



## wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 03:08 PM JST

PDB ID : 8JD3  
EMDB ID : EMD-36174  
Title : Cryo-EM structure of Gi1-bound mGlu2-mGlu3 heterodimer  
Authors : Wang, X.; Wang, M.; Xu, T.; Feng, Y.; Han, S.; Lin, S.; Zhao, Q.; Wu, B.  
Deposited on : 2023-05-12  
Resolution : 3.30 Å(reported)

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<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	: <b>FAILED</b>
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	: <b>FAILED</b>
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.39

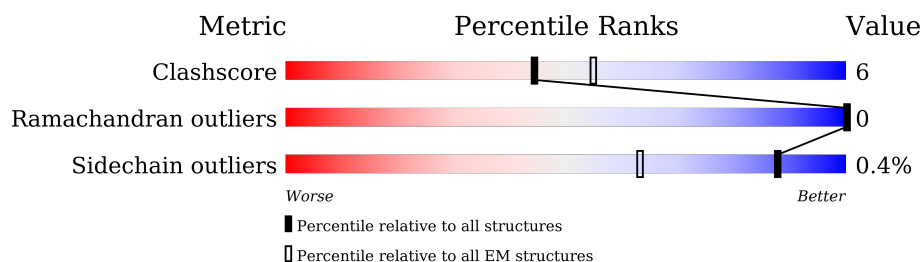
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	2	870	
2	3	894	
3	A	354	
4	B	351	
5	C	71	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15770 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 Metabotropic glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	774	Total	C	N	O	S	0	0
			5793	3730	990	1033	40		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	9	ASP	-	expression tag	UNP Q14416
2	10	TYR	-	expression tag	UNP Q14416
2	11	LYS	-	expression tag	UNP Q14416
2	12	ASP	-	expression tag	UNP Q14416
2	13	ASP	-	expression tag	UNP Q14416
2	14	ASP	-	expression tag	UNP Q14416
2	15	ASP	-	expression tag	UNP Q14416
2	16	GLY	-	expression tag	UNP Q14416
2	17	ALA	-	expression tag	UNP Q14416
2	18	PRO	-	expression tag	UNP Q14416
2	873	LEU	-	expression tag	UNP Q14416
2	874	GLU	-	expression tag	UNP Q14416
2	875	VAL	-	expression tag	UNP Q14416
2	876	LEU	-	expression tag	UNP Q14416
2	877	PHE	-	expression tag	UNP Q14416
2	878	GLN	-	expression tag	UNP Q14416

- Molecule 2 is a protein called Metabotropic glutamate receptor 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	763	Total	C	N	O	S	0	0
			5744	3685	963	1051	45		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-8	ASP	-	expression tag	UNP Q14832

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Chain	Residue	Modelled	Actual	Comment	Reference
3	-7	TYR	-	expression tag	UNP Q14832
3	-6	LYS	-	expression tag	UNP Q14832
3	-5	ASP	-	expression tag	UNP Q14832
3	-4	ASP	-	expression tag	UNP Q14832
3	-3	ASP	-	expression tag	UNP Q14832
3	-2	ASP	-	expression tag	UNP Q14832
3	-1	LYS	-	expression tag	UNP Q14832
3	0	GLY	-	expression tag	UNP Q14832
3	1	ALA	-	expression tag	UNP Q14832
3	2	PRO	-	expression tag	UNP Q14832
3	3	TRP	-	expression tag	UNP Q14832
3	4	SER	-	expression tag	UNP Q14832
3	5	HIS	-	expression tag	UNP Q14832
3	6	PRO	-	expression tag	UNP Q14832
3	7	GLN	-	expression tag	UNP Q14832
3	8	PHE	-	expression tag	UNP Q14832
3	9	GLU	-	expression tag	UNP Q14832
3	10	LYS	-	expression tag	UNP Q14832
3	11	GLY	-	expression tag	UNP Q14832
3	12	SER	-	expression tag	UNP Q14832
3	13	GLY	-	expression tag	UNP Q14832
3	14	SER	-	expression tag	UNP Q14832
3	15	TRP	-	expression tag	UNP Q14832
3	16	SER	-	expression tag	UNP Q14832
3	17	HIS	-	expression tag	UNP Q14832
3	18	PRO	-	expression tag	UNP Q14832
3	19	GLN	-	expression tag	UNP Q14832
3	20	PHE	-	expression tag	UNP Q14832
3	21	GLU	-	expression tag	UNP Q14832
3	22	LYS	-	expression tag	UNP Q14832
3	880	LEU	-	expression tag	UNP Q14832
3	881	GLU	-	expression tag	UNP Q14832
3	882	VAL	-	expression tag	UNP Q14832
3	883	LEU	-	expression tag	UNP Q14832
3	884	PHE	-	expression tag	UNP Q14832
3	885	GLN	-	expression tag	UNP Q14832

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	219	Total	C	N	O	S	0	0
			1491	948	251	282	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	conflict	UNP P63096
A	203	ALA	GLY	conflict	UNP P63096
A	245	ALA	GLU	conflict	UNP P63096
A	326	SER	ALA	conflict	UNP P63096

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	336	Total	C	N	O	S	0	0
			2220	1372	400	431	17		

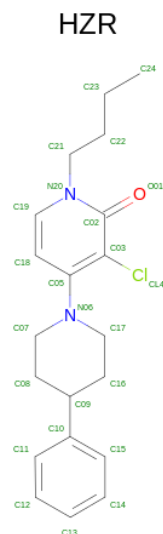
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	initiating methionine	UNP P62873
B	-9	HIS	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	GLY	-	expression tag	UNP P62873
B	-2	SER	-	expression tag	UNP P62873
B	-1	LEU	-	expression tag	UNP P62873
B	0	LEU	-	expression tag	UNP P62873
B	1	GLN	-	expression tag	UNP P62873

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

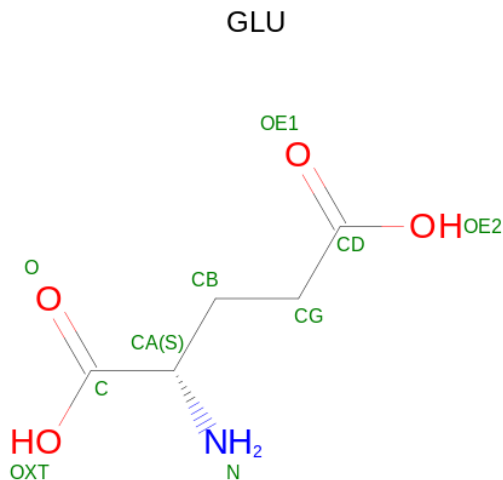
Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	54	Total	C	N	O	S	0	0
			347	216	63	65	3		

- Molecule 6 is 1-butyl-3-chloranyl-4-(4-phenylpiperidin-1-yl)pyridin-2-one (three-letter code: HZR) (formula: C<sub>20</sub>H<sub>25</sub>ClN<sub>2</sub>O) (labeled as "Ligand of Interest" by depositor).



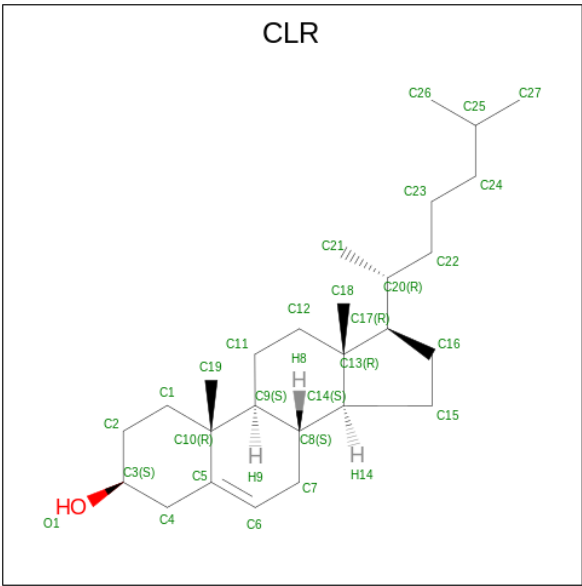
Mol	Chain	Residues	Atoms					AltConf
6	2	1	Total	C	Cl	N	O	0
			24	20	1	2	1	

- Molecule 7 is GLUTAMIC ACID (three-letter code: GLU) (formula:  $C_5H_9NO_4$ ) (labeled as "Ligand of Interest" by depositor).



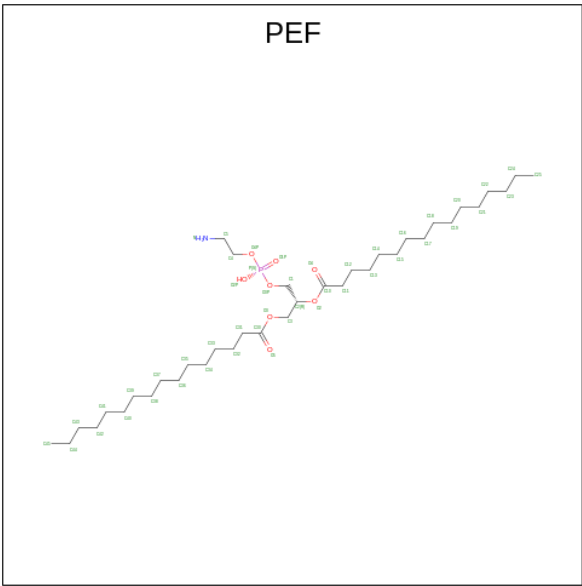
Mol	Chain	Residues	Atoms				AltConf
7	2	1	Total 10	C 5	N 1	O 4	0
7	3	1	Total 10	C 5	N 1	O 4	0

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



Mol	Chain	Residues	Atoms			AltConf
8	2	1	Total	C	O	0
			28	27	1	
8	3	1	Total	C	O	0
			28	27	1	
8	3	1	Total	C	O	0
			28	27	1	

- Molecule 9 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: C<sub>37</sub>H<sub>74</sub>NO<sub>8</sub>P).



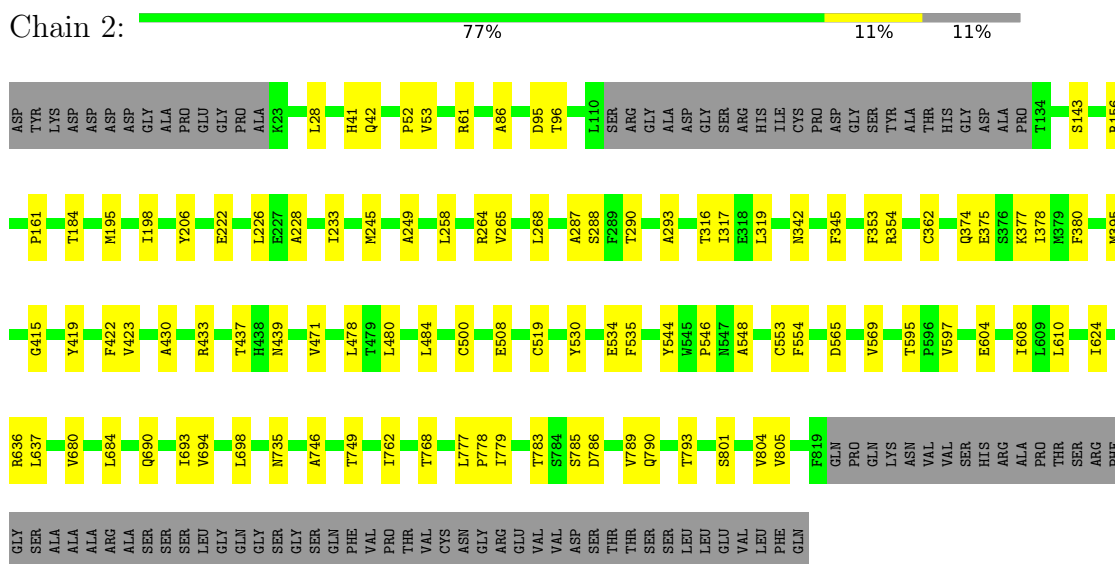
Mol	Chain	Residues	Atoms					AltConf
9	3	1	Total	C	N	O	P	0
			47	37	1	8	1	



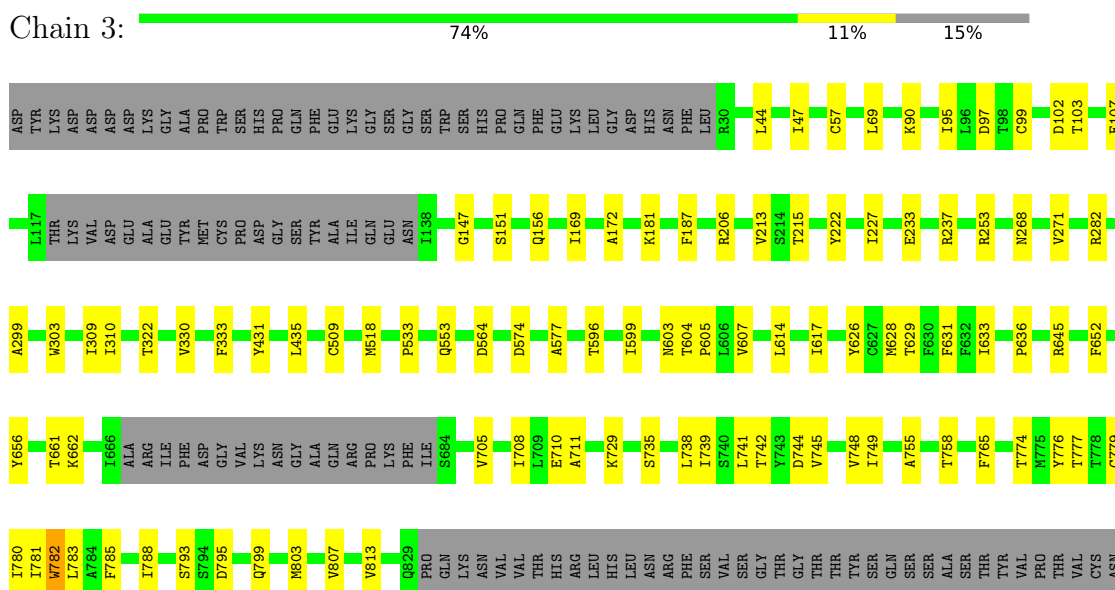
### 3 Residue-property plots

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: Metabotropic glutamate receptor 2



#### • Molecule 2: Metabotropic glutamate receptor 3



GLY
ARG
GLU
VAL
THR
LEU
ASP
SER
THR
THR
SER
SER
LEU
LEU
GLU
VAL
LEU
PHE
GLN

● Molecule 3: Guanine nucleotide-binding protein G(i) subunit alpha-1


Chain A:  56% 6% 38%

MET	GLY	CYS	THR	LEU	SER	ALA	E9	L37	M53	LYS	ILE	ILE	HIS	GLU	GLY	ALA	THR	SER	GLU	GLU	GLY	CYS	LYS	GLN	TYR	LYS	ALA	VAL	VAL	TYR	SER	ASN	THR	THR	ILE	GLN	SER	ILE	ILE	ALA	ARG	ILE	ARG	ALA	MET	GLY	ASP	LEU	LYS	ILE	ASP	PHE	GLY	ASP	SER	ALA	ASP	ARG	ALA
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ASP	ASP	ALA	ARG	GLN	LEU	PHE	VAL	LEU	ALA	GLY	ALA	ALA	GLU	GLU	GLY	PHE	THR	THR	ALA	GLU	SER	ALA	VAL	ILE	LYS	ARG	LEU	TRP	ALA	LYS	ASP	SER	GLY	VAL	ASN	GLN	ALA	CYS	PHE	ASN	ARG	ILE	ARG	GLU	TYR	GLN	LEU	ASP	ASN	SER	ALA	ALA	TYR	LEU	ASN	ASP	LEU	ASP	ARG	ARG
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ILE	ALA	GLN	PRO	ASN	TYR	ILE	PRO	THR	GLN	GLN	ASP	VAL	LEU	ARG	THR	VAL	LYS	THR	T192	E186	L194	H195	F196	V201	G202	A203	R206	K209	K210	W211	T212	H213	T221	L266	T295	E298	L310	N311	K312	T321	I344	L348	F354
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● Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:  77% 19% .

MET	HIS	HIS	HIS	HIS	HIS	HIS	GLY	SER	LEU	LEU	GLN	SER	GLU	L4	L7	R8	Q9	E10	Q13	N16	R19	R52	A56	K57	I58	Y59	S67	R68	Q75	D76	G77	L95	W99	Y100	M101	A104	M110	A113	L126	Y145	L146	S147	C148	C149
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G162	D163	T164	L168	W169	Q176	T177	T178	G182	H183	M188	D212	E215	I229	N230	A231	F235	F241	S245	D254	L255	R256	A257	I273	T274	S275	F278	D290	C294	N295	V296	W297	R304	A305	L308	A309	G310	N313	R314	G330
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S331	W332	D333	W339	ASN
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● Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain C:  70% 6% 24%

MET	ALA	SER	ASN	ASN	THR	ALA	SER	I9	K46	E47	D48	T52	P53	R62	GLU	LYS	PHE	PHE	CYS	ALA	ILE	LEU
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	994275	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 ( $e^-/\text{\AA}^2$ )	70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (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: CLR, HZR, PEF

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	2	0.25	0/5936	0.47	0/8095
2	3	0.25	0/5873	0.47	0/7997
3	A	0.24	0/1515	0.44	0/2069
4	B	0.24	0/2260	0.50	0/3099
5	C	0.24	0/352	0.46	0/483
All	All	0.24	0/15936	0.47	0/21743

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	2	5793	0	5597	63	0
2	3	5744	0	5464	67	0
3	A	1491	0	1253	13	0
4	B	2220	0	1846	41	0
5	C	347	0	298	2	0
6	2	24	0	0	1	0
7	2	10	0	5	0	0
7	3	10	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	2	28	0	46	3	0
8	3	56	0	92	3	0
9	3	47	0	73	7	0
All	All	15770	0	14679	190	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 190 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:745:VAL:HG22	2:3:782:TRP:HD1	1.49	0.77
1:2:265:VAL:HG12	1:2:290:THR:HB	1.73	0.69
2:3:614:LEU:HD23	2:3:662:LYS:HD2	1.74	0.69
1:2:768:THR:HG21	1:2:804:VAL:HG21	1.77	0.66
2:3:735:SER:O	2:3:739:ILE:HD12	1.95	0.66

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	2	770/870 (88%)	737 (96%)	33 (4%)	0	100	100
2	3	757/894 (85%)	732 (97%)	25 (3%)	0	100	100
3	A	215/354 (61%)	207 (96%)	8 (4%)	0	100	100
4	B	334/351 (95%)	317 (95%)	17 (5%)	0	100	100
5	C	52/71 (73%)	49 (94%)	3 (6%)	0	100	100
All	All	2128/2540 (84%)	2042 (96%)	86 (4%)	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	2	581/712 (82%)	580 (100%)	1 (0%)	92	95
2	3	588/781 (75%)	587 (100%)	1 (0%)	92	95
3	A	123/305 (40%)	122 (99%)	1 (1%)	79	87
4	B	180/293 (61%)	179 (99%)	1 (1%)	84	90
5	C	26/58 (45%)	25 (96%)	1 (4%)	28	56
All	All	1498/2149 (70%)	1493 (100%)	5 (0%)	88	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	354	ARG
2	3	782	TRP
3	A	209	LYS
4	B	19	ARG
5	C	46	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	13	GLN
4	B	230	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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 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	GLU	2	902	-	8,9,9	1.02	0	10,11,11	1.18	0
8	CLR	3	903	-	31,31,31	0.27	0	48,48,48	0.40	0
6	HZR	2	901	-	25,26,26	3.13	12 (48%)	31,35,35	1.80	8 (25%)
8	CLR	2	903	-	31,31,31	0.29	0	48,48,48	0.64	1 (2%)
9	PEF	3	904	-	46,46,46	1.30	4 (8%)	49,51,51	0.81	2 (4%)
8	CLR	3	902	-	31,31,31	0.27	0	48,48,48	0.40	0
7	GLU	3	901	-	8,9,9	1.02	0	10,11,11	1.17	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
7	GLU	2	902	-	-	4/9/9/9	-
8	CLR	3	903	-	-	4/10/68/68	0/4/4/4
6	HZR	2	901	-	-	7/12/22/22	0/3/3/3
8	CLR	2	903	-	-	5/10/68/68	0/4/4/4
9	PEF	3	904	-	-	34/50/50/50	-
8	CLR	3	902	-	-	4/10/68/68	0/4/4/4
7	GLU	3	901	-	-	6/9/9/9	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	901	HZR	C19-N20	7.93	1.48	1.37
6	2	901	HZR	C19-C18	7.70	1.53	1.35
6	2	901	HZR	C02-N20	5.57	1.48	1.39
6	2	901	HZR	C03-C02	4.62	1.53	1.44
6	2	901	HZR	C18-C05	4.30	1.49	1.41

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	901	HZR	C05-C03-C02	-4.15	119.76	123.11
6	2	901	HZR	C19-N20-C02	-3.83	120.05	122.89
9	3	904	PEF	O2-C10-C11	3.55	119.14	111.50
6	2	901	HZR	O01-C02-C03	-3.22	119.84	125.19
6	2	901	HZR	C07-C08-C09	2.91	114.48	111.04

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	2	902	GLU	N-CA-CB-CG
7	2	902	GLU	C-CA-CB-CG
8	2	903	CLR	C13-C17-C20-C21
9	3	904	PEF	O4-C10-O2-C2
9	3	904	PEF	C31-C30-O3-C3

There are no ring outliers.

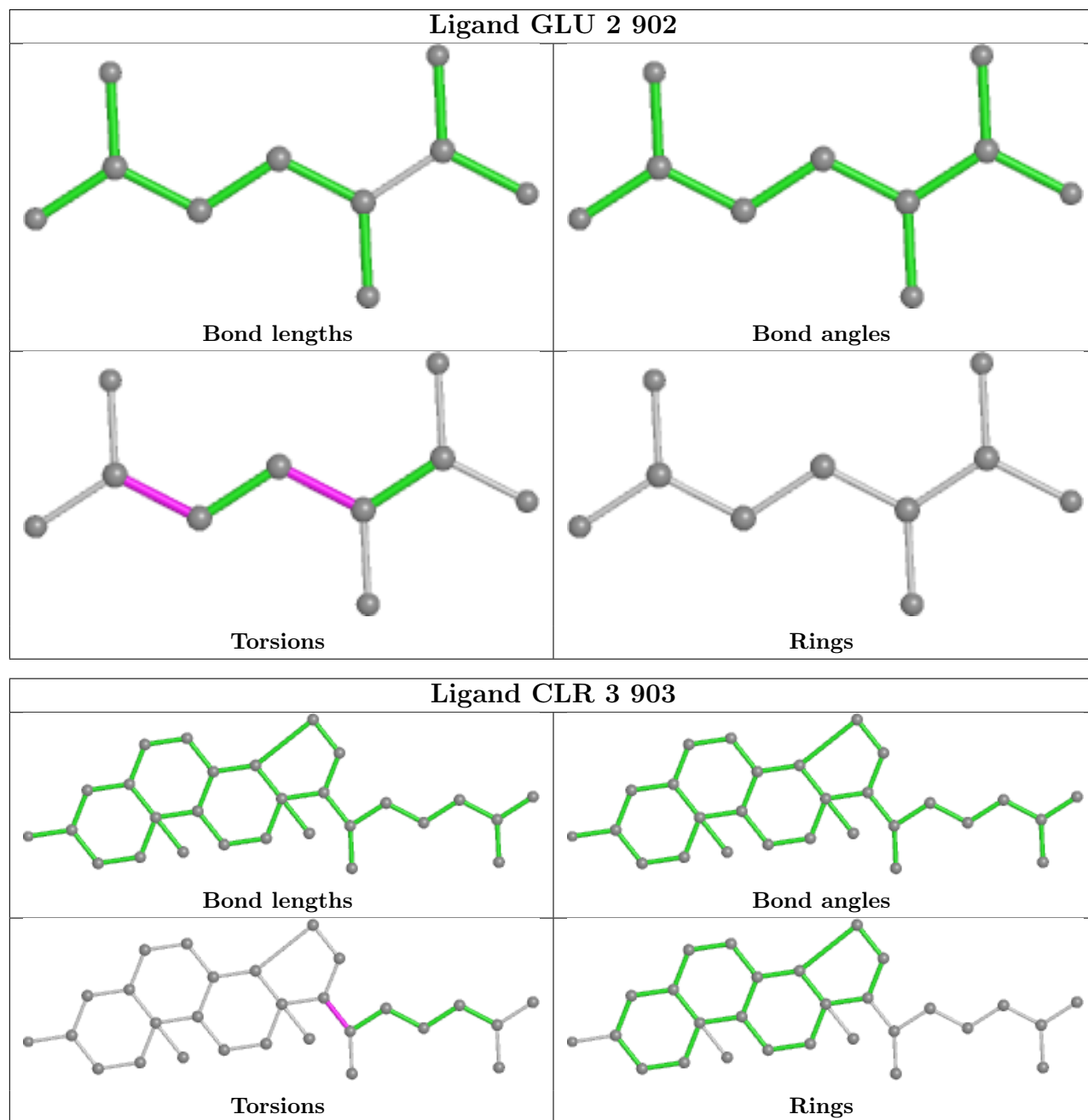
5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	3	903	CLR	3	0
6	2	901	HZR	1	0
8	2	903	CLR	3	0
9	3	904	PEF	7	0
7	3	901	GLU	1	0

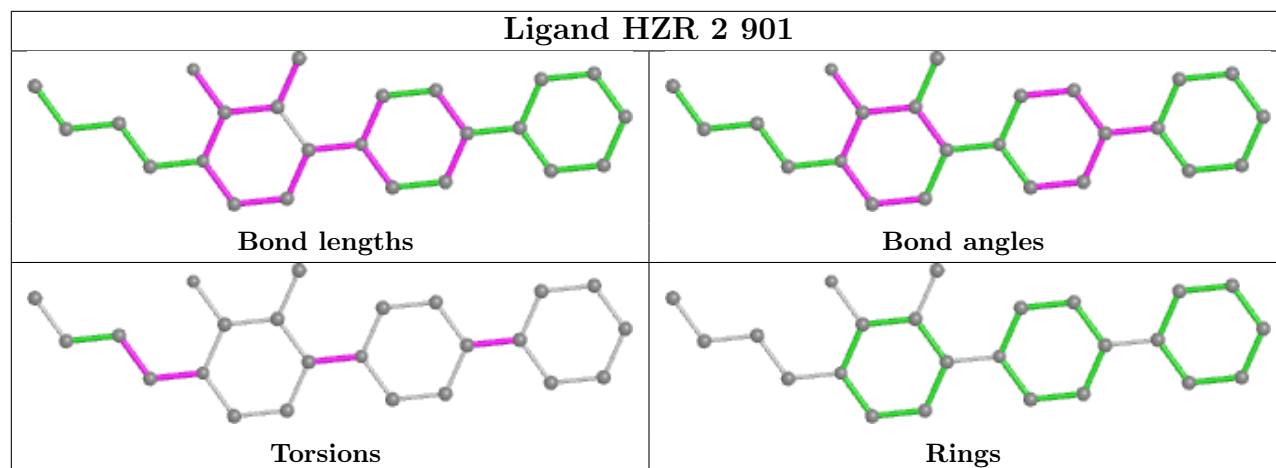
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



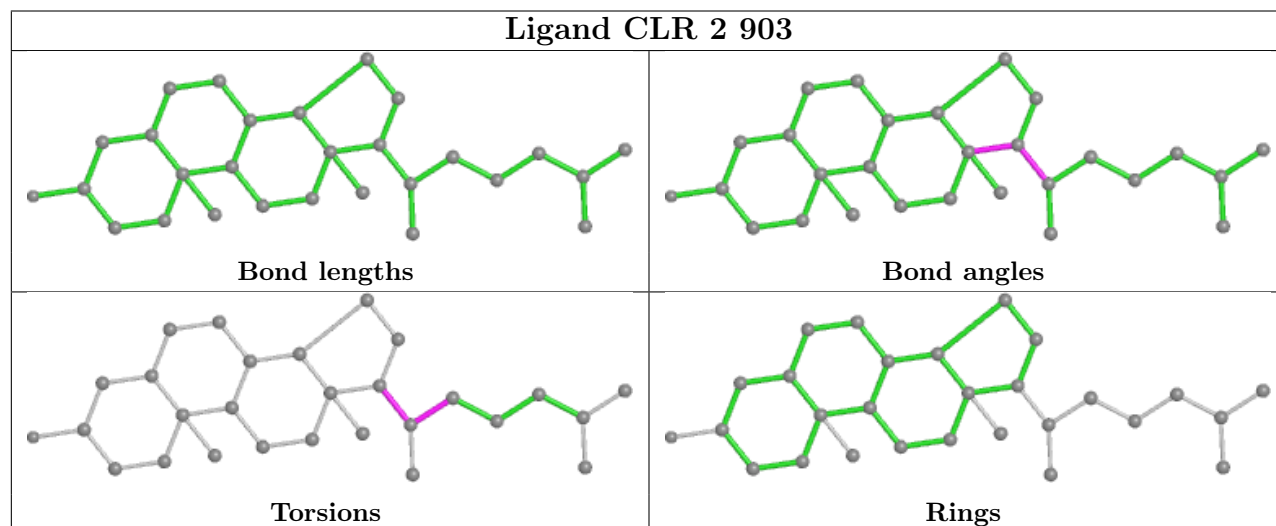
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



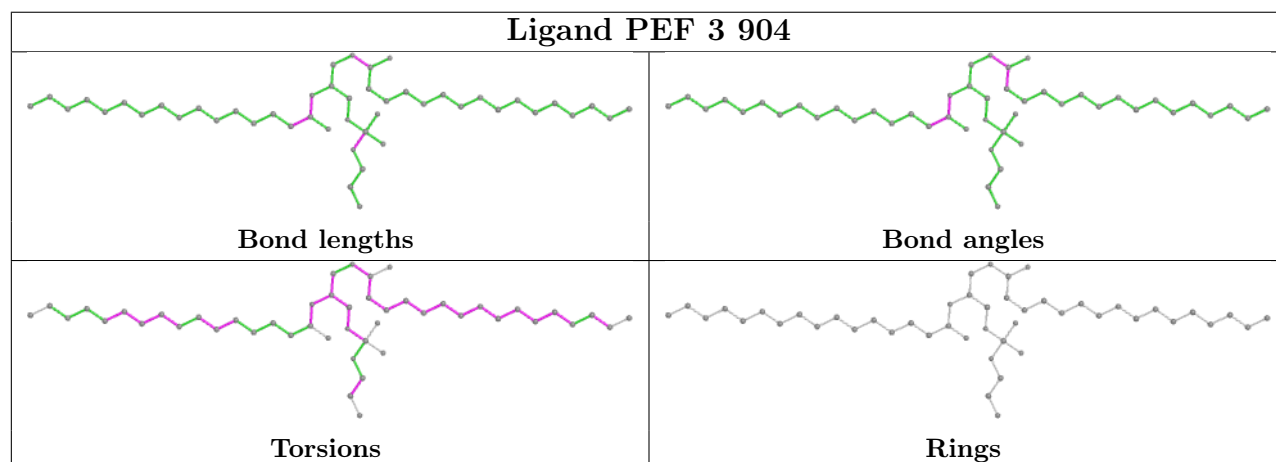
## Ligand HZR 2 901

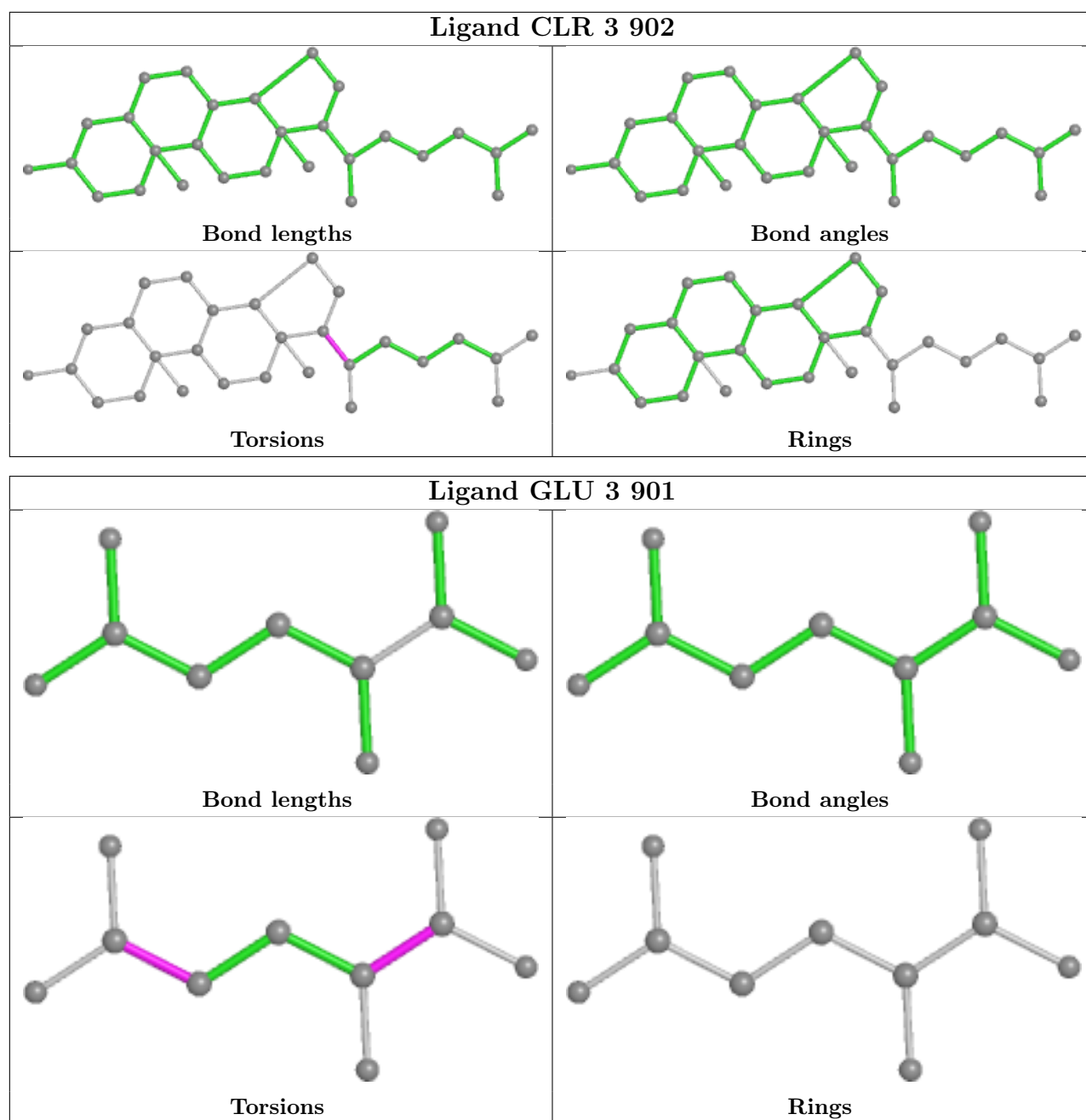


## Ligand CLR 2 903



## Ligand PEF 3 904





## 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.