



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 10, 2019 – 06:57 PM EDT

PDB ID : 6PV8  
EMDB ID: : EMD-20488  
Title : Human alpha3beta4 nicotinic acetylcholine receptor in complex with AT-1001  
Authors : Gharpure, A.; Teng, J.; Zhuang, Y.; Noviello, C.M.; Walsh, R.M.; Cabuco, R.; Howard, R.J.; Zaveri, N.T.; Lindahl, E.; Hibbs, R.E.  
Deposited on : 2019-07-19  
Resolution : 3.87 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB 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.

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MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

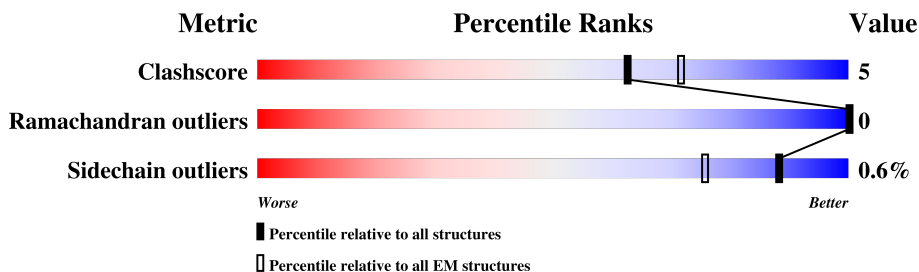
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.87 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	525	65% 9% 26%
1	D	525	64% 9% 26%
2	B	538	63% 9% 28%
2	C	538	61% 10% 28%
2	E	538	64% 8% 28%
3	F	219	50% 47%
3	H	219	52% 47%
4	G	213	42% 7% 51%
4	I	213	46% 51%

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 20051 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 Fusion protein of Neuronal acetylcholine receptor subunit alpha-3 and Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	387	Total	C	N	O	S	0	0
			3167	2096	489	562	20		
1	D	387	Total	C	N	O	S	0	0
			3167	2096	489	562	20		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	328A	TRP	MET	conflict	UNP A0A3W4NZ06
A	331R	ILE	HIS	conflict	UNP A0A3W4NZ06
A	331V	LEU	-	linker	UNP A0A3W4NZ06
D	328A	TRP	MET	conflict	UNP A0A3W4NZ06
D	331R	ILE	HIS	conflict	UNP A0A3W4NZ06
D	331V	LEU	-	linker	UNP A0A3W4NZ06

- Molecule 2 is a protein called Fusion protein of Neuronal acetylcholine receptor subunit beta-4 and Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	388	Total	C	N	O	S	0	0
			3149	2055	512	561	21		
2	C	385	Total	C	N	O	S	0	0
			3126	2041	506	558	21		
2	E	388	Total	C	N	O	S	0	0
			3149	2055	512	561	21		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	328S	TRP	MET	conflict	UNP A0A3W4NZ06
B	332J	ILE	HIS	conflict	UNP A0A3W4NZ06
B	332N	LEU	-	linker	UNP A0A3W4NZ06

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Chain	Residue	Modelled	Actual	Comment	Reference
B	478	SER	-	expression tag	UNP P30926
B	479	ALA	-	expression tag	UNP P30926
B	480	TRP	-	expression tag	UNP P30926
B	481	SER	-	expression tag	UNP P30926
B	482	HIS	-	expression tag	UNP P30926
B	483	PRO	-	expression tag	UNP P30926
B	484	GLN	-	expression tag	UNP P30926
B	485	PHE	-	expression tag	UNP P30926
B	486	GLU	-	expression tag	UNP P30926
B	487	LYS	-	expression tag	UNP P30926
C	328S	TRP	MET	conflict	UNP A0A3W4NZ06
C	332J	ILE	HIS	conflict	UNP A0A3W4NZ06
C	332N	LEU	-	linker	UNP A0A3W4NZ06
C	478	SER	-	expression tag	UNP P30926
C	479	ALA	-	expression tag	UNP P30926
C	480	TRP	-	expression tag	UNP P30926
C	481	SER	-	expression tag	UNP P30926
C	482	HIS	-	expression tag	UNP P30926
C	483	PRO	-	expression tag	UNP P30926
C	484	GLN	-	expression tag	UNP P30926
C	485	PHE	-	expression tag	UNP P30926
C	486	GLU	-	expression tag	UNP P30926
C	487	LYS	-	expression tag	UNP P30926
E	328S	TRP	MET	conflict	UNP A0A3W4NZ06
E	332J	ILE	HIS	conflict	UNP A0A3W4NZ06
E	332N	LEU	-	linker	UNP A0A3W4NZ06
E	478	SER	-	expression tag	UNP P30926
E	479	ALA	-	expression tag	UNP P30926
E	480	TRP	-	expression tag	UNP P30926
E	481	SER	-	expression tag	UNP P30926
E	482	HIS	-	expression tag	UNP P30926
E	483	PRO	-	expression tag	UNP P30926
E	484	GLN	-	expression tag	UNP P30926
E	485	PHE	-	expression tag	UNP P30926
E	486	GLU	-	expression tag	UNP P30926
E	487	LYS	-	expression tag	UNP P30926

- Molecule 3 is a protein called IgG2b Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	117	Total	C	N	O	S	0	0
			911	580	147	179	5		

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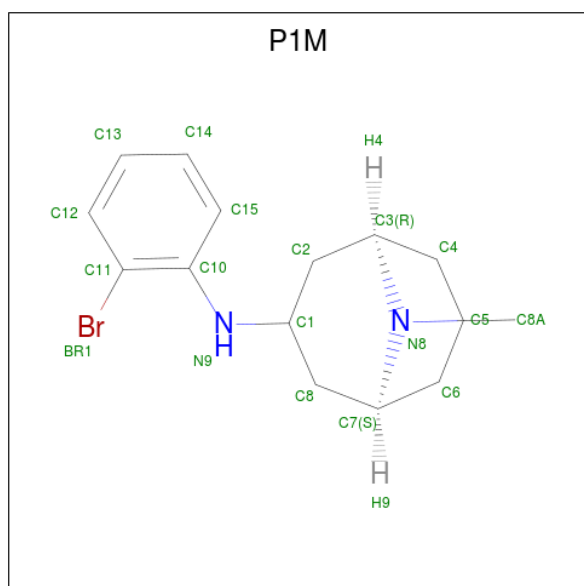
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	117	Total	C	N	O	S	0	0
			911	580	147	179	5		

- Molecule 4 is a protein called Kappa Fab light chain.

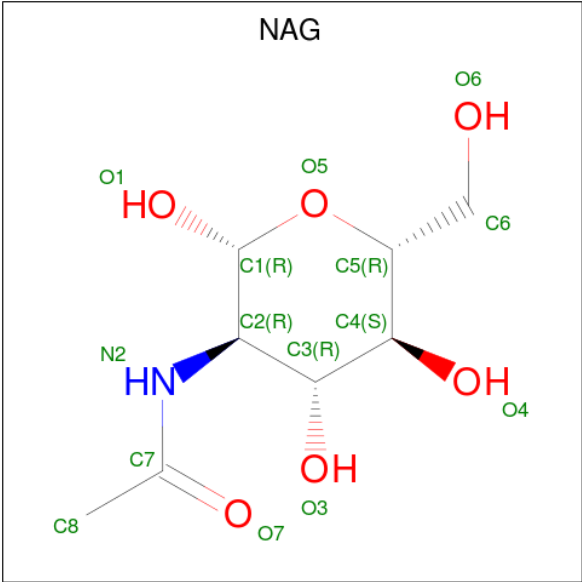
Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	105	Total	C	N	O	S	0	0
			792	494	131	160	7		
4	I	105	Total	C	N	O	S	0	0
			792	494	131	160	7		

- Molecule 5 is (3-endo)-N-(2-bromophenyl)-9-methyl-9-azabicyclo[3.3.1]nonan-3-amine (three-letter code: P1M) (formula:  $C_{15}H_{21}BrN_2$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	Br	C	N	0
			18	1	15	2	
5	D	1	Total	Br	C	N	0
			18	1	15	2	

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



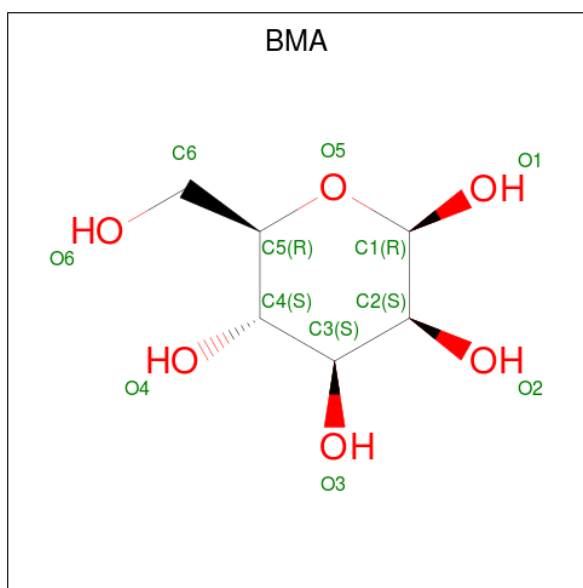
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			56	32	4	20	
6	A	1	Total	C	N	O	0
			56	32	4	20	
6	A	1	Total	C	N	O	0
			56	32	4	20	
6	A	1	Total	C	N	O	0
			56	32	4	20	
6	B	1	Total	C	N	O	0
			84	48	6	30	
6	B	1	Total	C	N	O	0
			84	48	6	30	
6	B	1	Total	C	N	O	0
			84	48	6	30	
6	B	1	Total	C	N	O	0
			84	48	6	30	
6	B	1	Total	C	N	O	0
			84	48	6	30	
6	B	1	Total	C	N	O	0
			84	48	6	30	
6	C	1	Total	C	N	O	0
			84	48	6	30	
6	C	1	Total	C	N	O	0
			84	48	6	30	
6	C	1	Total	C	N	O	0
			84	48	6	30	
6	C	1	Total	C	N	O	0
			84	48	6	30	

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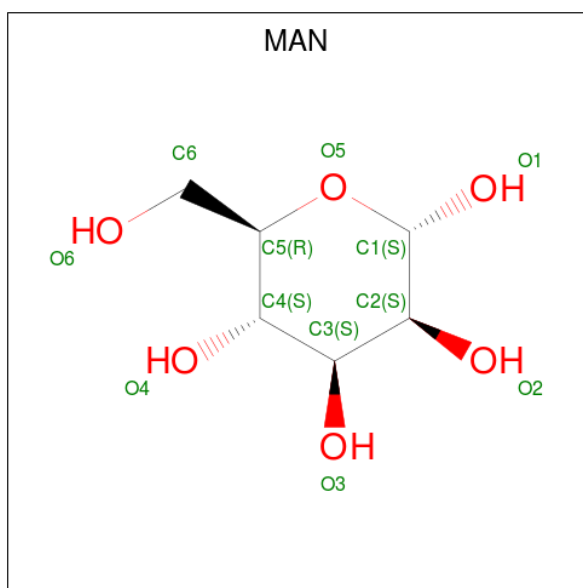
Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			84	48	6	30	
6	C	1	Total	C	N	O	0
			84	48	6	30	
6	D	1	Total	C	N	O	0
			56	32	4	20	
6	D	1	Total	C	N	O	0
			56	32	4	20	
6	D	1	Total	C	N	O	0
			56	32	4	20	
6	D	1	Total	C	N	O	0
			56	32	4	20	
6	E	1	Total	C	N	O	0
			84	48	6	30	
6	E	1	Total	C	N	O	0
			84	48	6	30	
6	E	1	Total	C	N	O	0
			84	48	6	30	
6	E	1	Total	C	N	O	0
			84	48	6	30	
6	E	1	Total	C	N	O	0
			84	48	6	30	
6	E	1	Total	C	N	O	0
			84	48	6	30	

- Molecule 7 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			11	6	5	
7	B	1	Total	C	O	0
			22	12	10	
7	B	1	Total	C	O	0
			22	12	10	
7	C	1	Total	C	O	0
			22	12	10	
7	C	1	Total	C	O	0
			22	12	10	
7	D	1	Total	C	O	0
			11	6	5	
7	E	1	Total	C	O	0
			22	12	10	
7	E	1	Total	C	O	0
			22	12	10	

- Molecule 8 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			22	12	10	
8	A	1	Total	C	O	0
			22	12	10	
8	B	1	Total	C	O	0
			22	12	10	
8	B	1	Total	C	O	0
			22	12	10	

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Mol	Chain	Residues	Atoms			AltConf
8	C	1	Total 22	C 12	O 10	0
8	C	1	Total 22	C 12	O 10	0
8	D	1	Total 22	C 12	O 10	0
8	D	1	Total 22	C 12	O 10	0
8	E	1	Total 22	C 12	O 10	0
8	E	1	Total 22	C 12	O 10	0

- # Y01

Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total 56	C 54	O 2	0
9	A	1	Total 56	C 54	O 2	0
9	B	1	Total 56	C 54	O 2	0
9	B	1	Total 56	C 54	O 2	0
9	C	1	Total 56	C 54	O 2	0




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Mol	Chain	Residues	Atoms			AltConf
9	C	1	Total	C	O	0
			56	54	2	
9	D	1	Total	C	O	0
			56	54	2	
9	D	1	Total	C	O	0
			56	54	2	
9	E	1	Total	C	O	0
			56	54	2	
9	E	1	Total	C	O	0
			56	54	2	

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
10	B	1	Total	Na	0
			1	1	

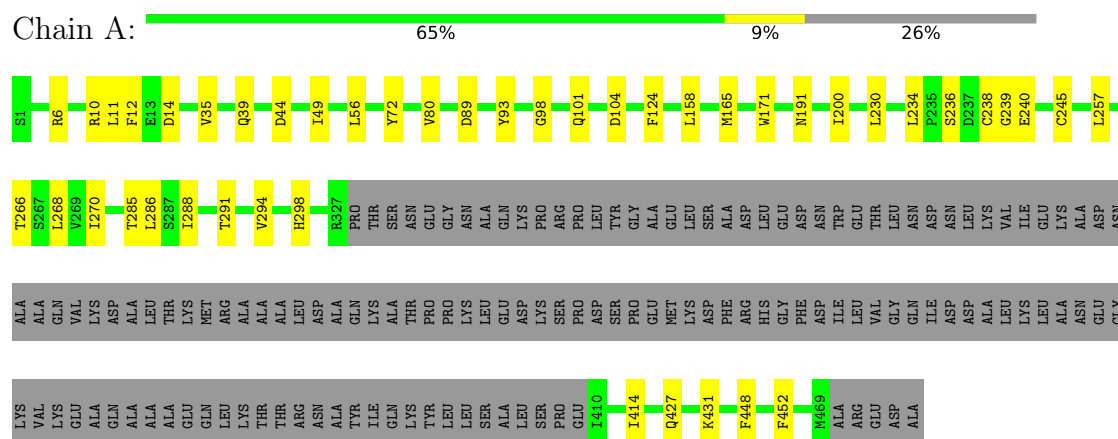
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	A	2	Total	O	0
			2	2	
11	B	3	Total	O	0
			3	3	
11	D	2	Total	O	0
			2	2	
11	E	1	Total	O	0
			1	1	

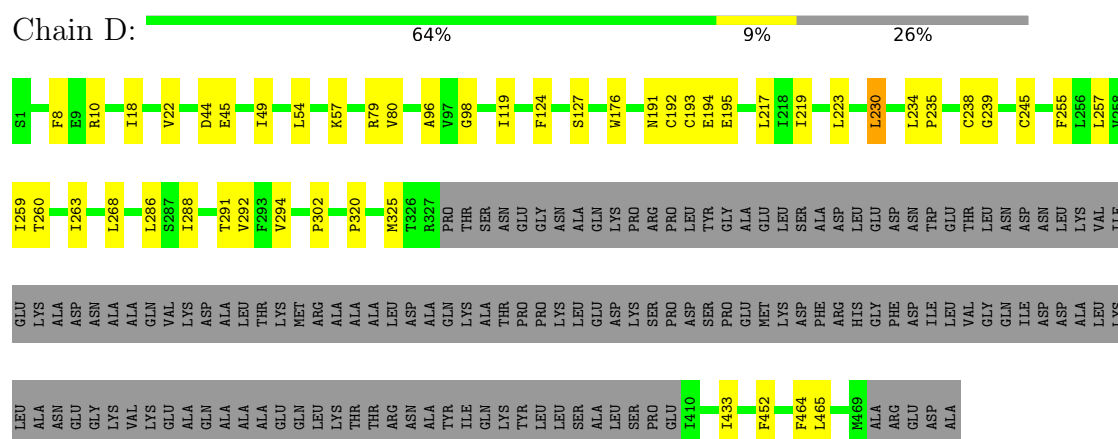
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

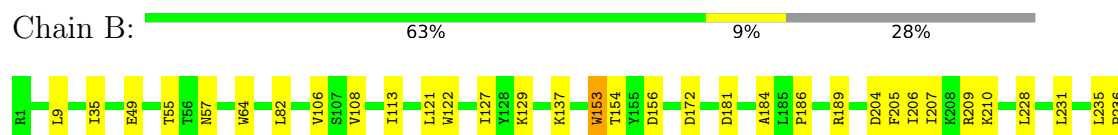
- Molecule 1: Fusion protein of Neuronal acetylcholine receptor subunit alpha-3 and Soluble cytochrome b562

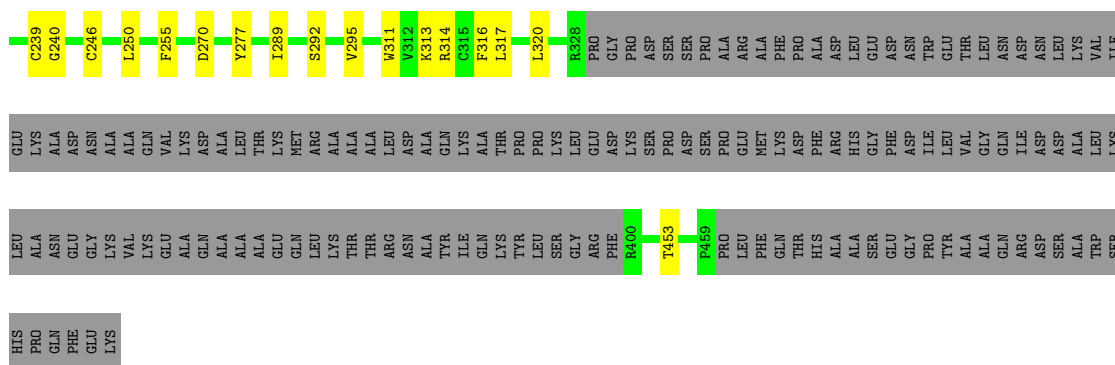


- Molecule 1: Fusion protein of Neuronal acetylcholine receptor subunit alpha-3 and Soluble cytochrome b562

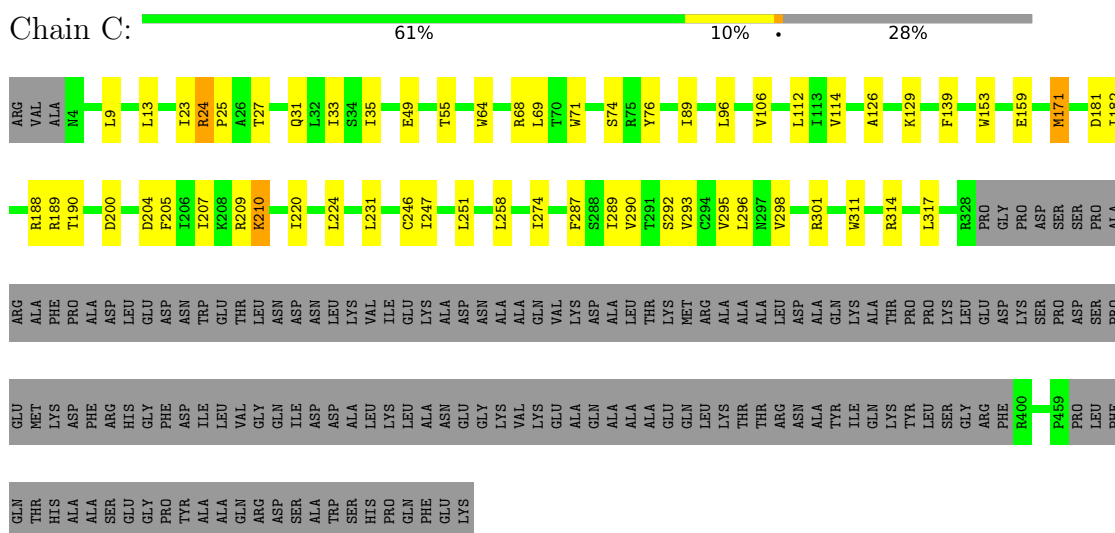


- Molecule 2: Fusion protein of Neuronal acetylcholine receptor subunit beta-4 and Soluble cytochrome b562

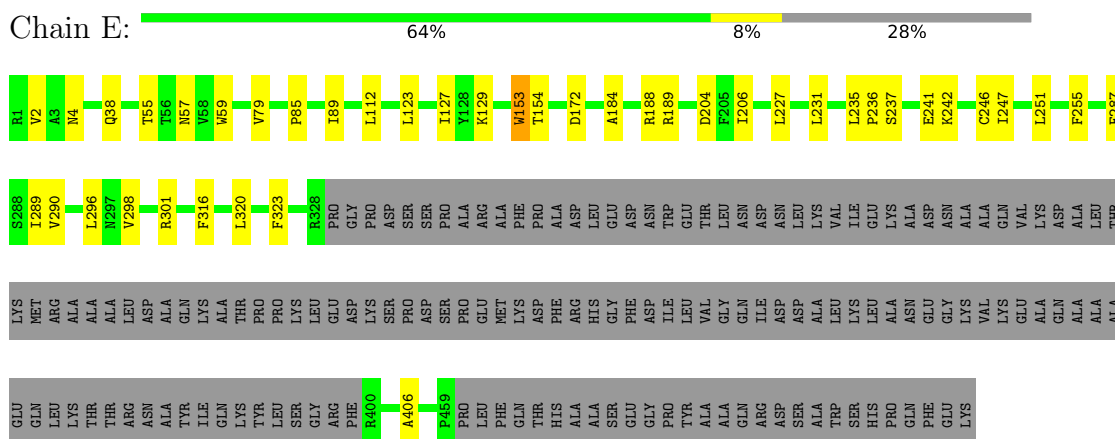




- Molecule 2: Fusion protein of Neuronal acetylcholine receptor subunit beta-4 and Soluble cytochrome b562

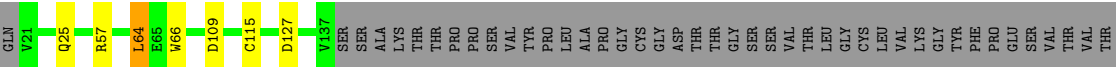


- Molecule 2: Fusion protein of Neuronal acetylcholine receptor subunit beta-4 and Soluble cytochrome b562

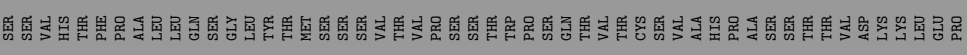
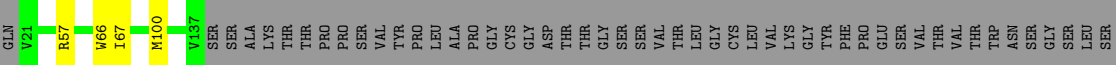


- Molecule 3: IgG2b Fab heavy chain

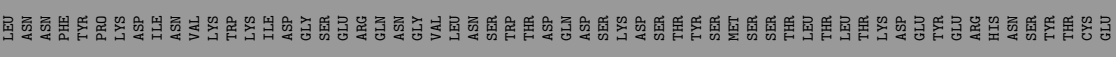




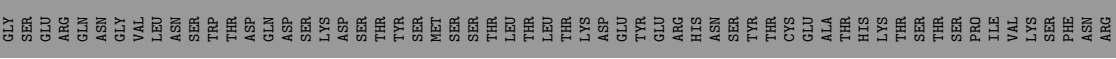
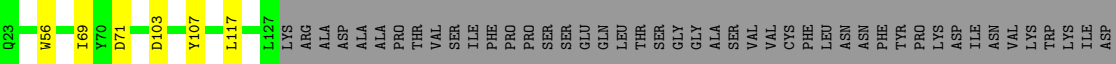
• Molecule 3: IgG2b Fab heavy chain



• Molecule 4: Kappa Fab light chain



• Molecule 4: Kappa Fab light chain



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	93080	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	59523	Depositor
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: BMA, NAG, NA, P1M, Y01, MAN

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.39	1/3252 (0.0%)	0.56	2/4431 (0.0%)
1	D	0.32	0/3252	0.55	1/4431 (0.0%)
2	B	0.30	0/3228	0.57	1/4402 (0.0%)
2	C	0.35	0/3205	0.60	2/4371 (0.0%)
2	E	0.30	0/3228	0.58	1/4402 (0.0%)
3	F	0.29	0/936	0.54	1/1273 (0.1%)
3	H	0.29	0/936	0.54	0/1273
4	G	0.29	0/811	0.56	0/1099
4	I	0.29	0/811	0.54	0/1099
All	All	0.33	1/19659 (0.0%)	0.57	8/26781 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	LEU	C-N	12.92	1.58	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	LEU	O-C-N	-6.34	109.06	121.10
2	E	231	LEU	CA-CB-CG	5.58	128.14	115.30
2	C	96	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	230	LEU	CA-CB-CG	5.49	127.92	115.30
1	D	230	LEU	CA-CB-CG	5.44	127.81	115.30

There are no chirality outliers.

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	3167	0	3214	33	0
1	D	3167	0	3214	37	0
2	B	3149	0	3203	35	0
2	C	3126	0	3173	47	0
2	E	3149	0	3203	26	0
3	F	911	0	865	7	0
3	H	911	0	865	2	0
4	G	792	0	757	10	0
4	I	792	0	757	4	0
5	A	18	0	0	2	0
5	D	18	0	0	0	0
6	A	56	0	49	0	0
6	B	84	0	74	0	0
6	C	84	0	74	5	0
6	D	56	0	49	0	0
6	E	84	0	74	0	0
7	A	11	0	8	0	0
7	B	22	0	18	0	0
7	C	22	0	18	1	0
7	D	11	0	8	0	0
7	E	22	0	18	1	0
8	A	22	0	20	0	0
8	B	22	0	20	0	0
8	C	22	0	20	1	0
8	D	22	0	20	0	0
8	E	22	0	20	1	0
9	A	56	0	90	4	0
9	B	56	0	90	2	0
9	C	56	0	90	4	0
9	D	56	0	90	4	0
9	E	56	0	90	5	0
10	B	1	0	0	0	0
11	A	2	0	0	0	0
11	B	3	0	0	0	0
11	D	2	0	0	0	0
11	E	1	0	0	0	0
All	All	20051	0	20191	194	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 194 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:234:LEU:HD12	1:D:235:PRO:HD2	1.16	1.14
1:D:234:LEU:CD1	1:D:235:PRO:HD2	2.01	0.90
2:E:188:ARG:NH1	2:E:204:ASP:OD2	2.11	0.83
1:D:57:LYS:HG3	1:D:119:ILE:CD1	2.13	0.79
1:D:234:LEU:HD12	1:D:235:PRO:CD	2.08	0.76

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	383/525 (73%)	366 (96%)	17 (4%)	0	100	100
1	D	383/525 (73%)	366 (96%)	17 (4%)	0	100	100
2	B	384/538 (71%)	361 (94%)	23 (6%)	0	100	100
2	C	381/538 (71%)	363 (95%)	18 (5%)	0	100	100
2	E	384/538 (71%)	368 (96%)	16 (4%)	0	100	100
3	F	115/219 (52%)	109 (95%)	6 (5%)	0	100	100
3	H	115/219 (52%)	112 (97%)	3 (3%)	0	100	100
4	G	103/213 (48%)	94 (91%)	9 (9%)	0	100	100
4	I	103/213 (48%)	96 (93%)	7 (7%)	0	100	100
All	All	2351/3528 (67%)	2235 (95%)	116 (5%)	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	359/470 (76%)	359 (100%)	0	100	100
1	D	359/470 (76%)	358 (100%)	1 (0%)	93	96
2	B	362/482 (75%)	360 (99%)	2 (1%)	87	94
2	C	360/482 (75%)	354 (98%)	6 (2%)	63	84
2	E	362/482 (75%)	358 (99%)	4 (1%)	76	88
3	F	98/188 (52%)	98 (100%)	0	100	100
3	H	98/188 (52%)	97 (99%)	1 (1%)	78	89
4	G	88/187 (47%)	88 (100%)	0	100	100
4	I	88/187 (47%)	88 (100%)	0	100	100
All	All	2174/3136 (69%)	2160 (99%)	14 (1%)	88	94

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	210	LYS
2	C	317	LEU
2	E	153	TRP
2	C	189	ARG
2	E	79	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	144	GLN
1	D	317	ASN
1	D	16	ASN
1	A	191	ASN
1	D	191	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 57 ligands modelled in this entry, 1 is monoatomic - leaving 56 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$
5	P1M	A	701	-	20,20,20	1.69	2 (10%)	27,28,28	1.82	4 (14%)
6	NAG	A	702	1,6	14,14,15	0.37	0	17,19,21	0.58	0
6	NAG	A	703	6	14,14,15	0.26	0	17,19,21	0.43	0
6	NAG	A	704	1,6	14,14,15	0.20	0	17,19,21	0.55	0
6	NAG	A	705	7,6	14,14,15	0.28	0	17,19,21	0.71	1 (5%)
7	BMA	A	706	8,6	11,11,12	0.84	0	15,15,17	0.93	0
8	MAN	A	707	7	11,11,12	0.81	0	15,15,17	1.09	2 (13%)
8	MAN	A	708	7	11,11,12	0.76	0	15,15,17	1.19	2 (13%)
9	Y01	A	709	-	31,31,38	0.61	0	48,48,57	1.43	7 (14%)
9	Y01	A	710	-	31,31,38	0.68	0	48,48,57	1.37	7 (14%)
6	NAG	B	701	2	14,14,15	0.47	0	17,19,21	0.54	0
6	NAG	B	702	2	14,14,15	0.33	0	17,19,21	0.56	0
6	NAG	B	703	2,6	14,14,15	0.52	0	17,19,21	1.08	2 (11%)
6	NAG	B	704	7,6	14,14,15	0.34	0	17,19,21	0.99	1 (5%)
7	BMA	B	705	6	11,11,12	0.77	0	15,15,17	0.91	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	B	706	2,6	14,14,15	0.22	0	17,19,21	0.69	0
6	NAG	B	707	7,6	14,14,15	0.28	0	17,19,21	0.54	0
7	BMA	B	708	8,6	11,11,12	0.86	0	15,15,17	1.21	1 (6%)
8	MAN	B	709	7	11,11,12	0.25	0	15,15,17	0.63	0
8	MAN	B	710	7	11,11,12	0.82	1 (9%)	15,15,17	1.25	2 (13%)
9	Y01	B	711	-	31,31,38	0.66	0	48,48,57	1.20	5 (10%)
9	Y01	B	712	-	31,31,38	0.67	1 (3%)	48,48,57	1.22	5 (10%)
6	NAG	C	701	2	14,14,15	0.48	0	17,19,21	0.54	0
6	NAG	C	702	2	14,14,15	0.27	0	17,19,21	0.65	0
6	NAG	C	703	2,6	14,14,15	0.39	0	17,19,21	1.24	1 (5%)
6	NAG	C	704	7,6	14,14,15	0.31	0	17,19,21	0.68	0
7	BMA	C	705	6	11,11,12	0.83	0	15,15,17	0.97	1 (6%)
6	NAG	C	706	2,6	14,14,15	0.38	0	17,19,21	0.61	0
6	NAG	C	707	7,6	14,14,15	0.38	0	17,19,21	1.06	1 (5%)
7	BMA	C	708	8,6	11,11,12	0.71	0	15,15,17	0.96	0
8	MAN	C	709	7	11,11,12	0.88	1 (9%)	15,15,17	1.11	2 (13%)
8	MAN	C	710	7	11,11,12	0.80	0	15,15,17	1.32	2 (13%)
9	Y01	C	711	-	31,31,38	0.62	0	48,48,57	1.40	6 (12%)
9	Y01	C	712	-	31,31,38	0.66	0	48,48,57	1.27	5 (10%)
5	P1M	D	701	-	20,20,20	1.74	2 (10%)	27,28,28	1.87	5 (18%)
6	NAG	D	702	1,6	14,14,15	0.32	0	17,19,21	0.63	1 (5%)
6	NAG	D	703	6	14,14,15	0.75	1 (7%)	17,19,21	2.22	3 (17%)
6	NAG	D	704	1,6	14,14,15	0.20	0	17,19,21	0.58	0
6	NAG	D	705	7,6	14,14,15	0.28	0	17,19,21	0.78	1 (5%)
7	BMA	D	706	8,6	11,11,12	0.90	0	15,15,17	0.87	0
8	MAN	D	707	7	11,11,12	0.85	0	15,15,17	1.06	2 (13%)
8	MAN	D	708	7	11,11,12	0.87	0	15,15,17	1.10	2 (13%)
9	Y01	D	709	-	31,31,38	0.63	0	48,48,57	1.35	6 (12%)
9	Y01	D	710	-	31,31,38	0.64	0	48,48,57	1.34	5 (10%)
6	NAG	E	701	2	14,14,15	0.55	0	17,19,21	0.97	1 (5%)
6	NAG	E	702	2	14,14,15	0.32	0	17,19,21	0.57	0
6	NAG	E	703	2,6	14,14,15	0.53	0	17,19,21	1.10	1 (5%)
6	NAG	E	704	7,6	14,14,15	0.32	0	17,19,21	0.98	1 (5%)
7	BMA	E	705	6	11,11,12	0.92	1 (9%)	15,15,17	1.30	1 (6%)
6	NAG	E	706	2,6	14,14,15	0.34	0	17,19,21	0.64	1 (5%)
6	NAG	E	707	7,6	14,14,15	0.36	0	17,19,21	1.17	2 (11%)
7	BMA	E	708	8,6	11,11,12	0.93	0	15,15,17	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MAN	E	709	7	11,11,12	1.12	2 (18%)	15,15,17	1.11	2 (13%)
8	MAN	E	710	7	11,11,12	0.78	0	15,15,17	1.14	2 (13%)
9	Y01	E	711	-	31,31,38	0.66	1 (3%)	48,48,57	1.25	4 (8%)
9	Y01	E	712	-	31,31,38	0.65	1 (3%)	48,48,57	1.41	6 (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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	P1M	A	701	-	-	0/4/26/26	0/4/3/3
6	NAG	A	702	1,6	-	1/6/23/26	0/1/1/1
6	NAG	A	703	6	-	2/6/23/26	0/1/1/1
6	NAG	A	704	1,6	-	2/6/23/26	0/1/1/1
6	NAG	A	705	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	706	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	707	7	-	0/2/19/22	0/1/1/1
8	MAN	A	708	7	-	0/2/19/22	0/1/1/1
9	Y01	A	709	-	-	4/10/68/77	0/4/4/4
9	Y01	A	710	-	-	7/10/68/77	0/4/4/4
6	NAG	B	701	2	-	2/6/23/26	0/1/1/1
6	NAG	B	702	2	-	2/6/23/26	0/1/1/1
6	NAG	B	703	2,6	-	3/6/23/26	0/1/1/1
6	NAG	B	704	7,6	-	3/6/23/26	0/1/1/1
7	BMA	B	705	6	-	1/2/19/22	0/1/1/1
6	NAG	B	706	2,6	-	2/6/23/26	0/1/1/1
6	NAG	B	707	7,6	-	2/6/23/26	0/1/1/1
7	BMA	B	708	8,6	-	2/2/19/22	0/1/1/1
8	MAN	B	709	7	-	0/2/19/22	0/1/1/1
8	MAN	B	710	7	-	2/2/19/22	0/1/1/1
9	Y01	B	711	-	-	6/10/68/77	0/4/4/4
9	Y01	B	712	-	-	4/10/68/77	0/4/4/4
6	NAG	C	701	2	-	2/6/23/26	0/1/1/1
6	NAG	C	702	2	-	4/6/23/26	0/1/1/1
6	NAG	C	703	2,6	-	1/6/23/26	0/1/1/1
6	NAG	C	704	7,6	-	3/6/23/26	0/1/1/1
7	BMA	C	705	6	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	706	2,6	-	1/6/23/26	0/1/1/1
6	NAG	C	707	7,6	-	3/6/23/26	0/1/1/1
7	BMA	C	708	8,6	-	0/2/19/22	0/1/1/1
8	MAN	C	709	7	-	2/2/19/22	0/1/1/1
8	MAN	C	710	7	-	0/2/19/22	0/1/1/1
9	Y01	C	711	-	-	6/10/68/77	0/4/4/4
9	Y01	C	712	-	-	6/10/68/77	0/4/4/4
5	P1M	D	701	-	-	3/4/26/26	0/4/3/3
6	NAG	D	702	1,6	-	2/6/23/26	0/1/1/1
6	NAG	D	703	6	-	5/6/23/26	0/1/1/1
6	NAG	D	704	1,6	-	2/6/23/26	0/1/1/1
6	NAG	D	705	7,6	-	0/6/23/26	0/1/1/1
7	BMA	D	706	8,6	-	0/2/19/22	0/1/1/1
8	MAN	D	707	7	-	0/2/19/22	0/1/1/1
8	MAN	D	708	7	-	1/2/19/22	0/1/1/1
9	Y01	D	709	-	-	6/10/68/77	0/4/4/4
9	Y01	D	710	-	-	4/10/68/77	0/4/4/4
6	NAG	E	701	2	-	2/6/23/26	0/1/1/1
6	NAG	E	702	2	-	2/6/23/26	0/1/1/1
6	NAG	E	703	2,6	-	3/6/23/26	0/1/1/1
6	NAG	E	704	7,6	-	1/6/23/26	0/1/1/1
7	BMA	E	705	6	-	1/2/19/22	0/1/1/1
6	NAG	E	706	2,6	-	2/6/23/26	0/1/1/1
6	NAG	E	707	7,6	-	3/6/23/26	0/1/1/1
7	BMA	E	708	8,6	-	0/2/19/22	0/1/1/1
8	MAN	E	709	7	-	0/2/19/22	0/1/1/1
8	MAN	E	710	7	-	0/2/19/22	0/1/1/1
9	Y01	E	711	-	-	4/10/68/77	0/4/4/4
9	Y01	E	712	-	-	6/10/68/77	0/4/4/4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	701	P1M	C3-N8	5.22	1.53	1.47
5	A	701	P1M	C3-N8	5.17	1.53	1.47
5	D	701	P1M	C7-N8	4.17	1.52	1.47
5	A	701	P1M	C7-N8	3.71	1.51	1.47
8	E	709	MAN	C1-C2	2.61	1.58	1.52

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	703	NAG	C2-N2-C7	7.73	134.00	122.92
5	A	701	P1M	BR1-C11-C10	-5.50	114.80	119.81
5	D	701	P1M	C2-C1-N9	4.61	117.69	110.57
9	C	711	Y01	CBI-CBE-CBB	-4.35	112.56	119.48
5	D	701	P1M	BR1-C11-C10	-4.22	115.96	119.81

There are no chirality outliers.

5 of 121 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	702	NAG	O7-C7-N2-C2
5	D	701	P1M	C2-C1-N9-C10
5	D	701	P1M	C11-C10-N9-C1
5	D	701	P1M	C15-C10-N9-C1
9	D	710	Y01	CAC-CBB-CBE-CBI

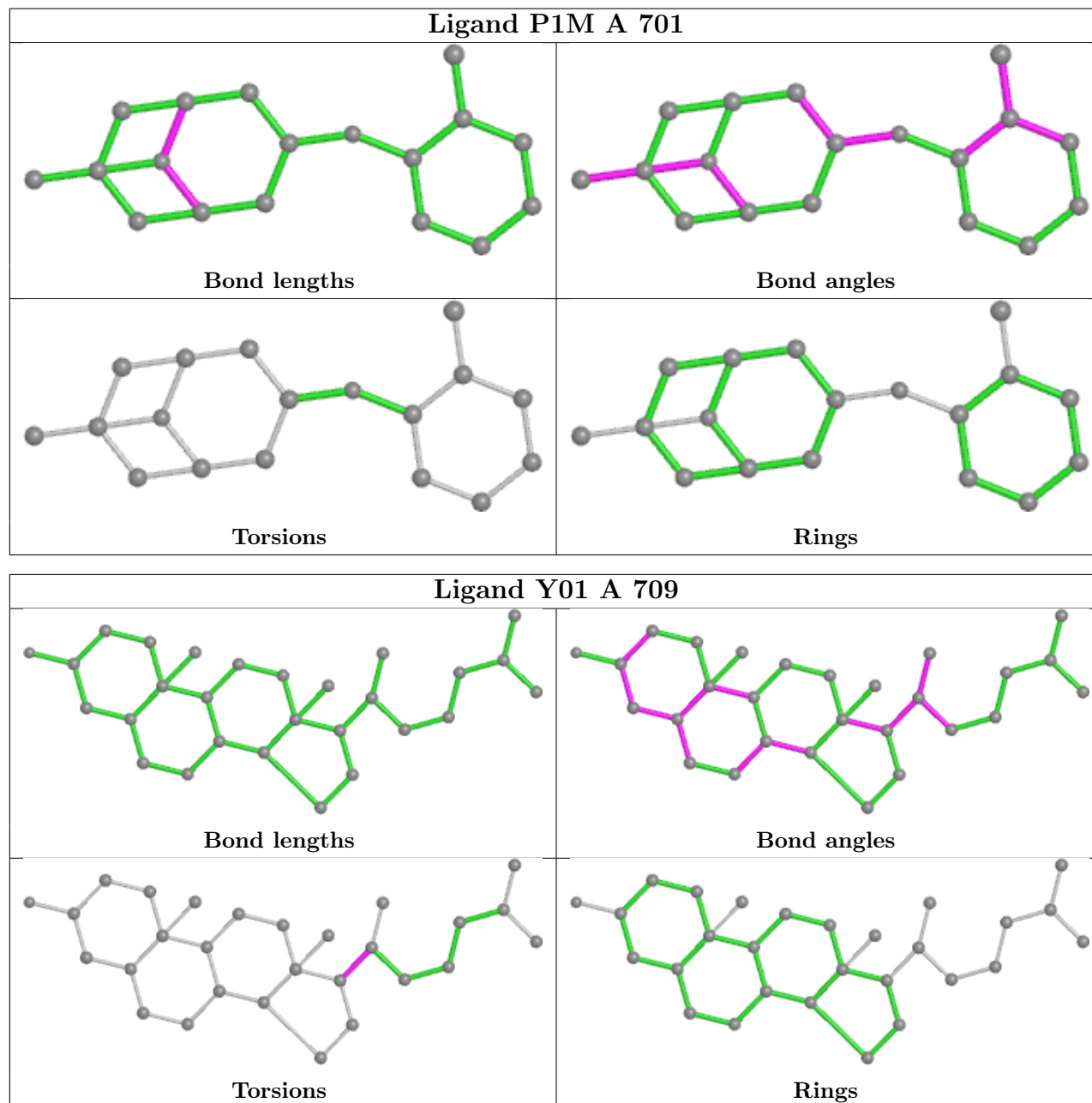
There are no ring outliers.

18 monomers are involved in 27 short contacts:

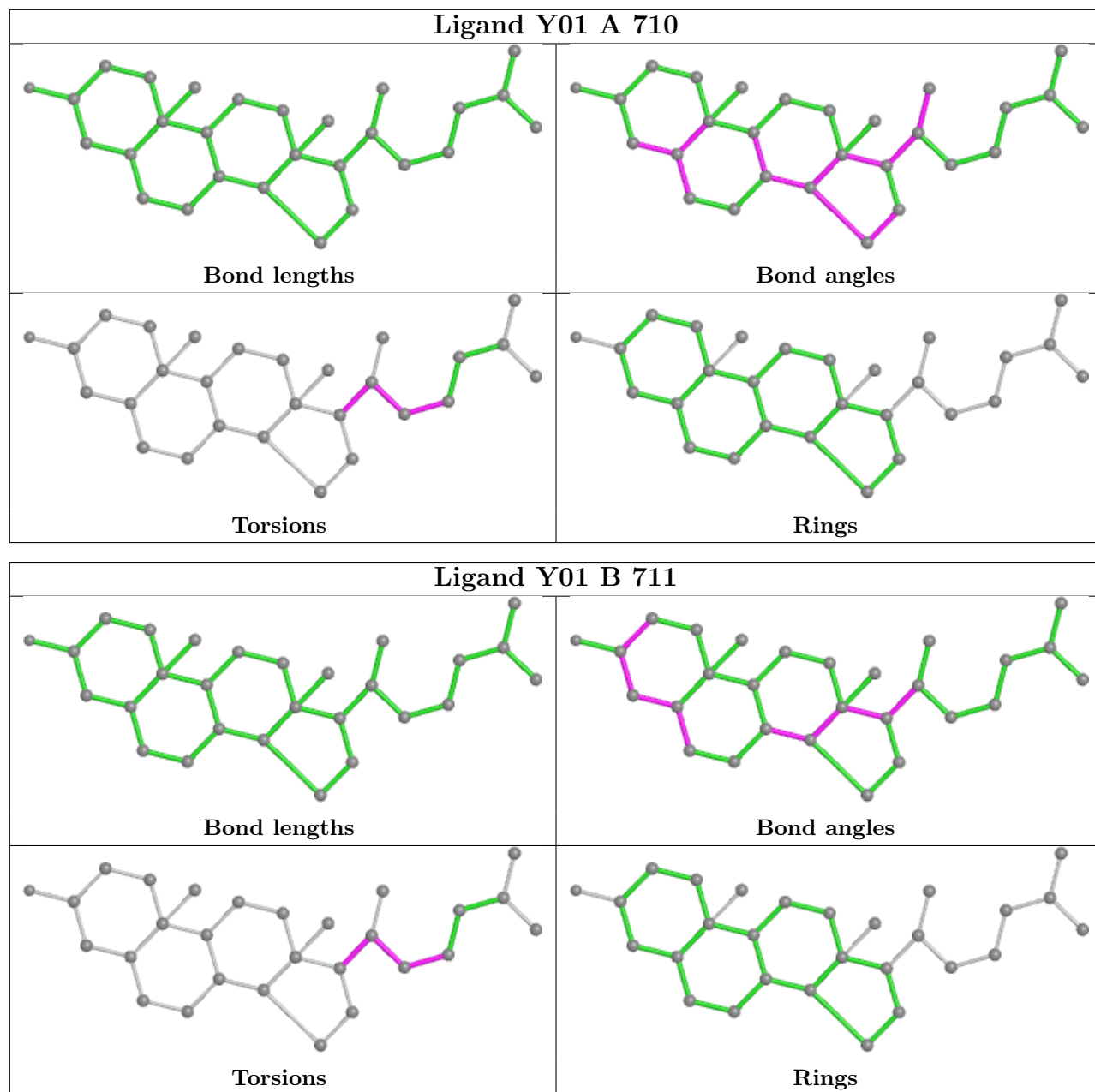
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	P1M	2	0
9	A	709	Y01	2	0
9	A	710	Y01	2	0
9	B	711	Y01	1	0
9	B	712	Y01	1	0
6	C	702	NAG	3	0
6	C	703	NAG	2	0
6	C	704	NAG	1	0
7	C	708	BMA	1	0
8	C	709	MAN	1	0
9	C	711	Y01	2	0
9	C	712	Y01	2	0
9	D	709	Y01	1	0
9	D	710	Y01	3	0
7	E	708	BMA	1	0
8	E	709	MAN	1	0
9	E	711	Y01	2	0
9	E	712	Y01	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

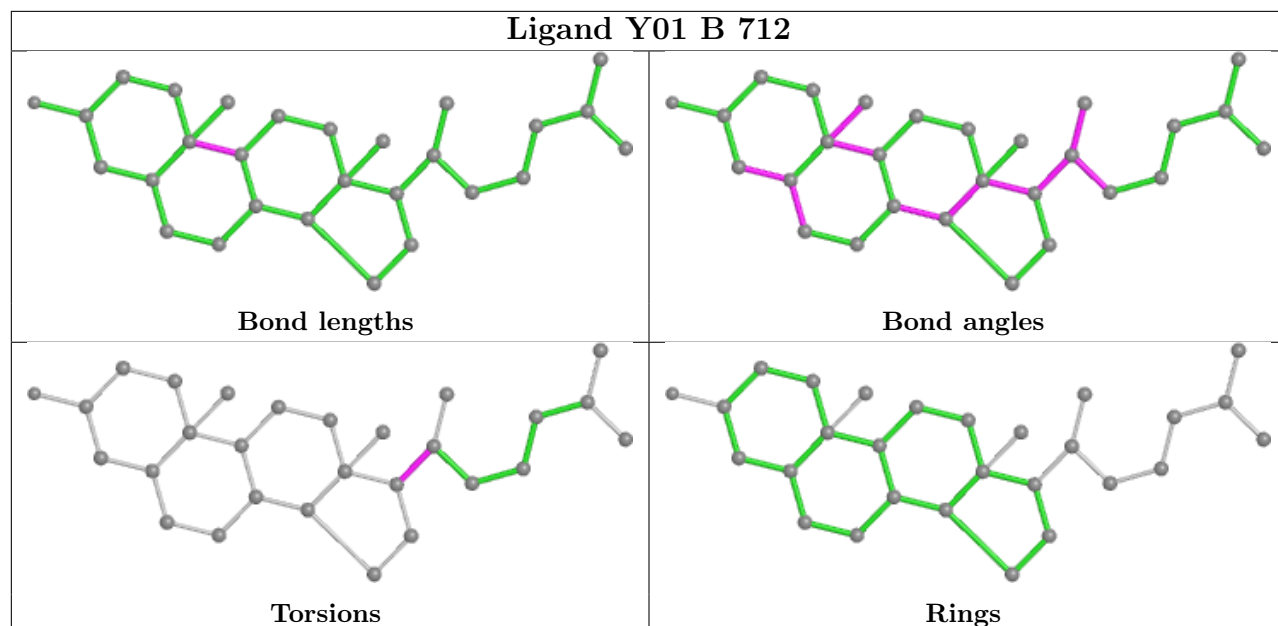
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.



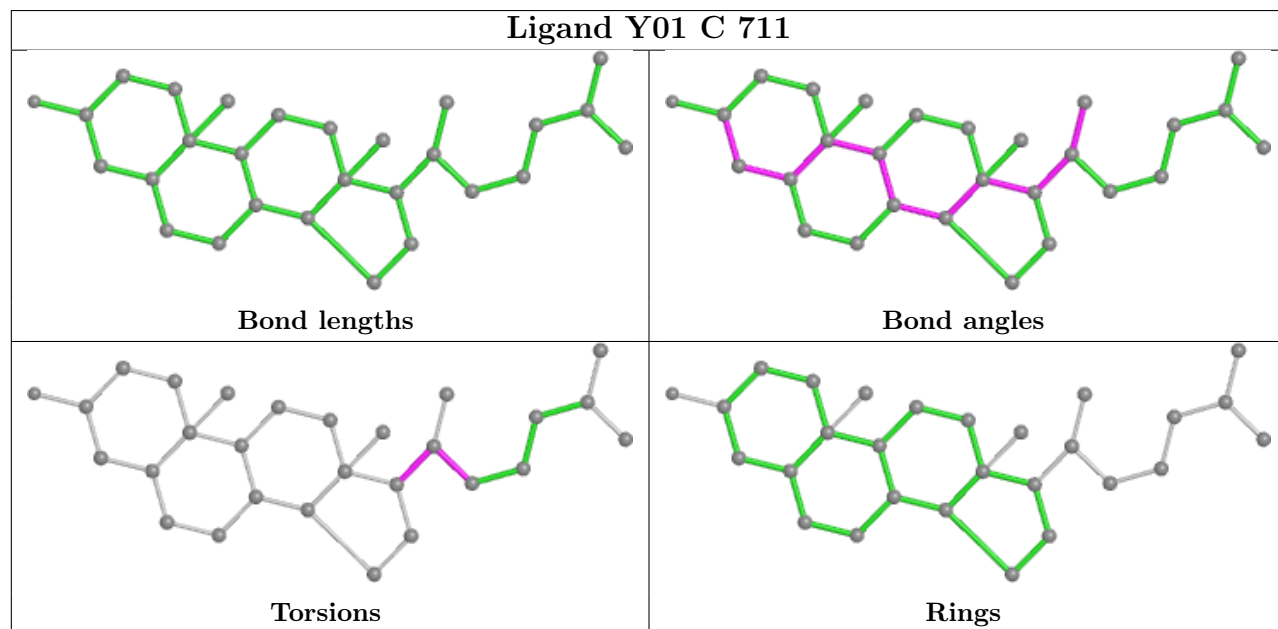




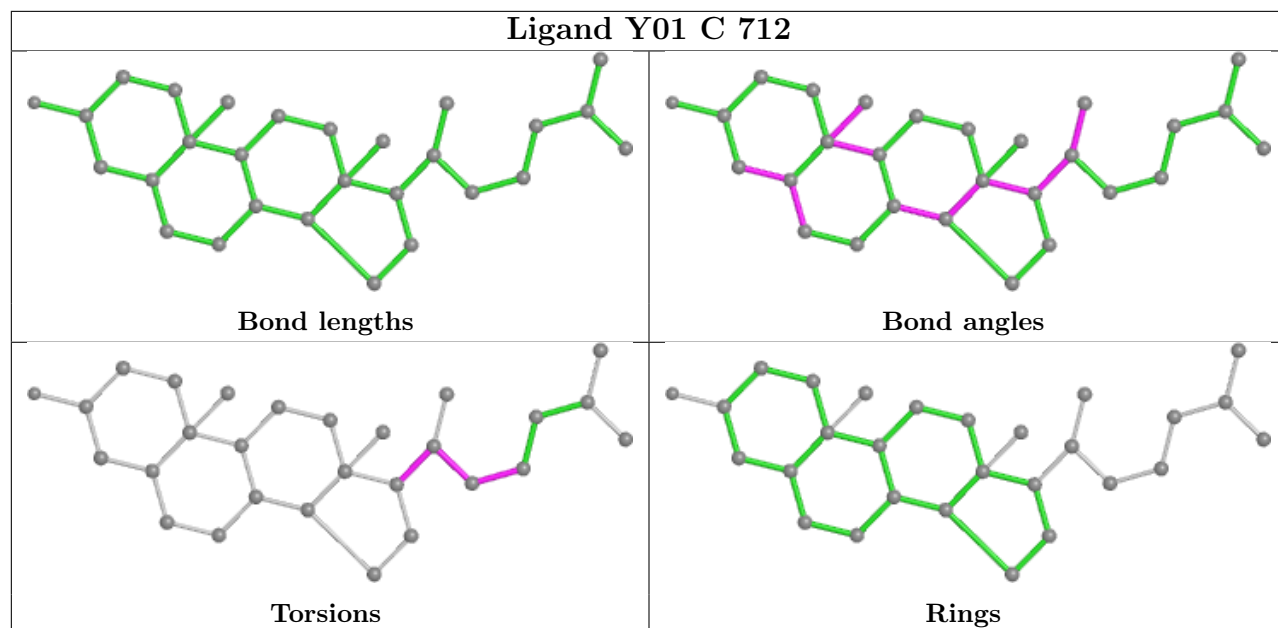
## Ligand Y01 B 712



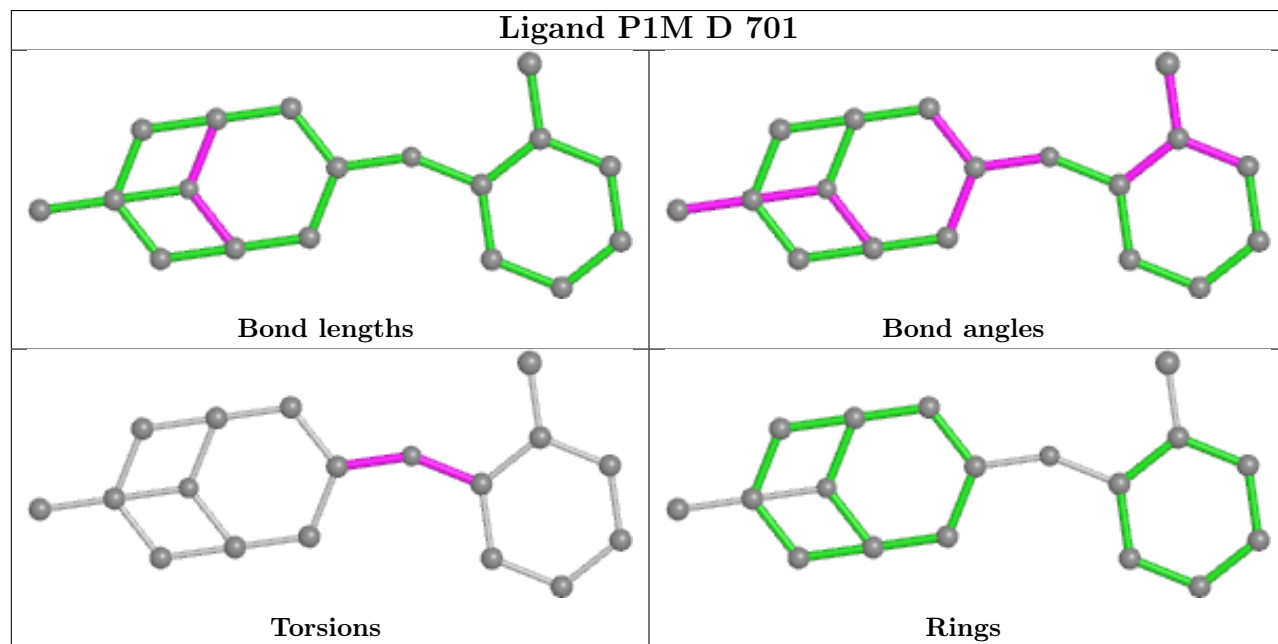
## Ligand Y01 C 711



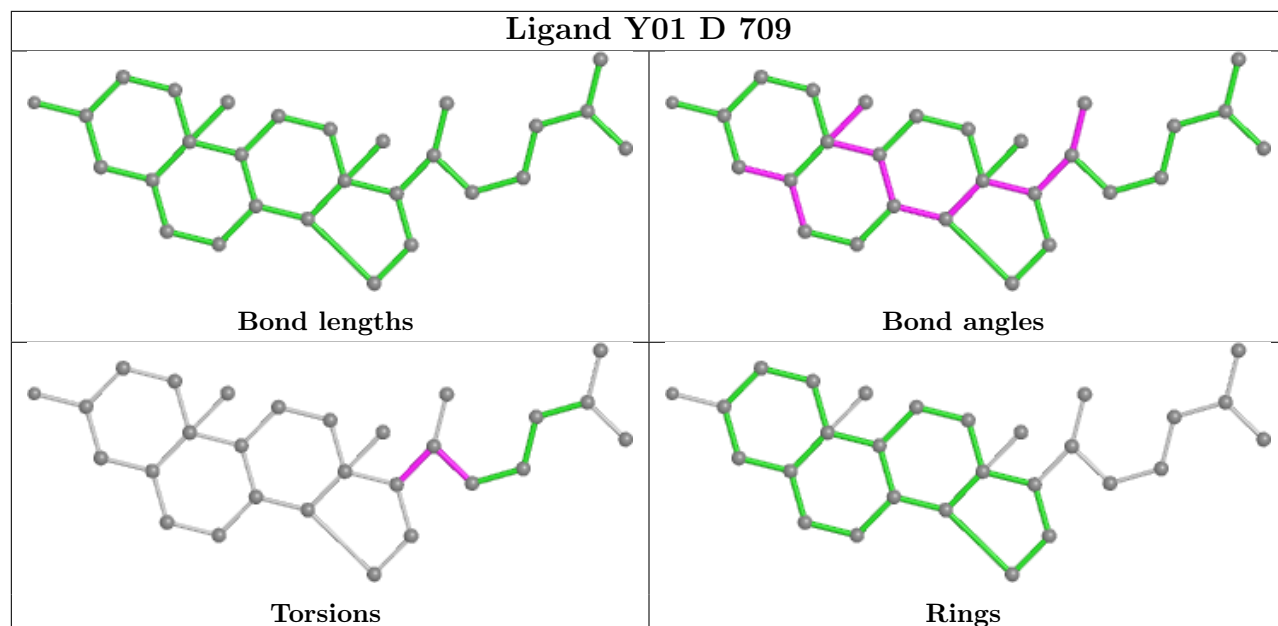
## Ligand Y01 C 712



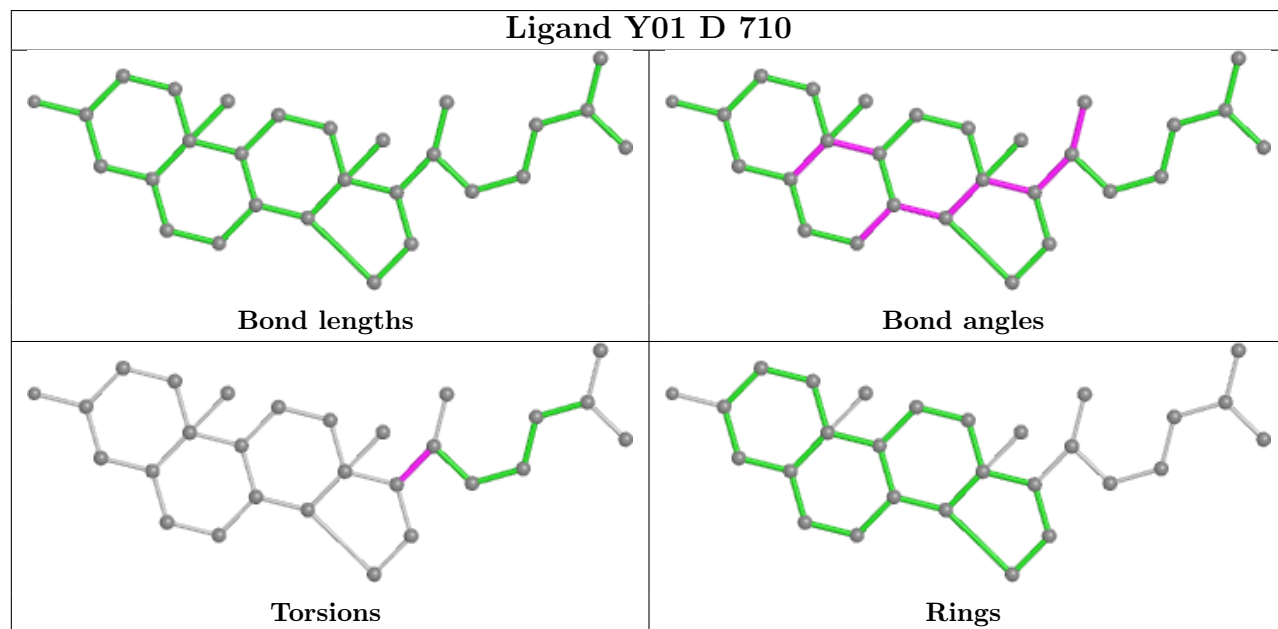
## Ligand P1M D 701

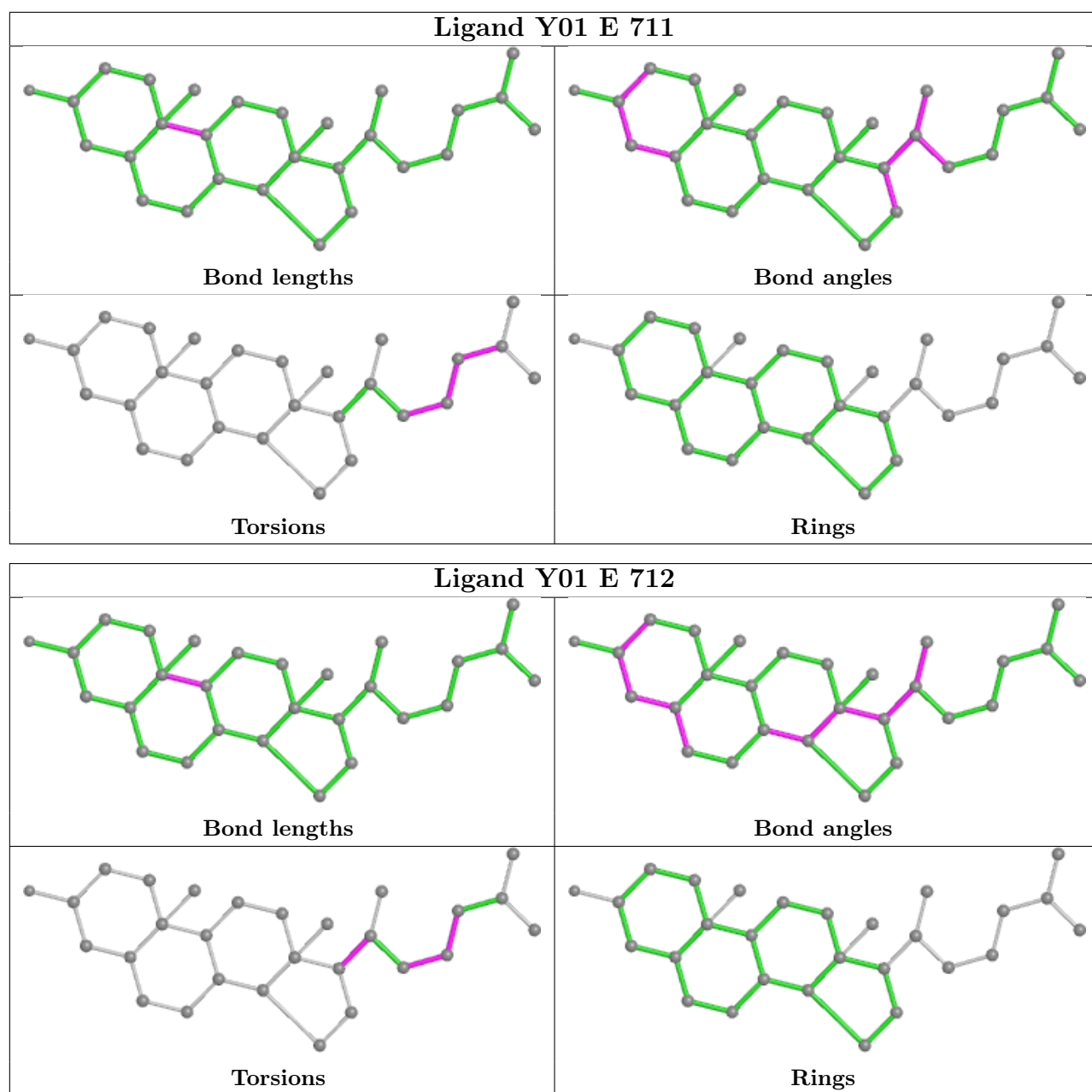


## Ligand Y01 D 709



## Ligand Y01 D 710





## 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.