



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Sep 10, 2019 – 06:47 PM EDT

PDB ID : 6PV7
EMDB ID: : EMD-20487
Title : Human alpha3beta4 nicotinic acetylcholine receptor in complex with nicotine
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 : 3.34 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

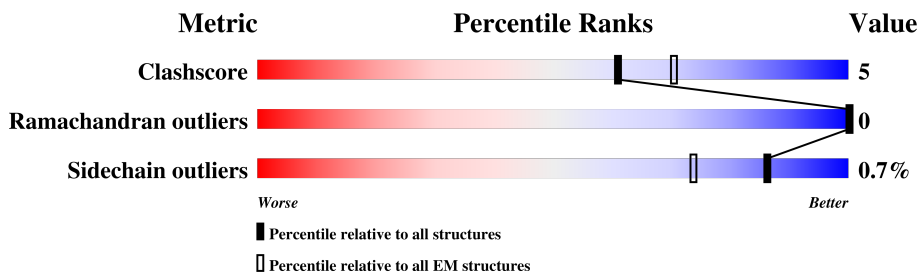
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.34 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 ≥ 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	67% 6% 26%
1	D	525	65% 9% 26%
2	B	538	63% 9% 28%
2	C	538	59% 12% 28%
2	E	538	63% 9% 28%
3	F	219	48% 5% 47%
3	H	219	51% 47%
4	G	213	41% 8% 51%
4	I	213	45% 5% 51%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 20048 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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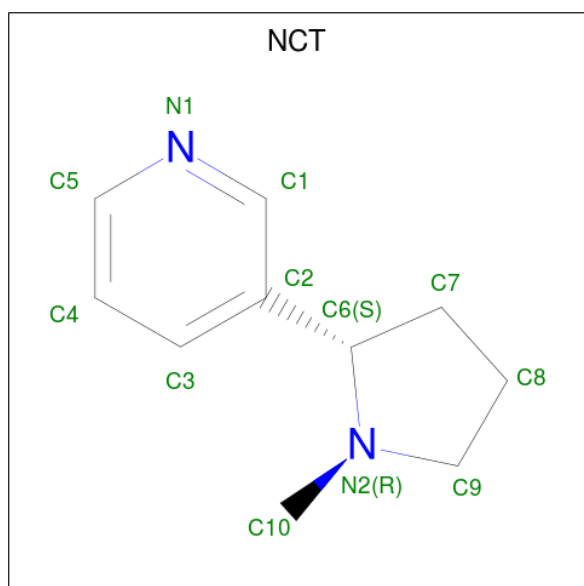
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	117	Total	C	N	O	S	0	0
			911	580	147	179	5		

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

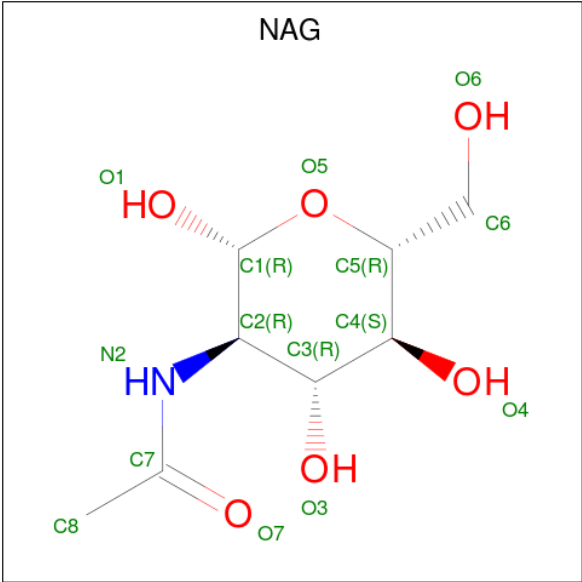
Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	105	Total	C	N	O	S	0	0
			792	494	131	160	7		
4	I	105	Total	C	N	O	S	0	0
			792	494	131	160	7		

- Molecule 5 is (S)-3-(1-METHYLPYRROLIDIN-2-YL)PYRIDINE (three-letter code: NCT) (formula: $C_{10}H_{14}N_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	N	0
			12	10	2	
5	D	1	Total	C	N	0
			12	10	2	

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



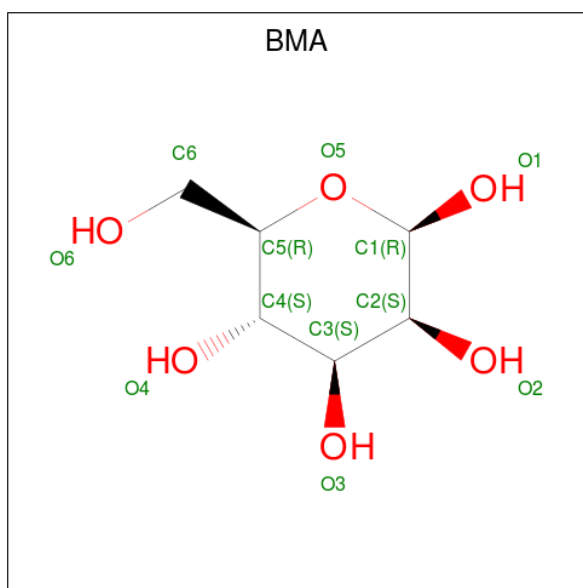
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			56	32	4	20	
6	A	1	Total	C	N	O	0
			56	32	4	20	
6	A	1	Total	C	N	O	0
			56	32	4	20	
6	A	1	Total	C	N	O	0
			56	32	4	20	
6	B	1	Total	C	N	O	0
			84	48	6	30	
6	B	1	Total	C	N	O	0
			84	48	6	30	
6	B	1	Total	C	N	O	0
			84	48	6	30	
6	B	1	Total	C	N	O	0
			84	48	6	30	
6	B	1	Total	C	N	O	0
			84	48	6	30	
6	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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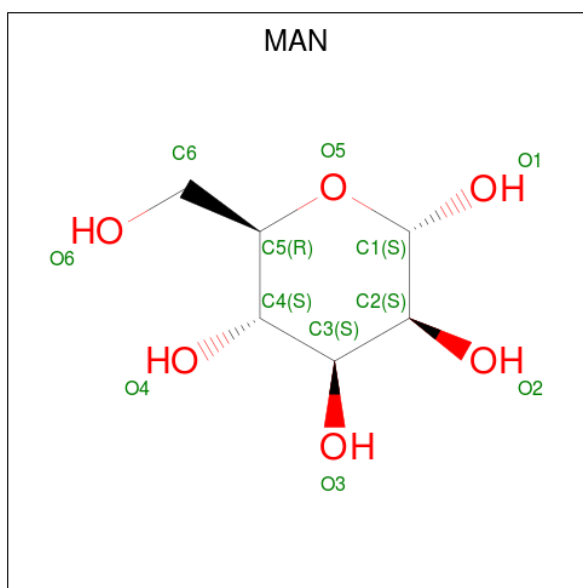
Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			84	48	6	30	
6	C	1	Total	C	N	O	0
			84	48	6	30	
6	D	1	Total	C	N	O	0
			56	32	4	20	
6	D	1	Total	C	N	O	0
			56	32	4	20	
6	D	1	Total	C	N	O	0
			56	32	4	20	
6	D	1	Total	C	N	O	0
			56	32	4	20	
6	E	1	Total	C	N	O	0
			84	48	6	30	
6	E	1	Total	C	N	O	0
			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: $C_6H_{12}O_6$).



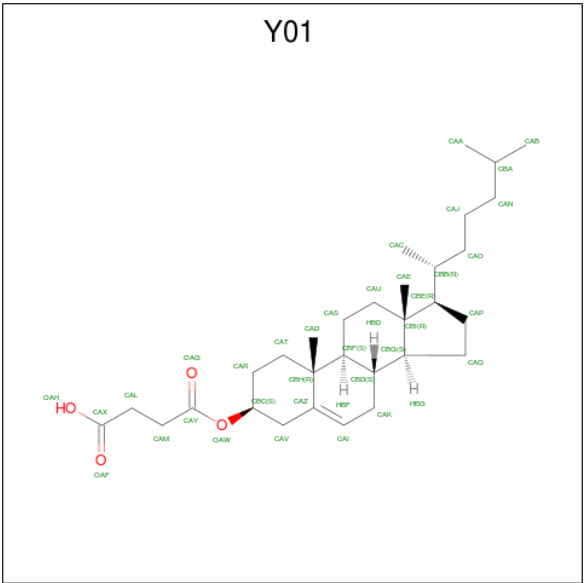
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			22	12	10	
8	A	1	Total	C	O	0
			22	12	10	
8	B	1	Total	C	O	0
			22	12	10	
8	B	1	Total	C	O	0
			22	12	10	

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

- Molecule 9 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



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

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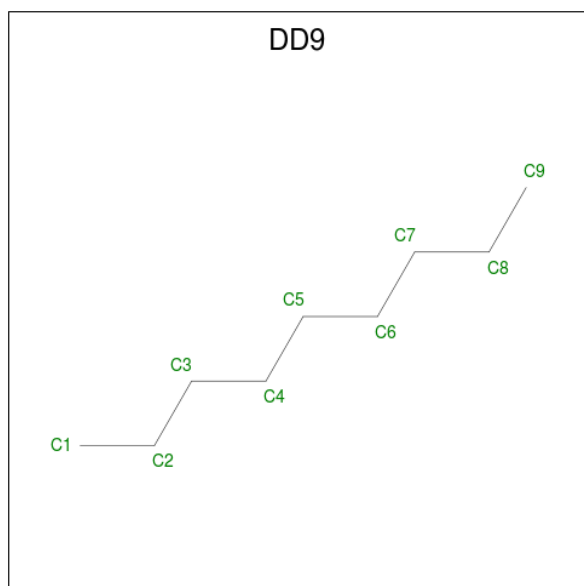
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Mol	Chain	Residues	Atoms			AltConf
9	C	1	Total	C	O	0
			56	54	2	
9	D	1	Total	C	O	0
			56	54	2	
9	D	1	Total	C	O	0
			56	54	2	
9	E	1	Total	C	O	0
			56	54	2	
9	E	1	Total	C	O	0
			56	54	2	

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

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

- Molecule 11 is nonane (three-letter code: DD9) (formula: C₉H₂₀).



Mol	Chain	Residues	Atoms		AltConf
11	C	1	Total	C	0
			9	9	

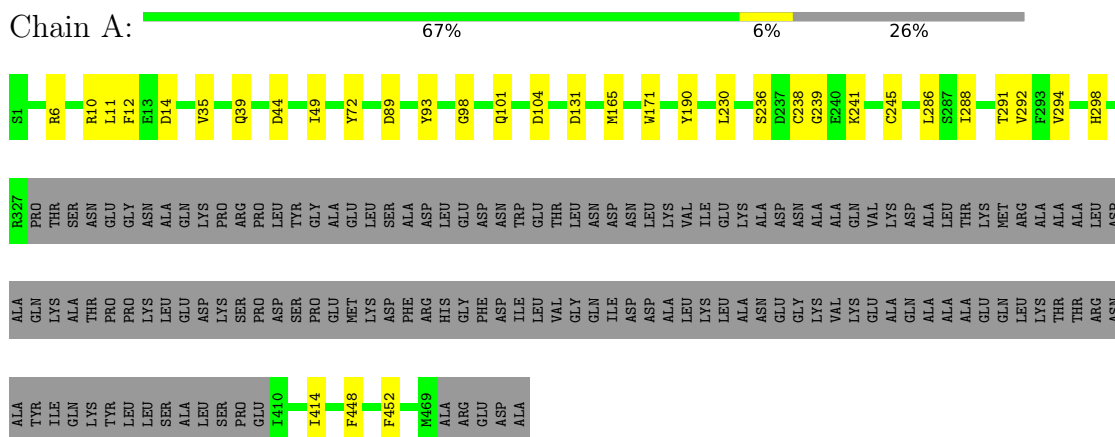
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	B	2	Total 2	O 2	0
12	C	2	Total 2	O 2	0
12	D	1	Total 1	O 1	0
12	E	3	Total 3	O 3	0

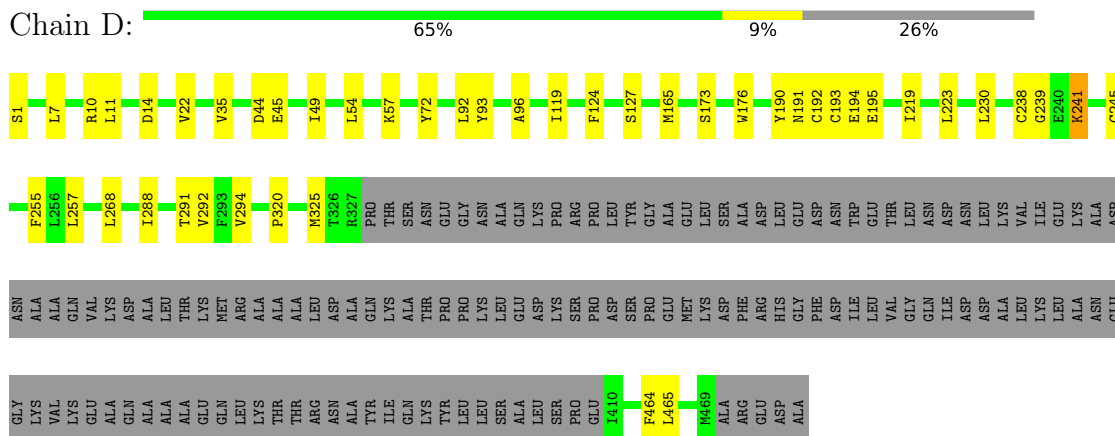
3 Residue-property plots

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.

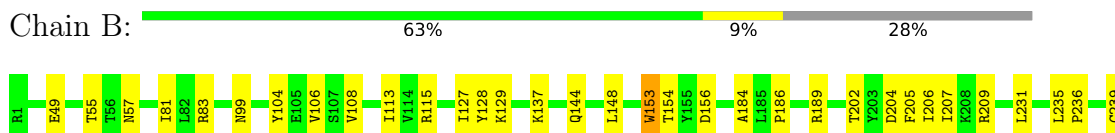
- Molecule 1: Fusion protein of Neuronal acetylcholine receptor subunit alpha-3 and Soluble cytochrome b562

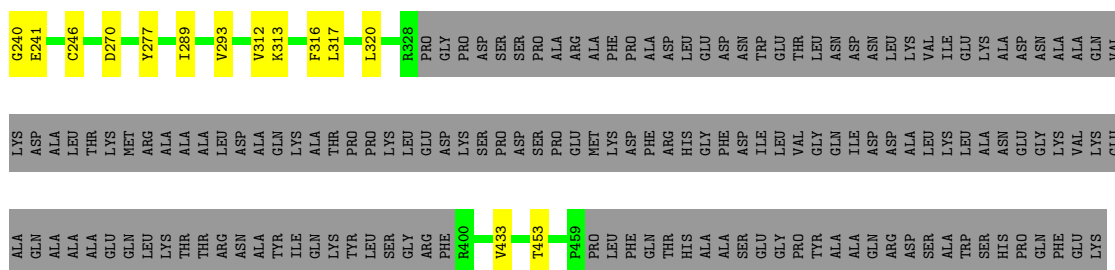


- Molecule 1: Fusion protein of Neuronal acetylcholine receptor subunit alpha-3 and Soluble cytochrome b562

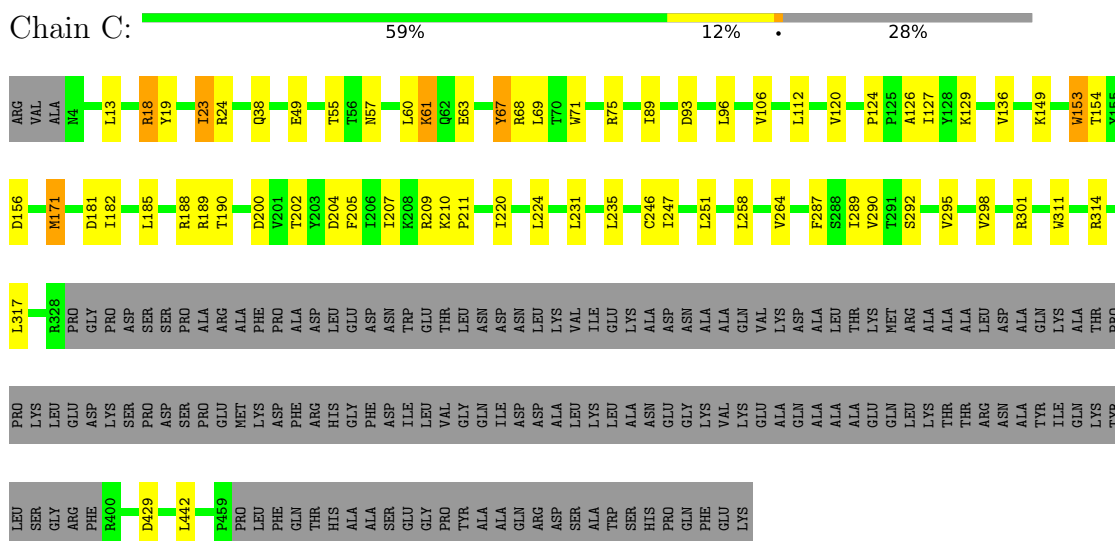


- Molecule 2: Fusion protein of Neuronal acetylcholine receptor subunit beta-4 and Soluble cytochrome b562

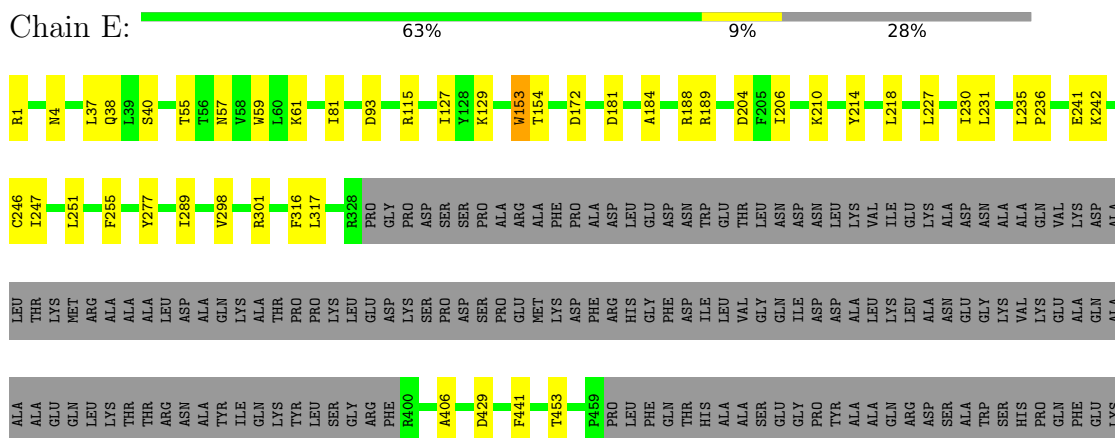




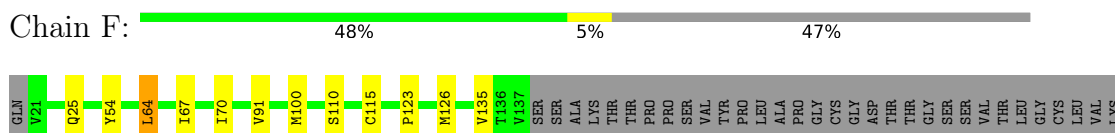
- Molecule 2: Fusion protein of Neuronal acetylcholine receptor subunit beta-4 and Soluble cytochrome b562



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



- Molecule 3: IgG2b Fab heavy chain



GLY	TYR	PHE	PRO	PRO	GLU	SER	VAL	THR	THR	TRP	ASN	SER	GLY	SER	SER	LEU	HIS	THR	PHE	PRO	ALA	LEU	LEU	GLN	SER	SER	GLY	LEU	THR	THR	MET	SER	SER	SER	VAL	THR	THR	PRO	SER	SER	TRP	PRO	CYS	GLN	THR	VAL	ALA	HIS	PRO	ALA	SER	SER
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THR
THR
VAL
ASP
LYS
LYS
LEU
GLU
PRO

- Molecule 3: IgG2b Fab heavy chain

Chain H: 51% . 47%

CLN	V21		R57	I66	I67	M100	S110	V135	T136	V137	SER	SER	ALA	LYS	THR	THR	PRO	PRO	SER	SER	VAL	TYR	LEU	ALA	ALA	GLY	CYS	GLY	ASP	THR	THR	GLY	SER	SER	VAL	VAL	LYS	GLY	TYR	PHE	PRO	GLU	SER	SER	VAL	THR	THR	TRP	ASN	SER
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GLY	SER	LEU	SER	SER	SER	VAL	HIS	THR	PHE	PRO	ALA	LEU	GLN	SER	GLY	LEU	TYR	THR	MET	SER	SER	SER	VAL	VAL	PRO	SER	SER	THR	THR	TRP	PRO	SER	SER	GLN	THR	THR	VAL	THR	CYS	SER	VAL	ALA	ALA	HIS	PRO	ALA	SER	SER	SER	THR	THR	THR	THR	VAL	ASP	LYS	LYS	LEU	LEU	GLU	PRO
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- Molecule 4: Kappa Fab light chain

Chain G:  41% 8% 51%

G23		P37	G38	V41	W66	I69	Y70	D71	R82		S97	M99	E100	D103	A104	W112	L117	F118	T119	L125	E126	L127	LVS	ARG	ALA	ASP	ALA	ALA	ALA	ALA	PRO	THR	THR	VAL	ILE	SER	LEU	GLN	GLU	SER	SER	SER	THR	GLY	GLY	ALA	ALA	VAL	VAL
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CYS PHE LEU ASN ASN PHE TYR PRO LYS ASP ASP ILE ASN VAL VAL LYS TRP LYS LYS ILE ASP GLY SER SER ARG ARG GLN ASN GLY VAL LEU LEU ASN ASN SER SER TRP THR THR GLN ASP ASP ASP SER SER LYS LYS ASP SER SER THR TYR TYR SER SER MET SER SER THR THR LEU LEU LEU LEU LEU THR THR LYS ASP ASP GLU TYR TYR GLU ARG HIS ASN ASN SER SER TYR THR

CYS
GLU
ALA
THR
HIS
LYS
THR
SER
THR
SER
PRO
ILE
VAL
LYS
SER
PHE
ASN
ARG
ASN
GLU
CYS

- Molecule 4: Kappa Fab light chain

Chain I: 45% 5% 51%

V23	V41	W56	I69	Y70	D71	R82	I96	S97	S98	A104	L117	L125	L127	LYS	ARG	ALA	ASP	ALA	ALA	ALA	ALA	PRO	THR	THR	VAL	SER	SER	ILE	PHE	PRO	PRO	PRO	SER	SER	SER	GLU	GLN	LEU	THR	SER	SER	GLY	GLY	ALA	SER	VAL	VAL	CYS	PHE	LEU	ASN	ASN	TYR	PRO	PRO	LYS	ASP
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[illegible]

PRO
ILE
VAL
LYS
SER
PHE
ASN
ARG
ASN
GLU
CYS

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	112737	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 ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	46730	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: DD9, Y01, NAG, NA, NCT, BMA, 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	0.35	0/3252	0.57	1/4431 (0.0%)
1	D	0.37	1/3252 (0.0%)	0.58	3/4431 (0.1%)
2	B	0.33	0/3228	0.61	1/4402 (0.0%)
2	C	0.35	0/3205	0.61	2/4371 (0.0%)
2	E	0.35	0/3228	0.61	1/4402 (0.0%)
3	F	0.32	0/936	0.55	1/1273 (0.1%)
3	H	0.34	0/936	0.55	0/1273
4	G	0.33	0/811	0.58	0/1099
4	I	0.33	0/811	0.57	0/1099
All	All	0.35	1/19659 (0.0%)	0.59	9/26781 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	241	LYS	C-N	5.96	1.47	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	96	LEU	CA-CB-CG	6.45	130.13	115.30
2	E	231	LEU	CA-CB-CG	6.19	129.54	115.30
2	B	231	LEU	CA-CB-CG	5.94	128.96	115.30
1	D	230	LEU	CA-CB-CG	5.72	128.45	115.30
1	D	241	LYS	O-C-N	-5.59	113.76	122.70

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	26	0
1	D	3167	0	3214	32	0
2	B	3149	0	3203	32	0
2	C	3126	0	3173	50	0
2	E	3149	0	3203	32	0
3	F	911	0	865	9	0
3	H	911	0	865	3	0
4	G	792	0	757	11	0
4	I	792	0	757	6	0
5	A	12	0	14	0	0
5	D	12	0	14	0	0
6	A	56	0	49	0	0
6	B	84	0	74	1	0
6	C	84	0	74	1	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	1	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	1	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	4	0
9	C	56	0	90	5	0
9	D	56	0	90	4	0
9	E	56	0	90	6	0
10	A	1	0	0	0	0
11	C	9	0	20	0	0
12	B	2	0	0	0	0
12	C	2	0	0	0	0
12	D	1	0	0	0	0
12	E	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20048	0	20239	200	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 200 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:C:171:MET:SD	2:C:182:ILE:CD1	2.64	0.85
2:B:313:LYS:HA	2:B:317:LEU:HD12	1.60	0.84
1:A:239:GLY:O	2:B:241:GLU:OE2	1.95	0.83
2:C:171:MET:SD	2:C:182:ILE:HD12	2.22	0.79
2:E:153:TRP:CD1	2:E:154:THR:HG23	2.26	0.70

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%)	369 (96%)	14 (4%)	0	100	100
2	B	384/538 (71%)	361 (94%)	23 (6%)	0	100	100
2	C	381/538 (71%)	360 (94%)	21 (6%)	0	100	100
2	E	384/538 (71%)	367 (96%)	17 (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%)	95 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2351/3528 (67%)	2233 (95%)	118 (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%)	359 (100%)	0	100	100
2	B	362/482 (75%)	360 (99%)	2 (1%)	87	94
2	C	360/482 (75%)	352 (98%)	8 (2%)	55	79
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	88
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%)	2159 (99%)	15 (1%)	86	92

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	67	TYR
2	C	153	TRP
2	E	189	ARG
2	C	61	LYS
2	E	153	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	144	GLN
1	D	317	ASN
1	D	191	ASN
1	A	298	HIS
1	D	298	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 1 is monoatomic - leaving 57 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	NCT	A	701	-	13,13,13	0.49	0	17,17,17	1.60	5 (29%)
6	NAG	A	702	1,6	14,14,15	0.28	0	17,19,21	0.66	1 (5%)
6	NAG	A	703	6	14,14,15	0.40	0	17,19,21	0.41	0
6	NAG	A	704	1,6	14,14,15	0.19	0	17,19,21	0.59	0
6	NAG	A	705	7,6	14,14,15	0.32	0	17,19,21	0.60	0
7	BMA	A	706	8,6	11,11,12	0.70	0	15,15,17	0.89	0
8	MAN	A	707	7	11,11,12	0.86	0	15,15,17	1.07	2 (13%)
8	MAN	A	708	7	11,11,12	0.79	0	15,15,17	1.22	2 (13%)
9	Y01	A	709	-	31,31,38	0.62	0	48,48,57	1.41	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	Y01	A	710	-	31,31,38	0.71	1 (3%)	48,48,57	1.22	5 (10%)
6	NAG	B	701	2	14,14,15	0.44	0	17,19,21	0.56	0
6	NAG	B	702	2	14,14,15	0.32	0	17,19,21	0.56	0
6	NAG	B	703	2,6	14,14,15	0.55	0	17,19,21	1.06	2 (11%)
6	NAG	B	704	7,6	14,14,15	0.39	0	17,19,21	1.01	1 (5%)
7	BMA	B	705	6	11,11,12	0.83	0	15,15,17	0.92	1 (6%)
6	NAG	B	706	2,6	14,14,15	0.26	0	17,19,21	0.66	1 (5%)
6	NAG	B	707	7,6	14,14,15	0.26	0	17,19,21	0.55	0
7	BMA	B	708	8,6	11,11,12	0.26	0	15,15,17	0.72	1 (6%)
8	MAN	B	709	7	11,11,12	0.25	0	15,15,17	0.69	0
8	MAN	B	710	7	11,11,12	1.00	1 (9%)	15,15,17	1.25	2 (13%)
9	Y01	B	711	-	31,31,38	0.66	0	48,48,57	1.21	6 (12%)
9	Y01	B	712	-	31,31,38	0.67	1 (3%)	48,48,57	1.26	4 (8%)
6	NAG	C	701	2	14,14,15	0.45	0	17,19,21	0.56	0
6	NAG	C	702	2	14,14,15	0.29	0	17,19,21	0.50	0
6	NAG	C	703	2,6	14,14,15	0.31	0	17,19,21	0.97	1 (5%)
6	NAG	C	704	7,6	14,14,15	0.28	0	17,19,21	0.61	0
7	BMA	C	705	6	11,11,12	0.79	0	15,15,17	0.98	1 (6%)
6	NAG	C	706	2,6	14,14,15	0.49	0	17,19,21	0.65	1 (5%)
6	NAG	C	707	7,6	14,14,15	0.34	0	17,19,21	1.08	1 (5%)
7	BMA	C	708	8,6	11,11,12	0.73	0	15,15,17	0.97	0
8	MAN	C	709	7	11,11,12	0.99	1 (9%)	15,15,17	1.11	2 (13%)
8	MAN	C	710	7	11,11,12	0.76	0	15,15,17	1.26	2 (13%)
9	Y01	C	711	-	31,31,38	0.63	0	48,48,57	1.40	7 (14%)
9	Y01	C	712	-	31,31,38	0.67	1 (3%)	48,48,57	1.35	5 (10%)
11	DD9	C	713	-	8,8,8	0.32	0	7,7,7	0.78	0
5	NCT	D	701	-	13,13,13	0.52	0	17,17,17	1.64	5 (29%)
6	NAG	D	702	1,6	14,14,15	0.34	0	17,19,21	0.62	1 (5%)
6	NAG	D	703	6	14,14,15	0.80	1 (7%)	17,19,21	2.21	3 (17%)
6	NAG	D	704	1,6	14,14,15	0.19	0	17,19,21	0.63	0
6	NAG	D	705	7,6	14,14,15	0.27	0	17,19,21	0.76	1 (5%)
7	BMA	D	706	8,6	11,11,12	0.75	0	15,15,17	0.90	1 (6%)
8	MAN	D	707	7	11,11,12	0.80	0	15,15,17	1.04	2 (13%)
8	MAN	D	708	7	11,11,12	0.84	0	15,15,17	1.09	2 (13%)
9	Y01	D	709	-	31,31,38	0.65	0	48,48,57	1.36	6 (12%)
9	Y01	D	710	-	31,31,38	0.63	0	48,48,57	1.41	7 (14%)
6	NAG	E	701	2	14,14,15	0.56	0	17,19,21	0.96	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	E	702	2	14,14,15	0.37	0	17,19,21	0.57	0
6	NAG	E	703	2,6	14,14,15	0.51	0	17,19,21	1.07	1 (5%)
6	NAG	E	704	7,6	14,14,15	0.35	0	17,19,21	1.01	1 (5%)
7	BMA	E	705	6	11,11,12	0.78	0	15,15,17	1.38	1 (6%)
6	NAG	E	706	2,6	14,14,15	0.33	0	17,19,21	0.71	1 (5%)
6	NAG	E	707	7,6	14,14,15	0.26	0	17,19,21	1.24	3 (17%)
7	BMA	E	708	8,6	11,11,12	0.69	0	15,15,17	0.97	0
8	MAN	E	709	7	11,11,12	1.12	1 (9%)	15,15,17	1.05	0
8	MAN	E	710	7	11,11,12	0.80	0	15,15,17	1.12	2 (13%)
9	Y01	E	711	-	31,31,38	0.64	0	48,48,57	1.28	8 (16%)
9	Y01	E	712	-	31,31,38	0.67	0	48,48,57	1.36	4 (8%)

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	NCT	A	701	-	-	0/4/14/14	0/2/2/2
6	NAG	A	702	1,6	-	2/6/23/26	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	-	1/6/23/26	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	Y01	B	711	-	-	7/10/68/77	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	-	2/6/23/26	0/1/1/1
6	NAG	C	703	2,6	-	1/6/23/26	0/1/1/1
6	NAG	C	704	7,6	-	1/6/23/26	0/1/1/1
7	BMA	C	705	6	-	1/2/19/22	0/1/1/1
6	NAG	C	706	2,6	-	2/6/23/26	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	-	-	5/10/68/77	0/4/4/4
11	DD9	C	713	-	-	0/6/6/6	-
5	NCT	D	701	-	-	0/4/14/14	0/2/2/2
6	NAG	D	702	1,6	-	2/6/23/26	0/1/1/1
6	NAG	D	703	6	-	3/6/23/26	0/1/1/1
6	NAG	D	704	1,6	-	0/6/23/26	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	-	-	5/10/68/77	0/4/4/4
6	NAG	E	701	2	-	3/6/23/26	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	-	3/6/23/26	0/1/1/1
7	BMA	E	705	6	-	1/2/19/22	0/1/1/1
6	NAG	E	706	2,6	-	0/6/23/26	0/1/1/1
6	NAG	E	707	7,6	-	3/6/23/26	0/1/1/1
7	BMA	E	708	8,6	-	1/2/19/22	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 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	710	MAN	C1-C2	2.90	1.58	1.52
8	E	709	MAN	C1-C2	2.82	1.58	1.52
8	C	709	MAN	C1-C2	2.64	1.58	1.52
6	D	703	NAG	C1-C2	2.35	1.55	1.52
9	A	710	Y01	CBH-CBF	-2.17	1.52	1.56

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	703	NAG	C2-N2-C7	7.66	133.89	122.92
9	C	712	Y01	CBI-CBE-CBB	-4.06	113.01	119.48
9	C	711	Y01	CBI-CBE-CBB	-4.05	113.03	119.48
9	E	712	Y01	CBI-CBE-CBB	-3.88	113.31	119.48
8	C	710	MAN	C1-O5-C5	3.84	117.42	112.20

There are no chirality outliers.

5 of 114 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	710	Y01	CAC-CBB-CBE-CBI
9	E	712	Y01	CAC-CBB-CBE-CBI
9	C	712	Y01	CAC-CBB-CBE-CBI
9	C	711	Y01	CAC-CBB-CBE-CBI
9	B	712	Y01	CAC-CBB-CBE-CAP

There are no ring outliers.

18 monomers are involved in 27 short contacts:

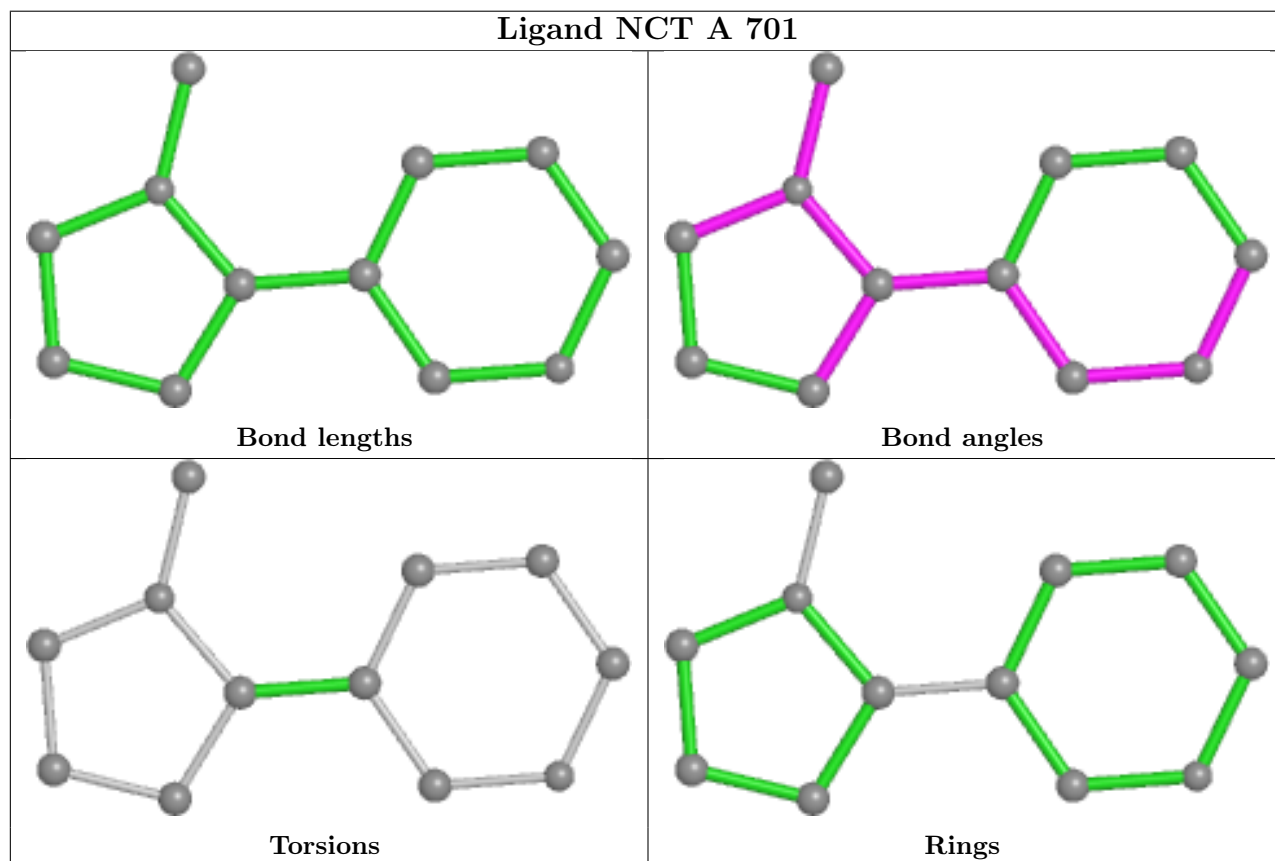
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	709	Y01	2	0
9	A	710	Y01	2	0
6	B	703	NAG	1	0
7	B	708	BMA	1	0
8	B	709	MAN	1	0
9	B	711	Y01	2	0
9	B	712	Y01	2	0
6	C	702	NAG	1	0
7	C	708	BMA	1	0
8	C	709	MAN	1	0
9	C	711	Y01	3	0

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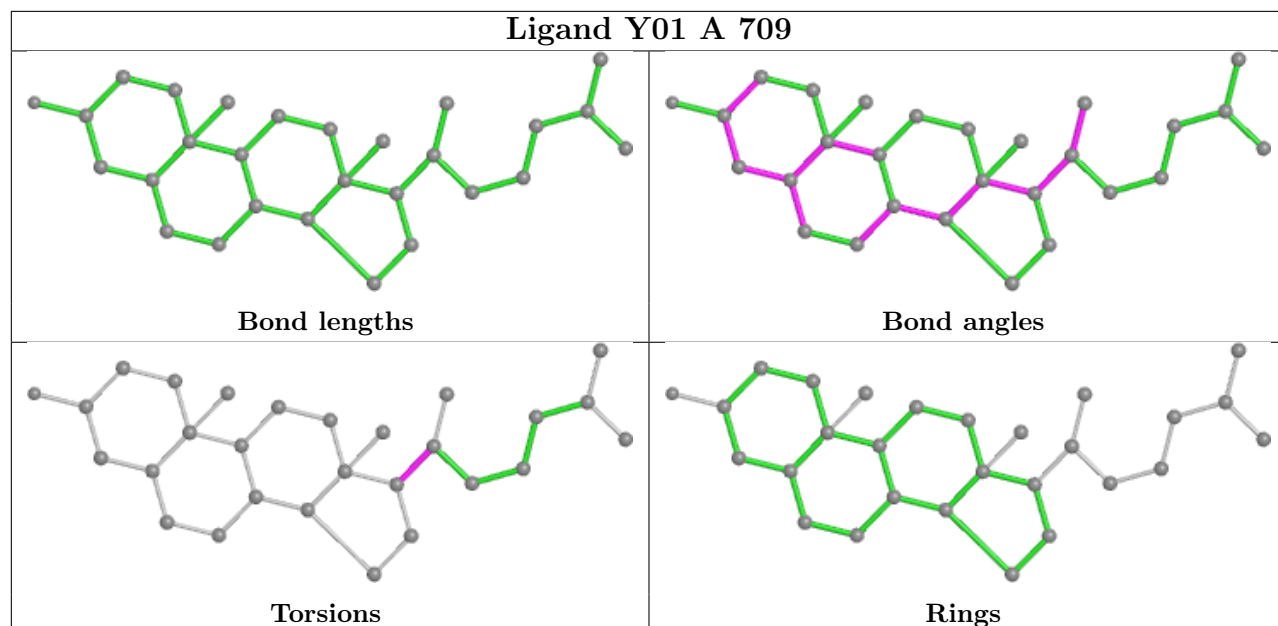
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	712	Y01	2	0
9	D	709	Y01	1	0
9	D	710	Y01	3	0
7	E	708	BMA	1	0
8	E	709	MAN	1	0
9	E	711	Y01	2	0
9	E	712	Y01	4	0

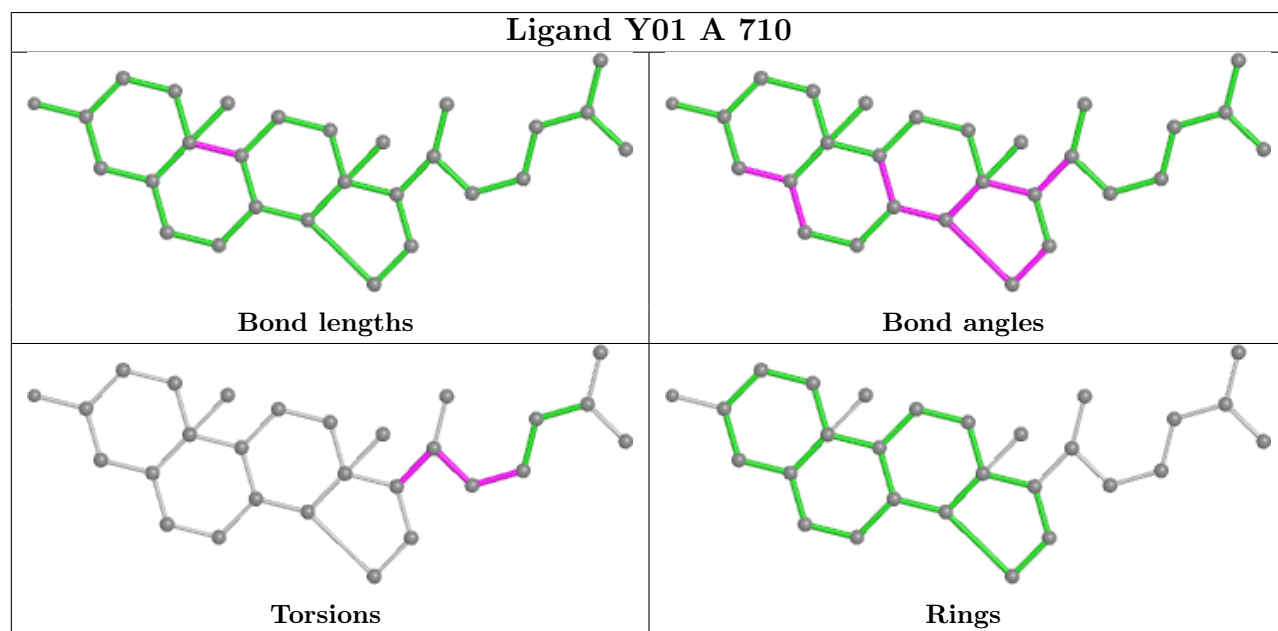
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



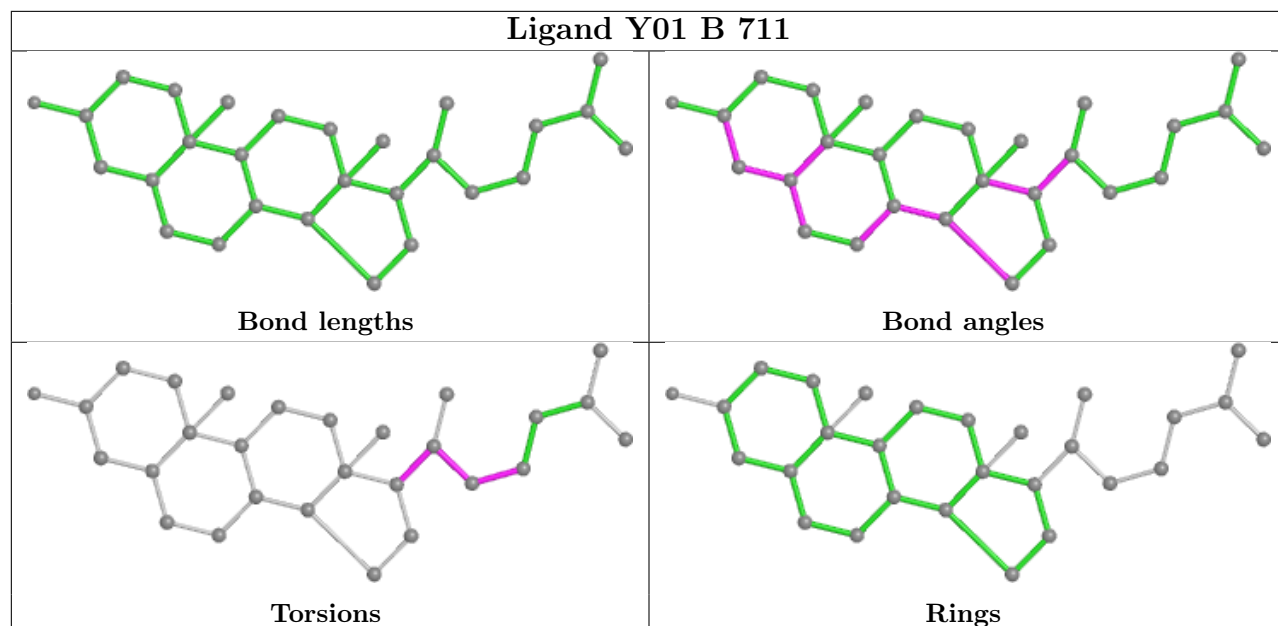
Ligand Y01 A 709



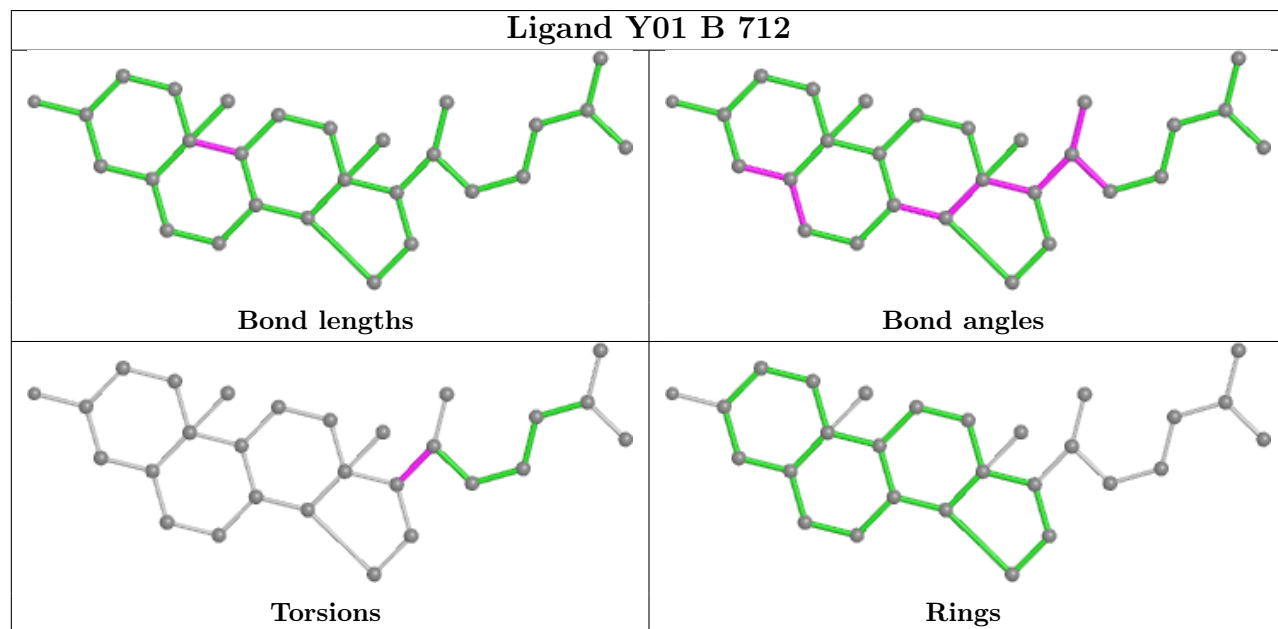
Ligand Y01 A 710

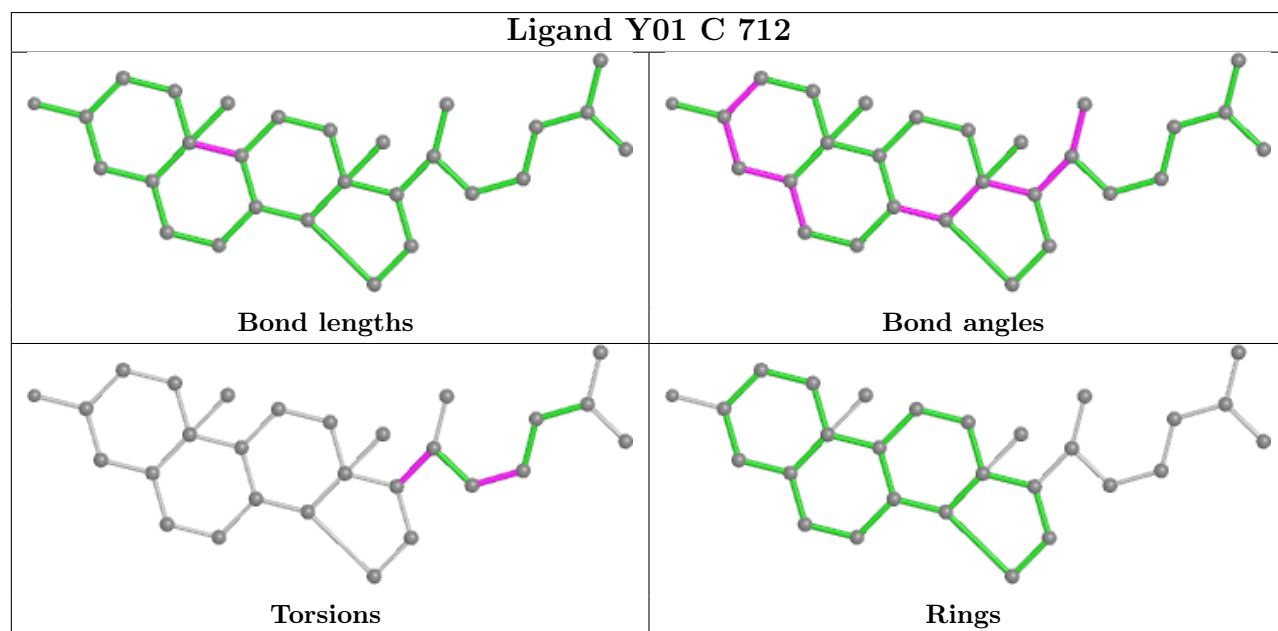
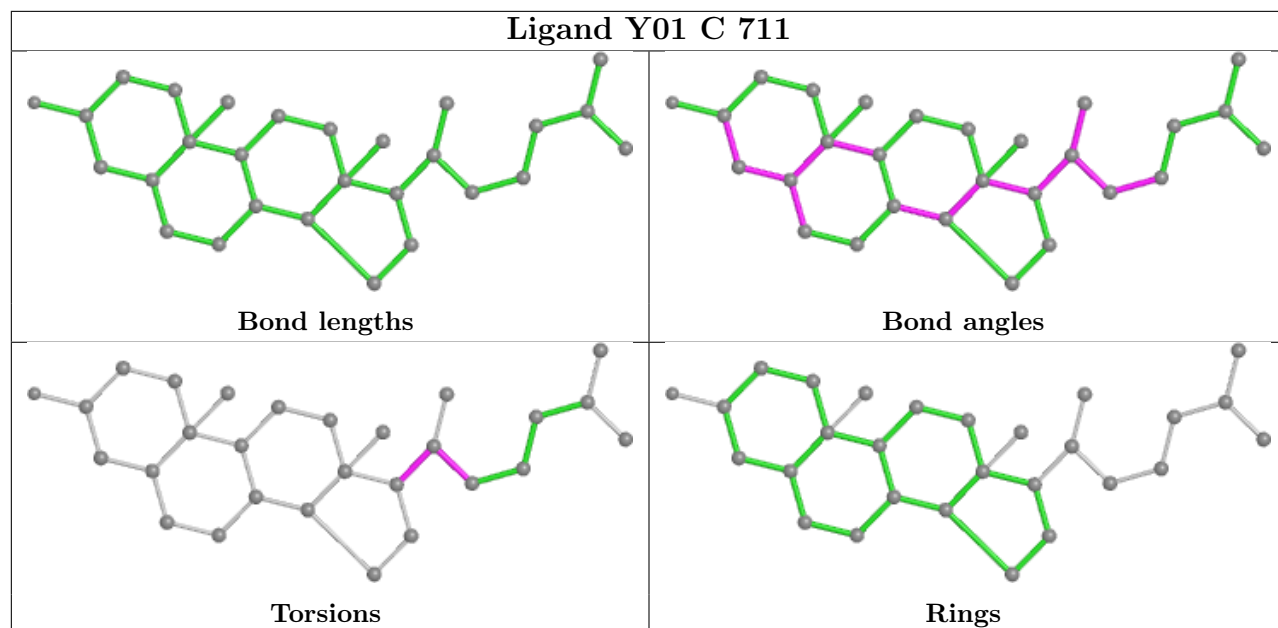


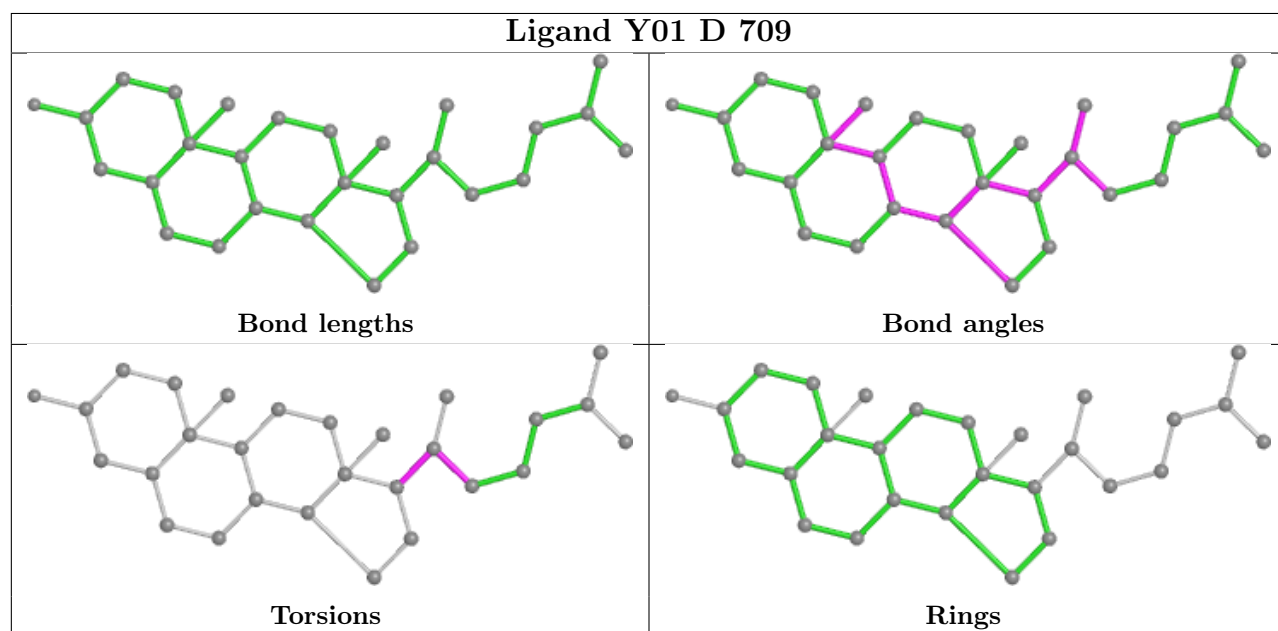
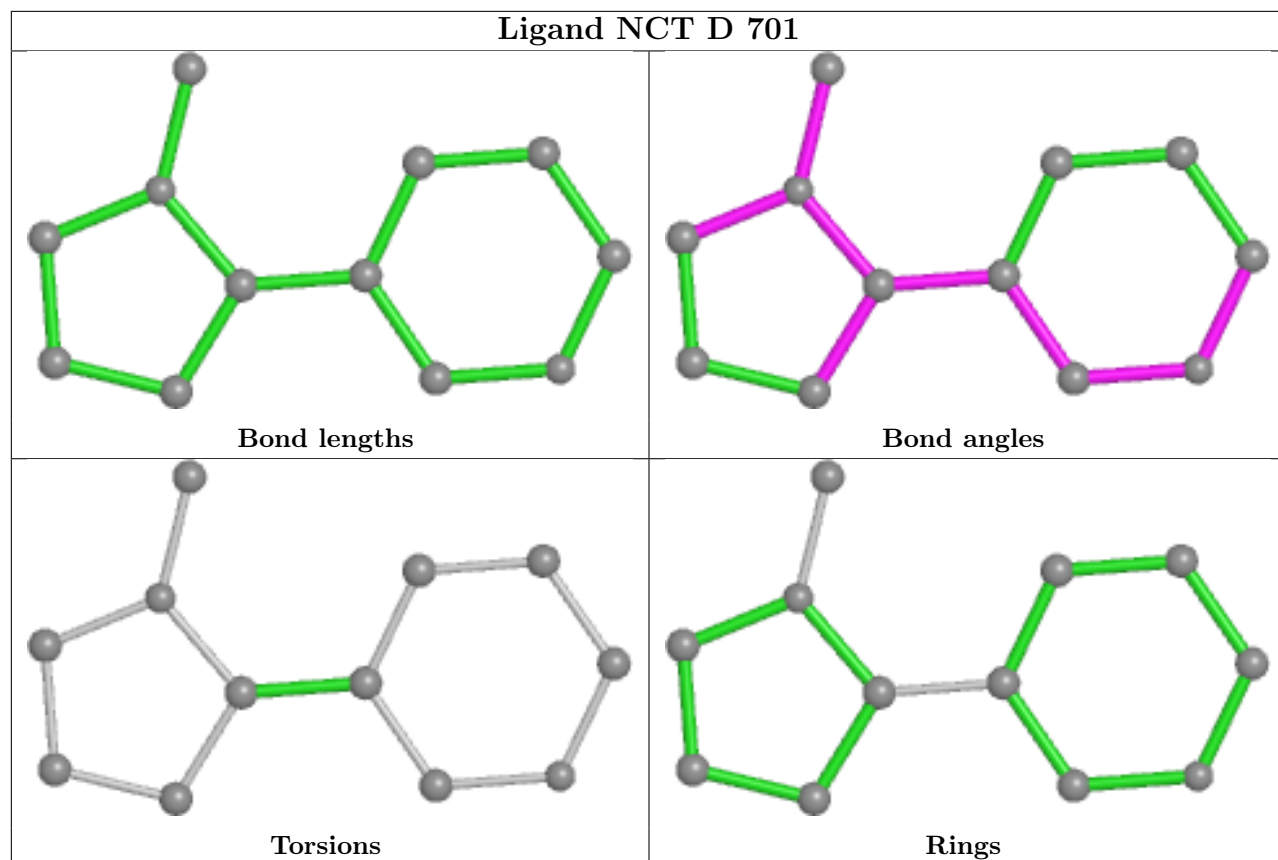
Ligand Y01 B 711



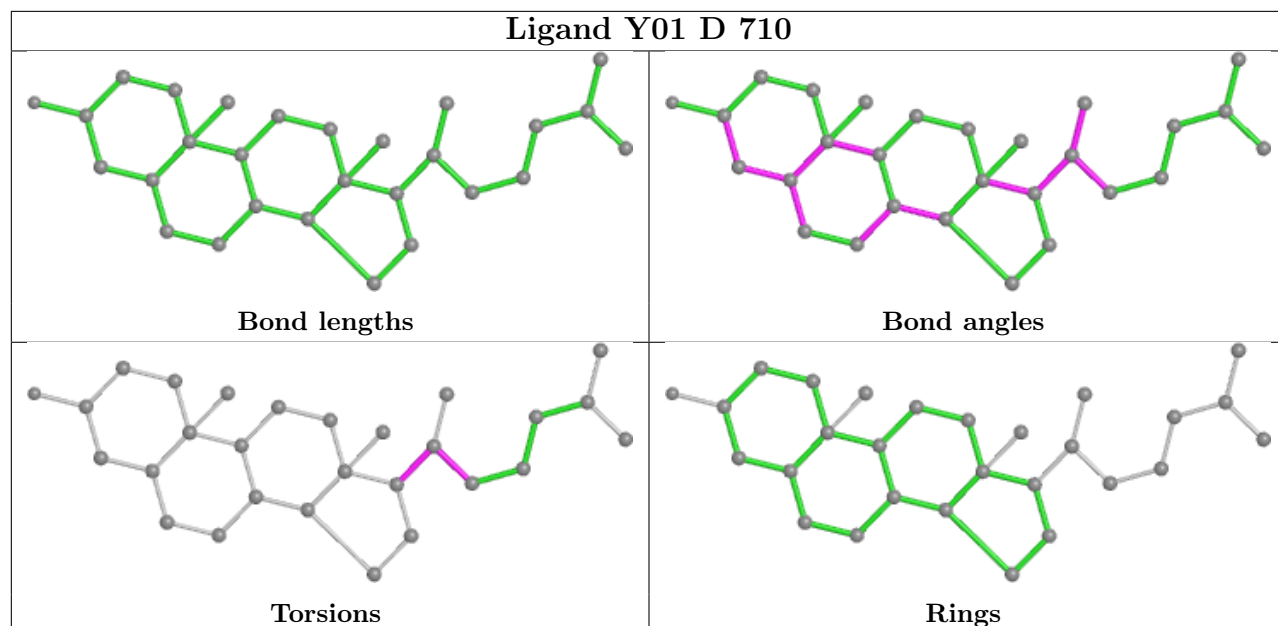
Ligand Y01 B 712



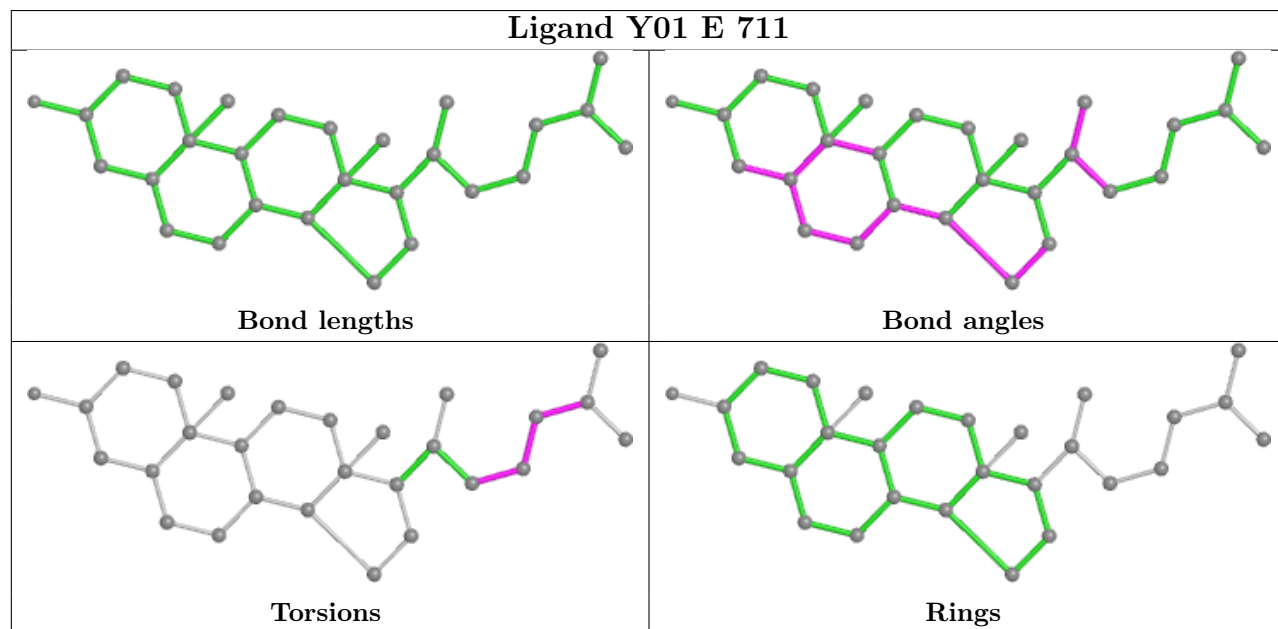


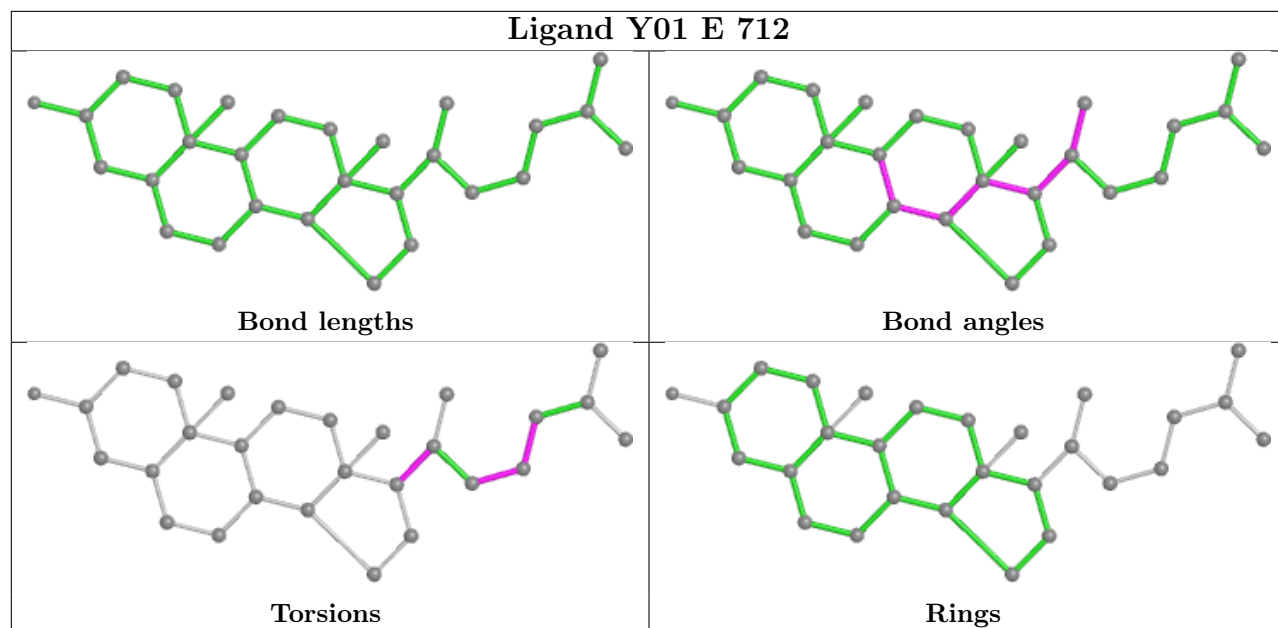


Ligand Y01 D 710



Ligand Y01 E 711





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.