



## wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 07:39 PM UTC

PDB ID : 6PLS / pdb\_00006pls  
EMDB ID : EMD-20374  
Title : CryoEM structure of zebra fish alpha-1 glycine receptor bound with taurine  
in nanodisc, desensitized state  
Authors : Yu, J.; Zhu, H.; Gouaux, E.  
Deposited on : 2019-07-01  
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>.

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
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

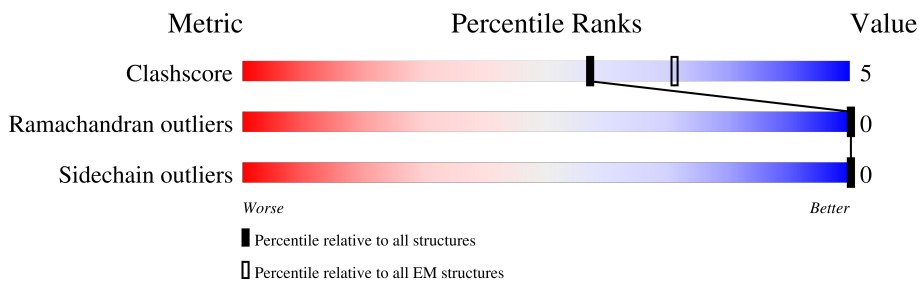
# 1 Overall quality at a glance i

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)
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  $\geq 3$ , 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	458	64% 11% 25%
1	B	458	65% 10% 25%
1	C	458	64% 11% 25%
1	D	458	64% 11% 25%
1	E	458	64% 11% 25%
2	F	2	50% 50%
2	G	2	50% 50%
2	H	2	50% 50%
2	I	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	J	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TAU	A	503	-	X	-	-
3	TAU	A	510	-	X	-	-
3	TAU	B	609	-	X	-	-
3	TAU	C	609	-	X	-	-
3	TAU	D	609	-	X	-	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 14610 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 Glycine receptor subunit alphaZ1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	344	2761	1802	446	493	20	0	0
1	B	344	2761	1802	446	493	20	0	0
1	C	344	2761	1802	446	493	20	0	0
1	D	344	2761	1802	446	493	20	0	0
1	E	344	2761	1802	446	493	20	0	0

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	437	LEU	-	expression tag	UNP O93430
A	438	VAL	-	expression tag	UNP O93430
A	439	PRO	-	expression tag	UNP O93430
A	440	ARG	-	expression tag	UNP O93430
A	441	GLY	-	expression tag	UNP O93430
A	442	SER	-	expression tag	UNP O93430
A	443	HIS	-	expression tag	UNP O93430
A	444	HIS	-	expression tag	UNP O93430
A	445	HIS	-	expression tag	UNP O93430
A	446	HIS	-	expression tag	UNP O93430
A	447	HIS	-	expression tag	UNP O93430
A	448	HIS	-	expression tag	UNP O93430
A	449	HIS	-	expression tag	UNP O93430
A	450	HIS	-	expression tag	UNP O93430
B	437	LEU	-	expression tag	UNP O93430
B	438	VAL	-	expression tag	UNP O93430
B	439	PRO	-	expression tag	UNP O93430
B	440	ARG	-	expression tag	UNP O93430
B	441	GLY	-	expression tag	UNP O93430
B	442	SER	-	expression tag	UNP O93430

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Chain	Residue	Modelled	Actual	Comment	Reference
B	443	HIS	-	expression tag	UNP O93430
B	444	HIS	-	expression tag	UNP O93430
B	445	HIS	-	expression tag	UNP O93430
B	446	HIS	-	expression tag	UNP O93430
B	447	HIS	-	expression tag	UNP O93430
B	448	HIS	-	expression tag	UNP O93430
B	449	HIS	-	expression tag	UNP O93430
B	450	HIS	-	expression tag	UNP O93430
C	437	LEU	-	expression tag	UNP O93430
C	438	VAL	-	expression tag	UNP O93430
C	439	PRO	-	expression tag	UNP O93430
C	440	ARG	-	expression tag	UNP O93430
C	441	GLY	-	expression tag	UNP O93430
C	442	SER	-	expression tag	UNP O93430
C	443	HIS	-	expression tag	UNP O93430
C	444	HIS	-	expression tag	UNP O93430
C	445	HIS	-	expression tag	UNP O93430
C	446	HIS	-	expression tag	UNP O93430
C	447	HIS	-	expression tag	UNP O93430
C	448	HIS	-	expression tag	UNP O93430
C	449	HIS	-	expression tag	UNP O93430
C	450	HIS	-	expression tag	UNP O93430
D	437	LEU	-	expression tag	UNP O93430
D	438	VAL	-	expression tag	UNP O93430
D	439	PRO	-	expression tag	UNP O93430
D	440	ARG	-	expression tag	UNP O93430
D	441	GLY	-	expression tag	UNP O93430
D	442	SER	-	expression tag	UNP O93430
D	443	HIS	-	expression tag	UNP O93430
D	444	HIS	-	expression tag	UNP O93430
D	445	HIS	-	expression tag	UNP O93430
D	446	HIS	-	expression tag	UNP O93430
D	447	HIS	-	expression tag	UNP O93430
D	448	HIS	-	expression tag	UNP O93430
D	449	HIS	-	expression tag	UNP O93430
D	450	HIS	-	expression tag	UNP O93430
E	437	LEU	-	expression tag	UNP O93430
E	438	VAL	-	expression tag	UNP O93430
E	439	PRO	-	expression tag	UNP O93430
E	440	ARG	-	expression tag	UNP O93430
E	441	GLY	-	expression tag	UNP O93430
E	442	SER	-	expression tag	UNP O93430

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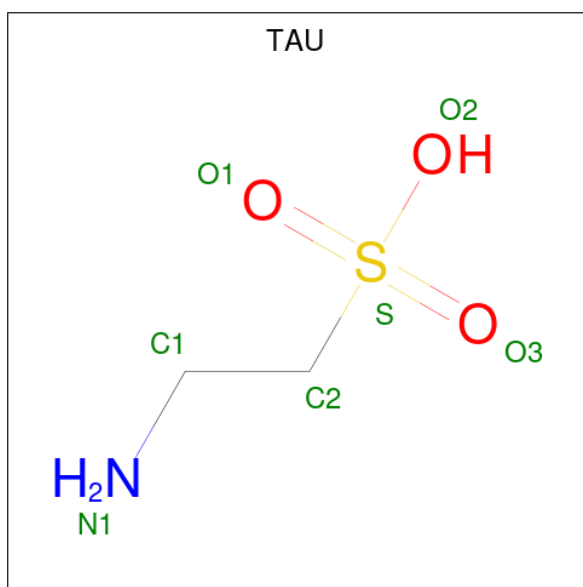
Chain	Residue	Modelled	Actual	Comment	Reference
E	443	HIS	-	expression tag	UNP O93430
E	444	HIS	-	expression tag	UNP O93430
E	445	HIS	-	expression tag	UNP O93430
E	446	HIS	-	expression tag	UNP O93430
E	447	HIS	-	expression tag	UNP O93430
E	448	HIS	-	expression tag	UNP O93430
E	449	HIS	-	expression tag	UNP O93430
E	450	HIS	-	expression tag	UNP O93430

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	F	2	28	16	2	10	0	0
2	G	2	28	16	2	10	0	0
2	H	2	28	16	2	10	0	0
2	I	2	28	16	2	10	0	0
2	J	2	28	16	2	10	0	0

- Molecule 3 is 2-AMINOETHANESULFONIC ACID (CCD ID: TAU) (formula: C<sub>2</sub>H<sub>7</sub>NO<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
3	A	1	7	2	1	3	1	0
3	A	1	7	2	1	3	1	0
3	B	1	7	2	1	3	1	0
3	C	1	7	2	1	3	1	0
3	D	1	7	2	1	3	1	0


- Molecule 4 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ).

Mol	Chain	Residues	Atoms		AltConf
			Total	C	
4	A	12	126	126	0
4	B	12	126	126	0
4	C	12	126	126	0
4	D	12	126	126	0
4	E	12	126	126	0






- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

MAG1  
MAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

MAG1  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	79709	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	61	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k 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, TAU, UNL

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	0.30	0/2830	0.53	2/3843 (0.1%)
1	B	0.30	0/2830	0.54	2/3843 (0.1%)
1	C	0.30	0/2830	0.54	2/3843 (0.1%)
1	D	0.30	0/2830	0.53	2/3843 (0.1%)
1	E	0.30	0/2830	0.53	2/3843 (0.1%)
All	All	0.30	0/14150	0.54	10/19215 (0.1%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	127	VAL	CA-C-N	6.81	134.54	121.54
1	B	127	VAL	C-N-CA	6.81	134.54	121.54
1	D	127	VAL	CA-C-N	6.80	134.53	121.54
1	D	127	VAL	C-N-CA	6.80	134.53	121.54
1	A	127	VAL	CA-C-N	6.79	134.51	121.54

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	2761	0	2755	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2761	0	2755	32	0
1	C	2761	0	2755	36	0
1	D	2761	0	2755	34	0
1	E	2761	0	2755	35	0
2	F	28	0	25	1	0
2	G	28	0	25	1	0
2	H	28	0	25	1	0
2	I	28	0	25	1	0
2	J	28	0	25	1	0
3	A	14	0	14	0	0
3	B	7	0	7	0	0
3	C	7	0	7	0	0
3	D	7	0	7	0	0
4	A	126	0	0	0	0
4	B	126	0	0	0	0
4	C	126	0	0	0	0
4	D	126	0	0	0	0
4	E	126	0	0	0	0
All	All	14610	0	13935	138	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.

The worst 5 of 138 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:D:235:GLN:HB3	1:E:294:SER:HB3	1.84	0.60
1:A:114:LEU:HD11	1:A:172:LEU:HD23	1.85	0.59
1:B:210:ASP:HB2	1:B:229:ARG:HB2	1.85	0.59
1:C:210:ASP:HB2	1:C:229:ARG:HB2	1.85	0.58
1:B:114:LEU:HD11	1:B:172:LEU:HD23	1.85	0.58

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	340/458 (74%)	331 (97%)	9 (3%)	0	100	100
1	B	340/458 (74%)	331 (97%)	9 (3%)	0	100	100
1	C	340/458 (74%)	331 (97%)	9 (3%)	0	100	100
1	D	340/458 (74%)	331 (97%)	9 (3%)	0	100	100
1	E	340/458 (74%)	331 (97%)	9 (3%)	0	100	100
All	All	1700/2290 (74%)	1655 (97%)	45 (3%)	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	303/400 (76%)	303 (100%)	0	100	100
1	B	303/400 (76%)	303 (100%)	0	100	100
1	C	303/400 (76%)	303 (100%)	0	100	100
1	D	303/400 (76%)	303 (100%)	0	100	100
1	E	303/400 (76%)	303 (100%)	0	100	100
All	All	1515/2000 (76%)	1515 (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. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	231	HIS
1	E	231	HIS
1	E	83	GLN
1	C	85	ASN
1	D	131	ASN

### 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](#)

10 monosaccharides 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
2	NAG	F	1	2,1	14,14,15	1.83	5 (35%)	17,19,21	1.83	6 (35%)
2	NAG	F	2	2	14,14,15	2.00	4 (28%)	17,19,21	1.34	3 (17%)
2	NAG	G	1	2,1	14,14,15	1.83	5 (35%)	17,19,21	1.83	6 (35%)
2	NAG	G	2	2	14,14,15	2.00	4 (28%)	17,19,21	1.33	3 (17%)
2	NAG	H	1	2,1	14,14,15	1.84	5 (35%)	17,19,21	1.83	6 (35%)
2	NAG	H	2	2	14,14,15	2.01	4 (28%)	17,19,21	1.33	3 (17%)
2	NAG	I	1	2,1	14,14,15	1.84	5 (35%)	17,19,21	1.83	6 (35%)
2	NAG	I	2	2	14,14,15	2.01	4 (28%)	17,19,21	1.33	3 (17%)
2	NAG	J	1	2,1	14,14,15	1.84	5 (35%)	17,19,21	1.83	6 (35%)
2	NAG	J	2	2	14,14,15	2.00	4 (28%)	17,19,21	1.34	3 (17%)

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
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	4/6/23/26	0/1/1/1

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	2	NAG	O5-C1	4.39	1.51	1.43
2	F	2	NAG	O5-C1	4.38	1.51	1.43
2	H	2	NAG	O5-C1	4.37	1.51	1.43
2	I	2	NAG	O5-C1	4.36	1.51	1.43
2	G	2	NAG	O5-C1	4.32	1.51	1.43

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	NAG	C2-N2-C7	-3.53	118.17	122.90
2	F	1	NAG	C2-N2-C7	-3.49	118.23	122.90
2	H	1	NAG	C2-N2-C7	-3.48	118.24	122.90
2	G	1	NAG	C2-N2-C7	-3.48	118.24	122.90
2	J	1	NAG	C2-N2-C7	-3.47	118.25	122.90

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

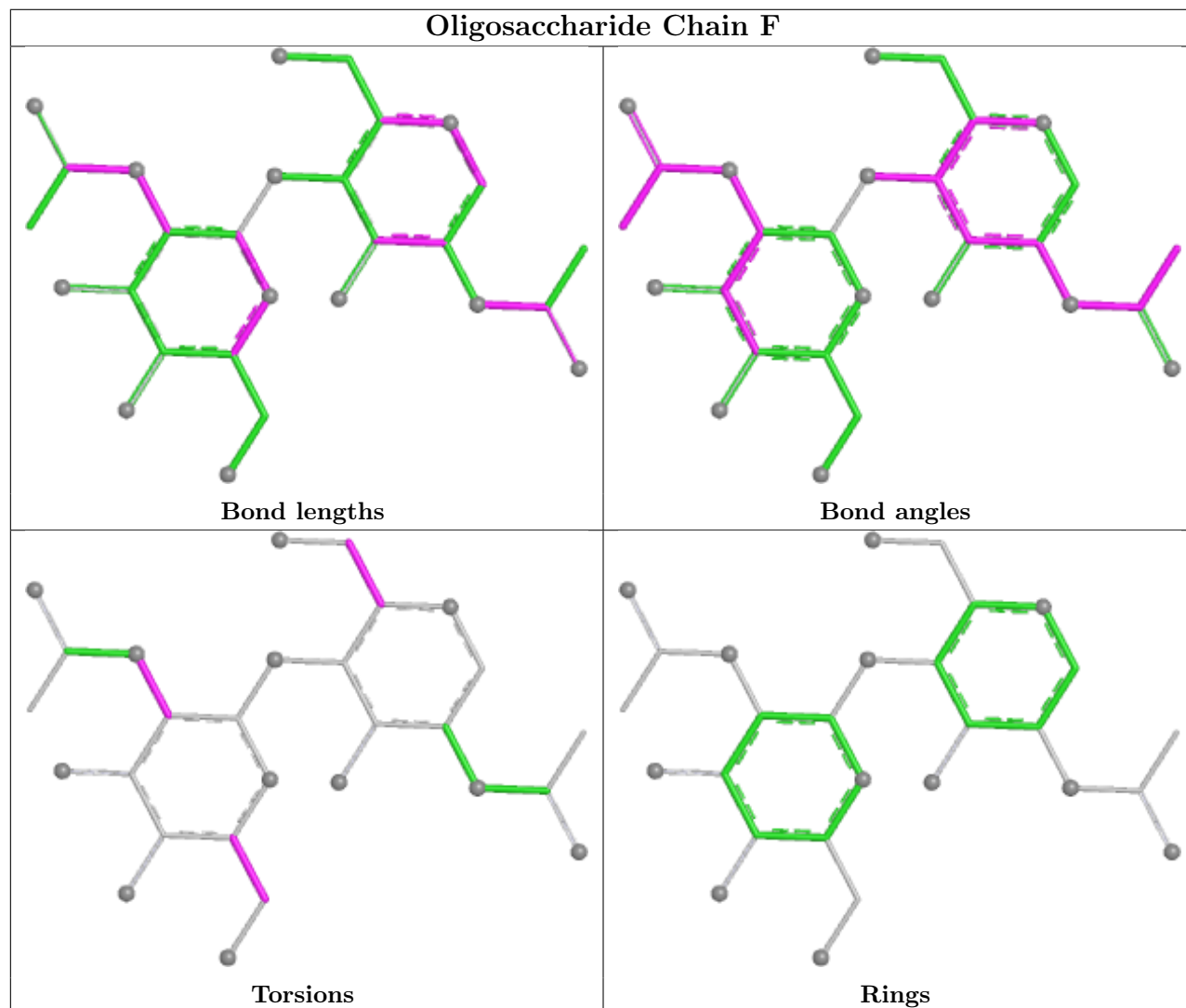
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6

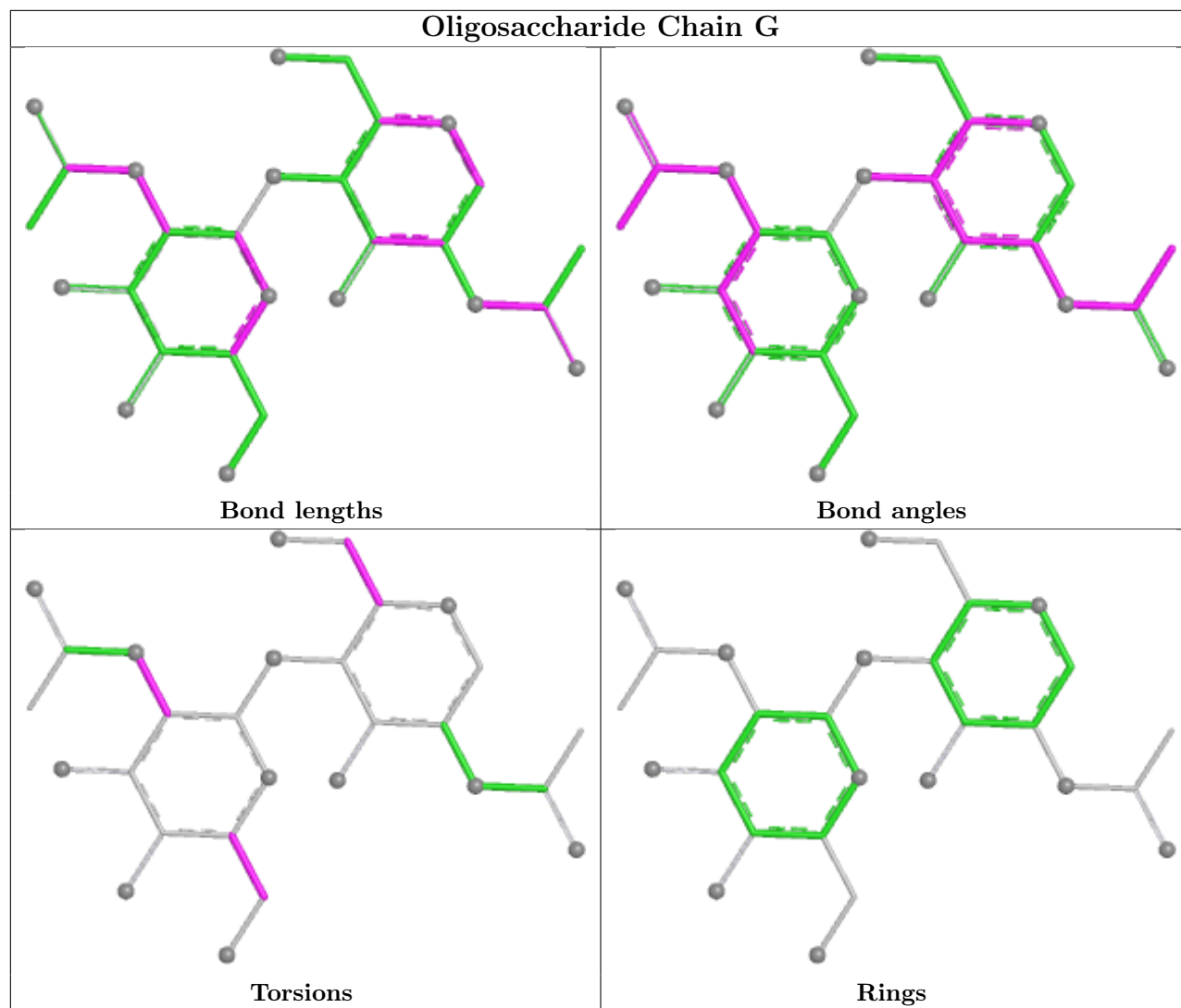
There are no ring outliers.

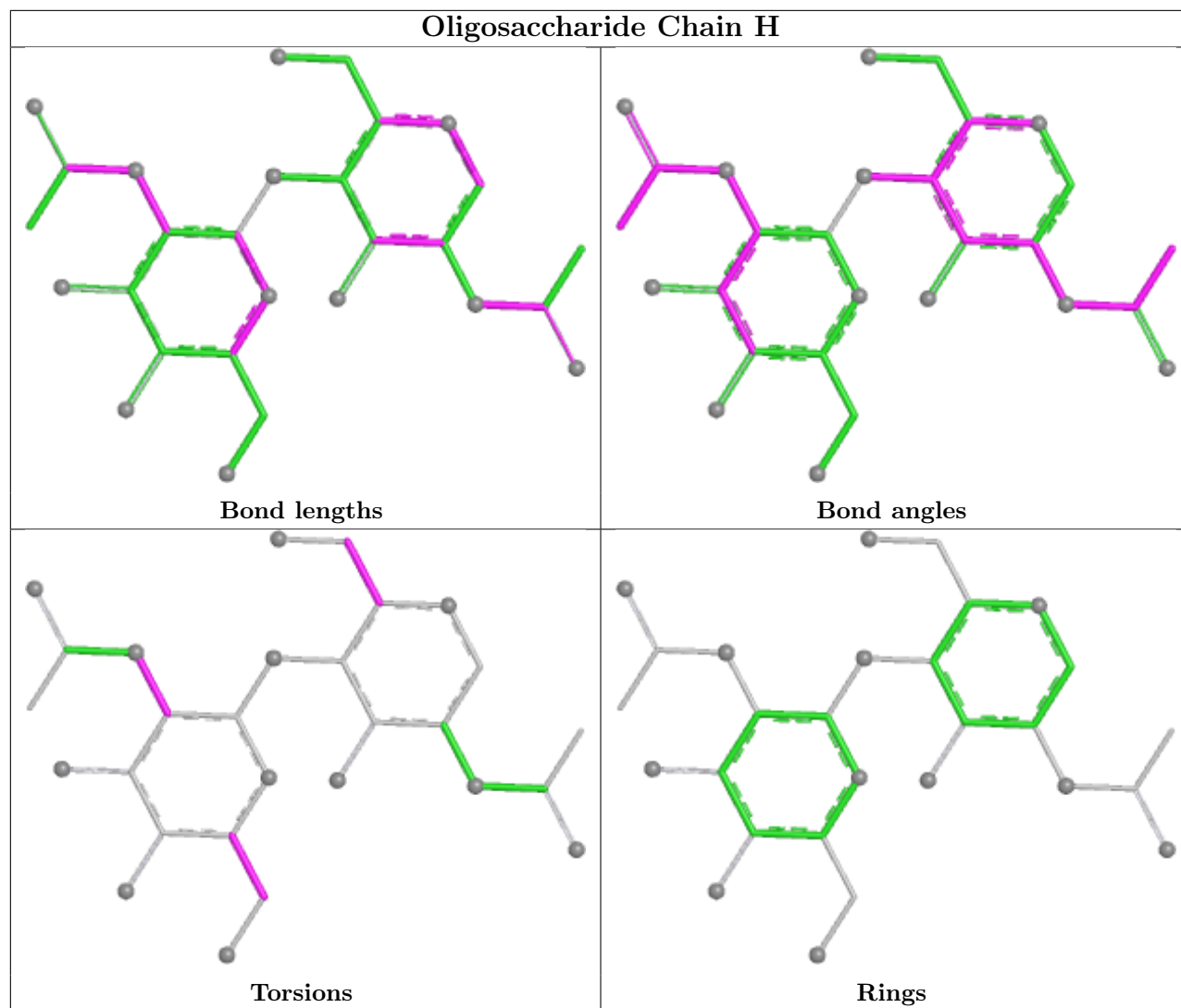
5 monomers are involved in 5 short contacts:

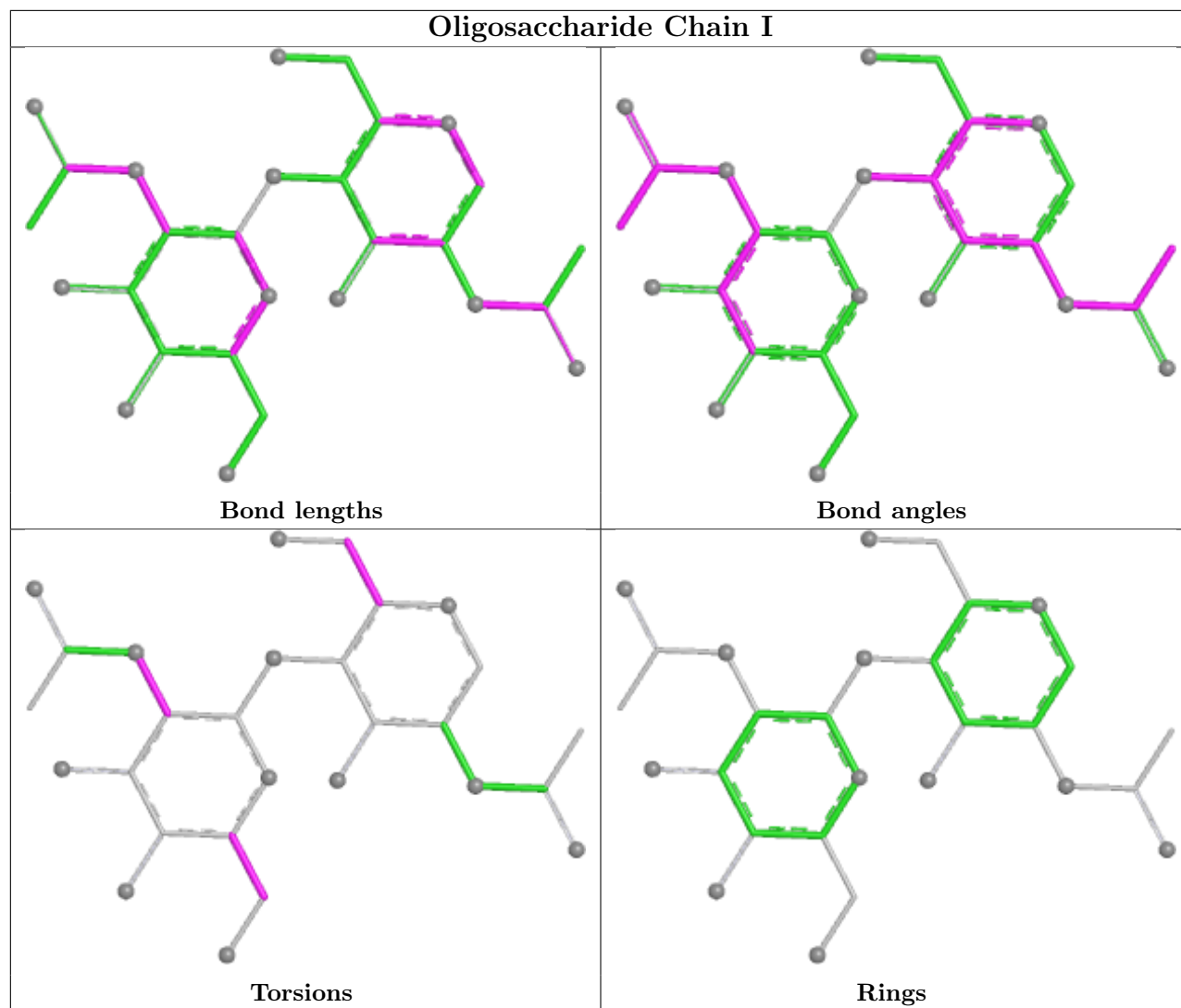
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	NAG	1	0
2	F	1	NAG	1	0
2	H	1	NAG	1	0
2	I	1	NAG	1	0
2	G	1	NAG	1	0

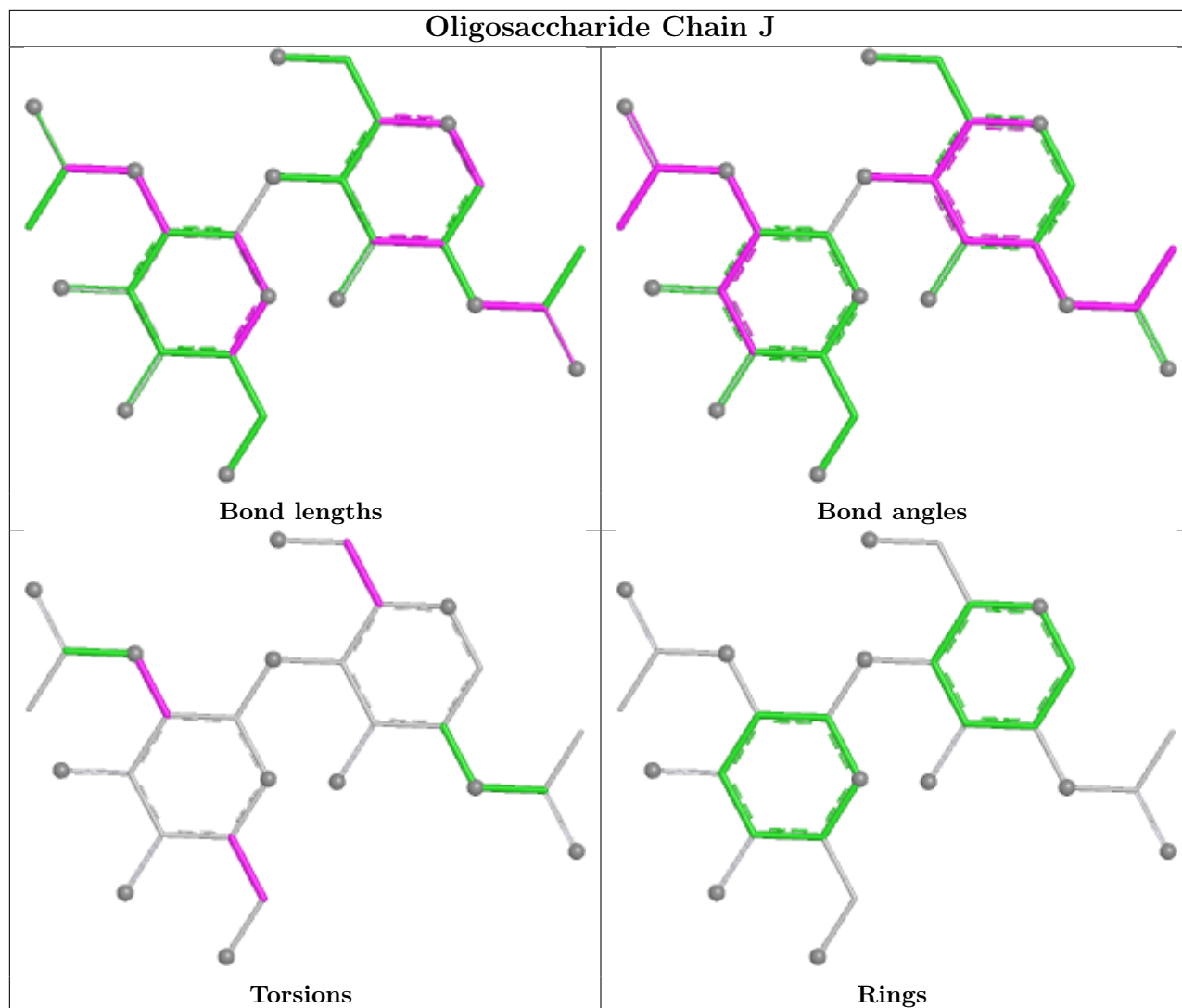
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 65 ligands modelled in this entry, 60 are unknown - leaving 5 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$
3	TAU	A	503	-	6,6,6	1.47	1 (16%)	7,8,8	2.65	4 (57%)
3	TAU	B	609	-	6,6,6	1.48	1 (16%)	7,8,8	2.65	4 (57%)
3	TAU	D	609	-	6,6,6	1.46	1 (16%)	7,8,8	2.64	4 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TAU	A	510	-	6,6,6	1.46	1 (16%)	7,8,8	2.66	4 (57%)
3	TAU	C	609	-	6,6,6	1.47	1 (16%)	7,8,8	2.66	4 (57%)

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	TAU	A	503	-	-	3/4/4/4	-
3	TAU	B	609	-	-	3/4/4/4	-
3	TAU	D	609	-	-	3/4/4/4	-
3	TAU	A	510	-	-	3/4/4/4	-
3	TAU	C	609	-	-	3/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	609	TAU	C2-S	2.39	1.80	1.77
3	A	503	TAU	C2-S	2.38	1.80	1.77
3	C	609	TAU	C2-S	2.36	1.80	1.77
3	D	609	TAU	C2-S	2.35	1.80	1.77
3	A	510	TAU	C2-S	2.33	1.80	1.77

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	510	TAU	O2-S-O3	-4.17	100.96	111.40
3	A	503	TAU	O2-S-O3	-4.17	100.98	111.40
3	C	609	TAU	O2-S-O3	-4.15	101.02	111.40
3	B	609	TAU	O2-S-O3	-4.15	101.03	111.40
3	D	609	TAU	O2-S-O3	-4.14	101.05	111.40

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	TAU	C1-C2-S-O2
3	A	510	TAU	C1-C2-S-O2
3	B	609	TAU	C1-C2-S-O2

*Continued on next page...*

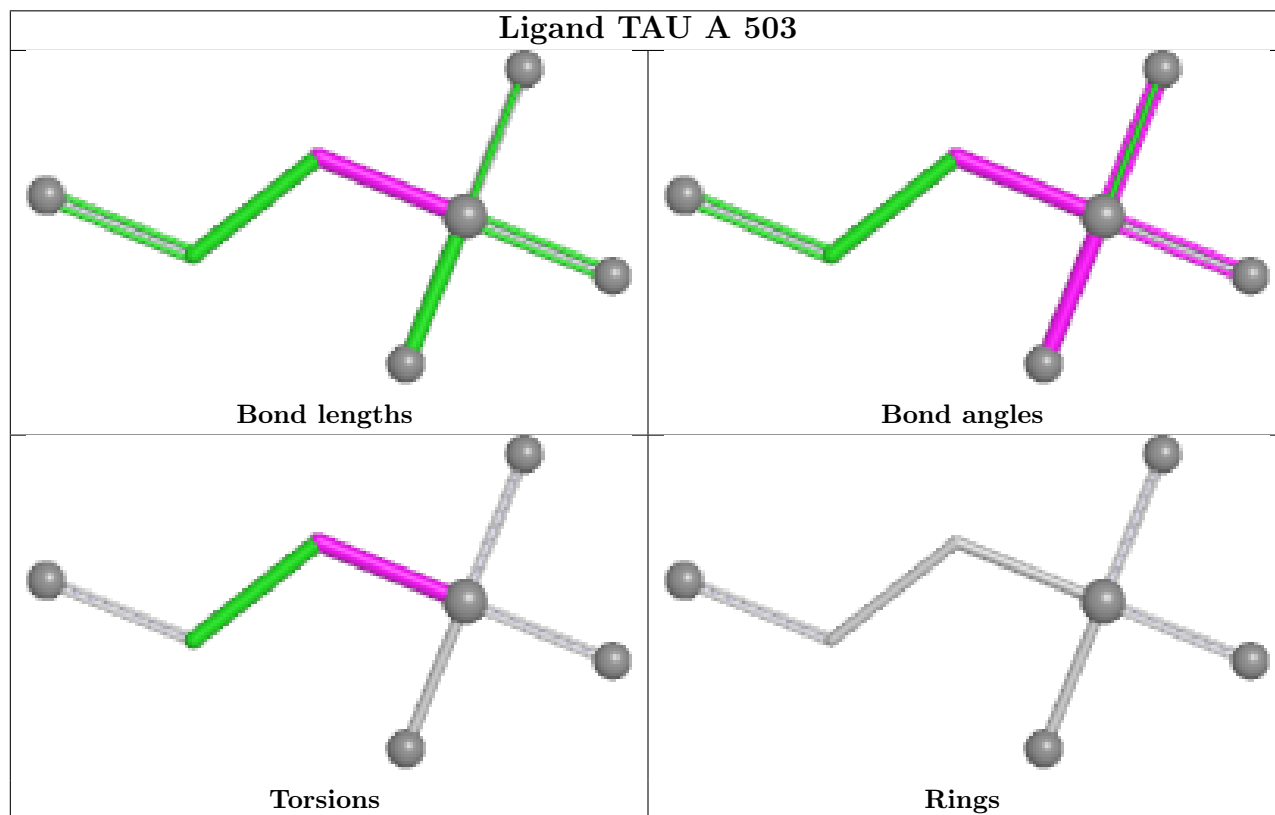
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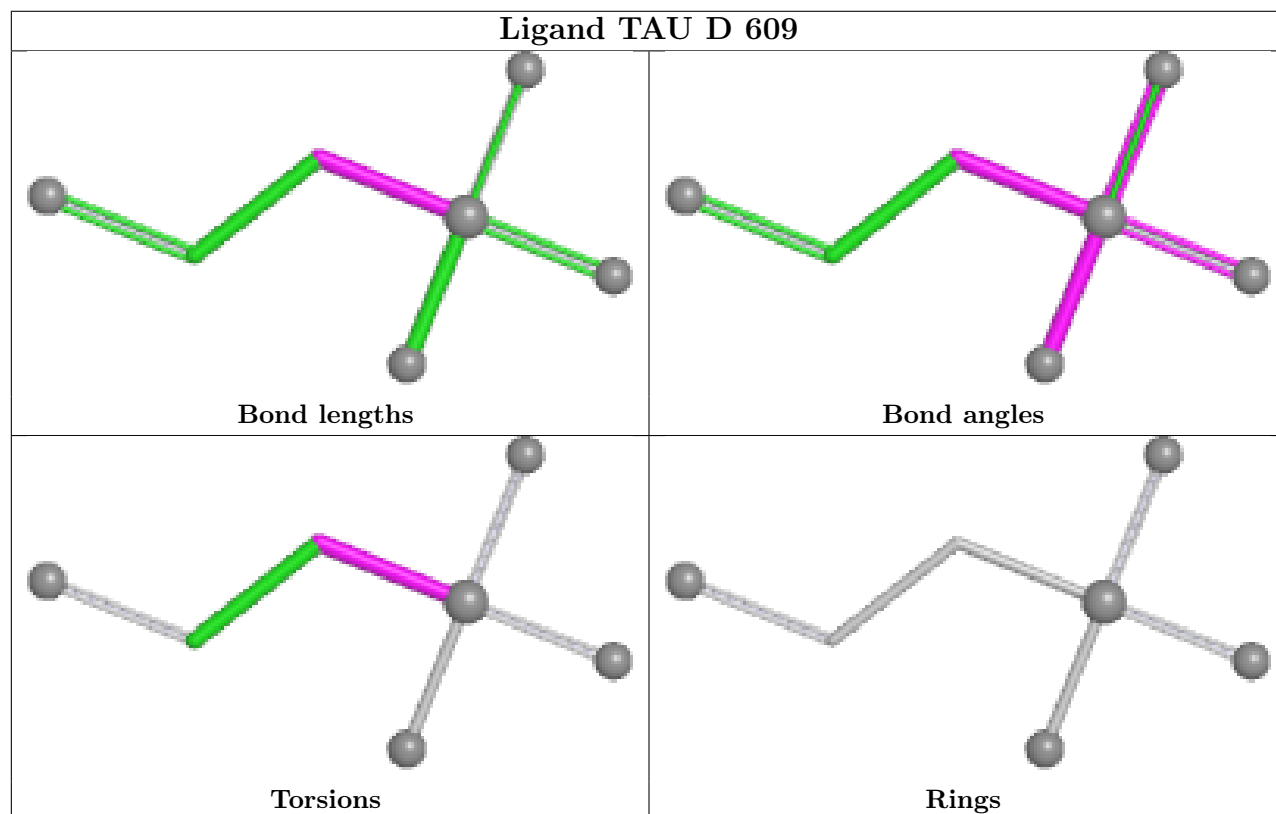
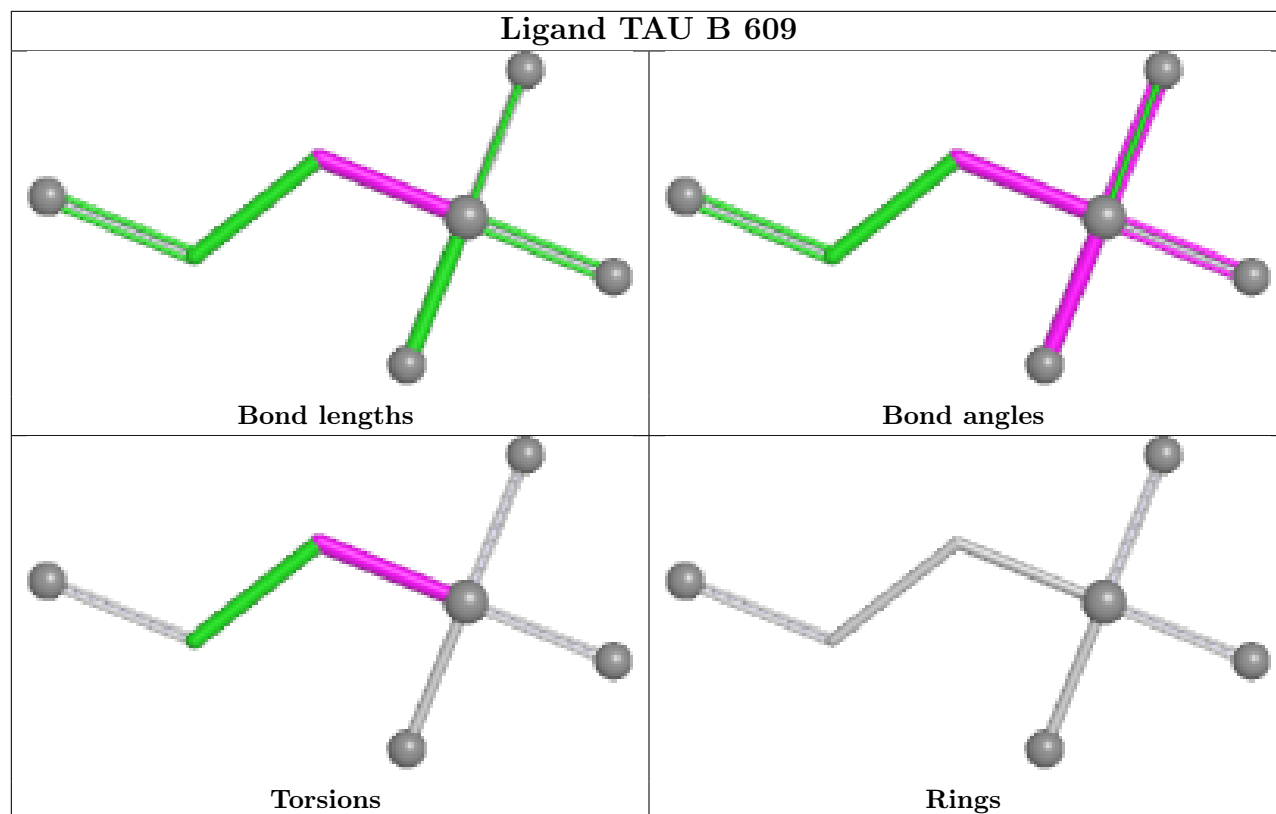
Mol	Chain	Res	Type	Atoms
3	C	609	TAU	C1-C2-S-O2
3	D	609	TAU	C1-C2-S-O2

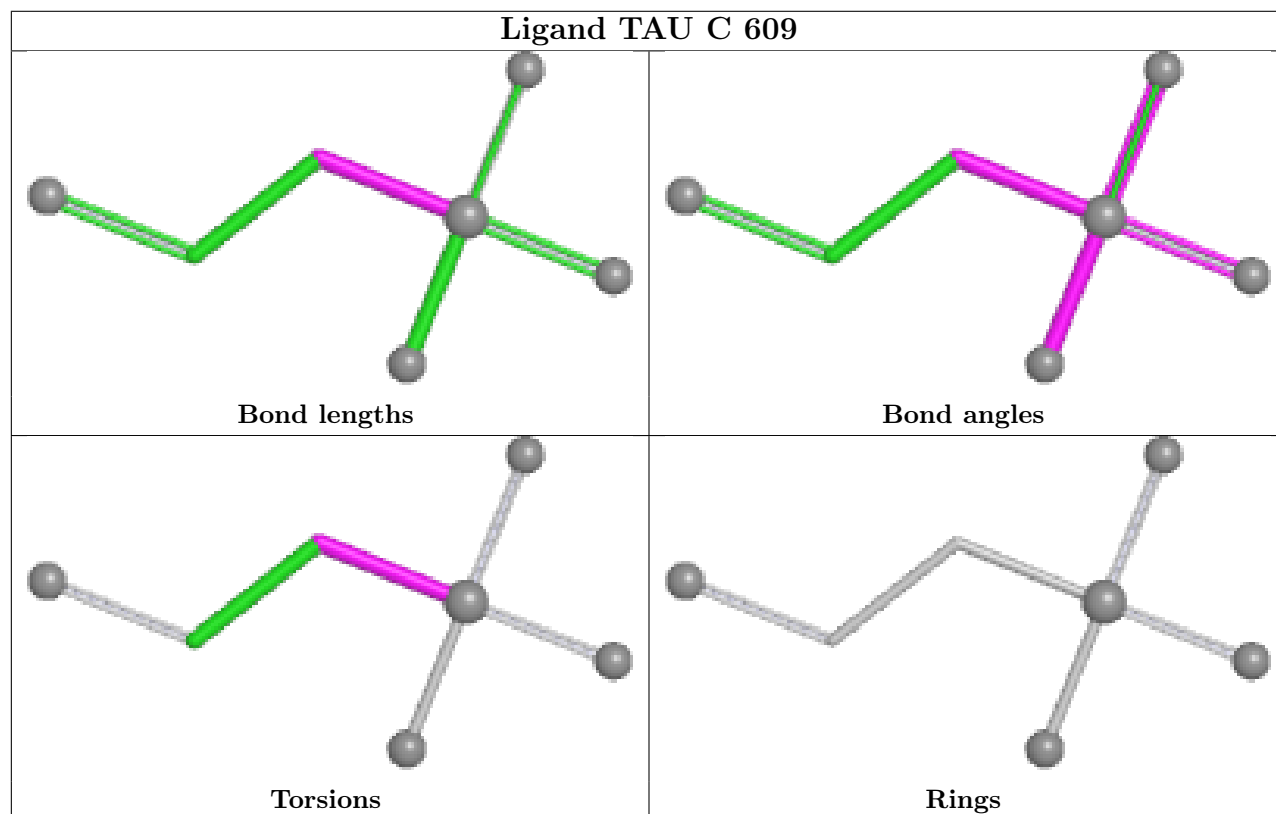
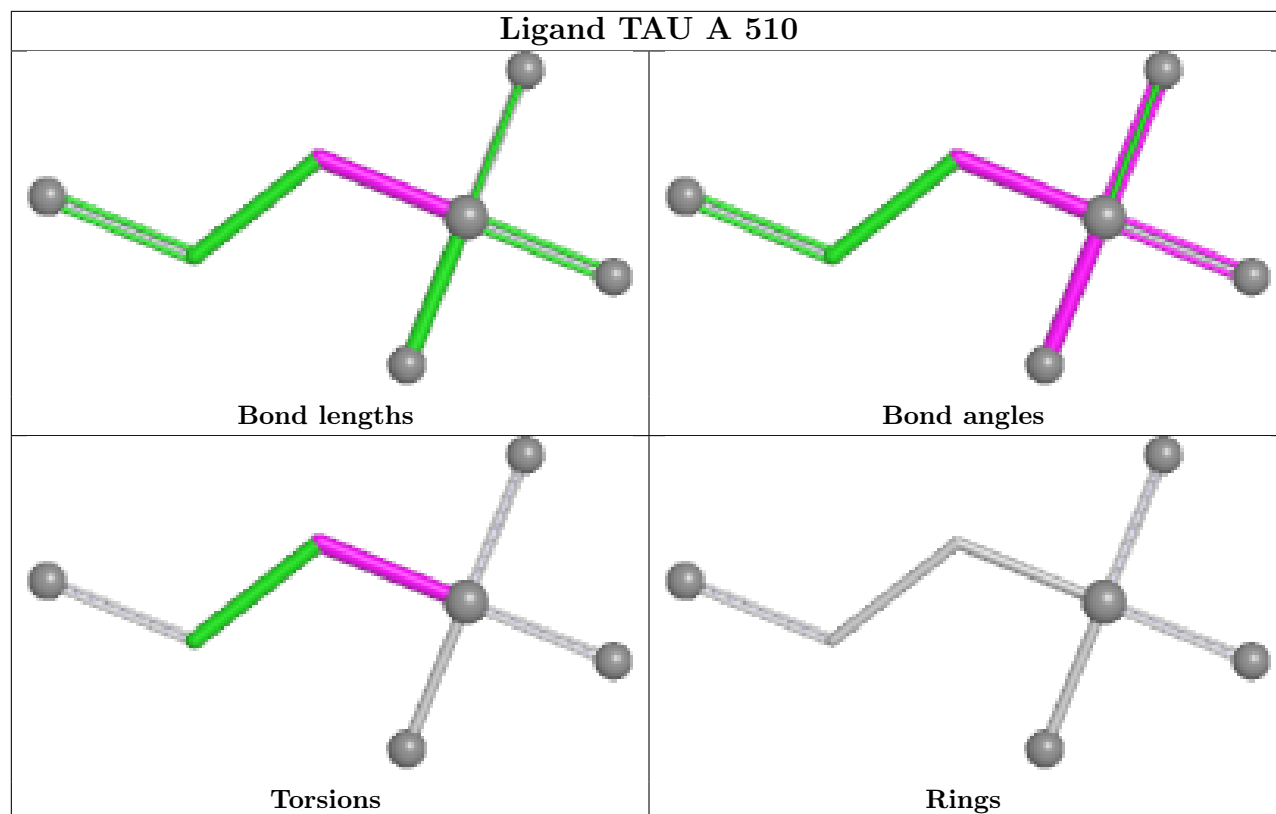
There are no ring outliers.

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 [i](#)

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20374. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis

This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution

This section was not generated.

### 7.2 Volume estimate versus contour level

This section was not generated.

### 7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit

This section was not generated.