



# wwPDB EM Validation Summary Report ⓘ

Jan 14, 2024 – 12:12 AM JST

PDB ID : 8IYL  
EMDB ID : EMD-35825  
Title : Tail tip conformation 2 of phage lambda tail  
Authors : Wang, J.W.; Wang, C.  
Deposited on : 2023-04-05  
Resolution : 3.00 Å(reported)

This is a wwPDB EM Validation Summary 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>.

---

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

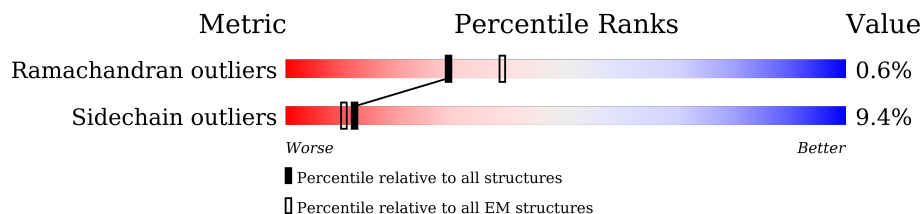
EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 3.00 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.



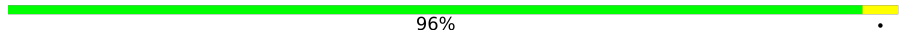
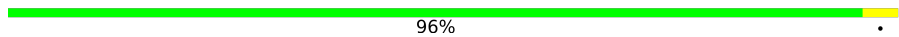
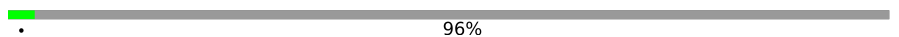
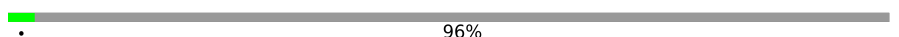






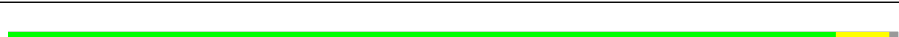


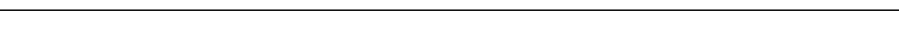
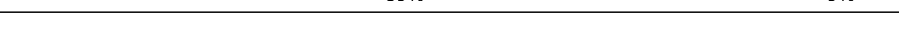
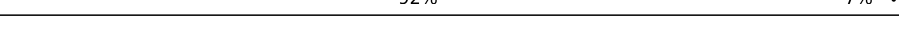
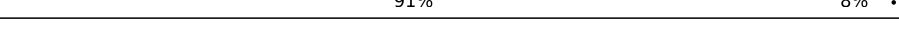
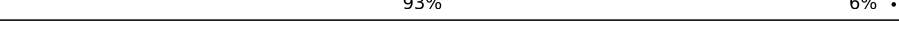
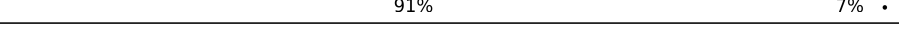
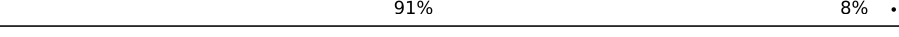
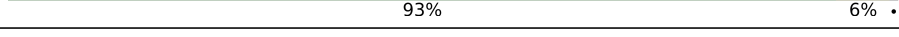
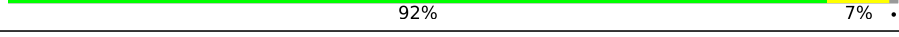

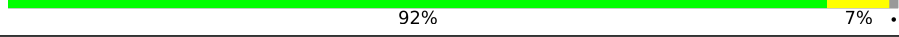

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	D	109	
1	F	109	
1	M	109	
1	X	109	
1	Z	109	
1	m	109	
2	E	1132	
2	J	1132	
2	Y	1132	
3	G	232	

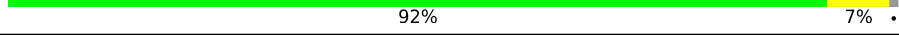
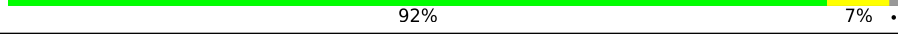
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	232	 96% .
3	d	232	 96% .
4	H	853	 96% .
4	K	853	 96% .
4	e	853	 96% .
5	I	223	 49% . 45%
5	N	223	 48% 6% 45%
5	f	223	 47% 7% 45%
6	A	246	 88% 11% .
6	B	246	 91% 8% .
6	C	246	 93% 6% .
6	O	246	 89% 10% .
6	P	246	 90% 9% .
6	Q	246	 89% 9% .
6	R	246	 92% 7% .
6	S	246	 91% 8% .
6	T	246	 93% 6% .
6	U	246	 91% 7% .
6	V	246	 91% 8% .
6	W	246	 93% 6% .
6	a	246	 92% 7% .
6	b	246	 91% 8% .
6	c	246	 92% 7% .
6	g	246	 91% 7% .
6	h	246	 93% 6% .

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
6	i	246	 90% 9%
6	j	246	 91% 7%
6	k	246	 91% 7%
6	l	246	 90% 9%
6	n	246	 93% 6%
6	o	246	 92% 7%
6	v	246	 92% 7%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 77370 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 Tail tip protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	M	109	884	569	154	157	4	0	0
1	m	109	884	569	154	157	4	0	0
1	D	109	884	569	154	157	4	0	0
1	F	109	884	569	154	157	4	0	0
1	X	109	884	569	154	157	4	0	0
1	Z	109	884	569	154	157	4	0	0

- Molecule 2 is a protein called Tip attachment protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	J	861	6720	4212	1171	1317	20	0	0
2	E	861	6720	4212	1171	1317	20	0	0
2	Y	861	6720	4212	1171	1317	20	0	0

- Molecule 3 is a protein called Tail tip protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	232	1801	1117	309	362	13	0	0
3	G	232	1801	1117	309	362	13	0	0
3	d	232	1801	1117	309	362	13	0	0

- Molecule 4 is a protein called Tape measure protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	33	Total	C	N	O	S	0	0
			250	154	47	47	2		
4	K	33	Total	C	N	O	S	0	0
			250	154	47	47	2		
4	e	33	Total	C	N	O	S	0	0
			250	154	47	47	2		

- Molecule 5 is a protein called Tail tip assembly protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	122	Total	C	N	O	S	0	0
			865	544	151	165	5		
5	N	122	Total	C	N	O	S	0	0
			865	544	151	165	5		
5	f	122	Total	C	N	O	S	0	0
			865	544	151	165	5		

- Molecule 6 is a protein called Tail tube protein.

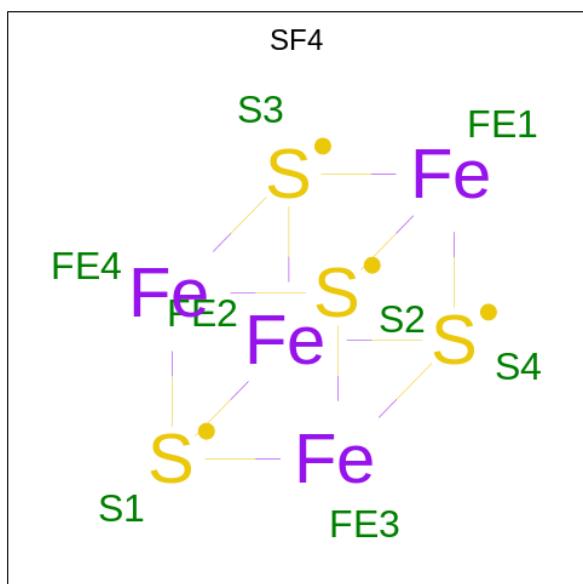
Mol	Chain	Residues	Atoms					AltConf	Trace
6	V	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
6	v	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
6	B	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	b	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	A	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	a	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	C	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	c	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	O	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
6	P	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
6	Q	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	R	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	T	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	U	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	W	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	g	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
6	h	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
6	i	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	j	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	k	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	l	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	n	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
6	o	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).




<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>AltConf</b>
7	L	1	Total 8	Fe 4	S 4	0
7	G	1	Total 8	Fe 4	S 4	0
7	d	1	Total 8	Fe 4	S 4	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: Tail tip protein M

Chain M:  90% 10%



- Molecule 1: Tail tip protein M

Chain m:  95% 5%



- Molecule 1: Tail tip protein M

Chain D:  92% 8%



- Molecule 1: Tail tip protein M

Chain F:  95% 5%



- Molecule 1: Tail tip protein M

Chain X:  87% 13%

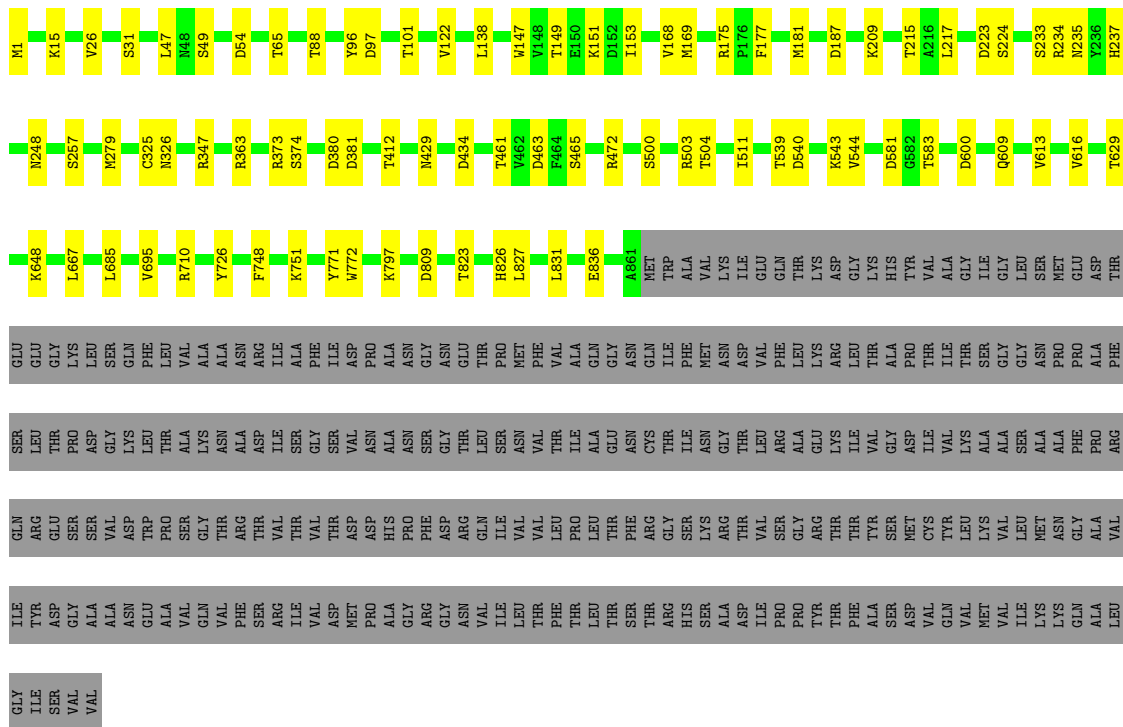


- Molecule 1: Tail tip protein M

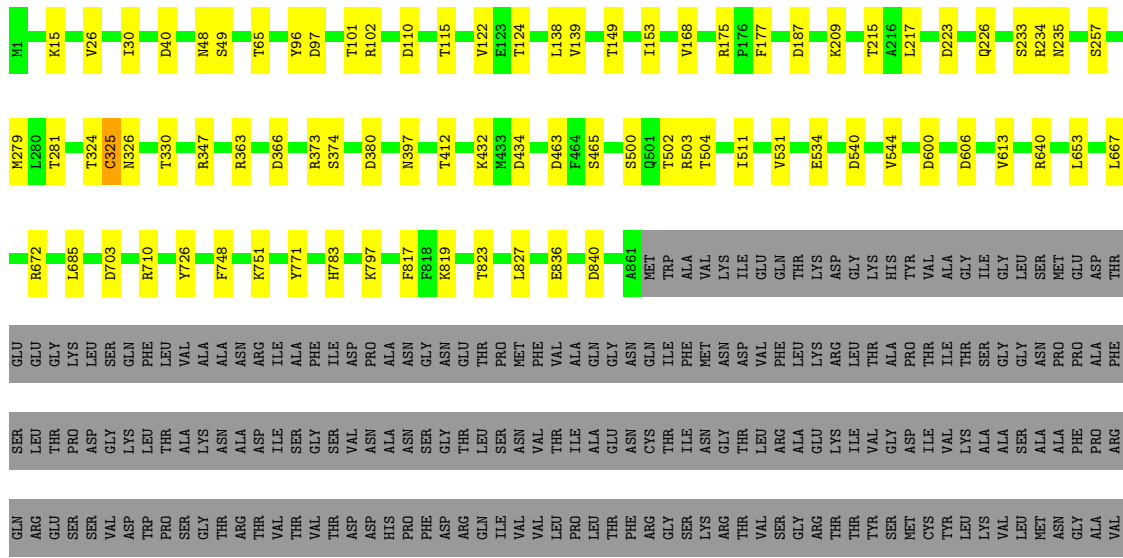
Chain Z:  93% 7%



• Molecule 2: Tip attachment protein J



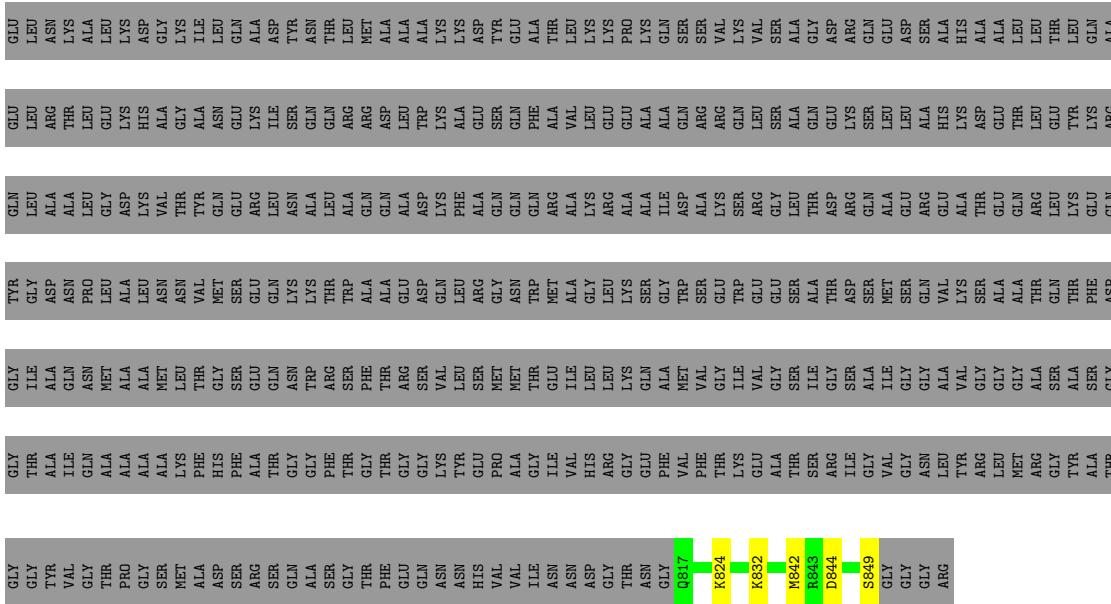
• Molecule 2: Tip attachment protein J



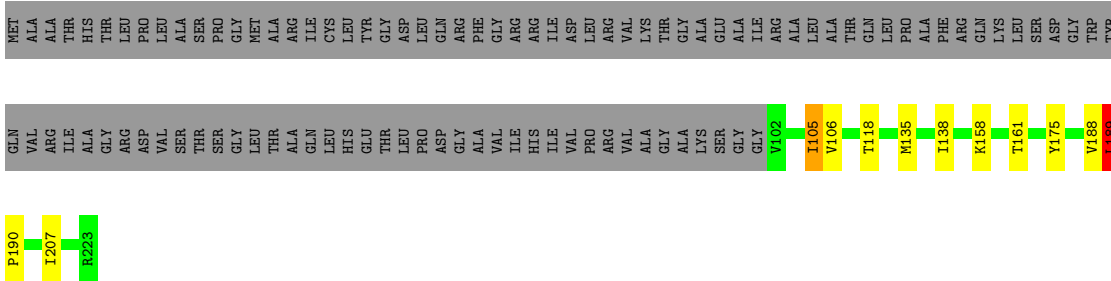




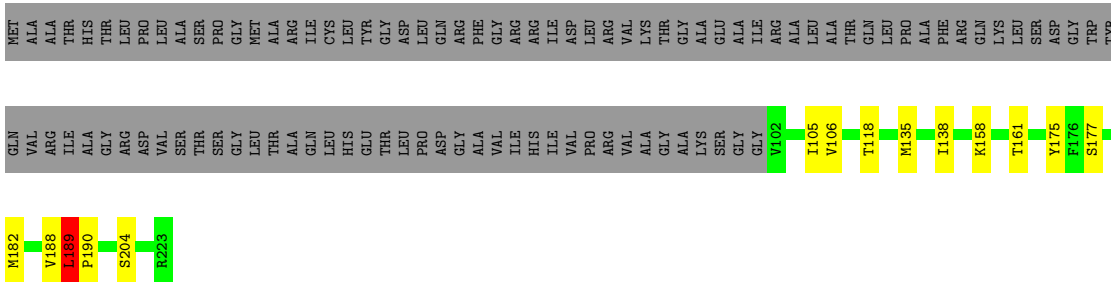




• Molecule 5: Tail tip assembly protein I

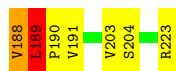
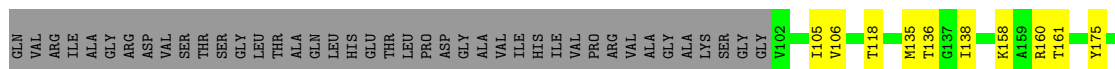


• Molecule 5: Tail tip assembly protein I



• Molecule 5: Tail tip assembly protein I





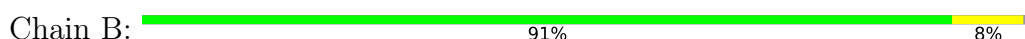
• Molecule 6: Tail tube protein



• Molecule 6: Tail tube protein



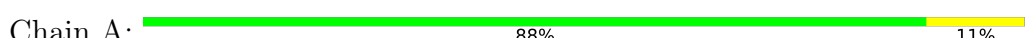
• Molecule 6: Tail tube protein



• Molecule 6: Tail tube protein



• Molecule 6: Tail tube protein

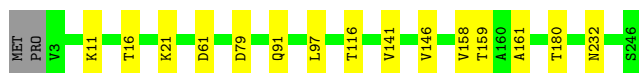


• Molecule 6: Tail tube protein




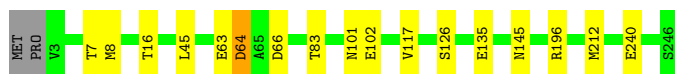
• Molecule 6: Tail tube protein

Chain C:  93% 6%




• Molecule 6: Tail tube protein

Chain c:  92% 7%




• Molecule 6: Tail tube protein

Chain O:  89% 10%




• Molecule 6: Tail tube protein

Chain P:  90% 9%



• Molecule 6: Tail tube protein

Chain Q:  89% 9%




• Molecule 6: Tail tube protein

Chain R:  92% 7%



• Molecule 6: Tail tube protein

Chain S:  91% 8%




• Molecule 6: Tail tube protein



Chain T:  93% 6%



• Molecule 6: Tail tube protein

Chain U:  91% 7%




• Molecule 6: Tail tube protein

Chain W:  93% 6%



• Molecule 6: Tail tube protein

Chain g:  91% 7%




• Molecule 6: Tail tube protein

Chain h:  93% 6%




• Molecule 6: Tail tube protein

Chain i:  90% 9%

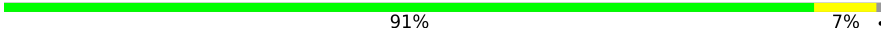


• Molecule 6: Tail tube protein

Chain j:  91% 7%




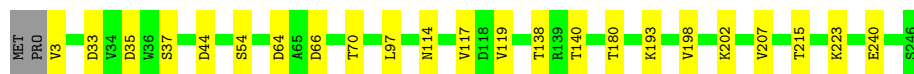
• Molecule 6: Tail tube protein

Chain k:  91% 7%



• Molecule 6: Tail tube protein

Chain l:  90% 9%



• Molecule 6: Tail tube protein

Chain n:  93% 6%



• Molecule 6: Tail tube protein

Chain o:  92% 7%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	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: SF4

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	D	0.30	0/909	0.56	0/1231
1	F	0.30	0/909	0.54	0/1231
1	M	0.31	0/909	0.55	0/1231
1	X	0.30	0/909	0.55	0/1231
1	Z	0.30	0/909	0.54	0/1231
1	m	0.30	0/909	0.54	0/1231
2	E	0.27	0/6866	0.54	1/9348 (0.0%)
2	J	0.27	0/6866	0.54	1/9348 (0.0%)
2	Y	0.27	0/6866	0.54	0/9348
3	G	0.29	0/1836	0.50	0/2487
3	L	0.29	0/1836	0.50	0/2487
3	d	0.29	0/1836	0.51	0/2487
4	H	0.29	0/252	0.52	0/335
4	K	0.30	0/252	0.56	0/335
4	e	0.35	0/252	0.57	0/335
5	I	0.29	0/876	0.65	2/1186 (0.2%)
5	N	0.28	0/876	0.65	2/1186 (0.2%)
5	f	0.29	0/876	0.65	2/1186 (0.2%)
6	A	0.28	0/1834	0.56	2/2505 (0.1%)
6	B	0.28	0/1834	0.55	1/2505 (0.0%)
6	C	0.28	0/1834	0.53	0/2505
6	O	0.28	0/1827	0.53	0/2494
6	P	0.28	0/1827	0.51	0/2494
6	Q	0.28	0/1834	0.55	1/2505 (0.0%)
6	R	0.28	0/1834	0.57	2/2505 (0.1%)
6	S	0.28	0/1834	0.56	1/2505 (0.0%)
6	T	0.28	0/1834	0.54	0/2505
6	U	0.26	0/1834	0.54	1/2505 (0.0%)
6	V	0.28	0/1827	0.52	0/2494
6	W	0.27	0/1834	0.55	1/2505 (0.0%)
6	a	0.29	0/1834	0.55	1/2505 (0.0%)
6	b	0.28	0/1834	0.56	2/2505 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
6	c	0.27	0/1834	0.56	1/2505 (0.0%)
6	g	0.28	0/1827	0.52	0/2494
6	h	0.28	0/1827	0.51	0/2494
6	i	0.28	0/1834	0.55	0/2505
6	j	0.28	0/1834	0.56	2/2505 (0.1%)
6	k	0.29	0/1834	0.56	1/2505 (0.0%)
6	l	0.29	0/1834	0.54	1/2505 (0.0%)
6	n	0.27	0/1834	0.55	0/2505
6	o	0.27	0/1834	0.55	0/2505
6	v	0.28	0/1827	0.51	0/2494
All	All	0.28	0/78918	0.54	25/107508 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
2	J	0	1
2	Y	0	1
5	I	0	1
5	N	0	1
5	f	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	f	189	LEU	CA-CB-CG	7.53	132.62	115.30
6	j	212	MET	CA-CB-CG	6.57	124.47	113.30
6	R	212	MET	CA-CB-CG	6.38	124.15	113.30
5	I	189	LEU	C-N-CD	-6.28	106.78	120.60
6	c	64	ASP	CB-CG-OD1	6.04	123.73	118.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	175	ARG	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
5	I	189	LEU	Peptide
2	J	175	ARG	Peptide
5	N	189	LEU	Peptide
2	Y	175	ARG	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	D	107/109 (98%)	94 (88%)	13 (12%)	0	100	100
1	F	107/109 (98%)	93 (87%)	13 (12%)	1 (1%)	17	55
1	M	107/109 (98%)	94 (88%)	13 (12%)	0	100	100
1	X	107/109 (98%)	94 (88%)	13 (12%)	0	100	100
1	Z	107/109 (98%)	95 (89%)	11 (10%)	1 (1%)	17	55
1	m	107/109 (98%)	92 (86%)	14 (13%)	1 (1%)	17	55
2	E	859/1132 (76%)	780 (91%)	75 (9%)	4 (0%)	29	68
2	J	859/1132 (76%)	773 (90%)	82 (10%)	4 (0%)	29	68
2	Y	859/1132 (76%)	775 (90%)	81 (9%)	3 (0%)	41	76
3	G	230/232 (99%)	222 (96%)	8 (4%)	0	100	100
3	L	230/232 (99%)	222 (96%)	8 (4%)	0	100	100
3	d	230/232 (99%)	224 (97%)	6 (3%)	0	100	100
4	H	31/853 (4%)	25 (81%)	6 (19%)	0	100	100
4	K	31/853 (4%)	25 (81%)	6 (19%)	0	100	100
4	e	31/853 (4%)	26 (84%)	5 (16%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	120/223 (54%)	97 (81%)	17 (14%)	6 (5%)	2	12
5	N	120/223 (54%)	97 (81%)	17 (14%)	6 (5%)	2	12
5	f	120/223 (54%)	97 (81%)	17 (14%)	6 (5%)	2	12
6	A	242/246 (98%)	225 (93%)	14 (6%)	3 (1%)	13	48
6	B	242/246 (98%)	223 (92%)	18 (7%)	1 (0%)	34	72
6	C	242/246 (98%)	224 (93%)	16 (7%)	2 (1%)	19	57
6	O	241/246 (98%)	227 (94%)	13 (5%)	1 (0%)	34	72
6	P	241/246 (98%)	229 (95%)	12 (5%)	0	100	100
6	Q	242/246 (98%)	223 (92%)	18 (7%)	1 (0%)	34	72
6	R	242/246 (98%)	228 (94%)	13 (5%)	1 (0%)	34	72
6	S	242/246 (98%)	224 (93%)	15 (6%)	3 (1%)	13	48
6	T	242/246 (98%)	231 (96%)	10 (4%)	1 (0%)	34	72
6	U	242/246 (98%)	225 (93%)	14 (6%)	3 (1%)	13	48
6	V	241/246 (98%)	228 (95%)	12 (5%)	1 (0%)	34	72
6	W	242/246 (98%)	228 (94%)	14 (6%)	0	100	100
6	a	242/246 (98%)	232 (96%)	9 (4%)	1 (0%)	34	72
6	b	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	34	72
6	c	242/246 (98%)	230 (95%)	12 (5%)	0	100	100
6	g	241/246 (98%)	229 (95%)	11 (5%)	1 (0%)	34	72
6	h	241/246 (98%)	228 (95%)	13 (5%)	0	100	100
6	i	242/246 (98%)	224 (93%)	17 (7%)	1 (0%)	34	72
6	j	242/246 (98%)	229 (95%)	12 (5%)	1 (0%)	34	72
6	k	242/246 (98%)	224 (93%)	15 (6%)	3 (1%)	13	48
6	l	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	34	72
6	n	242/246 (98%)	225 (93%)	15 (6%)	2 (1%)	19	57
6	o	242/246 (98%)	229 (95%)	12 (5%)	1 (0%)	34	72
6	v	241/246 (98%)	228 (95%)	13 (5%)	0	100	100
All	All	10164/13878 (73%)	9378 (92%)	725 (7%)	61 (1%)	29	64

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	105	ILE

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
5	I	188	VAL
5	I	190	PRO
6	V	158	VAL
6	B	158	VAL

### 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	D	96/96 (100%)	87 (91%)	9 (9%)	8	32
1	F	96/96 (100%)	92 (96%)	4 (4%)	30	66
1	M	96/96 (100%)	85 (88%)	11 (12%)	5	24
1	X	96/96 (100%)	82 (85%)	14 (15%)	3	15
1	Z	96/96 (100%)	89 (93%)	7 (7%)	14	44
1	m	96/96 (100%)	92 (96%)	4 (4%)	30	66
2	E	734/958 (77%)	658 (90%)	76 (10%)	7	27
2	J	734/958 (77%)	657 (90%)	77 (10%)	7	27
2	Y	734/958 (77%)	653 (89%)	81 (11%)	6	25
3	G	198/198 (100%)	187 (94%)	11 (6%)	21	56
3	L	198/198 (100%)	188 (95%)	10 (5%)	24	60
3	d	198/198 (100%)	189 (96%)	9 (4%)	27	64
4	H	24/648 (4%)	20 (83%)	4 (17%)	2	11
4	K	24/648 (4%)	20 (83%)	4 (17%)	2	11
4	e	24/648 (4%)	19 (79%)	5 (21%)	1	5
5	I	86/162 (53%)	79 (92%)	7 (8%)	11	40
5	N	86/162 (53%)	78 (91%)	8 (9%)	9	33
5	f	86/162 (53%)	74 (86%)	12 (14%)	3	16
6	A	194/196 (99%)	170 (88%)	24 (12%)	4	20
6	B	194/196 (99%)	176 (91%)	18 (9%)	9	33

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	C	194/196 (99%)	181 (93%)	13 (7%)	16	49
6	O	193/196 (98%)	170 (88%)	23 (12%)	5	22
6	P	193/196 (98%)	172 (89%)	21 (11%)	6	25
6	Q	194/196 (99%)	171 (88%)	23 (12%)	5	22
6	R	194/196 (99%)	177 (91%)	17 (9%)	10	36
6	S	194/196 (99%)	176 (91%)	18 (9%)	9	33
6	T	194/196 (99%)	180 (93%)	14 (7%)	14	45
6	U	194/196 (99%)	177 (91%)	17 (9%)	10	36
6	V	193/196 (98%)	175 (91%)	18 (9%)	9	33
6	W	194/196 (99%)	179 (92%)	15 (8%)	13	42
6	a	194/196 (99%)	177 (91%)	17 (9%)	10	36
6	b	194/196 (99%)	173 (89%)	21 (11%)	6	26
6	c	194/196 (99%)	177 (91%)	17 (9%)	10	36
6	g	193/196 (98%)	176 (91%)	17 (9%)	10	36
6	h	193/196 (98%)	178 (92%)	15 (8%)	12	42
6	i	194/196 (99%)	173 (89%)	21 (11%)	6	26
6	j	194/196 (99%)	176 (91%)	18 (9%)	9	33
6	k	194/196 (99%)	178 (92%)	16 (8%)	11	39
6	l	194/196 (99%)	173 (89%)	21 (11%)	6	26
6	n	194/196 (99%)	182 (94%)	12 (6%)	18	52
6	o	194/196 (99%)	177 (91%)	17 (9%)	10	36
6	v	193/196 (98%)	176 (91%)	17 (9%)	10	36
All	All	8352/11178 (75%)	7569 (91%)	783 (9%)	12	32

5 of 783 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	S	148	ARG
2	Y	366	ASP
6	T	84	LEU
6	S	146	VAL
1	X	27	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	38	ASN
5	f	169	ASN
6	o	74	GLN
6	n	94	GLN
2	E	75	GLN

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

3 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	$\# Z  > 2$
7	SF4	d	301	3	0,12,12	-	-	-		
7	SF4	L	301	3	0,12,12	-	-	-		
7	SF4	G	301	3	0,12,12	-	-	-		

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	d	301	3	-	-	0/6/5/5
7	SF4	L	301	3	-	-	0/6/5/5
7	SF4	G	301	3	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

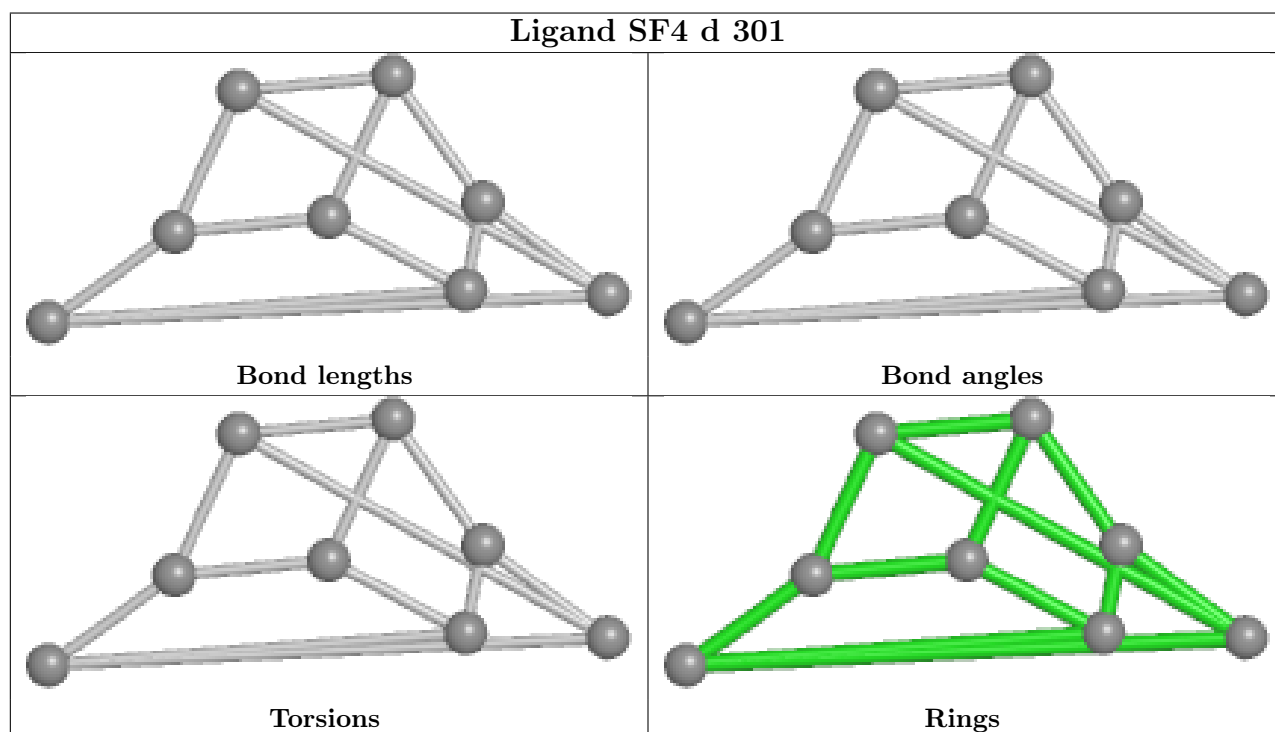
There are no chirality outliers.

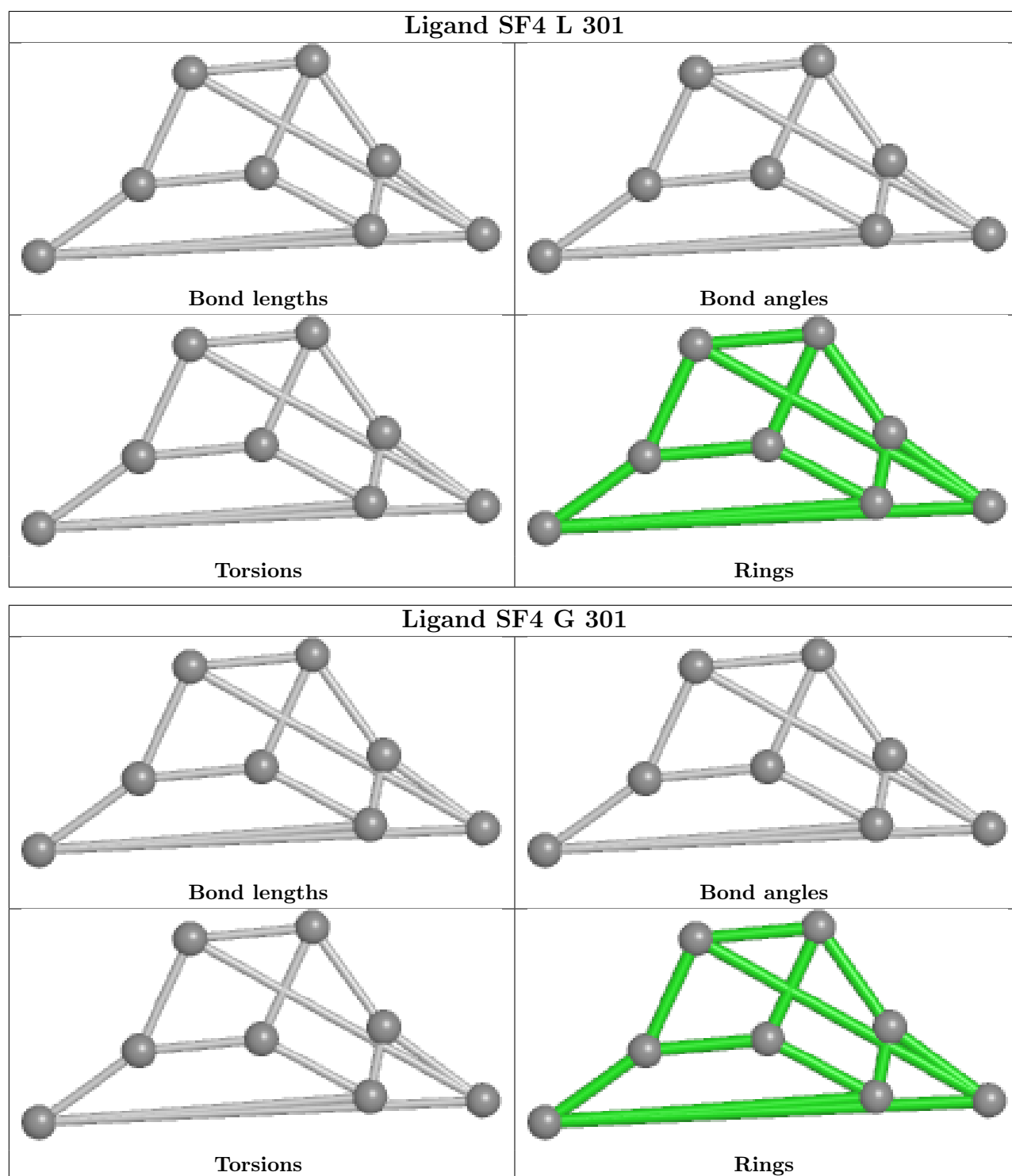
There are no torsion outliers.

There are no ring outliers.

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

There are no chain breaks in this entry.