



wwPDB EM Validation Summary Report ⓘ

Mar 3, 2025 – 06:04 pm GMT

PDB ID : 9GMR
EMDB ID : EMD-51453
Title : SIRT7-H3K36MTUnucleosome complex
Authors : Moreno-Yruela, C.; Ekundayo, B.; Foteva, P.; Calvino-Sanles, E.; Ni, D.;
Stahlberg, H.; Fierz, B.
Deposited on : 2024-08-29
Resolution : 2.80 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

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 : 1.8.4, 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

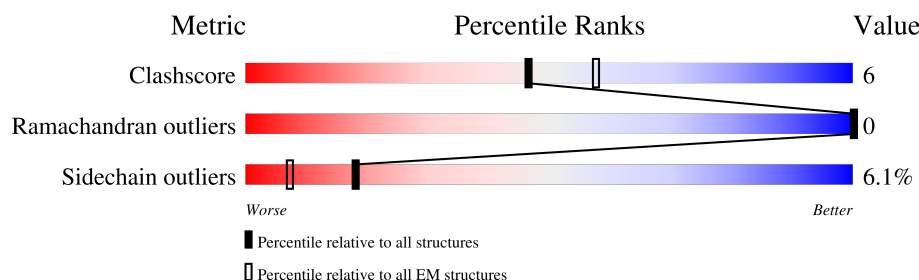
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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 ≥ 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	136	71% 26%
1	E	136	67% 29%
2	B	103	78% 19%
2	F	103	70% 6% 24%
3	C	129	65% 15% 19%
3	G	129	71% 11% 19%
4	D	126	61% 11% 28%
4	H	126	66% 8% 25%
5	I	149	62% 38%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	J	149	 60% 40%
7	K	401	 58% 23% • 17%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14763 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	100	Total	C	N	O	S	0	0
			821	519	159	141	2		
1	E	97	Total	C	N	O	S	0	0
			799	503	155	139	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	CYS	ALA	conflict	UNP Q71DI3
A	110	ALA	CYS	conflict	UNP Q71DI3
E	47	CYS	ALA	conflict	UNP Q71DI3
E	110	ALA	CYS	conflict	UNP Q71DI3

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
2	F	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

- Molecule 3 is a protein called Histone H2A type 2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	104	Total	C	N	O	S	0	0
			801	506	155	139	1		
3	G	105	Total	C	N	O	S	0	0
			806	509	156	140	1		

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	91	Total	C	N	O	S	0	0
			707	446	125	134	2		
4	H	94	Total	C	N	O	S	0	0
			733	461	132	138	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	31	LYS	ARG	conflict	UNP P06899
H	31	LYS	ARG	conflict	UNP P06899

- Molecule 5 is a DNA chain called DNA (149-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	149	Total	C	N	O	P	0	0
			3033	1441	551	892	149		

- Molecule 6 is a DNA chain called DNA (149-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	149	Total	C	N	O	P	0	0
			3076	1456	575	896	149		

- Molecule 7 is a protein called NAD-dependent protein deacetylase sirtuin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	334	Total	C	N	O	S	0	0
			2662	1642	516	489	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	0	GLY	-	expression tag	UNP Q9NRC8

- Molecule 8 is [[(2 {R},3 {a} {R},5 {R},6 {R},6 {a} {R})-2-(methylamino)-6-oxidanyl-2-(propylamino)-3 {a},5,6,6 {a}-tetrahydrofuro[2,3-d][1,3]oxathiol-5-yl]methoxy-oxidanyl-phosphoryl] [(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl hydrogen phosphate (three-letter code: A1IY0) (formula: C₂₀H₃₃N₇O₁₃P₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
8	A	1	Total 43	C 20	N 7	O 13	P 2	S 1	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

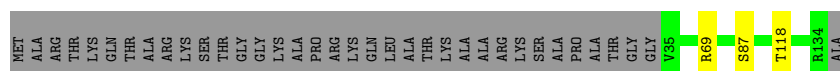
Mol	Chain	Residues	Atoms	AltConf
9	K	1	Total Zn 1 1	0

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.

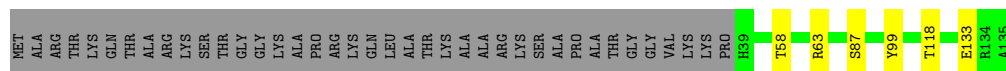
- Molecule 1: Histone H3.2

Chain A:  71% 26%




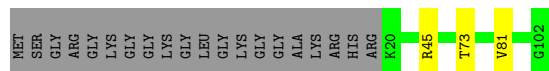
- Molecule 1: Histone H3.2

Chain E:  67% 29%



- Molecule 2: Histone H4

Chain B:  78% 19%



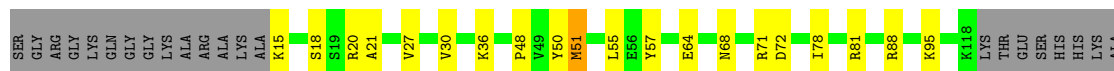
- Molecule 2: Histone H4

Chain F:  70% 6% 24%



- Molecule 3: Histone H2A type 2-A

Chain C:  65% 15% 19%



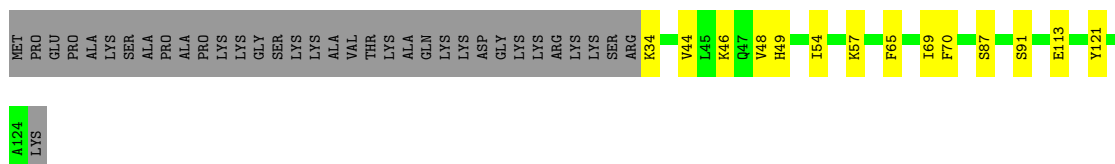
- Molecule 3: Histone H2A type 2-A

Chain G:  71% 11% 19%



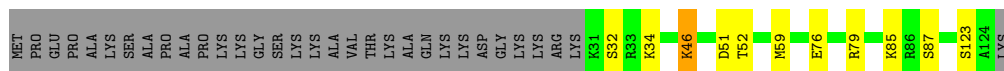
- Molecule 4: Histone H2B type 1-J

Chain D:  61% 11% 28%



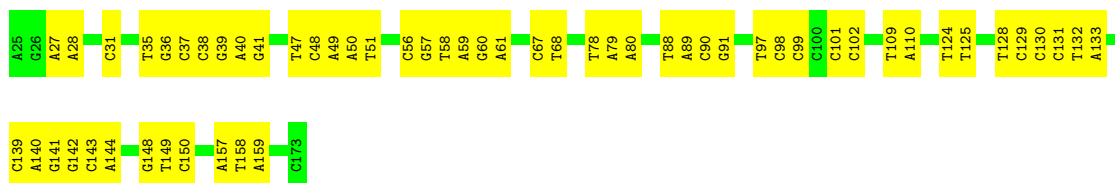
- Molecule 4: Histone H2B type 1-J

Chain H:  66% 8% 25%



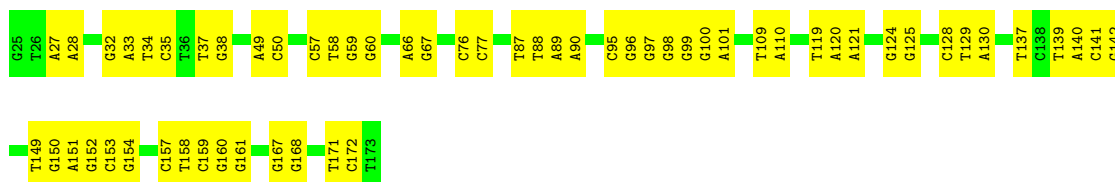
- Molecule 5: DNA (149-MER)

Chain I:  62% 38%



- Molecule 6: DNA (149-MER)

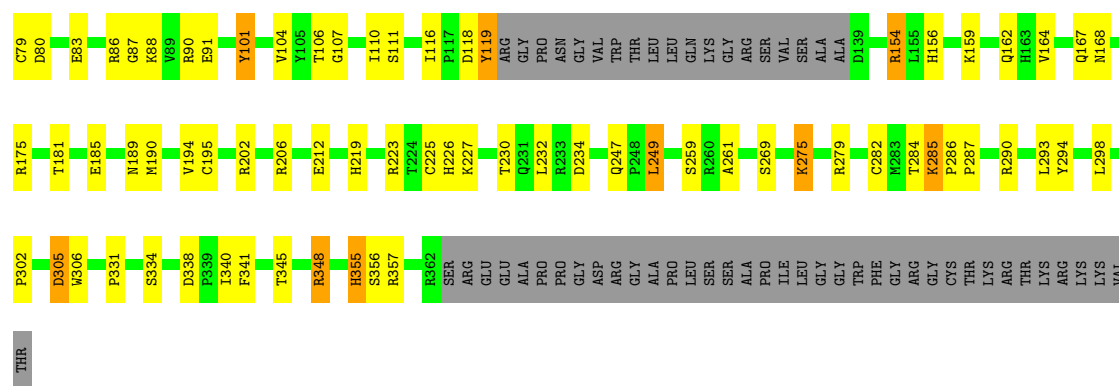
Chain J:  60% 40%



- Molecule 7: NAD-dependent protein deacetylase sirtuin-7

Chain K:  58% 23% 17%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	337476	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k 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: ZN, A1IY0

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/833	0.54	0/1118
1	E	0.29	0/810	0.55	0/1085
2	B	0.29	0/669	0.56	0/894
2	F	0.29	0/626	0.55	0/837
3	C	0.27	0/811	0.51	0/1093
3	G	0.27	0/816	0.51	0/1100
4	D	0.30	0/718	0.49	0/967
4	H	0.31	0/744	0.51	0/1000
5	I	0.56	0/3398	0.92	0/5236
6	J	0.55	0/3454	0.90	0/5335
7	K	0.24	0/2706	0.55	0/3648
All	All	0.42	0/15585	0.74	0/22313

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
4	D	1	0
4	H	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	39	ILE	CB
4	H	39	ILE	CB

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	821	0	859	2	0
1	E	799	0	833	2	0
2	B	662	0	709	2	0
2	F	619	0	659	3	0
3	C	801	0	857	11	0
3	G	806	0	862	6	0
4	D	707	0	722	8	0
4	H	733	0	753	5	0
5	I	3033	0	1672	38	0
6	J	3076	0	1674	38	0
7	K	2662	0	2692	52	0
8	A	43	0	0	2	0
9	K	1	0	0	0	0
All	All	14763	0	12292	159	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.

The worst 5 of 159 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)
8:A:401:A1IY0:C02	8:A:401:A1IY0:O02	1.63	1.34
3:C:64:GLU:OE1	4:D:49:HIS:NE2	2.25	0.68
7:K:356:SER:O	7:K:357:ARG:NH1	2.28	0.66
7:K:206:ARG:NH1	7:K:345:THR:O	2.29	0.66
7:K:11:ARG:HB3	7:K:11:ARG:NH1	2.12	0.65

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	98/136 (72%)	93 (95%)	5 (5%)	0	100	100
1	E	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
2	B	81/103 (79%)	79 (98%)	2 (2%)	0	100	100
2	F	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
3	C	102/129 (79%)	101 (99%)	1 (1%)	0	100	100
3	G	103/129 (80%)	100 (97%)	3 (3%)	0	100	100
4	D	89/126 (71%)	85 (96%)	4 (4%)	0	100	100
4	H	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
7	K	330/401 (82%)	317 (96%)	13 (4%)	0	100	100
All	All	1066/1389 (77%)	1034 (97%)	32 (3%)	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	86/111 (78%)	85 (99%)	1 (1%)	67	89
1	E	83/111 (75%)	80 (96%)	3 (4%)	30	64
2	B	68/79 (86%)	68 (100%)	0	100	100
2	F	63/79 (80%)	62 (98%)	1 (2%)	58	85
3	C	82/98 (84%)	75 (92%)	7 (8%)	8	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	82/98 (84%)	77 (94%)	5 (6%)	15	43
4	D	76/105 (72%)	72 (95%)	4 (5%)	19	49
4	H	79/105 (75%)	74 (94%)	5 (6%)	15	42
7	K	286/335 (85%)	257 (90%)	29 (10%)	6	20
All	All	905/1121 (81%)	850 (94%)	55 (6%)	18	43

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	K	24	GLN
7	K	156	HIS
7	K	355	HIS
7	K	293	LEU
7	K	28	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
8	A1IY0	A	401	1	37,47,47	3.51	14 (37%)	38,72,72	1.89	10 (26%)

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
8	A1IY0	A	401	1	-	5/20/72/72	0/5/5/5

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	401	A1IY0	O02-C02	12.40	1.63	1.43
8	A	401	A1IY0	C08-S01	-9.48	1.64	1.82
8	A	401	A1IY0	O03-C08	6.77	1.54	1.43
8	A	401	A1IY0	C01-C02	-6.11	1.39	1.52
8	A	401	A1IY0	O09-C15	5.48	1.48	1.41

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	401	A1IY0	O02-C02-C08	5.54	110.12	103.79
8	A	401	A1IY0	N05-C19-N06	-5.05	120.79	128.68
8	A	401	A1IY0	C13-C14-C15	4.05	107.07	100.98
8	A	401	A1IY0	C18-C17-N04	-2.92	106.35	109.40
8	A	401	A1IY0	C02-C01-C09	2.90	108.29	101.99

There are no chirality outliers.

All (5) torsion outliers are listed below:

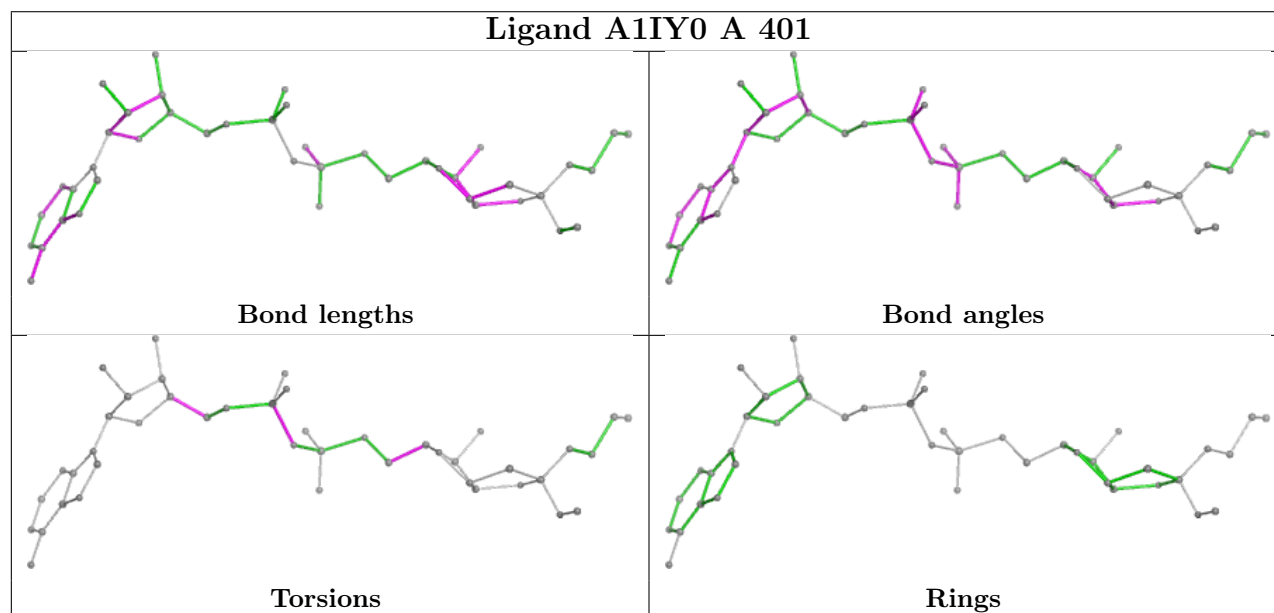
Mol	Chain	Res	Type	Atoms
8	A	401	A1IY0	C01-C09-C10-O04
8	A	401	A1IY0	O03-C09-C10-O04
8	A	401	A1IY0	O06-C11-C12-O09
8	A	401	A1IY0	O06-C11-C12-C13
8	A	401	A1IY0	P01-O05-P02-O11

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	401	A1IY0	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 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.