRP:HA	1:D:437:ALA:HB3	1.77	0.66
1:A:433:TRP:HA	1:A:437:ALA:HB3	1.78	0.66
1:C:278:VAL:HG11	1:C:320:MET:HE1	1.78	0.66
1:A:159:MET:O	1:A:163:THR:N	2.28	0.66
1:B:278:VAL:HG11	1:B:320:MET:HE1	1.78	0.66
1:B:338:ASN:OD1	1:B:339:ASN:N	2.29	0.65
1:D:397:THR:OG1	1:D:704:GLU:OE2	2.03	0.65
1:A:721:CYS:SG	1:A:722:LYS:NZ	2.70	0.65
1:B:721:CYS:SG	1:B:722:LYS:NZ	2.70	0.65
1:C:338:ASN:OD1	1:C:339:ASN:N	2.30	0.65
1:D:278:VAL:HG11	1:D:320:MET:HE1	1.78	0.64
1:C:433:TRP:HA	1:C:437:ALA:HB3	1.78	0.64
1:A:278:VAL:HG11	1:A:320:MET:HE1	1.78	0.64
1:A:431:MET:SD	1:A:716:ARG:NH1	2.71	0.64
1:C:721:CYS:SG	1:C:722:LYS:NZ	2.70	0.64
1:D:721:CYS:SG	1:D:722:LYS:NZ	2.71	0.64
1:C:431:MET:SD	1:C:716:ARG:NH1	2.71	0.64
1:B:431:MET:SD	1:B:716:ARG:NH1	2.71	0.63
1:D:167:THR:OG1	1:D:210:GLU:OE2	2.13	0.63
1:B:167:THR:OG1	1:B:210:GLU:OE2	2.13	0.63
1:D:431:MET:SD	1:D:716:ARG:NH1	2.71	0.63
1:C:167:THR:OG1	1:C:210:GLU:OE2	2.12	0.62
1:D:673:LEU:HD12	1:D:677:MET:HE2	1.75	0.62
1:C:270:ALA:HA	1:C:320:MET:HE2	1.82	0.62
1:D:270:ALA:HA	1:D:320:MET:HE2	1.82	0.61
1:B:270:ALA:HA	1:B:320:MET:HE2	1.82	0.61
1:A:176:LEU:HD21	1:A:230:ILE:HG21	1.83	0.60
1:C:176:LEU:CD2	1:C:230:ILE:HG21	2.32	0.60
1:C:673:LEU:HD12	1:C:677:MET:HE2	1.77	0.60
1:B:176:LEU:CD2	1:B:230:ILE:HG21	2.32	0.60
1:B:176:LEU:HD21	1:B:230:ILE:HG21	1.83	0.60
1:A:176:LEU:CD2	1:A:230:ILE:HG21	2.32	0.60
1:D:674:ILE:O	1:D:678:GLY:N	2.35	0.60
1:A:639:LEU:HD21	1:D:635:LEU:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:LEU:HD21	1:C:230:ILE:HG21	1.83	0.60
1:C:408:VAL:HG12	1:C:420:LEU:HD21	1.85	0.59
1:A:635:LEU:HD12	1:B:639:LEU:HD21	1.84	0.59
1:A:674:ILE:O	1:A:678:GLY:N	2.36	0.59
1:B:674:ILE:O	1:B:678:GLY:N	2.35	0.59
1:D:176:LEU:HD21	1:D:230:ILE:HG21	1.83	0.59
1:A:270:ALA:HA	1:A:320:MET:HE2	1.83	0.59
1:D:176:LEU:CD2	1:D:230:ILE:HG21	2.32	0.59
1:A:408:VAL:HG12	1:A:420:LEU:HD21	1.84	0.59
1:C:635:LEU:HD12	1:D:639:LEU:HD21	1.85	0.59
1:D:408:VAL:HG12	1:D:420:LEU:HD21	1.85	0.59
1:B:408:VAL:HG12	1:B:420:LEU:HD21	1.85	0.58
1:B:635:LEU:HD12	1:C:639:LEU:HD21	1.85	0.58
1:C:674:ILE:O	1:C:678:GLY:N	2.36	0.58
1:B:673:LEU:HD12	1:B:677:MET:HE2	1.76	0.57
1:D:673:LEU:CD1	1:D:677:MET:CE	2.63	0.56
1:C:299:ILE:CG1	1:C:324:ILE:HD13	2.37	0.55
1:D:299:ILE:CG1	1:D:324:ILE:HD13	2.37	0.55
1:A:673:LEU:HD12	1:A:677:MET:HE2	1.79	0.55
1:D:371:ARG:O	1:D:374:SER:OG	2.23	0.54
1:A:597:PHE:CG	1:A:664:LEU:HD21	2.43	0.54
1:D:597:PHE:CG	1:D:664:LEU:HD21	2.43	0.54
1:A:299:ILE:CG1	1:A:324:ILE:HD13	2.37	0.54
1:B:299:ILE:CG1	1:B:324:ILE:HD13	2.37	0.54
1:D:204:ILE:HD11	1:D:234:LEU:HD23	1.90	0.54
1:D:299:ILE:HG12	1:D:324:ILE:HD13	1.90	0.54
1:B:597:PHE:CG	1:B:664:LEU:HD21	2.43	0.54
1:C:204:ILE:HD11	1:C:234:LEU:HD23	1.89	0.54
1:C:299:ILE:HG12	1:C:324:ILE:HD13	1.90	0.53
1:B:204:ILE:HD11	1:B:234:LEU:HD23	1.90	0.53
1:A:204:ILE:HD11	1:A:234:LEU:HD23	1.89	0.53
1:A:597:PHE:CD1	1:A:664:LEU:HD21	2.44	0.53
1:C:597:PHE:CG	1:C:664:LEU:HD21	2.43	0.53
1:B:299:ILE:HG12	1:B:324:ILE:HD13	1.90	0.53
1:B:597:PHE:CD1	1:B:664:LEU:HD21	2.44	0.53
1:A:299:ILE:HG12	1:A:324:ILE:HD13	1.90	0.53
1:B:204:ILE:HD11	1:B:234:LEU:CD2	2.39	0.53
1:B:570:GLN:NE2	1:B:570:GLN:O	2.42	0.53
1:C:673:LEU:CG	1:C:677:MET:HE2	2.37	0.53
1:C:597:PHE:CD1	1:C:664:LEU:HD21	2.44	0.52
1:D:570:GLN:NE2	1:D:570:GLN:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:GLN:NE2	1:C:570:GLN:O	2.43	0.52
1:C:598:LEU:HD12	1:C:632:LEU:HD13	1.92	0.52
1:A:598:LEU:HD12	1:A:632:LEU:HD13	1.91	0.52
1:B:371:ARG:O	1:B:374:SER:OG	2.23	0.52
1:C:204:ILE:HD11	1:C:234:LEU:CD2	2.39	0.52
1:D:598:LEU:HD12	1:D:632:LEU:HD13	1.92	0.52
1:A:570:GLN:NE2	1:A:570:GLN:O	2.42	0.52
1:A:204:ILE:HD11	1:A:234:LEU:CD2	2.39	0.52
1:A:371:ARG:O	1:A:374:SER:OG	2.25	0.52
1:D:597:PHE:CD1	1:D:664:LEU:HD21	2.44	0.52
1:D:709:GLU:OE1	1:D:709:GLU:N	2.39	0.51
1:B:673:LEU:CD1	1:B:677:MET:CE	2.64	0.51
1:C:659:ILE:HD11	1:D:633:PHE:HB3	1.92	0.51
1:D:204:ILE:HD11	1:D:234:LEU:CD2	2.39	0.51
2:A:903:A1IPI:F5	2:A:903:A1IPI:F1	2.08	0.51
2:C:903:A1IPI:F5	2:C:903:A1IPI:F1	2.09	0.51
1:D:673:LEU:CG	1:D:677:MET:HE2	2.39	0.51
1:A:397:THR:HG21	1:A:701:LEU:CD1	2.40	0.51
1:B:709:GLU:OE1	1:B:709:GLU:N	2.39	0.51
1:A:659:ILE:HD11	1:B:633:PHE:HB3	1.92	0.51
1:C:397:THR:HG21	1:C:701:LEU:CD1	2.41	0.51
1:B:598:LEU:HD12	1:B:632:LEU:HD13	1.92	0.50
1:A:633:PHE:HB3	1:D:659:ILE:HD11	1.93	0.50
1:A:709:GLU:OE1	1:A:709:GLU:N	2.39	0.50
1:B:397:THR:HG21	1:B:701:LEU:CD1	2.41	0.50
1:B:659:ILE:HD11	1:C:633:PHE:HB3	1.93	0.50
1:C:179:ILE:HD13	1:D:744:THR:HG21	1.94	0.50
2:B:903:A1IPI:F5	2:B:903:A1IPI:F1	2.09	0.50
1:C:645:GLN:NE2	1:C:651:PRO:O	2.44	0.50
1:C:673:LEU:CD1	1:C:677:MET:CE	2.66	0.50
1:B:179:ILE:HD13	1:C:744:THR:HG21	1.94	0.50
1:B:673:LEU:CG	1:B:677:MET:HE2	2.40	0.50
1:B:645:GLN:NE2	1:B:651:PRO:O	2.44	0.50
1:A:179:ILE:HD13	1:B:744:THR:HG21	1.94	0.50
1:D:397:THR:HG21	1:D:701:LEU:CD1	2.41	0.50
1:A:321:TYR:OH	1:A:334:GLU:OE1	2.28	0.49
1:D:205:ASN:OD1	1:D:240:ASP:N	2.46	0.49
1:B:205:ASN:OD1	1:B:240:ASP:N	2.46	0.49
1:A:639:LEU:HD21	1:D:635:LEU:CD1	2.43	0.49
1:A:673:LEU:CD1	1:A:677:MET:CE	2.68	0.49
1:A:635:LEU:CD1	1:B:639:LEU:HD21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:645:GLN:NE2	1:D:651:PRO:O	2.44	0.48
1:A:226:ARG:NH1	1:A:272:THR:O	2.46	0.48
1:A:645:GLN:NE2	1:A:651:PRO:O	2.45	0.48
1:C:635:LEU:CD1	1:D:639:LEU:HD21	2.43	0.48
1:A:744:THR:HG21	1:D:179:ILE:HD13	1.95	0.48
1:B:635:LEU:CD1	1:C:639:LEU:HD21	2.43	0.48
1:C:205:ASN:OD1	1:C:240:ASP:N	2.45	0.48
1:C:226:ARG:NH1	1:C:272:THR:O	2.46	0.48
1:C:177:LEU:O	1:C:225:ARG:NH1	2.46	0.48
1:D:177:LEU:O	1:D:225:ARG:NH1	2.47	0.47
1:D:226:ARG:NH1	1:D:272:THR:O	2.46	0.47
2:A:901:A1IPI:F5	2:A:901:A1IPI:F1	2.09	0.47
1:B:226:ARG:NH1	1:B:272:THR:O	2.47	0.47
1:A:177:LEU:O	1:A:225:ARG:NH1	2.47	0.47
1:A:607:SER:O	1:A:611:LYS:NZ	2.48	0.47
1:D:432:LYS:NZ	1:D:704:GLU:OE1	2.45	0.47
1:D:607:SER:O	1:D:611:LYS:NZ	2.47	0.47
1:B:177:LEU:O	1:B:225:ARG:NH1	2.47	0.47
1:B:607:SER:O	1:B:611:LYS:NZ	2.47	0.47
1:C:290:THR:HG23	1:C:290:THR:O	2.15	0.47
1:B:513:LEU:O	1:B:513:LEU:HD12	2.15	0.47
1:C:513:LEU:HD12	1:C:513:LEU:O	2.15	0.46
1:D:513:LEU:O	1:D:513:LEU:HD12	2.15	0.46
1:A:673:LEU:CG	1:A:677:MET:HE2	2.40	0.46
1:B:290:THR:HG23	1:B:290:THR:O	2.15	0.46
1:C:607:SER:O	1:C:611:LYS:NZ	2.48	0.46
1:D:290:THR:HG23	1:D:290:THR:O	2.15	0.46
1:A:432:LYS:NZ	1:A:704:GLU:OE1	2.45	0.46
1:C:321:TYR:OH	1:C:334:GLU:OE1	2.29	0.46
1:B:321:TYR:OH	1:B:334:GLU:OE1	2.29	0.46
1:A:205:ASN:OD1	1:A:240:ASP:N	2.47	0.46
1:A:513:LEU:HD12	1:A:513:LEU:O	2.15	0.46
1:B:284:HIS:O	1:B:287:THR:HG22	2.16	0.46
1:C:709:GLU:OE1	1:C:709:GLU:N	2.39	0.46
1:A:290:THR:HG23	1:A:290:THR:O	2.15	0.45
1:C:284:HIS:O	1:C:287:THR:HG22	2.16	0.45
1:A:159:MET:O	1:A:163:THR:OG1	2.30	0.45
1:A:284:HIS:O	1:A:287:THR:HG22	2.16	0.45
1:D:284:HIS:O	1:D:287:THR:HG22	2.16	0.45
1:D:410:ASN:O	1:D:416:ARG:NE	2.51	0.44
1:B:432:LYS:NZ	1:B:704:GLU:OE1	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:GLU:OE1	1:D:367:GLU:N	2.51	0.44
1:C:410:ASN:O	1:C:416:ARG:NE	2.51	0.43
1:A:410:ASN:O	1:A:416:ARG:NE	2.50	0.43
1:B:410:ASN:O	1:B:416:ARG:NE	2.51	0.43
1:C:367:GLU:N	1:C:367:GLU:OE1	2.51	0.43
1:D:408:VAL:HG21	1:D:701:LEU:HG	2.01	0.43
1:A:367:GLU:N	1:A:367:GLU:OE1	2.52	0.43
1:B:367:GLU:OE1	1:B:367:GLU:N	2.51	0.43
1:B:408:VAL:CG1	1:B:420:LEU:HD21	2.49	0.43
1:D:408:VAL:CG1	1:D:420:LEU:HD21	2.49	0.43
1:C:395:VAL:HG12	1:C:395:VAL:O	2.19	0.43
1:A:397:THR:HG21	1:A:701:LEU:HD11	2.01	0.42
1:C:371:ARG:O	1:C:374:SER:OG	2.24	0.42
1:D:159:MET:O	1:D:163:THR:OG1	2.31	0.42
1:D:395:VAL:HG12	1:D:395:VAL:O	2.19	0.42
1:B:225:ARG:O	1:C:744:THR:HG23	2.20	0.42
1:A:744:THR:HG23	1:D:225:ARG:O	2.19	0.42
1:B:408:VAL:HG21	1:B:701:LEU:HG	2.00	0.42
1:C:264:THR:HG22	1:C:265:PRO:HD2	2.02	0.42
1:A:395:VAL:HG12	1:A:395:VAL:O	2.19	0.42
1:A:408:VAL:CG1	1:A:420:LEU:HD21	2.48	0.42
1:B:264:THR:HG22	1:B:265:PRO:HD2	2.02	0.42
1:B:397:THR:HG21	1:B:701:LEU:HD11	2.01	0.42
1:C:225:ARG:O	1:D:744:THR:HG23	2.20	0.42
1:A:225:ARG:O	1:B:744:THR:HG23	2.20	0.42
1:B:395:VAL:O	1:B:395:VAL:HG12	2.19	0.41
1:B:723:VAL:HG13	1:B:724:ALA:N	2.35	0.41
1:A:723:VAL:HG13	1:A:724:ALA:N	2.35	0.41
1:C:723:VAL:HG13	1:C:724:ALA:N	2.36	0.41
1:D:723:VAL:HG13	1:D:724:ALA:N	2.36	0.41
1:B:275:PRO:HA	1:B:278:VAL:HG12	2.03	0.41
1:D:264:THR:HG22	1:D:265:PRO:HD2	2.02	0.41
1:A:627:ASP:O	1:A:631:GLU:OE1	2.39	0.41
1:B:362:SER:O	1:B:362:SER:OG	2.38	0.41
1:C:397:THR:HG21	1:C:701:LEU:HD11	2.01	0.41
1:A:275:PRO:HA	1:A:278:VAL:HG12	2.02	0.41
1:B:159:MET:O	1:B:163:THR:OG1	2.31	0.41
1:B:752:ASP:OD1	1:B:752:ASP:N	2.54	0.41
1:C:432:LYS:NZ	1:C:704:GLU:OE1	2.45	0.41
1:D:397:THR:HG21	1:D:701:LEU:HD11	2.01	0.41
1:A:552:VAL:HG21	1:D:607:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:THR:HG22	1:A:265:PRO:HD2	2.02	0.40
1:B:243:ALA:O	1:B:244:HIS:ND1	2.54	0.40
3:D:902:POV:C311	3:D:902:POV:H214	2.52	0.40
1:A:607:SER:HB2	1:B:552:VAL:HG21	2.03	0.40
3:A:902:POV:C311	3:A:902:POV:H214	2.52	0.40
3:B:902:POV:C311	3:B:902:POV:H214	2.52	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	594/802 (74%)	548 (92%)	46 (8%)	0	100	100
1	B	594/802 (74%)	548 (92%)	46 (8%)	0	100	100
1	C	594/802 (74%)	548 (92%)	46 (8%)	0	100	100
1	D	594/802 (74%)	547 (92%)	47 (8%)	0	100	100
All	All	2376/3208 (74%)	2191 (92%)	185 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	532/712 (75%)	532 (100%)	0	100	100
1	B	532/712 (75%)	532 (100%)	0	100	100
1	C	532/712 (75%)	532 (100%)	0	100	100
1	D	532/712 (75%)	532 (100%)	0	100	100
All	All	2128/2848 (75%)	2128 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	HIS
1	A	286	GLN
1	A	297	ASN
1	A	412	ASN
1	B	197	ASN
1	B	284	HIS
1	B	286	GLN
1	B	297	ASN
1	B	412	ASN
1	C	197	ASN
1	C	297	ASN
1	C	412	ASN
1	D	197	ASN
1	D	297	ASN
1	D	412	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 oligosaccharides in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	POV	C	902	-	51,51,51	0.92	2 (3%)	57,59,59	1.06	5 (8%)
2	A1IPI	B	903	-	10,11,11	1.00	0	15,17,17	1.32	2 (13%)
3	POV	C	901	-	51,51,51	0.89	2 (3%)	57,59,59	2.60	8 (14%)
3	POV	D	902	-	51,51,51	0.92	2 (3%)	57,59,59	1.06	5 (8%)
3	POV	A	904	-	51,51,51	0.89	2 (3%)	57,59,59	2.60	8 (14%)
3	POV	A	902	-	51,51,51	0.92	2 (3%)	57,59,59	1.06	5 (8%)
2	A1IPI	C	903	-	10,11,11	1.00	0	15,17,17	1.32	2 (13%)
3	POV	B	901	-	51,51,51	0.90	2 (3%)	57,59,59	2.59	7 (12%)
2	A1IPI	A	903	-	10,11,11	1.00	0	15,17,17	1.31	2 (13%)
2	A1IPI	A	901	-	10,11,11	1.00	0	15,17,17	1.32	2 (13%)
3	POV	D	901	-	51,51,51	0.90	2 (3%)	57,59,59	2.58	7 (12%)
3	POV	B	902	-	51,51,51	0.92	2 (3%)	57,59,59	1.06	5 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	C	902	-	-	16/55/55/55	-
2	A1IPI	B	903	-	-	9/12/15/15	-
3	POV	C	901	-	-	23/55/55/55	-
3	POV	D	902	-	-	16/55/55/55	-
3	POV	A	904	-	-	23/55/55/55	-
3	POV	A	902	-	-	16/55/55/55	-
2	A1IPI	C	903	-	-	9/12/15/15	-
3	POV	B	901	-	-	23/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1IPI	A	903	-	-	10/12/15/15	-
2	A1IPI	A	901	-	-	10/12/15/15	-
3	POV	D	901	-	-	22/55/55/55	-
3	POV	B	902	-	-	16/55/55/55	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	901	POV	O31-C31	4.19	1.45	1.33
3	B	901	POV	O31-C31	4.19	1.45	1.33
3	C	901	POV	O31-C31	4.17	1.45	1.33
3	A	904	POV	O31-C31	4.17	1.45	1.33
3	D	902	POV	O31-C31	4.00	1.45	1.33
3	A	902	POV	O31-C31	3.99	1.45	1.33
3	B	901	POV	O21-C21	3.98	1.45	1.34
3	C	902	POV	O31-C31	3.97	1.44	1.33
3	C	901	POV	O21-C21	3.97	1.45	1.34
3	D	901	POV	O21-C21	3.97	1.45	1.34
3	B	902	POV	O31-C31	3.96	1.44	1.33
3	A	902	POV	O21-C21	3.95	1.45	1.34
3	A	904	POV	O21-C21	3.95	1.45	1.34
3	B	902	POV	O21-C21	3.94	1.45	1.34
3	C	902	POV	O21-C21	3.94	1.45	1.34
3	D	902	POV	O21-C21	3.93	1.45	1.34

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	901	POV	C15-N-C14	-11.14	80.32	108.97
3	A	904	POV	C15-N-C13	-11.07	80.51	108.97
3	C	901	POV	C15-N-C13	-11.06	80.53	108.97
3	A	904	POV	C15-N-C14	-11.05	80.57	108.97
3	B	901	POV	C15-N-C13	-11.05	80.57	108.97
3	B	901	POV	C15-N-C14	-11.05	80.57	108.97
3	C	901	POV	C15-N-C14	-11.04	80.60	108.97
3	D	901	POV	C15-N-C13	-11.02	80.65	108.97
3	B	901	POV	C15-N-C12	-7.23	80.33	109.92
3	C	901	POV	C15-N-C12	-7.21	80.40	109.92
3	A	904	POV	C15-N-C12	-7.21	80.43	109.92
3	D	901	POV	C15-N-C12	-7.19	80.50	109.92
3	B	902	POV	O21-C21-C22	4.40	120.99	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	POV	O21-C21-C22	4.40	120.99	111.50
3	D	902	POV	O21-C21-C22	4.40	120.99	111.50
3	C	902	POV	O21-C21-C22	4.39	120.96	111.50
3	A	904	POV	O21-C21-C22	4.10	120.34	111.50
3	C	901	POV	O21-C21-C22	4.08	120.29	111.50
3	B	901	POV	O21-C21-C22	4.01	120.15	111.50
3	D	901	POV	O21-C21-C22	3.75	119.58	111.50
3	C	901	POV	C11-C12-N	-3.40	104.43	115.78
3	A	904	POV	C11-C12-N	-3.40	104.43	115.78
3	B	901	POV	C11-C12-N	-3.38	104.51	115.78
3	D	901	POV	C14-N-C13	3.29	117.44	108.97
3	A	904	POV	C14-N-C13	3.26	117.35	108.97
3	C	901	POV	C14-N-C13	3.26	117.35	108.97
3	D	901	POV	C11-C12-N	-3.26	104.91	115.78
3	B	901	POV	C14-N-C13	3.25	117.32	108.97
3	B	902	POV	O31-C31-C32	2.91	121.04	111.91
3	D	902	POV	O31-C31-C32	2.91	121.04	111.91
3	A	902	POV	O31-C31-C32	2.90	121.02	111.91
3	C	902	POV	O31-C31-C32	2.89	120.99	111.91
2	A	901	A1IPI	O1-C2-C4	2.80	110.04	107.93
2	A	903	A1IPI	O1-C2-C4	2.79	110.03	107.93
2	B	903	A1IPI	O1-C2-C4	2.78	110.02	107.93
2	C	903	A1IPI	O1-C2-C4	2.76	110.01	107.93
3	A	904	POV	O31-C31-C32	2.68	120.32	111.91
3	C	901	POV	O31-C31-C32	2.65	120.22	111.91
3	B	901	POV	O31-C31-C32	2.63	120.15	111.91
3	D	901	POV	O31-C31-C32	2.48	119.70	111.91
3	D	902	POV	C2-O21-C21	-2.35	112.00	117.79
3	C	902	POV	C2-O21-C21	-2.35	112.00	117.79
3	A	902	POV	C2-O21-C21	-2.35	112.01	117.79
3	B	902	POV	C2-O21-C21	-2.34	112.03	117.79
3	B	902	POV	O21-C21-O22	-2.30	118.14	123.70
3	C	902	POV	O21-C21-O22	-2.30	118.15	123.70
3	A	902	POV	O21-C21-O22	-2.30	118.15	123.70
3	D	902	POV	O21-C21-O22	-2.30	118.15	123.70
3	D	902	POV	O31-C31-O32	-2.16	118.14	123.59
3	B	902	POV	O31-C31-O32	-2.16	118.14	123.59
3	A	902	POV	O31-C31-O32	-2.15	118.17	123.59
2	B	903	A1IPI	C4-C2-C3	-2.14	108.39	112.51
3	C	902	POV	O31-C31-O32	-2.13	118.20	123.59
3	A	904	POV	C2-O21-C21	-2.13	112.55	117.79
2	C	903	A1IPI	C4-C2-C3	-2.12	108.42	112.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	A1IPI	C4-C2-C3	-2.12	108.43	112.51
2	A	903	A1IPI	C4-C2-C3	-2.08	108.50	112.51
3	C	901	POV	C2-O21-C21	-2.06	112.72	117.79

There are no chirality outliers.

All (193) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	A1IPI	O1-C2-C3-F1
2	A	901	A1IPI	O1-C2-C3-F2
2	A	901	A1IPI	O1-C2-C3-F3
2	A	903	A1IPI	O1-C2-C3-F1
2	A	903	A1IPI	O1-C2-C3-F2
2	A	903	A1IPI	O1-C2-C3-F3
2	B	903	A1IPI	O1-C2-C3-F1
2	B	903	A1IPI	O1-C2-C3-F2
2	B	903	A1IPI	O1-C2-C3-F3
2	C	903	A1IPI	O1-C2-C3-F1
2	C	903	A1IPI	O1-C2-C3-F2
2	C	903	A1IPI	O1-C2-C3-F3
3	A	902	POV	C1-O11-P-O14
3	A	902	POV	C11-O12-P-O11
3	A	902	POV	O22-C21-O21-C2
3	A	904	POV	C11-O12-P-O11
3	A	904	POV	C11-O12-P-O13
3	A	904	POV	C11-O12-P-O14
3	A	904	POV	O12-C11-C12-N
3	B	901	POV	C11-O12-P-O11
3	B	901	POV	C11-O12-P-O13
3	B	901	POV	C11-O12-P-O14
3	B	901	POV	O12-C11-C12-N
3	B	902	POV	C1-O11-P-O14
3	B	902	POV	C11-O12-P-O11
3	B	902	POV	O22-C21-O21-C2
3	C	901	POV	C11-O12-P-O11
3	C	901	POV	C11-O12-P-O13
3	C	901	POV	C11-O12-P-O14
3	C	901	POV	O12-C11-C12-N
3	C	902	POV	C1-O11-P-O14
3	C	902	POV	C11-O12-P-O11
3	C	902	POV	O22-C21-O21-C2
3	D	901	POV	O12-C11-C12-N

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Mol	Chain	Res	Type	Atoms
3	D	902	POV	C1-O11-P-O14
3	D	902	POV	C11-O12-P-O11
3	D	902	POV	O22-C21-O21-C2
2	A	901	A1IPI	C4-C2-C3-F3
2	A	903	A1IPI	C4-C2-C3-F3
2	A	901	A1IPI	C4-C2-C3-F1
2	A	903	A1IPI	C4-C2-C3-F1
2	B	903	A1IPI	C4-C2-C3-F1
2	B	903	A1IPI	C4-C2-C3-F3
2	C	903	A1IPI	C4-C2-C3-F1
2	A	901	A1IPI	C4-C2-C3-F2
2	A	903	A1IPI	C4-C2-C3-F2
2	B	903	A1IPI	C4-C2-C3-F2
2	C	903	A1IPI	C4-C2-C3-F2
2	C	903	A1IPI	C4-C2-C3-F3
3	A	902	POV	C22-C21-O21-C2
3	B	902	POV	C22-C21-O21-C2
3	C	902	POV	C22-C21-O21-C2
3	D	902	POV	C22-C21-O21-C2
3	A	904	POV	C22-C21-O21-C2
3	C	901	POV	C22-C21-O21-C2
3	A	904	POV	C21-C22-C23-C24
3	B	901	POV	C21-C22-C23-C24
3	C	901	POV	C21-C22-C23-C24
3	D	901	POV	C21-C22-C23-C24
3	B	901	POV	C22-C21-O21-C2
3	A	904	POV	O22-C21-O21-C2
3	D	901	POV	C11-O12-P-O11
3	B	901	POV	O22-C21-O21-C2
3	C	901	POV	O22-C21-O21-C2
3	D	901	POV	C210-C211-C212-C213
3	D	901	POV	C22-C21-O21-C2
3	D	901	POV	O22-C21-O21-C2
3	A	904	POV	C210-C211-C212-C213
3	B	901	POV	C210-C211-C212-C213
3	C	901	POV	C210-C211-C212-C213
3	A	904	POV	C11-C12-N-C14
3	B	901	POV	C11-C12-N-C14
3	C	901	POV	C11-C12-N-C14
3	D	901	POV	C11-C12-N-C14
3	B	901	POV	C213-C214-C215-C216
3	C	901	POV	C213-C214-C215-C216

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Mol	Chain	Res	Type	Atoms
3	A	904	POV	C213-C214-C215-C216
3	D	901	POV	C213-C214-C215-C216
3	A	904	POV	C34-C35-C36-C37
3	B	901	POV	C34-C35-C36-C37
3	C	901	POV	C34-C35-C36-C37
3	A	902	POV	C35-C36-C37-C38
3	B	902	POV	C35-C36-C37-C38
3	C	902	POV	C35-C36-C37-C38
3	D	902	POV	C35-C36-C37-C38
3	D	901	POV	C34-C35-C36-C37
3	A	902	POV	C210-C211-C212-C213
3	B	902	POV	C210-C211-C212-C213
3	C	902	POV	C210-C211-C212-C213
3	D	902	POV	C210-C211-C212-C213
3	A	904	POV	C35-C36-C37-C38
3	B	901	POV	C35-C36-C37-C38
3	C	901	POV	C35-C36-C37-C38
3	D	901	POV	C35-C36-C37-C38
3	A	902	POV	C32-C31-O31-C3
3	B	902	POV	C32-C31-O31-C3
3	C	902	POV	C32-C31-O31-C3
3	D	902	POV	C32-C31-O31-C3
2	A	903	A1IPI	O1-C2-C4-F5
3	B	902	POV	C213-C214-C215-C216
3	A	902	POV	C213-C214-C215-C216
3	D	902	POV	C213-C214-C215-C216
3	A	902	POV	C1-O11-P-O12
3	B	902	POV	C1-O11-P-O12
3	C	902	POV	C1-O11-P-O12
3	D	902	POV	C1-O11-P-O12
3	A	904	POV	C32-C33-C34-C35
3	A	902	POV	C11-O12-P-O13
3	B	902	POV	C11-O12-P-O13
3	C	902	POV	C11-O12-P-O13
3	D	901	POV	C11-O12-P-O14
3	D	902	POV	C11-O12-P-O13
3	C	902	POV	C213-C214-C215-C216
3	B	901	POV	C32-C33-C34-C35
3	A	902	POV	C27-C28-C29-C210
3	B	902	POV	C27-C28-C29-C210
3	C	902	POV	C27-C28-C29-C210
3	D	902	POV	C27-C28-C29-C210

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Mol	Chain	Res	Type	Atoms
3	D	902	POV	O32-C31-O31-C3
3	C	901	POV	C32-C33-C34-C35
3	A	902	POV	O32-C31-O31-C3
3	B	902	POV	O32-C31-O31-C3
3	C	902	POV	O32-C31-O31-C3
3	D	901	POV	O31-C31-C32-C33
3	A	902	POV	O12-C11-C12-N
3	B	902	POV	O12-C11-C12-N
3	C	902	POV	O12-C11-C12-N
3	D	902	POV	O12-C11-C12-N
3	D	901	POV	C23-C24-C25-C26
3	B	901	POV	O31-C31-C32-C33
3	C	901	POV	O31-C31-C32-C33
3	A	904	POV	C1-O11-P-O12
3	B	901	POV	C1-O11-P-O12
3	C	901	POV	C1-O11-P-O12
3	D	901	POV	C1-O11-P-O12
3	C	901	POV	C23-C24-C25-C26
2	A	901	A1IPI	O1-C2-C4-F5
2	A	903	A1IPI	O1-C2-C4-F4
2	A	903	A1IPI	O1-C2-C4-F6
3	A	904	POV	O31-C31-C32-C33
3	B	901	POV	C23-C24-C25-C26
3	A	904	POV	C26-C27-C28-C29
3	B	901	POV	C26-C27-C28-C29
3	D	901	POV	C26-C27-C28-C29
3	C	901	POV	C26-C27-C28-C29
3	A	904	POV	C23-C24-C25-C26
2	B	903	A1IPI	O1-C2-C4-F5
3	D	901	POV	C32-C33-C34-C35
3	A	904	POV	C11-C12-N-C13
3	B	901	POV	C11-C12-N-C13
3	C	901	POV	C11-C12-N-C13
3	D	901	POV	C11-C12-N-C13
2	A	901	A1IPI	O1-C2-C4-F6
2	B	903	A1IPI	O1-C2-C4-F6
2	C	903	A1IPI	O1-C2-C4-F6
3	D	901	POV	C212-C213-C214-C215
3	B	901	POV	O21-C2-C3-O31
3	D	901	POV	O21-C2-C3-O31
3	A	904	POV	C212-C213-C214-C215
3	C	901	POV	C212-C213-C214-C215

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Mol	Chain	Res	Type	Atoms
3	B	901	POV	C212-C213-C214-C215
2	A	901	A1IPI	O1-C2-C4-F4
2	B	903	A1IPI	O1-C2-C4-F4
2	C	903	A1IPI	O1-C2-C4-F4
2	C	903	A1IPI	O1-C2-C4-F5
3	A	902	POV	O21-C2-C3-O31
3	B	902	POV	O21-C2-C3-O31
3	C	901	POV	O21-C2-C3-O31
3	C	902	POV	O21-C2-C3-O31
3	D	902	POV	O21-C2-C3-O31
3	A	904	POV	C27-C28-C29-C210
3	C	901	POV	C27-C28-C29-C210
2	A	903	A1IPI	C3-C2-C4-F5
3	A	904	POV	O21-C2-C3-O31
3	B	901	POV	C27-C28-C29-C210
3	C	901	POV	C211-C212-C213-C214
3	B	901	POV	C211-C212-C213-C214
3	D	901	POV	C27-C28-C29-C210
3	A	904	POV	C211-C212-C213-C214
3	A	904	POV	C1-O11-P-O14
3	B	901	POV	C1-O11-P-O14
3	C	901	POV	C1-O11-P-O14
3	D	901	POV	C1-O11-P-O14
3	D	901	POV	C211-C212-C213-C214
2	A	901	A1IPI	C3-C2-C4-F5
3	A	902	POV	O21-C21-C22-C23
3	D	902	POV	C310-C311-C312-C313
3	A	902	POV	C310-C311-C312-C313
3	B	902	POV	C310-C311-C312-C313
3	C	902	POV	C310-C311-C312-C313
3	B	902	POV	O21-C21-C22-C23
3	C	902	POV	O21-C21-C22-C23
3	D	902	POV	O21-C21-C22-C23

There are no ring outliers.

11 monomers are involved in 11 short contacts:

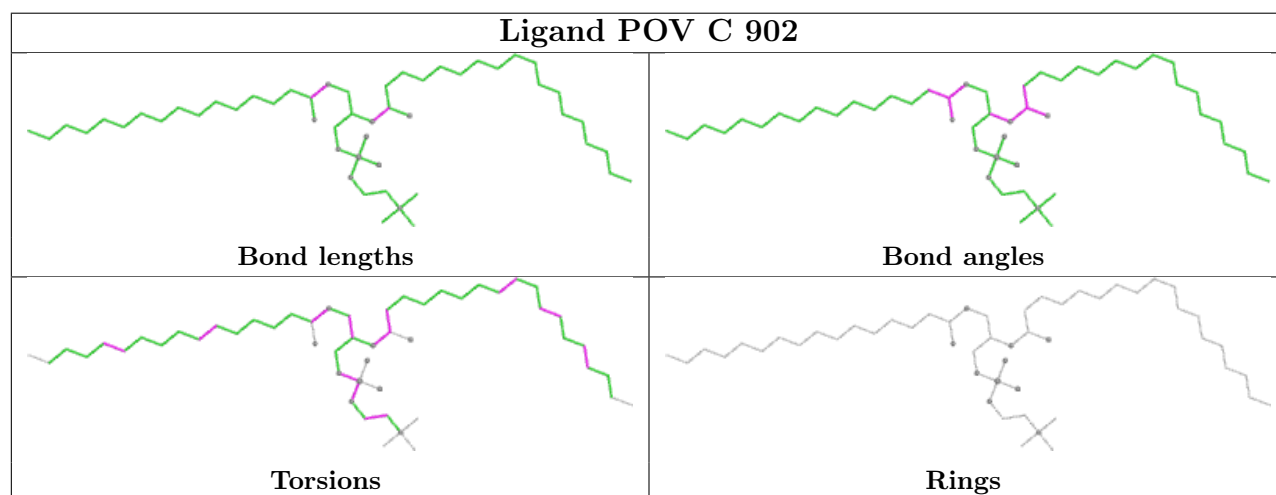
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	903	A1IPI	1	0
3	C	901	POV	1	0
3	D	902	POV	1	0
3	A	904	POV	1	0

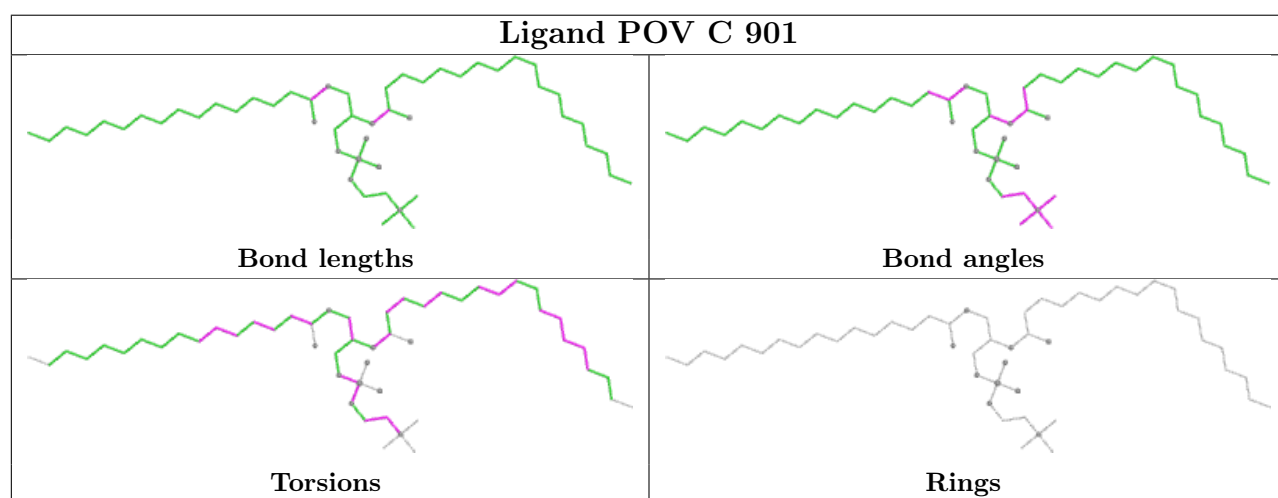
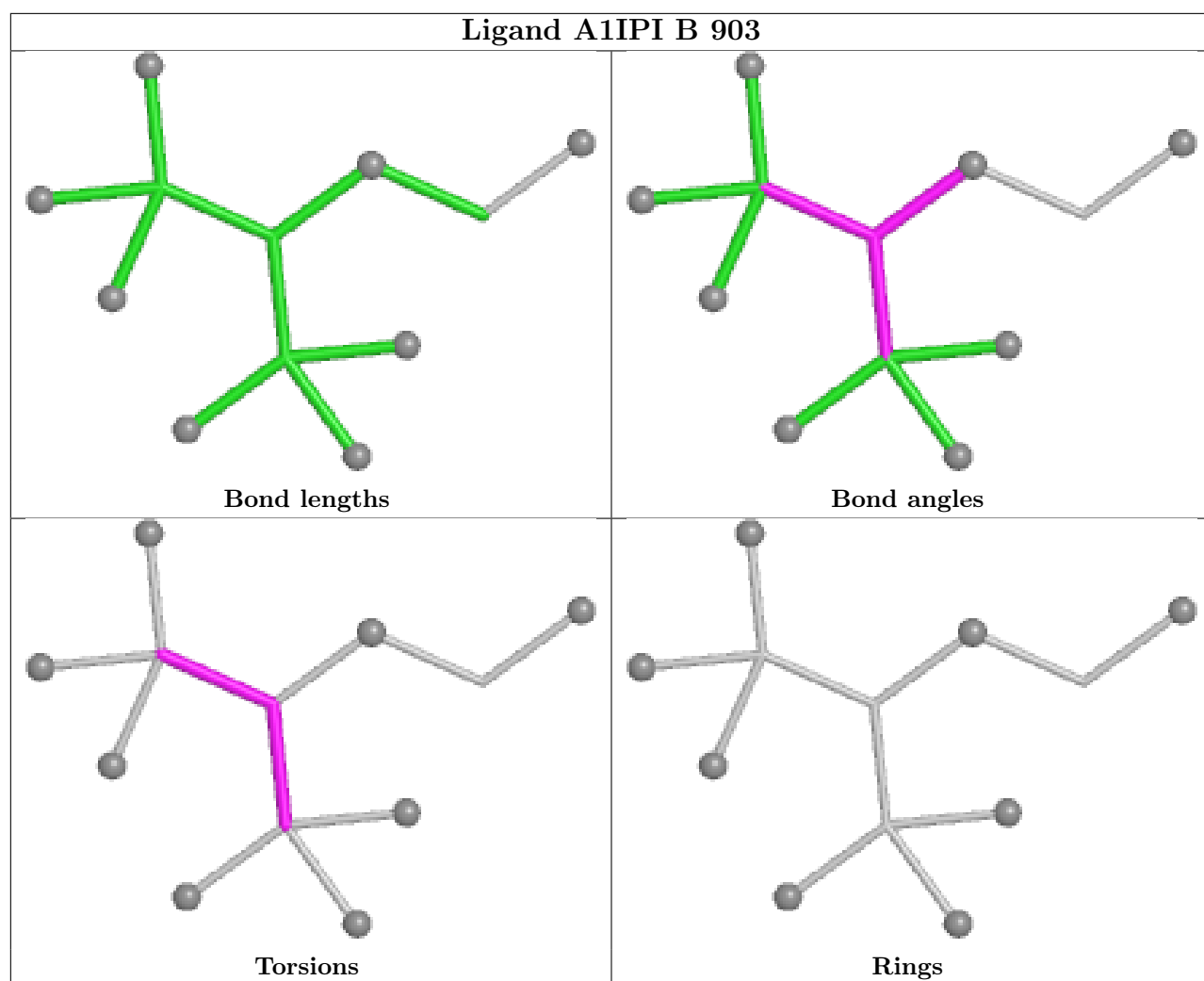
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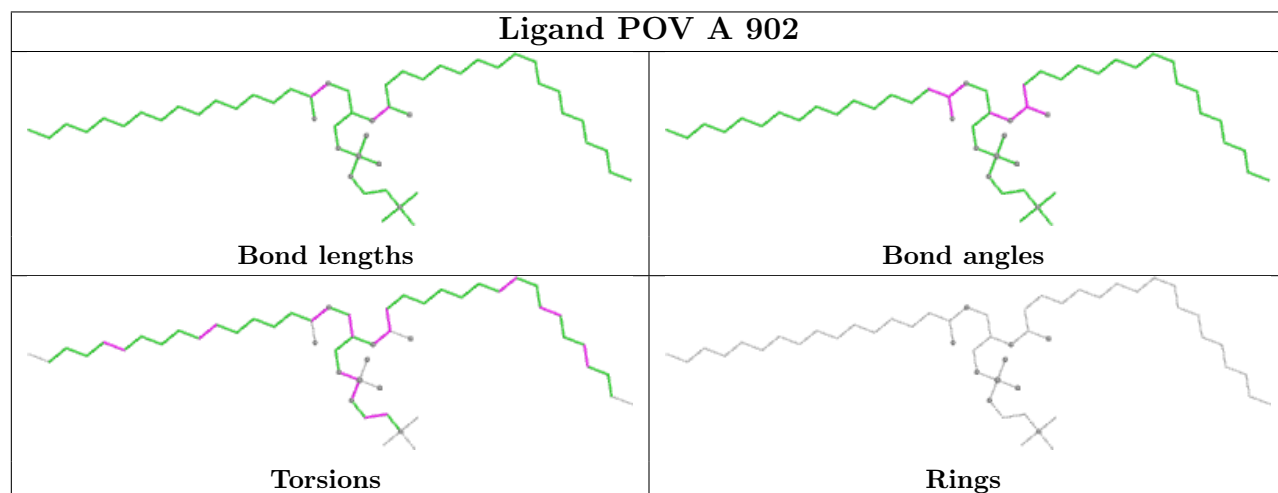
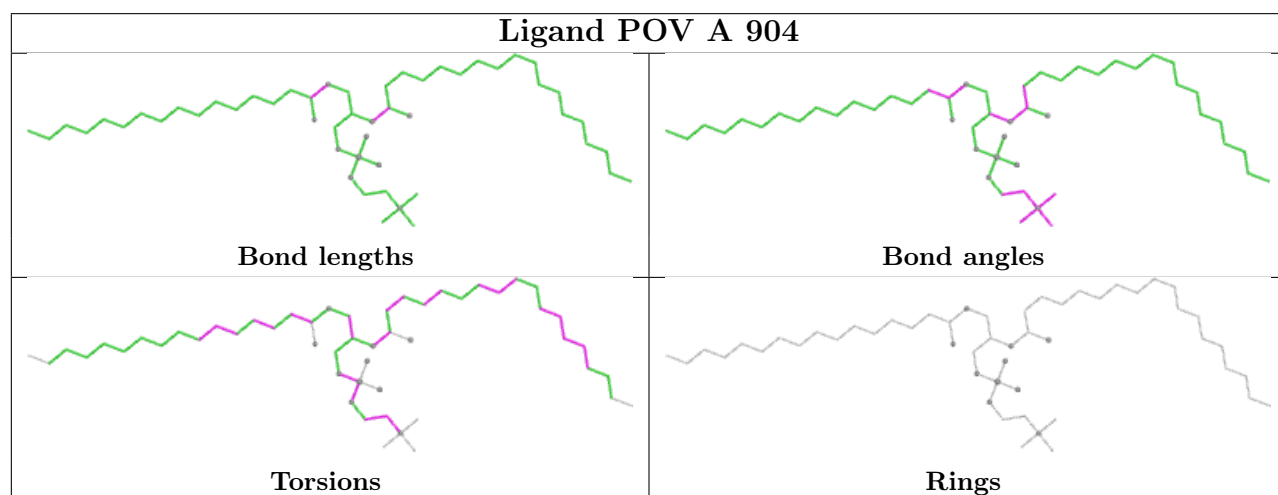
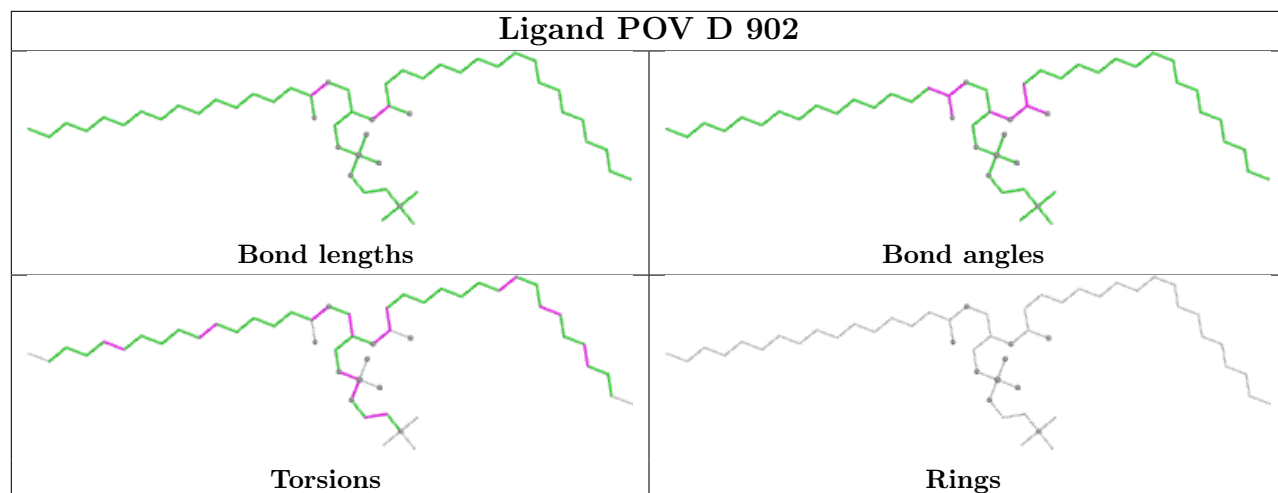
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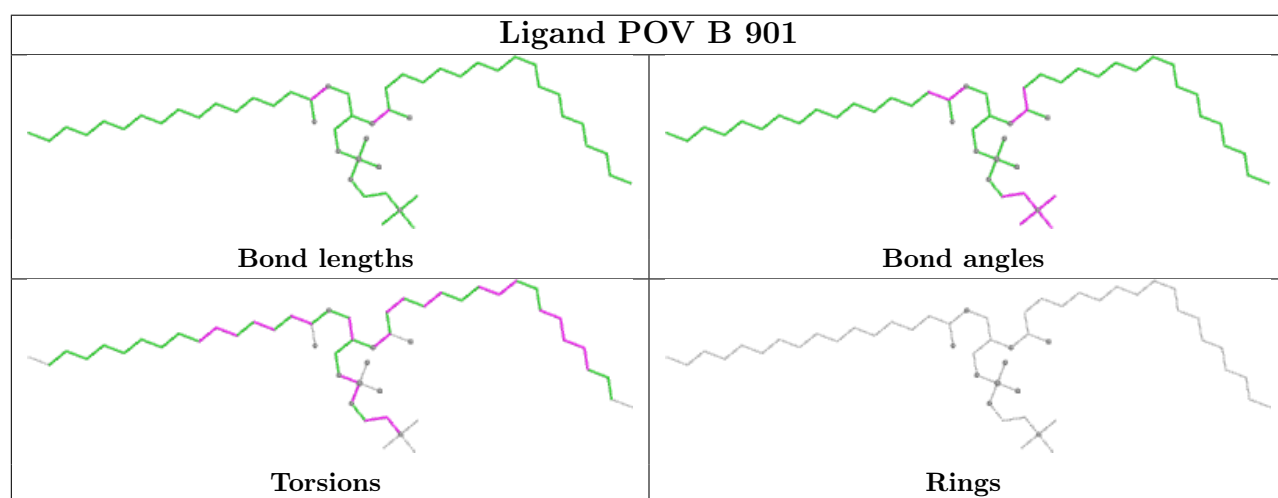
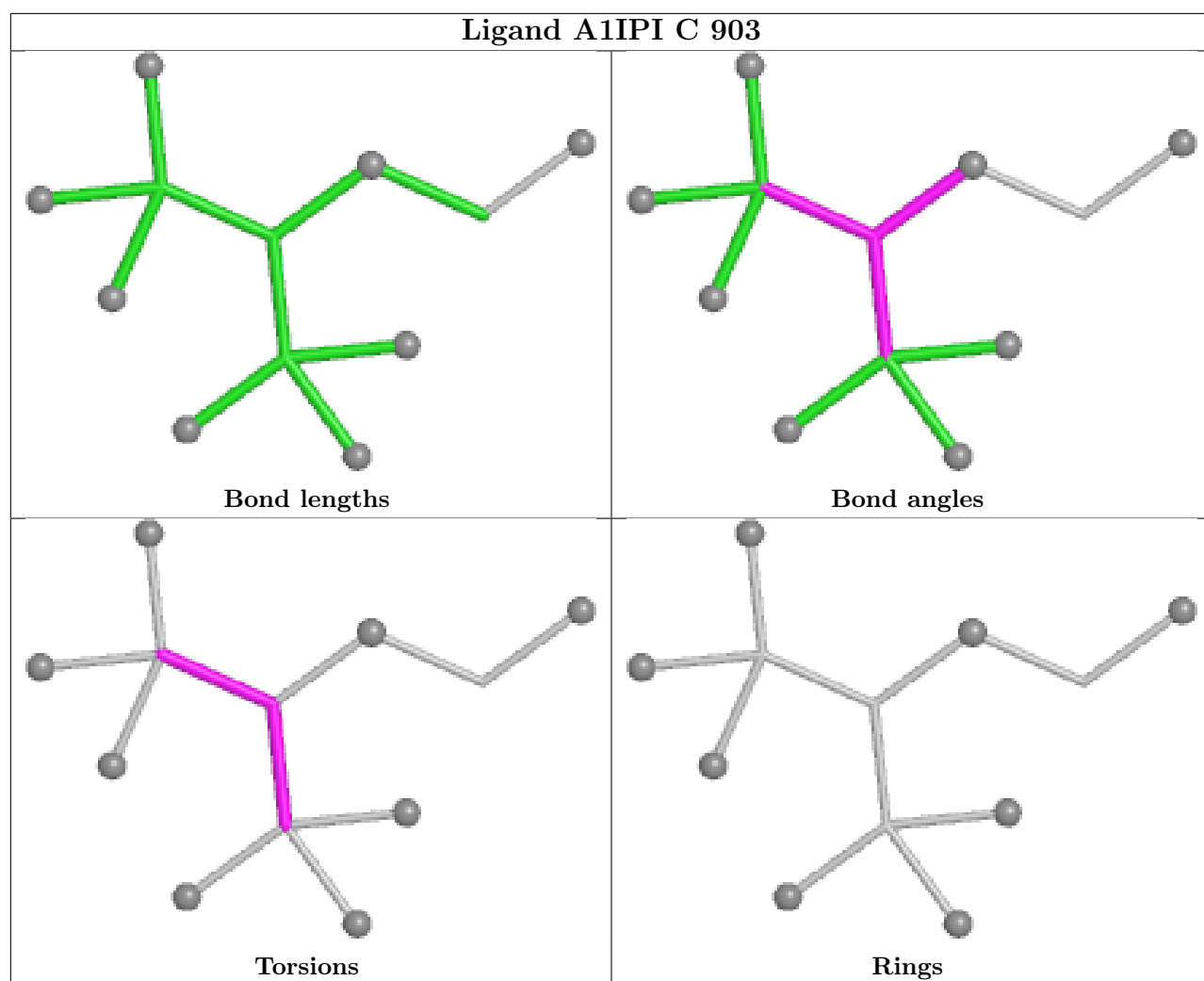
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	POV	1	0
2	C	903	A1IPI	1	0
3	B	901	POV	1	0
2	A	903	A1IPI	1	0
2	A	901	A1IPI	1	0
3	D	901	POV	1	0
3	B	902	POV	1	0

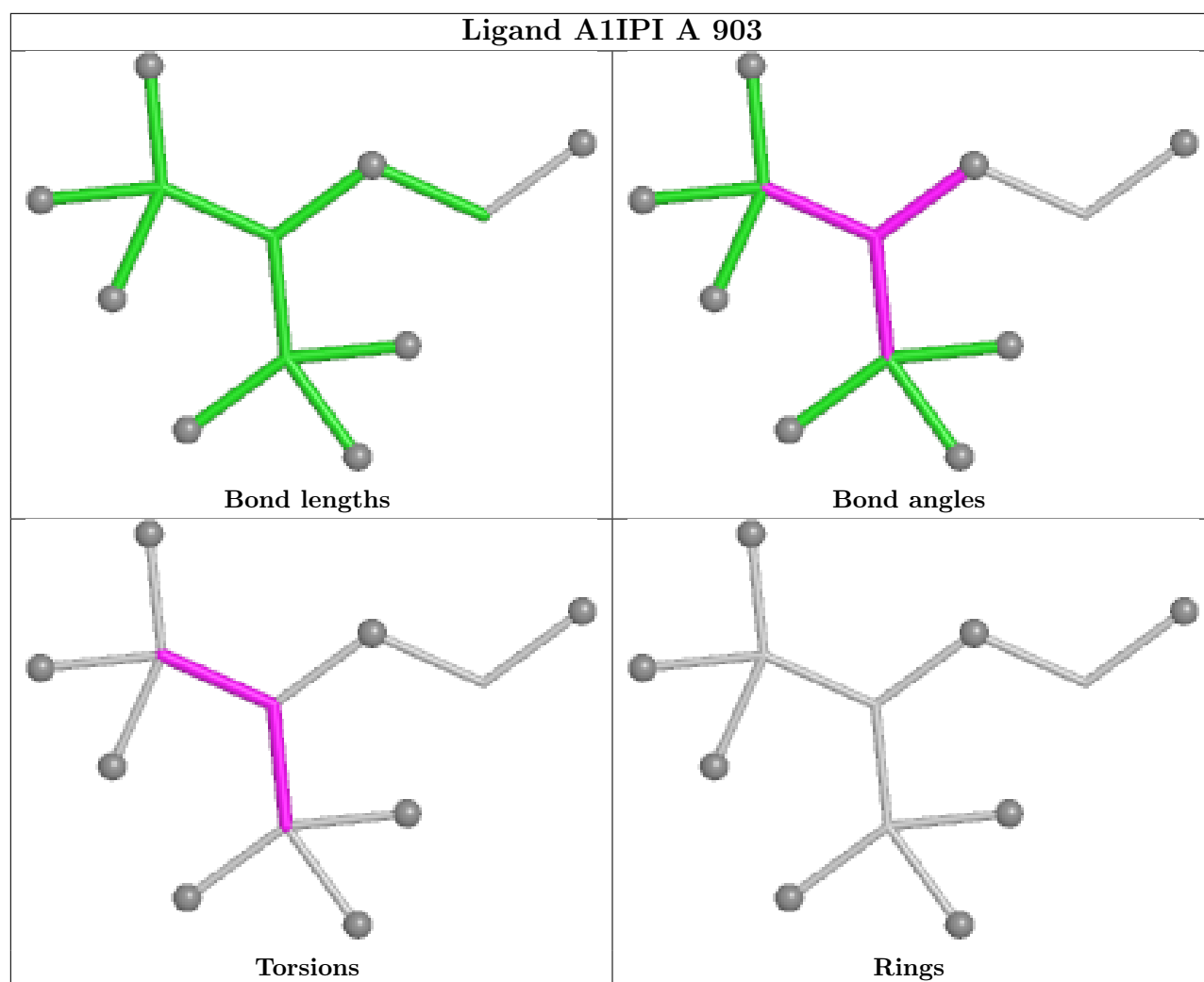
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

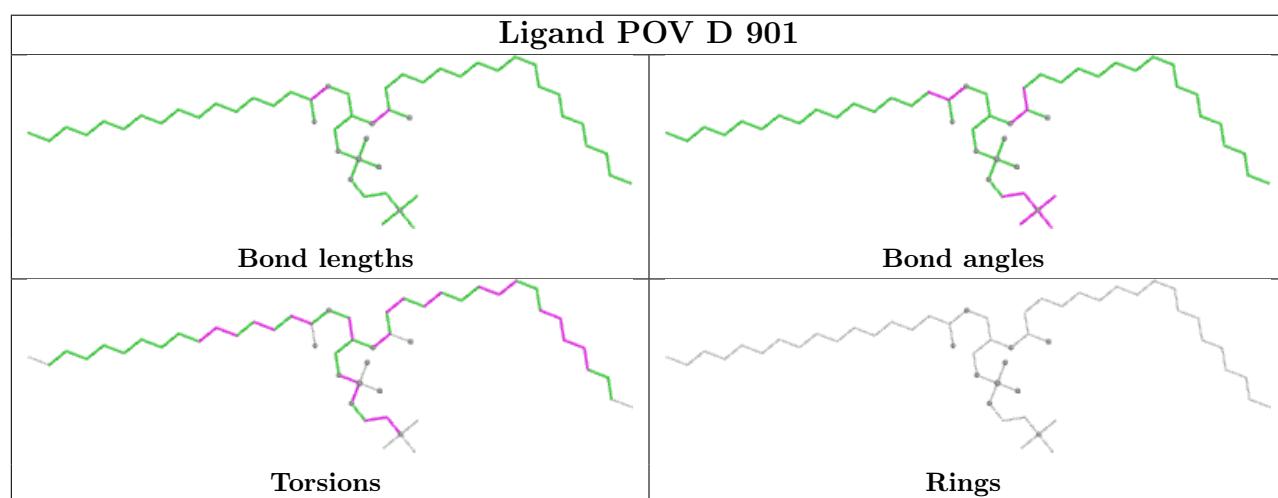
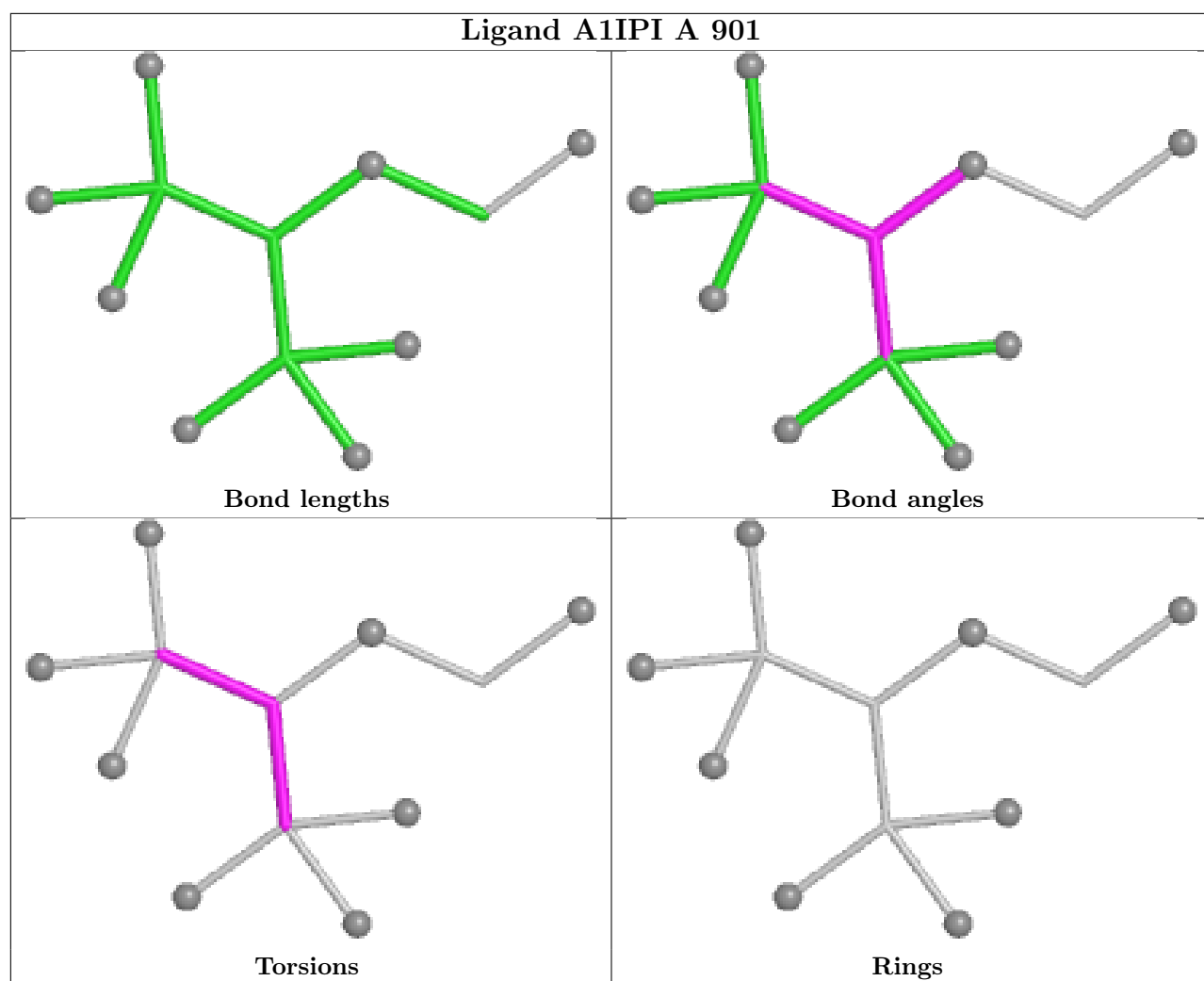


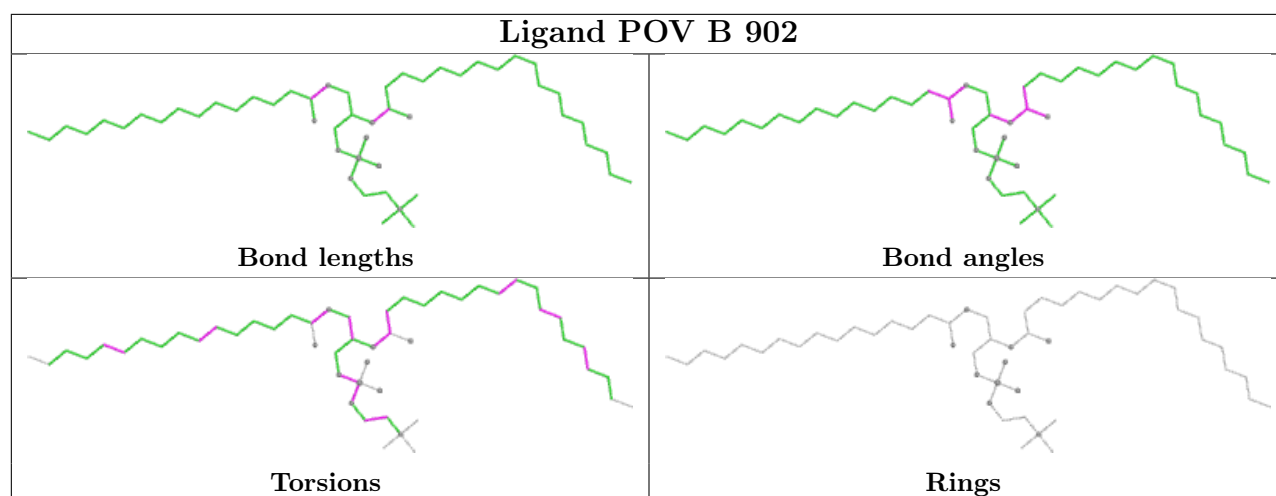












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.