



## Full wwPDB EM Validation Report ⓘ

Feb 25, 2025 – 06:06 pm GMT

PDB ID : 9GI3  
EMDB ID : EMD-51369  
Title : Truncated MmpL4 in nanodiscs in the presence of desferrated mycobactin  
Authors : Earp, J.C.; Garaeva, A.A.; Seeger, M.A.  
Deposited on : 2024-08-16  
Resolution : 3.50 Å(reported)  
Based on initial model : 9GI0

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

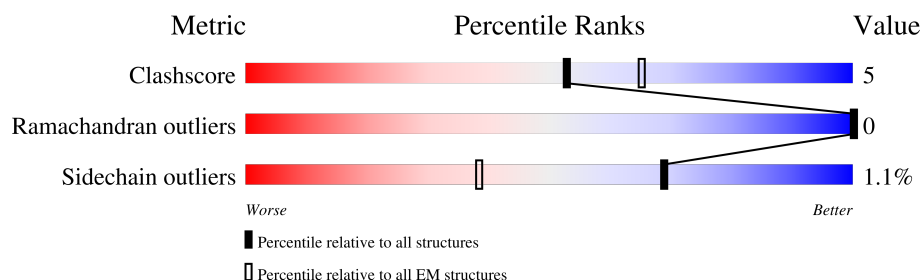
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	78	 74% 24% .
2	B	783	 81% 11% 8%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12384 atoms, of which 6282 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 Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	77	Total	C	H	N	O	S	0	0
			1169	368	572	93	135	1		

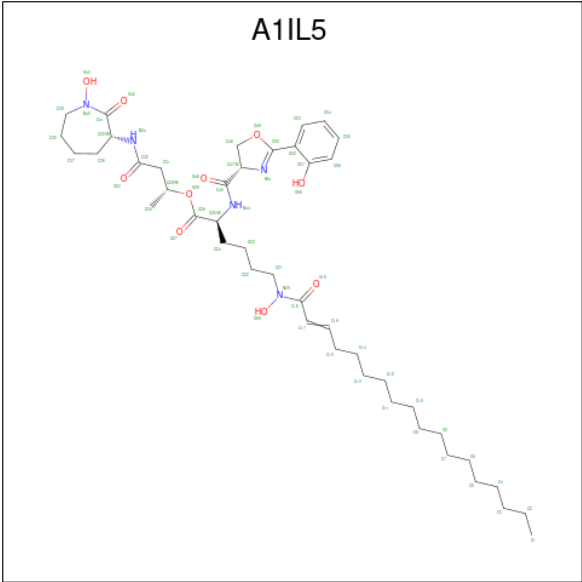
- Molecule 2 is a protein called Siderophore exporter MmpL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	722	Total	C	H	N	O	S	0	0
			11087	3524	5641	932	963	27		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	VAL	-	expression tag	UNP P9WJV2
B	682	GLY	-	linker	UNP P9WJV2
B	683	GLY	-	linker	UNP P9WJV2
B	684	SER	-	linker	UNP P9WJV2
B	685	SER	-	linker	UNP P9WJV2
B	686	SER	-	linker	UNP P9WJV2
B	968	ALA	-	expression tag	UNP P9WJV2
B	969	LEU	-	expression tag	UNP P9WJV2
B	970	GLU	-	expression tag	UNP P9WJV2
B	971	VAL	-	expression tag	UNP P9WJV2
B	972	LEU	-	expression tag	UNP P9WJV2
B	973	PHE	-	expression tag	UNP P9WJV2
B	974	GLN	-	expression tag	UNP P9WJV2

- Molecule 3 is Mycobactin S (three-letter code: A1IL5) (formula: C<sub>44</sub>H<sub>69</sub>N<sub>5</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
3	B	1	128	44	69	5	10	0

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

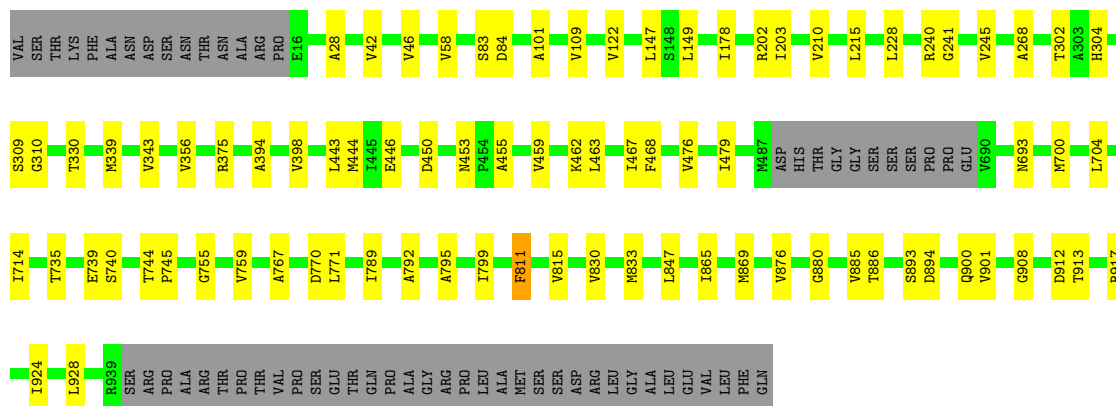
- Molecule 1: Acyl carrier protein

Chain A: 



- Molecule 2: Siderophore exporter MmpL4

Chain B: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	122605	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	64.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1IL5

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	0.26	0/601	0.52	0/812
2	B	0.25	0/5558	0.50	0/7557
All	All	0.25	0/6159	0.50	0/8369

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	597	572	571	13	0
2	B	5446	5641	5638	51	0
3	B	59	69	0	0	0
All	All	6102	6282	6209	63	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:880:GLY:HA3	2:B:913:THR:HG21	1.67	0.77
2:B:310:GLY:HA3	2:B:343:VAL:HG21	1.71	0.72
1:A:27:ALA:O	1:A:65:THR:OG1	2.07	0.70
2:B:770:ASP:OD1	2:B:771:LEU:N	2.28	0.66
2:B:109:VAL:HG23	2:B:122:VAL:HG11	1.81	0.62
1:A:15:GLN:OE1	2:B:375:ARG:NH2	2.34	0.61
2:B:744:THR:HG22	2:B:745:PRO:HD2	1.85	0.58
1:A:18:VAL:HG21	1:A:33:LEU:HD12	1.86	0.57
2:B:46:VAL:HG11	2:B:245:VAL:HG22	1.88	0.56
1:A:62:LYS:C	1:A:63:ILE:HD13	2.27	0.54
2:B:450:ASP:O	2:B:453:ASN:ND2	2.42	0.53
1:A:15:GLN:NE2	1:A:39:ASP:OD1	2.42	0.53
1:A:58:GLU:OE2	1:A:62:LYS:NZ	2.40	0.53
2:B:310:GLY:CA	2:B:343:VAL:HG21	2.38	0.53
2:B:42:VAL:HG11	2:B:241:GLY:HA3	1.92	0.52
2:B:394:ALA:O	2:B:398:VAL:HG13	2.10	0.51
2:B:833:MET:HE2	2:B:901:VAL:HG21	1.92	0.51
2:B:735:THR:O	2:B:739:GLU:HG3	2.11	0.51
2:B:202:ARG:NH2	2:B:894:ASP:OD1	2.42	0.50
2:B:122:VAL:HG13	2:B:147:LEU:HD23	1.92	0.50
2:B:908:GLY:O	2:B:912:ASP:OD2	2.30	0.50
2:B:203:ILE:HD11	2:B:893:SER:CB	2.43	0.49
2:B:755:GLY:O	2:B:759:VAL:HG23	2.13	0.49
2:B:83:SER:OG	2:B:149:LEU:O	2.19	0.48
2:B:203:ILE:HD11	2:B:893:SER:HB2	1.95	0.48
2:B:876:VAL:HG11	2:B:917:ARG:HD3	1.94	0.48
2:B:795:ALA:O	2:B:799:ILE:HG13	2.13	0.48
2:B:468:PHE:HD2	2:B:476:VAL:HG23	1.79	0.47
2:B:122:VAL:HG13	2:B:147:LEU:CD2	2.44	0.47
2:B:459:VAL:HG13	2:B:744:THR:HG21	1.96	0.47
2:B:443:LEU:HD23	2:B:444:MET:N	2.30	0.47
2:B:302:THR:O	2:B:302:THR:HG22	2.14	0.47
2:B:792:ALA:HB3	2:B:795:ALA:HB3	1.97	0.47
2:B:700:MET:CE	2:B:704:LEU:HD12	2.44	0.47
1:A:18:VAL:CG2	1:A:33:LEU:HD12	2.44	0.46
2:B:865:ILE:HG22	2:B:869:MET:CE	2.46	0.45
2:B:28:ALA:HB1	2:B:356:VAL:HG23	1.99	0.45
1:A:8:VAL:HA	1:A:11:ILE:HG22	1.98	0.45
1:A:7:ARG:HH11	1:A:7:ARG:HG2	1.81	0.45
2:B:339:MET:O	2:B:343:VAL:HG23	2.17	0.45
1:A:65:THR:HG23	1:A:68:ALA:H	1.81	0.44
2:B:42:VAL:O	2:B:46:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:789:ILE:HG21	2:B:847:LEU:HD11	2.00	0.44
1:A:9:LYS:NZ	1:A:20:GLN:OE1	2.50	0.44
2:B:84:ASP:O	2:B:84:ASP:OD1	2.36	0.43
2:B:880:GLY:CA	2:B:913:THR:HG21	2.45	0.43
2:B:463:LEU:O	2:B:467:ILE:HG22	2.19	0.43
2:B:479:ILE:HD11	2:B:700:MET:SD	2.57	0.43
2:B:811:PHE:CE2	2:B:815:VAL:HG21	2.53	0.43
2:B:714:ILE:N	2:B:714:ILE:HD13	2.33	0.43
2:B:215:LEU:HD13	2:B:228:LEU:HD23	2.00	0.43
2:B:101:ALA:HB2	2:B:178:ILE:HD11	2.00	0.43
1:A:4:ILE:O	1:A:8:VAL:HG13	2.19	0.42
2:B:210:VAL:HG11	2:B:885:VAL:CG1	2.49	0.42
2:B:811:PHE:HE2	2:B:815:VAL:HG21	1.84	0.42
2:B:455:ALA:O	2:B:459:VAL:HG23	2.20	0.42
2:B:767:ALA:O	2:B:770:ASP:OD1	2.38	0.41
2:B:830:VAL:HG21	2:B:900:GLN:HB3	2.02	0.41
2:B:58:VAL:HG11	2:B:330:THR:HG21	2.03	0.41
2:B:462:LYS:NZ	2:B:740:SER:O	2.54	0.41
2:B:268:ALA:HB2	2:B:886:THR:HG21	2.03	0.40
1:A:71:ASP:OD1	1:A:72:TYR:N	2.55	0.40
2:B:924:ILE:HG22	2:B:928:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
2	B	718/783 (92%)	707 (98%)	11 (2%)	0	100	100
All	All	793/861 (92%)	780 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	66/67 (98%)	65 (98%)	1 (2%)	60	77
2	B	570/621 (92%)	564 (99%)	6 (1%)	70	83
All	All	636/688 (92%)	629 (99%)	7 (1%)	69	83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
2	B	240	ARG
2	B	304	HIS
2	B	309	SER
2	B	446	GLU
2	B	693	ASN
2	B	811	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	123	GLN
2	B	153	GLN
2	B	304	HIS
2	B	722	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	A1IL5	B	1001	-	59,61,61	0.25	0	66,77,77	0.83	3 (4%)

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	A1IL5	B	1001	-	-	21/54/80/80	1/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	A1IL5	C41-C35-N34	-3.67	100.98	108.73
3	B	1001	A1IL5	C35-N34-C32	2.24	127.41	121.65
3	B	1001	A1IL5	C29-O28-C26	2.11	121.08	118.22

There are no chirality outliers.

All (21) torsion outliers are listed below:

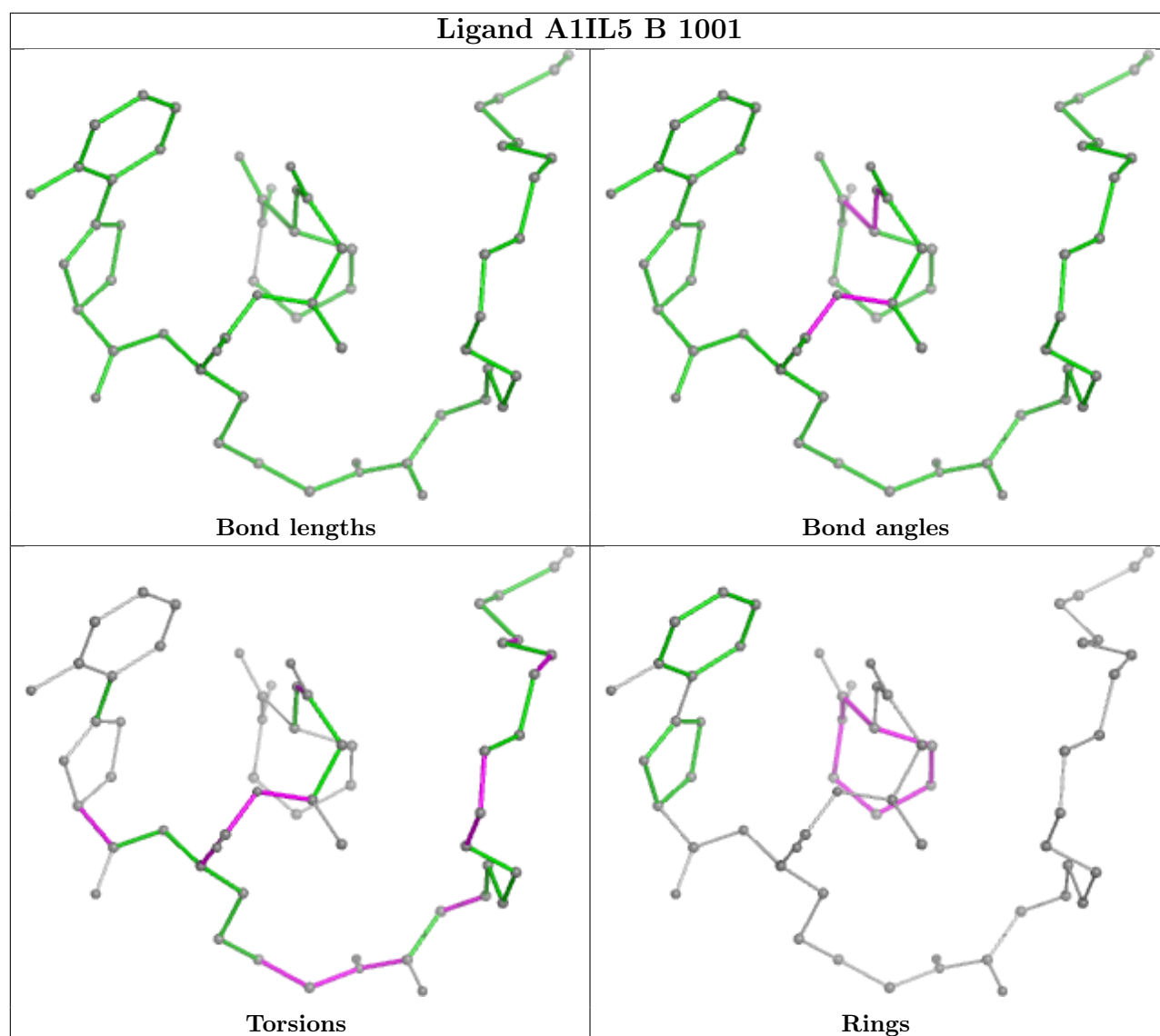
Mol	Chain	Res	Type	Atoms
3	B	1001	A1IL5	C15-C16-C17-C18
3	B	1001	A1IL5	N20-C21-C22-C23
3	B	1001	A1IL5	C22-C21-N20-O59
3	B	1001	A1IL5	C25-C26-O28-C29
3	B	1001	A1IL5	O19-C18-N20-C21
3	B	1001	A1IL5	O19-C18-N20-O59
3	B	1001	A1IL5	C30-C29-O28-C26
3	B	1001	A1IL5	C31-C32-N34-C35
3	B	1001	A1IL5	O33-C32-N34-C35
3	B	1001	A1IL5	N44-C45-C47-C48
3	B	1001	A1IL5	O46-C45-C47-C48
3	B	1001	A1IL5	O27-C26-O28-C29
3	B	1001	A1IL5	C10-C11-C12-C13
3	B	1001	A1IL5	C9-C10-C11-C12
3	B	1001	A1IL5	C22-C21-N20-C18
3	B	1001	A1IL5	N44-C25-C26-O27
3	B	1001	A1IL5	N44-C25-C26-O28
3	B	1001	A1IL5	C4-C5-C6-C7
3	B	1001	A1IL5	C6-C7-C8-C9
3	B	1001	A1IL5	O46-C45-C47-N51
3	B	1001	A1IL5	N44-C45-C47-N51

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1001	A1IL5	C35-C36-C37-C38-C39-C41-N40

No monomer is involved in short contacts.

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.