



wwPDB EM Validation Summary Report ⓘ

Nov 18, 2024 – 01:04 PM JST

PDB ID : 8YWA
EMDB ID : EMD-39627
Title : The structure of IgE receptor binding to IgE
Authors : Chen, M.Y.; Su, Q.; Shi, Y.G.
Deposited on : 2024-03-30
Resolution : 3.14 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 : 1.8.5 (274361), 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) : 2.39

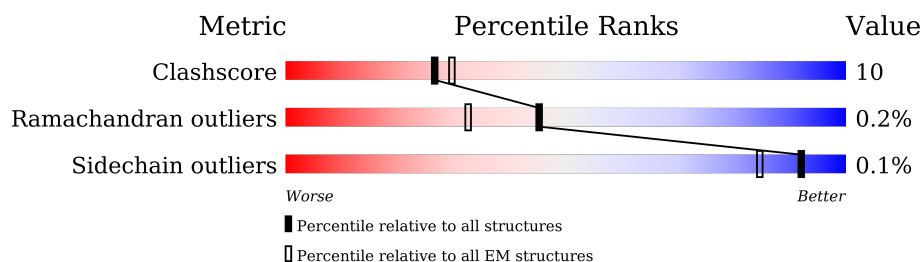
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.14 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	H	577	64% 10% 26%
1	X	577	62% 12% 26%
2	h	261	40% 60%
2	x	261	39% 60%
3	A	267	57% 20% 23%
4	B	283	53% 45%
5	C	86	37% 63%
5	D	86	37% 63%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16619 atoms, of which 6751 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 Immunoglobulin heavy constant epsilon.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	H	426	Total	C	H	N	O	S	0	0
			5579	1873	2551	552	592	11		
1	X	426	Total	C	H	N	O	S	0	0
			5565	1869	2546	550	589	11		

- Molecule 2 is a protein called Immunoglobulin kappa constant.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	h	104	Total	C	N	O	1	0
			518	310	104	104		
2	x	104	Total	C	N	O	1	0
			518	310	104	104		

- Molecule 3 is a protein called High affinity immunoglobulin epsilon receptor subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	205	Total	C	H	N	O	S	0	0
			2803	998	1232	263	305	5		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP P12319
A	5	ASP	-	expression tag	UNP P12319
A	6	MET	-	expression tag	UNP P12319
A	7	ARG	-	expression tag	UNP P12319
A	8	VAL	-	expression tag	UNP P12319
A	9	PRO	-	expression tag	UNP P12319
A	10	ALA	-	expression tag	UNP P12319
A	11	GLN	-	expression tag	UNP P12319
A	12	LEU	-	expression tag	UNP P12319
A	13	LEU	-	expression tag	UNP P12319
A	14	GLY	-	expression tag	UNP P12319

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Chain	Residue	Modelled	Actual	Comment	Reference
A	15	LEU	-	expression tag	UNP P12319
A	16	LEU	-	expression tag	UNP P12319
A	17	LEU	-	expression tag	UNP P12319
A	18	LEU	-	expression tag	UNP P12319
A	19	TRP	-	expression tag	UNP P12319
A	20	LEU	-	expression tag	UNP P12319
A	21	SER	-	expression tag	UNP P12319
A	22	GLY	-	expression tag	UNP P12319
A	23	ALA	-	expression tag	UNP P12319
A	24	ARG	-	expression tag	UNP P12319
A	25	CYS	-	expression tag	UNP P12319
A	258	GLY	-	expression tag	UNP P12319
A	259	GLY	-	expression tag	UNP P12319
A	260	GLY	-	expression tag	UNP P12319
A	261	SER	-	expression tag	UNP P12319
A	262	MET	-	expression tag	UNP P12319
A	263	ASP	-	expression tag	UNP P12319
A	264	TYR	-	expression tag	UNP P12319
A	265	LYS	-	expression tag	UNP P12319
A	266	ASP	-	expression tag	UNP P12319
A	267	ASP	-	expression tag	UNP P12319
A	268	ASP	-	expression tag	UNP P12319
A	269	ASP	-	expression tag	UNP P12319
A	270	LYS	-	expression tag	UNP P12319

- Molecule 4 is a protein called High affinity immunoglobulin epsilon receptor subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	157	Total	C	H	N	O	0	0
			1068	456	298	157	157		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-78	MET	-	initiating methionine	UNP Q01362
B	-77	GLY	-	expression tag	UNP Q01362
B	-76	ALA	-	expression tag	UNP Q01362
B	-75	SER	-	expression tag	UNP Q01362
B	-74	SER	-	expression tag	UNP Q01362
B	-73	ALA	-	expression tag	UNP Q01362
B	-72	TRP	-	expression tag	UNP Q01362
B	-71	SER	-	expression tag	UNP Q01362

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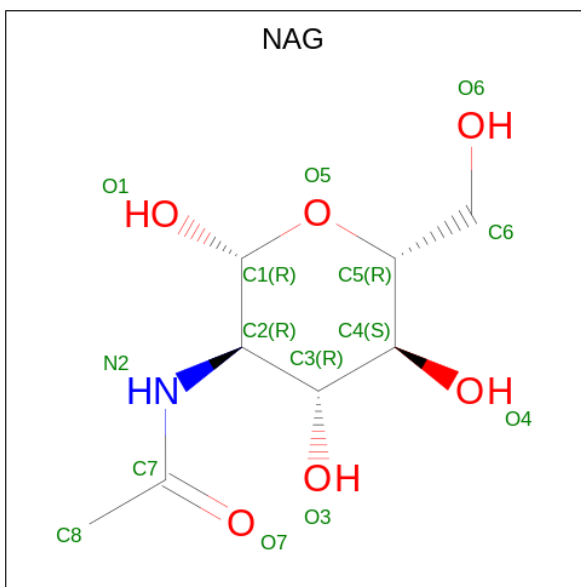
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-70	HIS	-	expression tag	UNP Q01362
B	-69	PRO	-	expression tag	UNP Q01362
B	-68	GLN	-	expression tag	UNP Q01362
B	-67	PHE	-	expression tag	UNP Q01362
B	-66	GLU	-	expression tag	UNP Q01362
B	-65	LYS	-	expression tag	UNP Q01362
B	-64	GLY	-	expression tag	UNP Q01362
B	-63	GLY	-	expression tag	UNP Q01362
B	-62	GLY	-	expression tag	UNP Q01362
B	-61	SER	-	expression tag	UNP Q01362
B	-60	GLY	-	expression tag	UNP Q01362
B	-59	GLY	-	expression tag	UNP Q01362
B	-58	GLY	-	expression tag	UNP Q01362
B	-57	SER	-	expression tag	UNP Q01362
B	-56	GLY	-	expression tag	UNP Q01362
B	-55	GLY	-	expression tag	UNP Q01362
B	-54	SER	-	expression tag	UNP Q01362
B	-53	ALA	-	expression tag	UNP Q01362
B	-52	TRP	-	expression tag	UNP Q01362
B	-51	SER	-	expression tag	UNP Q01362
B	-50	HIS	-	expression tag	UNP Q01362
B	-49	PRO	-	expression tag	UNP Q01362
B	-48	GLN	-	expression tag	UNP Q01362
B	-47	PHE	-	expression tag	UNP Q01362
B	-46	GLU	-	expression tag	UNP Q01362
B	-45	LYS	-	expression tag	UNP Q01362
B	-44	GLY	-	expression tag	UNP Q01362
B	-43	SER	-	expression tag	UNP Q01362
B	-42	ALA	-	expression tag	UNP Q01362
B	-41	ALA	-	expression tag	UNP Q01362
B	-40	ALA	-	expression tag	UNP Q01362

- Molecule 5 is a protein called High affinity immunoglobulin epsilon receptor subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	32	Total	C	H	N	O	0	0
			221	95	62	32	32		
5	C	32	Total	C	H	N	O	0	0
			221	95	62	32	32		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

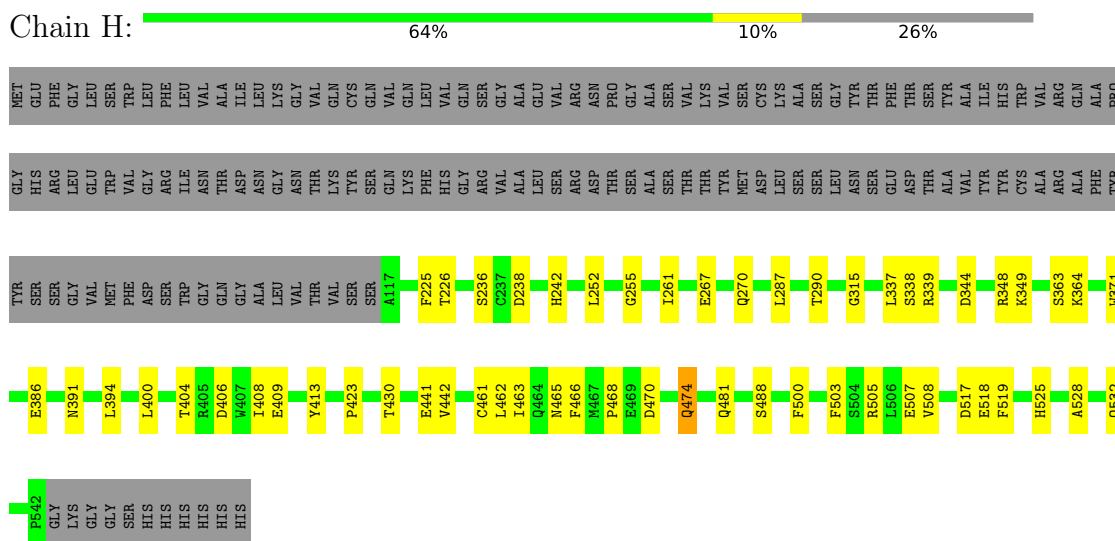


Mol	Chain	Residues	Atoms				AltConf
6	H	1	Total	C	N	O	0
			14	8	1	5	
6	X	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	

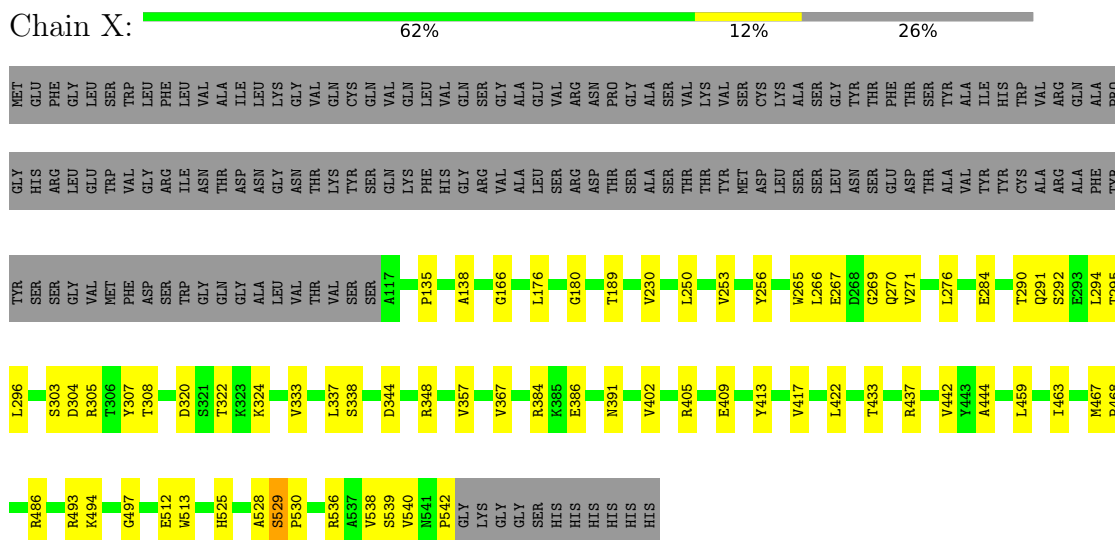
3 Residue-property plots

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: Immunoglobulin heavy constant epsilon

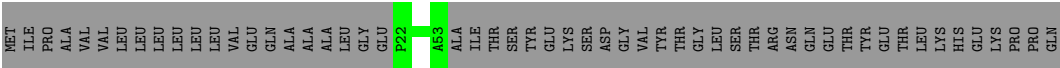


- Molecule 1: Immunoglobulin heavy constant epsilon

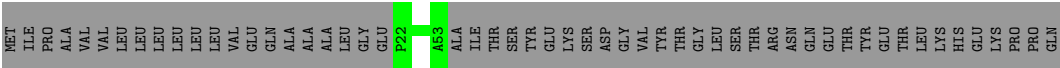


- Molecule 2: Immunoglobulin kappa constant





- Molecule 5: High affinity immunoglobulin epsilon receptor subunit gamma



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	920752	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)	-1200	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (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: NAG

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	H	0.26	0/3090	0.52	0/4227
1	X	0.27	0/3081	0.52	0/4217
2	h	0.26	0/520	0.47	0/724
2	x	0.26	0/520	0.45	0/724
3	A	0.39	1/1611 (0.1%)	0.50	0/2198
4	B	0.26	0/769	0.45	0/1066
5	C	0.22	0/158	0.33	0/219
5	D	0.22	0/158	0.32	0/219
All	All	0.29	1/9907 (0.0%)	0.50	0/13594

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	29	LYS	N-CA	5.68	1.57	1.46

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	H	3028	2551	2679	39	0
1	X	3019	2546	2667	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	h	518	0	237	0	0
2	x	518	0	237	0	0
3	A	1571	1232	1382	66	0
4	B	770	298	360	5	0
5	C	159	62	70	0	0
5	D	159	62	70	0	0
6	A	98	0	91	13	0
6	H	14	0	13	2	0
6	X	14	0	13	2	0
All	All	9868	6751	7819	157	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 10.

The worst 5 of 157 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)
3:A:46:ASN:HD21	6:A:305:NAG:C1	1.50	1.23
3:A:99:ASN:HD21	6:A:306:NAG:C1	1.60	1.15
3:A:75:ASN:ND2	6:A:301:NAG:C1	2.20	1.05
3:A:27:PRO:HB2	3:A:98:VAL:HG21	1.39	1.03
3:A:75:ASN:HD21	6:A:301:NAG:C1	1.73	1.01

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	H	424/577 (74%)	398 (94%)	26 (6%)	0	100	100
1	X	424/577 (74%)	406 (96%)	17 (4%)	1 (0%)	44	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	h	103/261 (40%)	99 (96%)	4 (4%)	0	100	100
2	x	103/261 (40%)	99 (96%)	3 (3%)	1 (1%)	13	40
3	A	201/267 (75%)	172 (86%)	28 (14%)	1 (0%)	25	55
4	B	155/283 (55%)	148 (96%)	7 (4%)	0	100	100
5	C	30/86 (35%)	30 (100%)	0	0	100	100
5	D	30/86 (35%)	29 (97%)	1 (3%)	0	100	100
All	All	1470/2398 (61%)	1381 (94%)	86 (6%)	3 (0%)	45	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	x	145	TYR
3	A	29	LYS
1	X	529	SER

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	H	285/500 (57%)	284 (100%)	1 (0%)	89	94
1	X	282/500 (56%)	282 (100%)	0	100	100
3	A	156/242 (64%)	156 (100%)	0	100	100
All	All	723/1242 (58%)	722 (100%)	1 (0%)	92	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	474	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	160	ASN
3	A	191	ASN
3	A	46	ASN
3	A	67	ASN
3	A	75	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 ⓘ

9 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	$\# Z > 2$
6	NAG	A	302	-	14,14,15	0.23	0	17,19,21	0.45	0
6	NAG	A	303	-	14,14,15	0.30	0	17,19,21	0.38	0
6	NAG	X	601	-	14,14,15	0.47	0	17,19,21	0.80	1 (5%)
6	NAG	A	306	-	14,14,15	0.26	0	17,19,21	0.40	0
6	NAG	H	601	-	14,14,15	0.29	0	17,19,21	0.62	0
6	NAG	A	304	-	14,14,15	0.26	0	17,19,21	0.36	0
6	NAG	A	307	-	14,14,15	0.20	0	17,19,21	0.58	0
6	NAG	A	305	-	14,14,15	0.17	0	17,19,21	0.45	0
6	NAG	A	301	-	14,14,15	0.19	0	17,19,21	0.40	0

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
6	NAG	A	302	-	-	2/6/23/26	0/1/1/1
6	NAG	A	303	-	-	2/6/23/26	0/1/1/1
6	NAG	X	601	-	-	3/6/23/26	0/1/1/1
6	NAG	A	306	-	-	1/6/23/26	0/1/1/1
6	NAG	H	601	-	-	3/6/23/26	0/1/1/1
6	NAG	A	304	-	-	2/6/23/26	0/1/1/1
6	NAG	A	307	-	-	0/6/23/26	0/1/1/1
6	NAG	A	305	-	-	2/6/23/26	0/1/1/1
6	NAG	A	301	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	601	NAG	C1-O5-C5	2.76	115.94	112.19

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	601	NAG	C8-C7-N2-C2
6	H	601	NAG	O7-C7-N2-C2
6	A	302	NAG	C3-C2-N2-C7
6	A	301	NAG	C4-C5-C6-O6
6	A	305	NAG	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 17 short contacts:

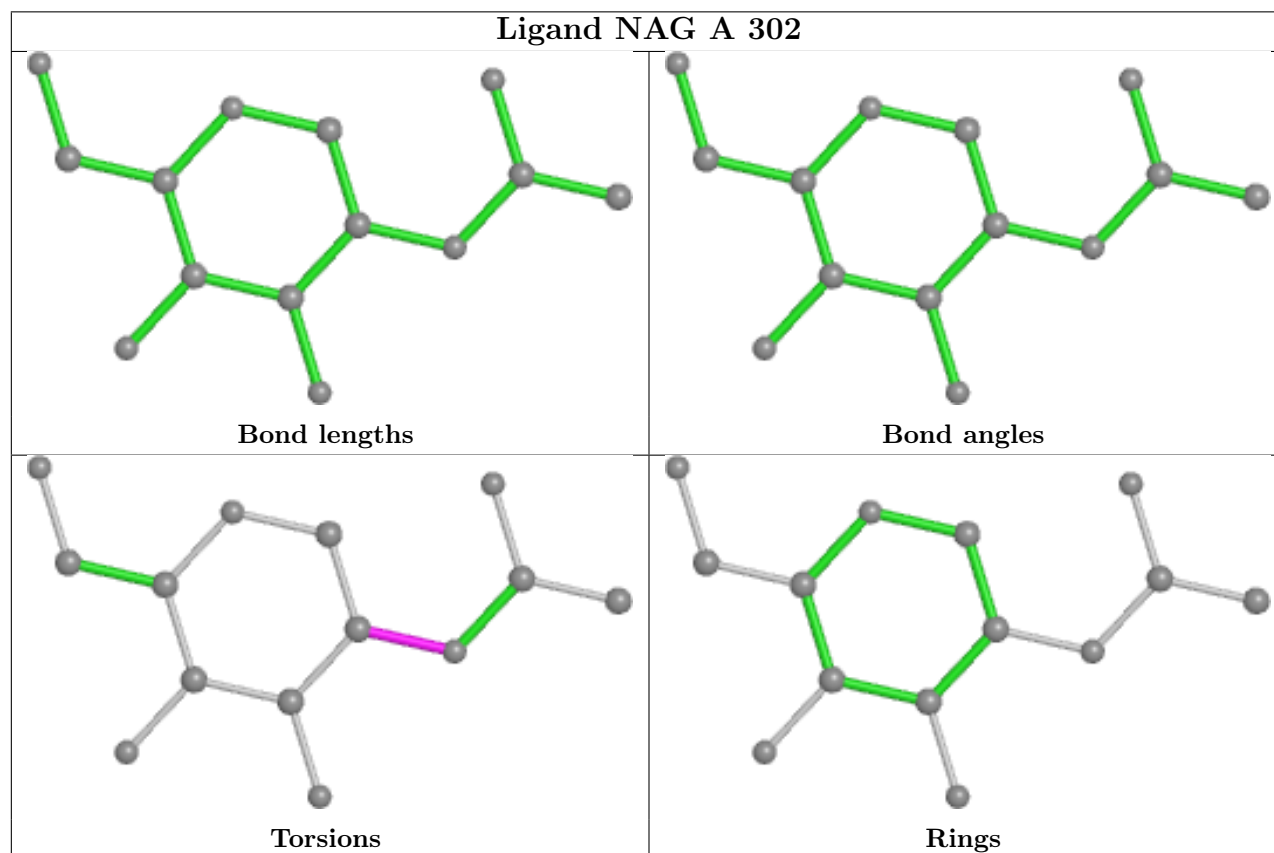
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	303	NAG	1	0
6	X	601	NAG	2	0
6	A	306	NAG	2	0
6	H	601	NAG	2	0
6	A	304	NAG	3	0

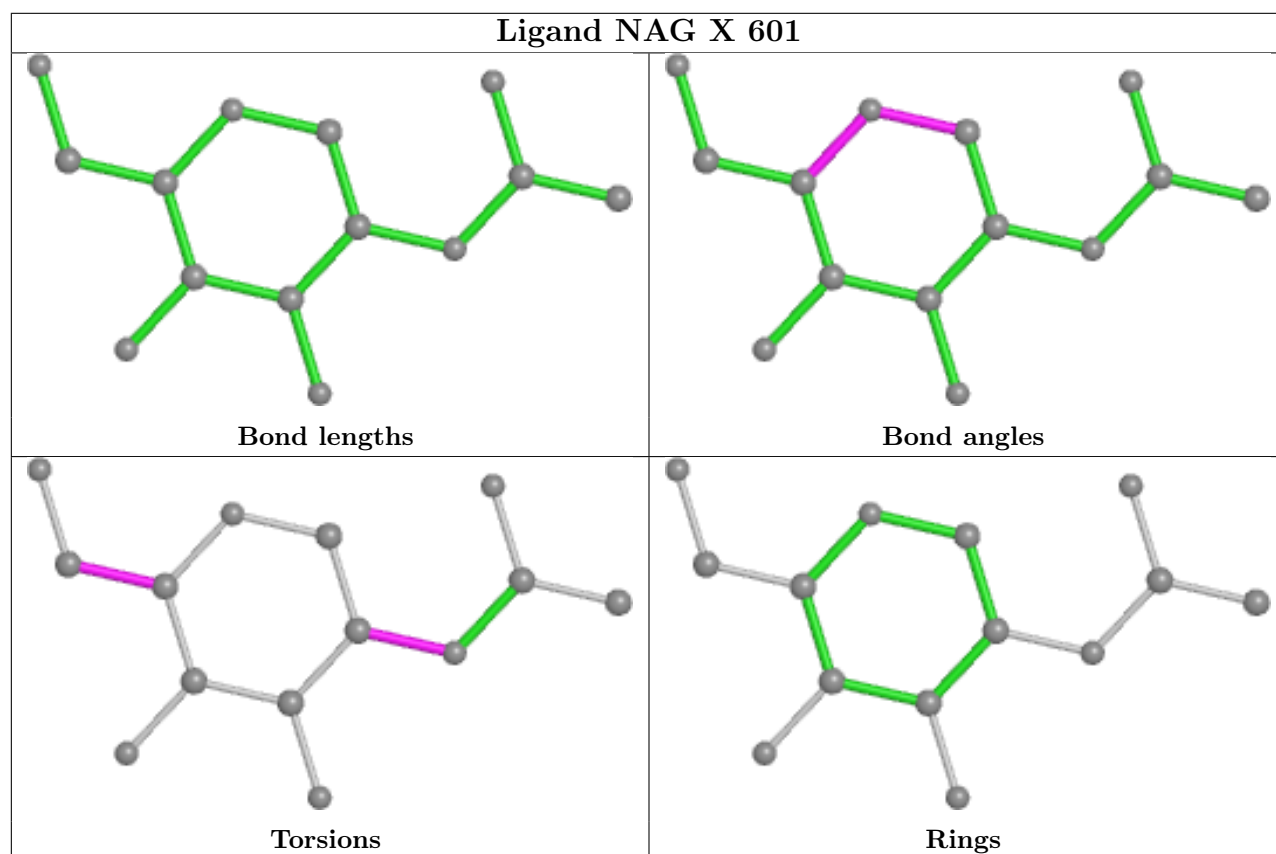
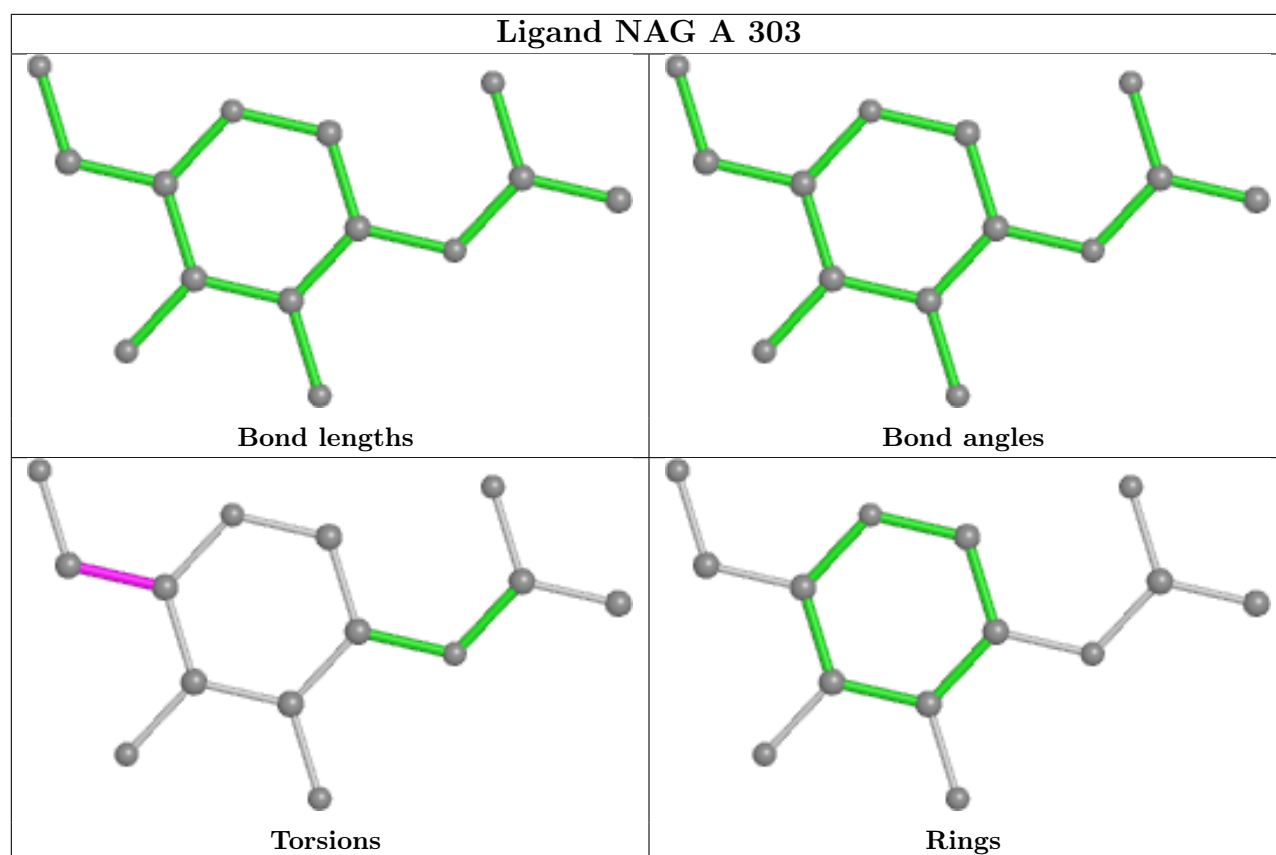
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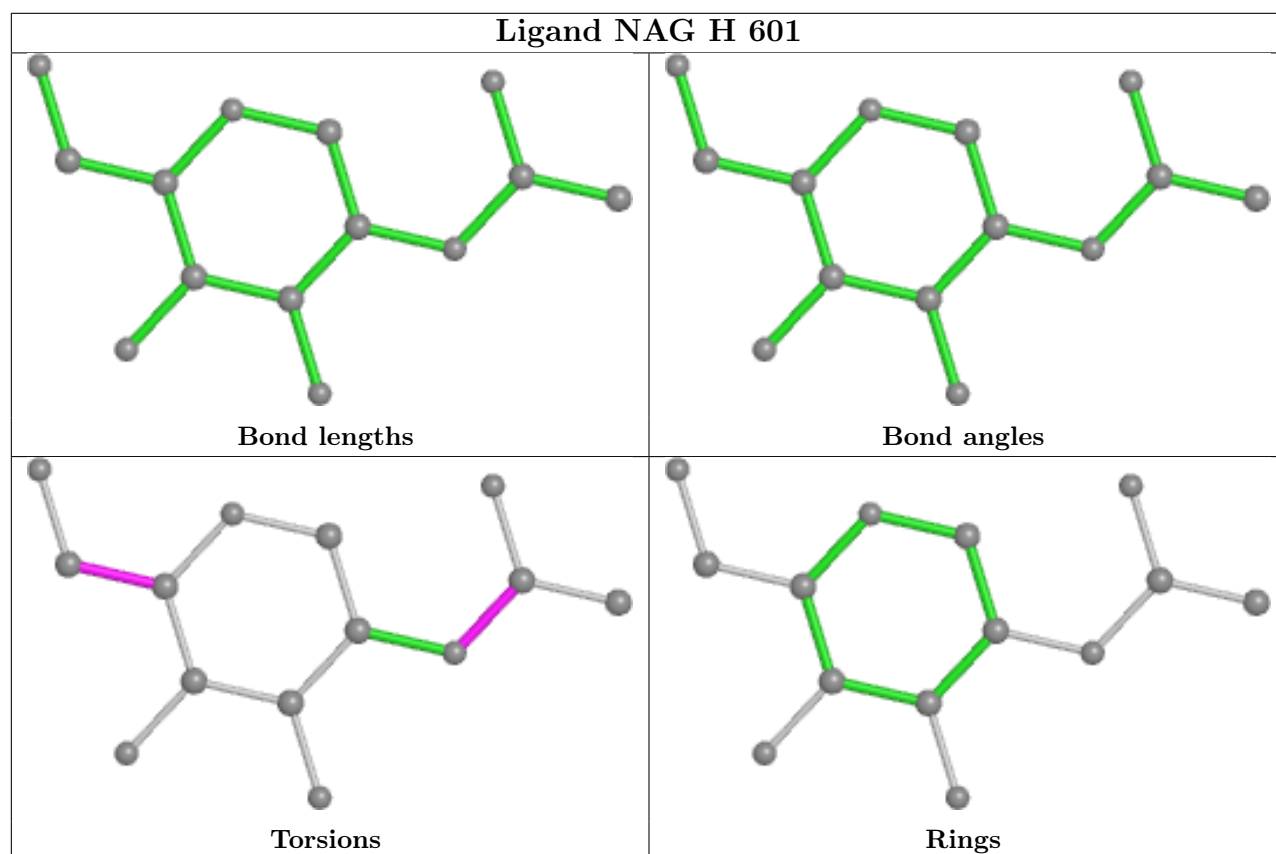
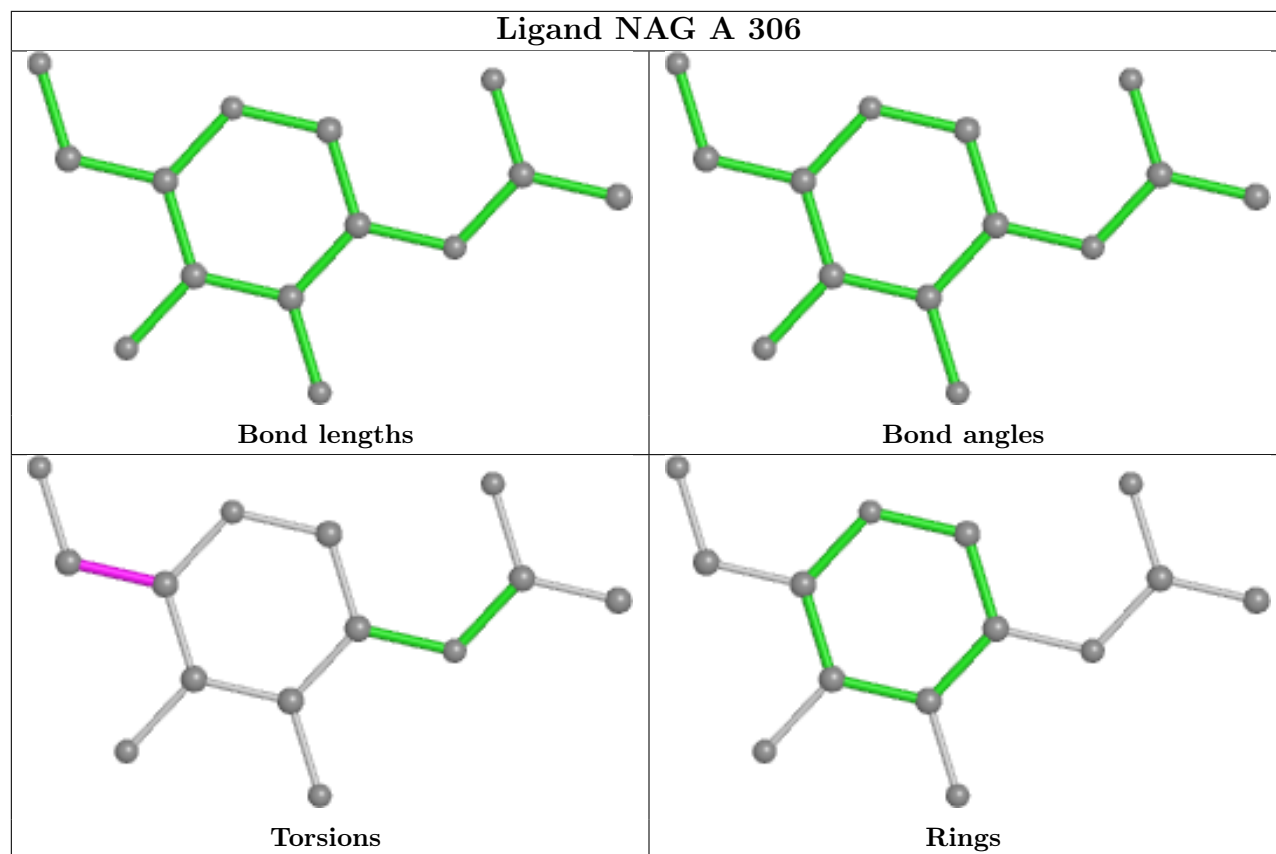
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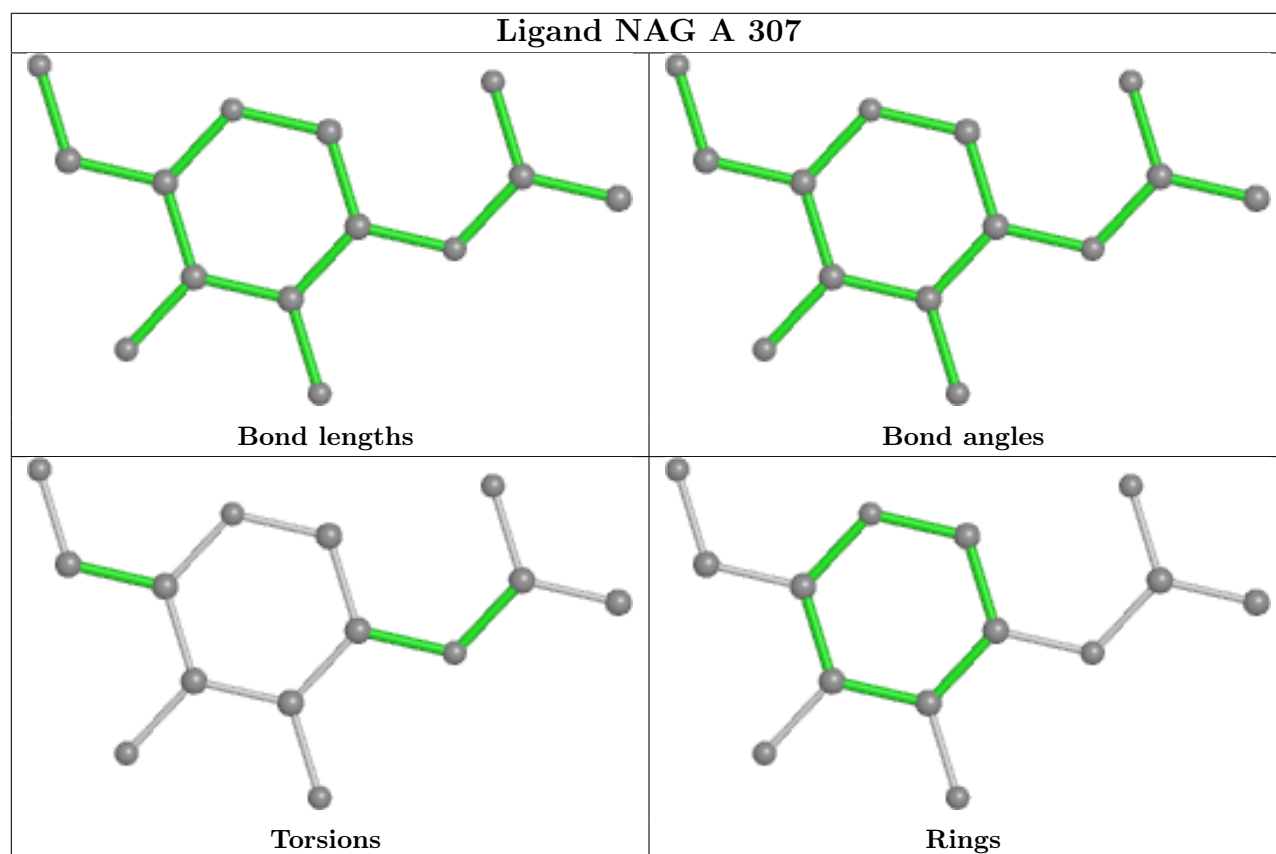
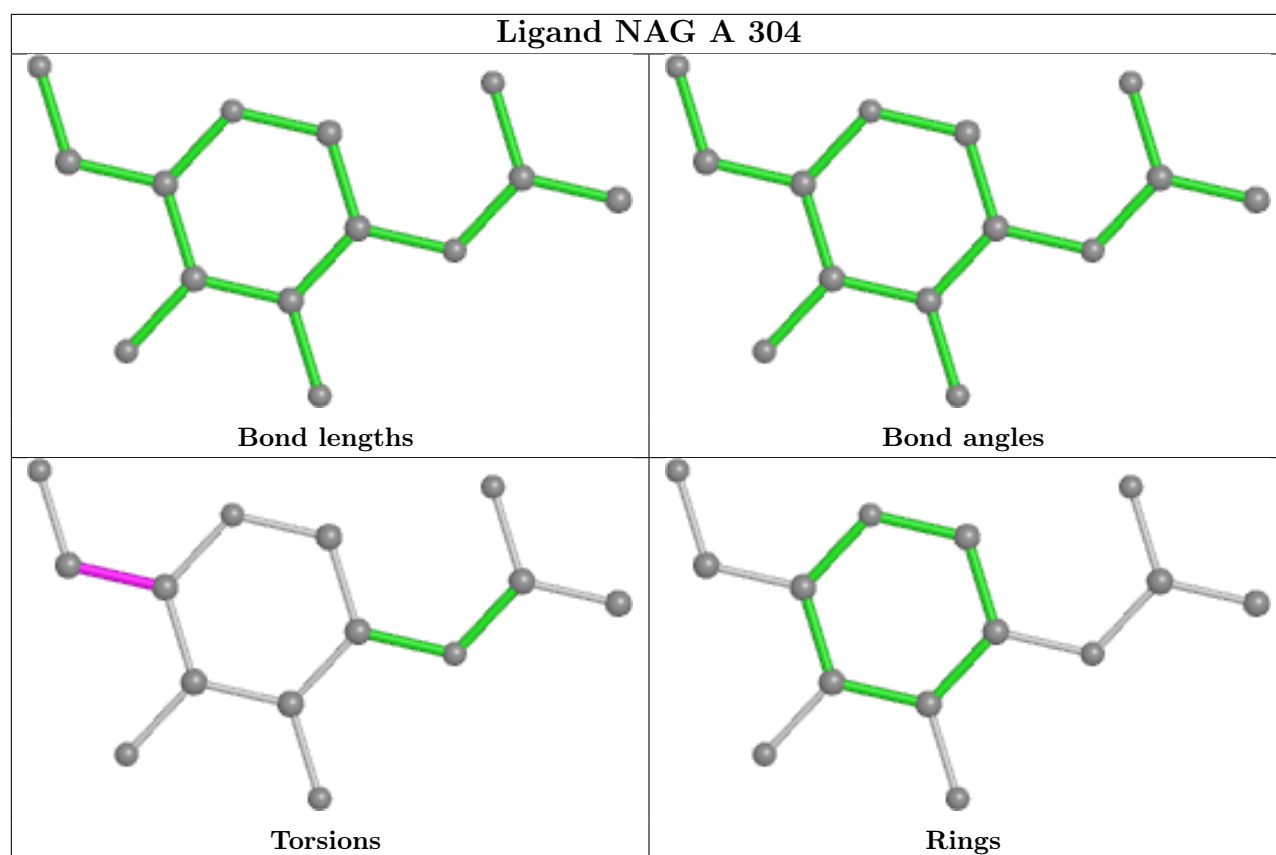
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	307	NAG	2	0
6	A	305	NAG	2	0
6	A	301	NAG	3	0

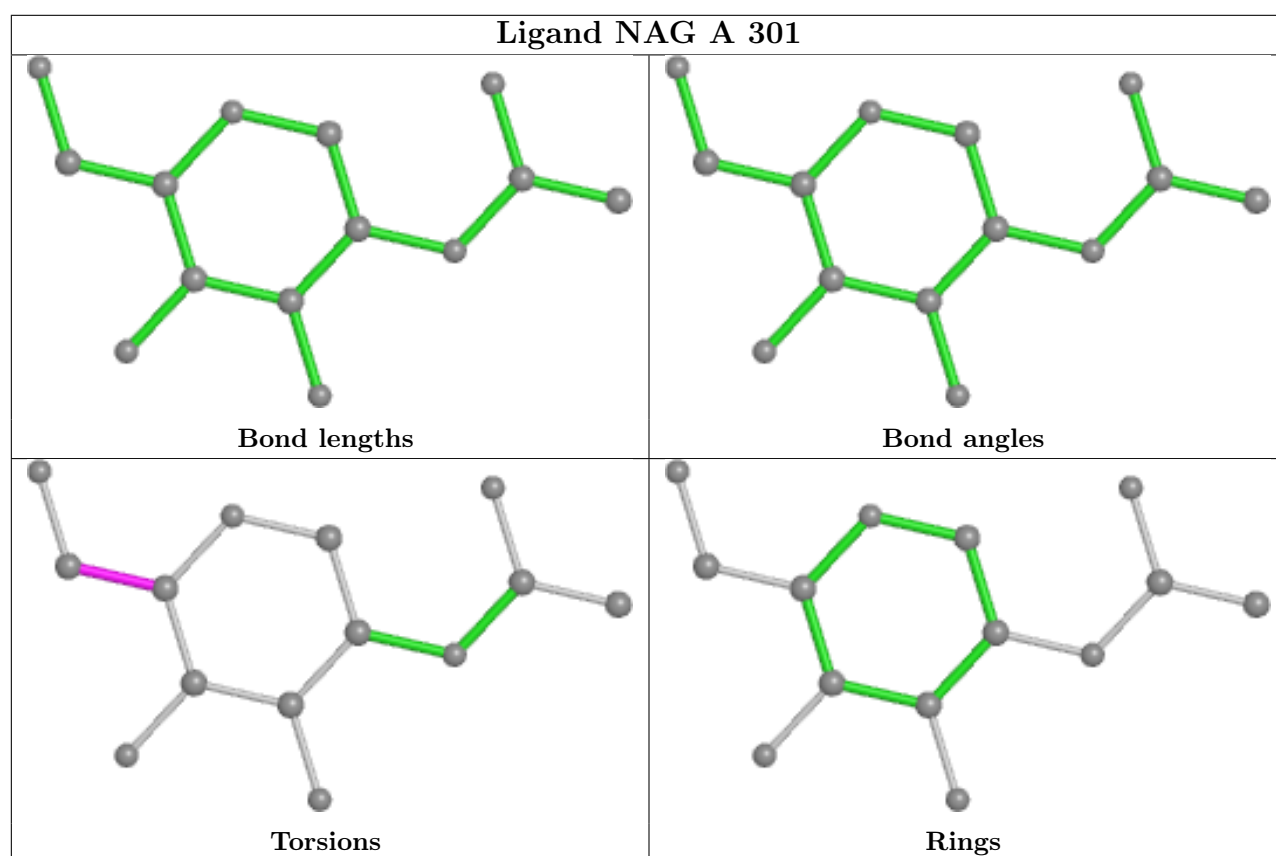
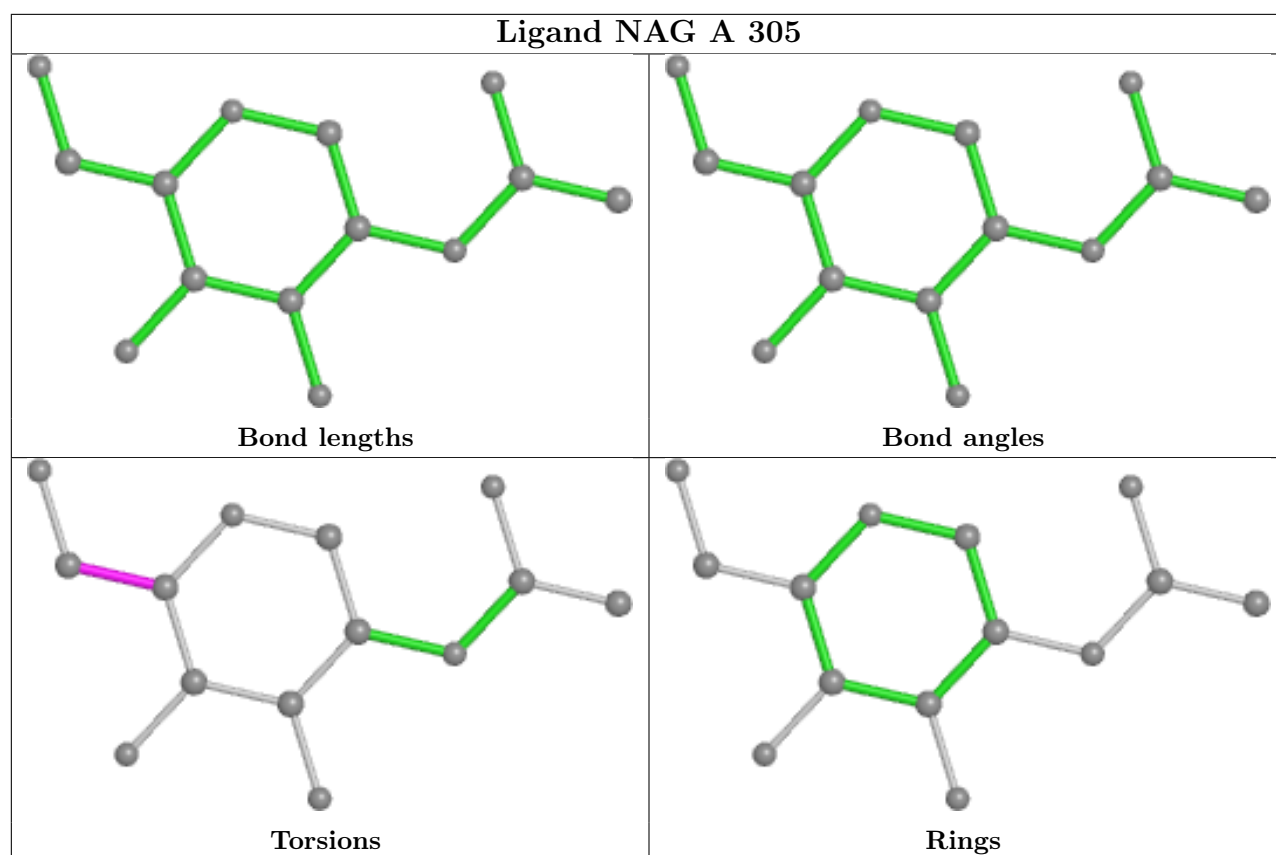
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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