



## Full wwPDB EM Validation Report ⓘ

Nov 30, 2025 – 12:19 AM JST

PDB ID : 9KDA / pdb\_00009kda  
EMDB ID : EMD-62267  
Title : Cryo-EM structure of lipid-mediated dimer of human norepinephrine transporter NET in the presence of the antidepressant vilazodone in an inward-open state at resolution of 2.44 angstrom.  
Authors : Zhang, H.; Xu, E.H.; Jiang, Y.  
Deposited on : 2024-11-03  
Resolution : 2.44 Å(reported)

This is a Full wwPDB EM Validation 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 : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

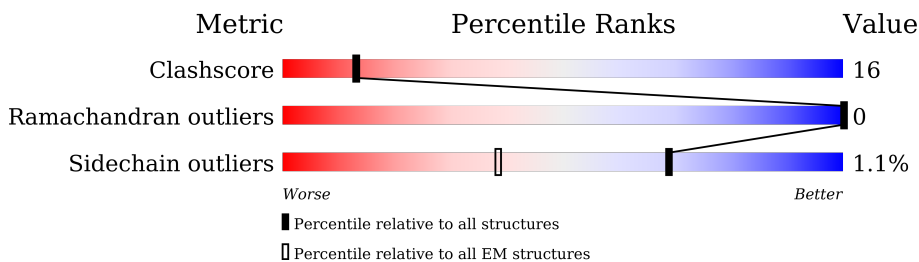
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.44 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	A	629	
1	B	629	

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	CLR	A	702	-	-	X	-
3	CLR	A	707	-	-	X	-
3	CLR	A	708	-	-	X	-
3	CLR	B	703	-	-	X	-
3	CLR	B	708	-	-	X	-
3	CLR	B	709	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9494 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 Sodium-dependent noradrenaline transporter.

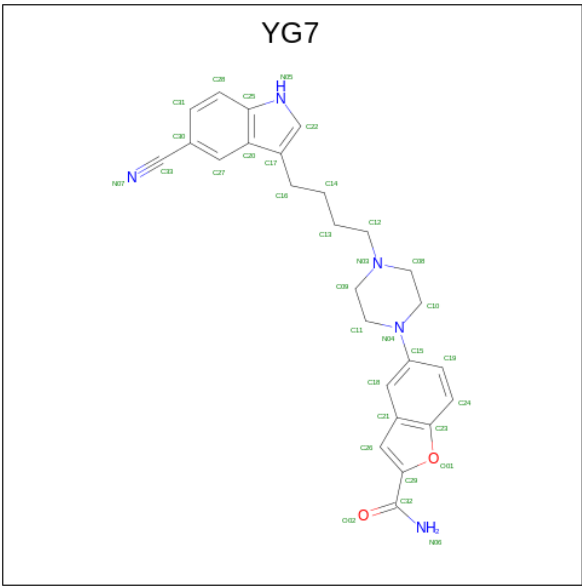
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	558	Total	C	N	O	S	0	0
			4449	2980	696	753	20		
1	B	558	Total	C	N	O	S	0	0
			4449	2980	696	753	20		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P23975
A	-10	ASP	-	expression tag	UNP P23975
A	-9	TYR	-	expression tag	UNP P23975
A	-8	LYS	-	expression tag	UNP P23975
A	-7	ASP	-	expression tag	UNP P23975
A	-6	ASP	-	expression tag	UNP P23975
A	-5	ASP	-	expression tag	UNP P23975
A	-4	ASP	-	expression tag	UNP P23975
A	-3	LYS	-	expression tag	UNP P23975
A	-2	GLY	-	expression tag	UNP P23975
A	-1	SER	-	expression tag	UNP P23975
A	0	GLY	-	expression tag	UNP P23975
B	-11	MET	-	initiating methionine	UNP P23975
B	-10	ASP	-	expression tag	UNP P23975
B	-9	TYR	-	expression tag	UNP P23975
B	-8	LYS	-	expression tag	UNP P23975
B	-7	ASP	-	expression tag	UNP P23975
B	-6	ASP	-	expression tag	UNP P23975
B	-5	ASP	-	expression tag	UNP P23975
B	-4	ASP	-	expression tag	UNP P23975
B	-3	LYS	-	expression tag	UNP P23975
B	-2	GLY	-	expression tag	UNP P23975
B	-1	SER	-	expression tag	UNP P23975
B	0	GLY	-	expression tag	UNP P23975

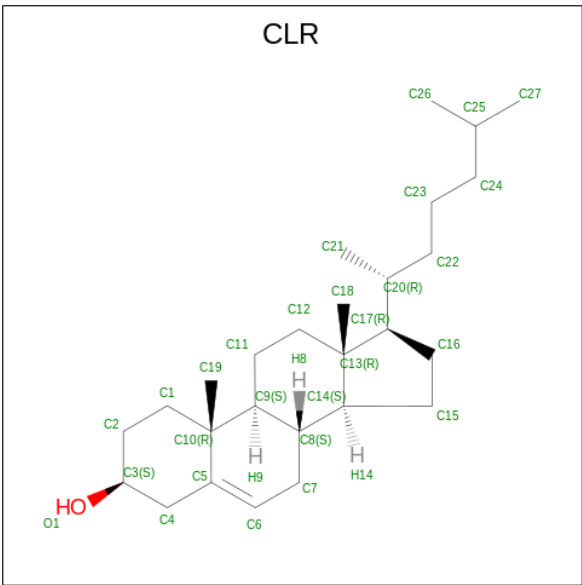
- Molecule 2 is 5-{4-[4-(5-cyano-1H-indol-3-yl)butyl]piperazin-1-yl}-1-benzofuran-2-carboxam

ide (CCD ID: YG7) (formula: C<sub>26</sub>H<sub>27</sub>N<sub>5</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



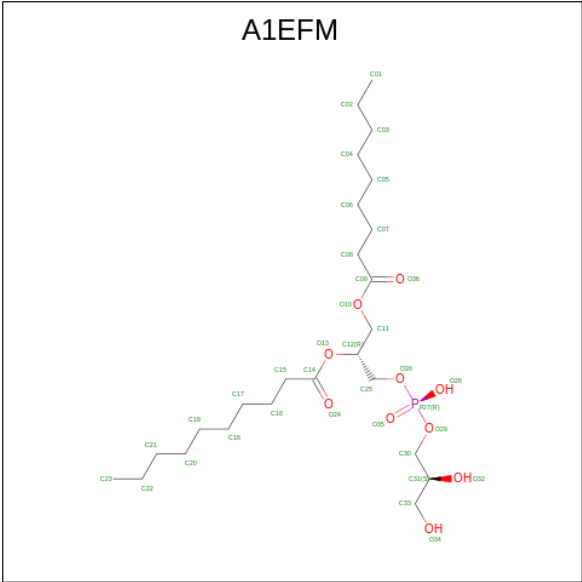
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			33	26	5	2	
2	B	1	Total	C	N	O	0
			33	26	5	2	

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	

- Molecule 4 is [(2 {R})-1-[(2 {S})-2,3-bis(oxidanyl)propoxy]-oxidanyl-phosphoryl]oxy-3-nonanoyloxy-propan-2-yl] decanoate (CCD ID: A1EFM) (formula: C<sub>25</sub>H<sub>49</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			36	25	10	1	
4	B	1	Total	C	O	P	0
			36	25	10	1	

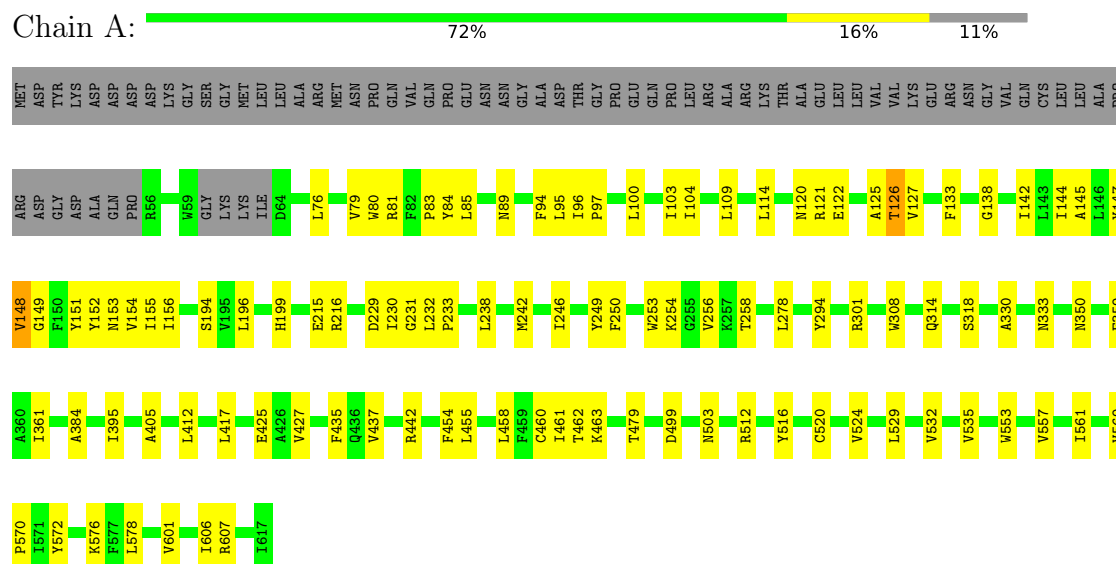
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	5	Total	O	0
			5	5	
5	B	5	Total	O	0
			5	5	

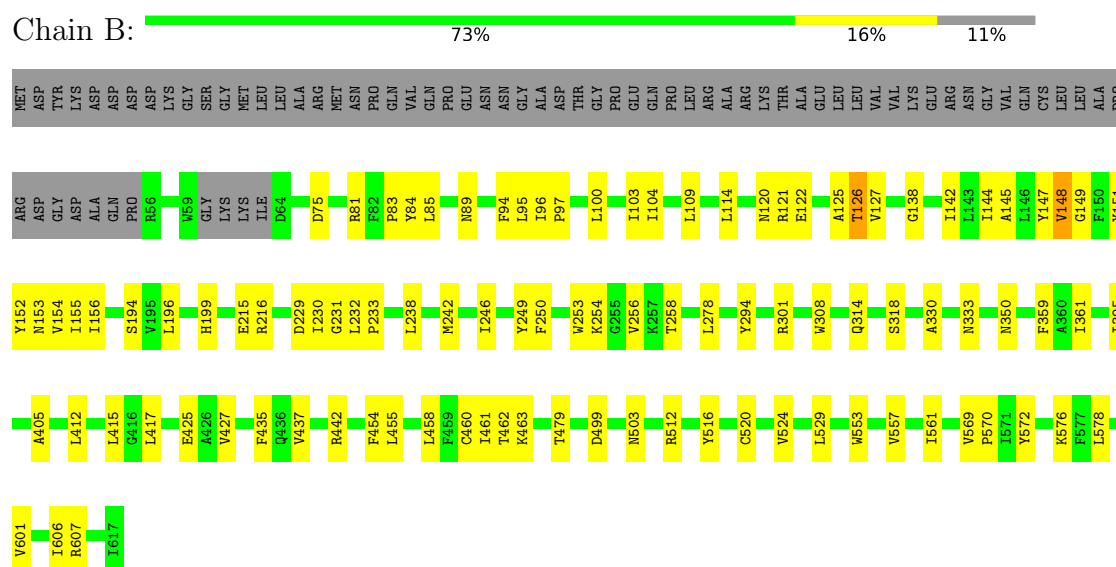
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Sodium-dependent noradrenaline transporter



- Molecule 1: Sodium-dependent noradrenaline transporter



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	247021	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: YG7, CLR, A1EFM

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	0.25	0/4593	0.41	0/6267
1	B	0.25	0/4593	0.41	0/6267
All	All	0.25	0/9186	0.41	0/12534

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

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	4449	0	4408	115	0
1	B	4449	0	4408	112	0
2	A	33	0	0	1	0
2	B	33	0	0	1	0
3	A	224	0	368	128	0
3	B	224	0	368	128	0
4	A	36	0	0	2	0
4	B	36	0	0	2	0
5	A	5	0	0	1	0
5	B	5	0	0	1	0
All	All	9494	0	9552	306	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 16.

All (306) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:707:CLR:C18	3:B:708:CLR:H152	1.38	1.50
3:A:707:CLR:H152	3:B:708:CLR:C18	1.38	1.49
1:B:250:PHE:CZ	3:B:709:CLR:H112	1.87	1.10
3:A:707:CLR:C15	3:B:708:CLR:H181	1.82	1.09
1:A:250:PHE:CZ	3:A:708:CLR:H112	1.86	1.08
3:A:707:CLR:H181	3:B:708:CLR:C15	1.82	1.06
3:A:707:CLR:C18	3:B:708:CLR:C15	2.33	1.05
3:A:707:CLR:C15	3:B:708:CLR:C18	2.33	1.04
1:A:553:TRP:CZ3	3:B:703:CLR:H22	1.93	1.02
1:A:455:LEU:HD21	3:A:704:CLR:H272	1.41	1.02
3:A:702:CLR:H22	1:B:553:TRP:CZ3	1.93	1.02
3:A:707:CLR:H181	3:B:708:CLR:H152	1.03	1.02
1:B:455:LEU:HD21	3:B:705:CLR:H272	1.41	1.02
3:A:707:CLR:H212	3:B:707:CLR:H12	1.44	1.00
3:A:707:CLR:H152	3:B:708:CLR:H183	1.41	0.99
3:A:707:CLR:H152	3:B:708:CLR:H181	1.03	0.99
3:A:706:CLR:H12	3:B:708:CLR:H212	1.43	0.98
3:A:707:CLR:H183	3:B:708:CLR:H152	1.41	0.97
3:A:702:CLR:H11	3:B:704:CLR:H6	1.47	0.95
3:A:703:CLR:H6	3:B:703:CLR:H11	1.48	0.95
1:A:553:TRP:CE3	3:B:703:CLR:H22	2.03	0.94
3:A:703:CLR:C6	3:B:703:CLR:H112	1.99	0.93
3:A:703:CLR:H6	3:B:703:CLR:H112	1.48	0.93
3:A:702:CLR:H22	1:B:553:TRP:CE3	2.04	0.93
3:A:702:CLR:H112	3:B:704:CLR:C6	1.99	0.92
3:A:702:CLR:H112	3:B:704:CLR:H6	1.49	0.92
1:A:250:PHE:HE2	3:A:708:CLR:C1	1.84	0.91
3:A:707:CLR:H181	3:B:708:CLR:H181	1.52	0.91
1:B:250:PHE:HE2	3:B:709:CLR:C1	1.84	0.89
1:A:250:PHE:HE2	3:A:708:CLR:H11	1.36	0.89
1:B:250:PHE:HE2	3:B:709:CLR:H11	1.36	0.89
1:A:242:MET:CE	3:A:708:CLR:H271	2.03	0.88
1:B:242:MET:CE	3:B:709:CLR:H271	2.03	0.87
1:B:437:VAL:HG13	3:B:708:CLR:H262	1.56	0.87
1:A:250:PHE:CZ	3:A:708:CLR:C11	2.57	0.87
1:A:437:VAL:HG13	3:A:707:CLR:H262	1.56	0.87
1:B:250:PHE:CZ	3:B:709:CLR:C11	2.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:PHE:HZ	3:A:708:CLR:C11	1.90	0.85
1:B:250:PHE:HZ	3:B:709:CLR:C11	1.90	0.85
1:A:561:ILE:HD11	3:A:703:CLR:H152	1.56	0.85
1:B:561:ILE:HD11	3:B:704:CLR:H152	1.56	0.84
1:A:553:TRP:CZ3	3:B:703:CLR:C2	2.62	0.82
1:A:557:VAL:HG21	3:B:703:CLR:H193	1.60	0.82
3:A:702:CLR:C2	1:B:553:TRP:CZ3	2.63	0.81
3:A:702:CLR:H193	1:B:557:VAL:HG21	1.60	0.81
3:A:707:CLR:H222	3:B:708:CLR:H222	1.61	0.81
1:B:249:TYR:CE2	3:B:706:CLR:H121	2.17	0.80
1:A:249:TYR:CE2	3:A:705:CLR:H121	2.17	0.80
1:A:455:LEU:HD21	3:A:704:CLR:C27	2.13	0.78
1:B:455:LEU:HD21	3:B:705:CLR:C27	2.13	0.78
1:B:250:PHE:CE2	3:B:709:CLR:H11	2.19	0.77
1:B:242:MET:HE2	3:B:709:CLR:H271	1.67	0.77
1:A:250:PHE:CE2	3:A:708:CLR:H11	2.19	0.77
1:B:578:LEU:HD12	3:B:701:CLR:H112	1.67	0.76
1:A:242:MET:HE2	3:A:708:CLR:H271	1.67	0.76
1:A:578:LEU:HD12	3:A:710:CLR:H112	1.67	0.76
3:A:710:CLR:H272	3:B:706:CLR:H221	1.68	0.76
1:A:572:TYR:HE1	4:A:709:A1EFM:C25	2.00	0.75
3:A:705:CLR:H221	3:B:701:CLR:H272	1.68	0.75
1:B:561:ILE:CD1	3:B:704:CLR:H181	2.17	0.75
1:A:561:ILE:CD1	3:A:703:CLR:H181	2.17	0.74
1:B:572:TYR:HE1	4:B:710:A1EFM:C25	2.00	0.74
3:A:706:CLR:H21	3:B:708:CLR:H211	1.68	0.74
1:A:462:THR:HG22	1:A:463:LYS:N	2.02	0.74
3:A:707:CLR:H211	3:B:707:CLR:H21	1.68	0.74
1:B:462:THR:HG22	1:B:463:LYS:N	2.02	0.73
3:A:702:CLR:C19	1:B:557:VAL:HG21	2.18	0.73
1:A:557:VAL:HG21	3:B:703:CLR:C19	2.18	0.73
3:A:702:CLR:C19	1:B:557:VAL:CG2	2.68	0.71
1:A:557:VAL:CG2	3:B:703:CLR:C19	2.68	0.71
1:A:561:ILE:HD11	3:A:703:CLR:H181	1.72	0.70
1:B:561:ILE:HD11	3:B:704:CLR:H181	1.72	0.69
1:B:83:PRO:HB3	1:B:361:ILE:HG13	1.75	0.68
1:A:83:PRO:HB3	1:A:361:ILE:HG13	1.75	0.68
1:B:250:PHE:CE2	3:B:709:CLR:C1	2.73	0.68
1:A:250:PHE:CE2	3:A:708:CLR:H112	2.28	0.68
1:B:103:ILE:HG13	1:B:104:ILE:HG23	1.76	0.68
1:B:250:PHE:CE2	3:B:709:CLR:H112	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:PHE:CE2	3:A:708:CLR:C1	2.73	0.67
3:A:707:CLR:C18	3:B:708:CLR:H181	2.24	0.67
1:A:557:VAL:CG2	3:B:703:CLR:H193	2.25	0.66
3:A:702:CLR:H193	1:B:557:VAL:CG2	2.25	0.66
3:A:706:CLR:H3	3:B:708:CLR:C21	2.26	0.66
1:A:103:ILE:HG13	1:A:104:ILE:HG23	1.76	0.66
3:A:707:CLR:H181	3:B:708:CLR:C18	2.24	0.66
3:A:707:CLR:C21	3:B:707:CLR:H3	2.25	0.65
1:B:250:PHE:HE2	3:B:709:CLR:H12	1.61	0.65
1:A:455:LEU:CD2	3:A:704:CLR:C27	2.76	0.64
3:A:707:CLR:H212	3:B:707:CLR:C1	2.26	0.64
1:A:121:ARG:NH2	1:A:333:ASN:O	2.25	0.64
3:A:705:CLR:H162	3:A:708:CLR:H232	1.79	0.64
1:B:250:PHE:HZ	3:B:709:CLR:C12	2.11	0.63
3:B:706:CLR:H162	3:B:709:CLR:H232	1.79	0.63
1:A:250:PHE:CZ	3:A:708:CLR:C12	2.82	0.63
1:A:250:PHE:HE2	3:A:708:CLR:H12	1.61	0.63
1:A:455:LEU:CD2	3:A:704:CLR:H272	2.25	0.63
3:A:702:CLR:H112	3:B:704:CLR:C7	2.28	0.63
1:B:455:LEU:CD2	3:B:705:CLR:C27	2.76	0.63
3:A:703:CLR:C7	3:B:703:CLR:H112	2.29	0.63
3:A:706:CLR:C2	3:B:708:CLR:H211	2.29	0.62
3:A:707:CLR:H211	3:B:707:CLR:C2	2.29	0.62
1:B:249:TYR:OH	3:B:706:CLR:H112	2.00	0.62
1:B:250:PHE:CZ	3:B:709:CLR:C12	2.82	0.62
1:A:249:TYR:OH	3:A:705:CLR:H112	2.00	0.61
1:A:462:THR:HG22	1:A:463:LYS:H	1.64	0.61
1:A:250:PHE:HZ	3:A:708:CLR:C12	2.11	0.61
1:B:455:LEU:CD2	3:B:705:CLR:H272	2.25	0.61
3:A:703:CLR:H41	3:B:703:CLR:H11	1.83	0.61
1:B:462:THR:HG22	1:B:463:LYS:H	1.64	0.60
1:B:109:LEU:HD11	1:B:529:LEU:HD11	1.84	0.60
1:A:561:ILE:HD11	3:A:703:CLR:C15	2.31	0.60
3:A:702:CLR:H11	3:B:704:CLR:H41	1.84	0.60
1:B:121:ARG:NH2	1:B:333:ASN:O	2.25	0.59
3:A:710:CLR:H12	3:B:706:CLR:H3	1.84	0.59
3:A:705:CLR:H3	3:B:701:CLR:H12	1.84	0.59
1:B:561:ILE:HD11	3:B:704:CLR:C15	2.31	0.59
1:A:109:LEU:HD11	1:A:529:LEU:HD11	1.84	0.58
3:A:706:CLR:C1	3:B:708:CLR:H212	2.25	0.58
1:A:250:PHE:CZ	3:A:708:CLR:H122	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:THR:CG2	1:A:463:LYS:N	2.67	0.57
1:A:425:GLU:OE1	1:A:442:ARG:NH1	2.38	0.57
1:B:250:PHE:CZ	3:B:709:CLR:H122	2.39	0.57
1:B:462:THR:CG2	1:B:463:LYS:N	2.67	0.57
1:B:425:GLU:OE1	1:B:442:ARG:NH1	2.38	0.57
1:A:249:TYR:CE2	3:A:705:CLR:C11	2.88	0.57
1:B:250:PHE:HZ	3:B:709:CLR:H122	1.70	0.56
1:A:246:ILE:HD11	3:A:708:CLR:H272	1.88	0.56
1:A:250:PHE:HZ	3:A:708:CLR:H122	1.70	0.56
1:B:246:ILE:HD11	3:B:709:CLR:H272	1.88	0.56
1:A:249:TYR:CE2	3:A:705:CLR:C12	2.88	0.56
1:A:503:ASN:OD1	1:A:512:ARG:NH2	2.38	0.56
1:B:250:PHE:CE2	3:B:709:CLR:H12	2.39	0.56
1:B:249:TYR:CE2	3:B:706:CLR:C11	2.88	0.56
3:A:707:CLR:C21	3:B:707:CLR:C2	2.84	0.56
1:B:503:ASN:OD1	1:B:512:ARG:NH2	2.38	0.56
1:B:249:TYR:CE2	3:B:706:CLR:C12	2.88	0.55
1:A:250:PHE:CE2	3:A:708:CLR:H12	2.39	0.55
3:A:706:CLR:C2	3:B:708:CLR:C21	2.84	0.55
1:B:85:LEU:HD23	1:B:314:GLN:HB2	1.89	0.54
3:A:702:CLR:C11	3:B:704:CLR:C7	2.86	0.54
1:B:462:THR:CG2	1:B:463:LYS:H	2.20	0.54
3:A:703:CLR:C7	3:B:703:CLR:C11	2.86	0.54
3:A:703:CLR:H6	3:B:703:CLR:C11	2.30	0.54
3:A:706:CLR:H12	3:B:708:CLR:C21	2.29	0.54
1:B:253:TRP:CD1	1:B:254:LYS:H	2.26	0.54
1:A:253:TRP:CD1	1:A:254:LYS:H	2.26	0.54
1:A:215:GLU:HG3	1:A:216:ARG:HG3	1.90	0.53
1:A:238:LEU:HD21	3:A:704:CLR:H151	1.91	0.53
1:A:601:VAL:HA	1:A:606:ILE:HD11	1.90	0.53
1:B:215:GLU:HG3	1:B:216:ARG:HG3	1.90	0.53
1:B:238:LEU:HD21	3:B:705:CLR:H151	1.91	0.53
1:A:85:LEU:HD23	1:A:314:GLN:HB2	1.89	0.53
1:B:233:PRO:HA	1:B:462:THR:HA	1.90	0.53
1:B:154:VAL:HG21	1:B:460:CYS:HB2	1.91	0.53
1:B:148:VAL:HA	1:B:151:TYR:CE2	2.43	0.53
1:A:148:VAL:HA	1:A:151:TYR:CE2	2.43	0.53
1:A:479:THR:O	1:A:479:THR:HG22	2.09	0.53
1:A:462:THR:CG2	1:A:463:LYS:H	2.20	0.52
1:A:114:LEU:HD13	1:A:330:ALA:HB2	1.91	0.52
3:A:707:CLR:H222	3:B:708:CLR:C22	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:VAL:HA	1:B:606:ILE:HD11	1.90	0.52
1:A:230:ILE:O	1:A:462:THR:HG22	2.10	0.52
1:A:103:ILE:O	1:A:516:TYR:OH	2.28	0.52
1:A:233:PRO:HA	1:A:462:THR:HA	1.90	0.52
1:B:458:LEU:HD23	1:B:461:ILE:HD11	1.92	0.52
1:A:154:VAL:HG21	1:A:460:CYS:HB2	1.91	0.51
1:B:103:ILE:O	1:B:516:TYR:OH	2.28	0.51
1:B:114:LEU:HD13	1:B:330:ALA:HB2	1.91	0.51
1:B:230:ILE:O	1:B:462:THR:HG22	2.10	0.51
1:B:557:VAL:HG11	3:B:704:CLR:H72	1.93	0.51
1:B:479:THR:HG22	1:B:479:THR:O	2.09	0.51
1:A:557:VAL:HG11	3:A:703:CLR:H72	1.93	0.51
1:A:120:ASN:HB2	1:A:127:VAL:HG12	1.93	0.51
3:A:702:CLR:C11	3:B:704:CLR:H6	2.31	0.51
1:A:232:LEU:O	1:A:463:LYS:NZ	2.44	0.51
1:A:569:VAL:HB	1:A:570:PRO:HD3	1.93	0.51
1:A:194:SER:HB2	1:A:196:LEU:HD13	1.94	0.50
1:A:458:LEU:HD23	1:A:461:ILE:HD11	1.92	0.50
1:A:435:PHE:HD1	3:A:707:CLR:H273	1.77	0.50
1:B:120:ASN:HB2	1:B:127:VAL:HG12	1.93	0.50
1:B:499:ASP:OD2	1:B:607:ARG:NH1	2.40	0.50
1:B:318:SER:HB2	1:B:350:ASN:HD21	1.76	0.50
1:B:569:VAL:HB	1:B:570:PRO:HD3	1.93	0.50
1:B:435:PHE:HD1	3:B:708:CLR:H273	1.77	0.50
1:A:242:MET:CE	3:A:708:CLR:C27	2.86	0.49
1:B:520:CYS:HA	1:B:524:VAL:HB	1.93	0.49
1:A:151:TYR:O	1:A:155:ILE:HG13	2.13	0.49
1:A:454:PHE:O	1:A:458:LEU:HG	2.13	0.49
1:A:520:CYS:HA	1:A:524:VAL:HB	1.93	0.49
1:A:249:TYR:HE2	3:A:705:CLR:C11	2.26	0.49
1:A:318:SER:HB2	1:A:350:ASN:HD21	1.76	0.49
1:B:435:PHE:CE1	3:B:708:CLR:H213	2.48	0.49
1:A:435:PHE:CE1	3:A:707:CLR:H213	2.48	0.49
3:A:702:CLR:C11	3:B:704:CLR:H71	2.43	0.49
1:B:454:PHE:O	1:B:458:LEU:HG	2.13	0.49
1:B:194:SER:HB2	1:B:196:LEU:HD13	1.93	0.49
1:A:230:ILE:HB	1:A:462:THR:HG21	1.95	0.49
1:B:100:LEU:HD23	1:B:308:TRP:HZ3	1.78	0.48
1:B:125:ALA:HA	1:B:138:GLY:HA3	1.95	0.48
1:B:249:TYR:HE2	3:B:706:CLR:C11	2.26	0.48
1:B:151:TYR:O	1:B:155:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LEU:O	1:B:463:LYS:NZ	2.44	0.48
3:A:703:CLR:H71	3:B:703:CLR:C11	2.43	0.48
1:B:232:LEU:HD23	3:B:703:CLR:H41	1.95	0.48
1:A:499:ASP:OD2	1:A:607:ARG:NH1	2.40	0.48
1:A:278:LEU:HD21	1:A:359:PHE:HD2	1.79	0.48
1:B:230:ILE:HB	1:B:462:THR:HG21	1.95	0.48
1:A:89:ASN:HB2	1:A:94:PHE:HB2	1.96	0.48
1:A:125:ALA:HA	1:A:138:GLY:HA3	1.96	0.48
1:B:89:ASN:HB2	1:B:94:PHE:HB2	1.96	0.48
3:A:707:CLR:C22	3:B:708:CLR:H222	2.37	0.47
1:A:246:ILE:HD13	3:A:708:CLR:C21	2.44	0.47
1:A:100:LEU:HD23	1:A:308:TRP:HZ3	1.78	0.47
1:B:278:LEU:HD21	1:B:359:PHE:HD2	1.79	0.47
1:B:572:TYR:OH	4:B:710:A1EFM:O28	2.25	0.47
1:A:231:GLY:O	3:A:702:CLR:H41	2.14	0.47
1:A:232:LEU:HD23	3:A:702:CLR:H41	1.95	0.47
1:B:249:TYR:HE2	3:B:706:CLR:H111	1.79	0.47
1:B:246:ILE:HD13	3:B:709:CLR:C21	2.44	0.47
1:B:231:GLY:O	3:B:703:CLR:H41	2.14	0.47
1:A:96:ILE:HB	1:A:97:PRO:HD3	1.96	0.46
1:A:435:PHE:CD1	3:A:707:CLR:H17	2.51	0.46
3:B:707:CLR:H212	3:B:708:CLR:H6	1.97	0.46
1:A:142:ILE:HG23	1:A:427:VAL:HG22	1.98	0.46
1:A:249:TYR:HE2	3:A:705:CLR:H111	1.80	0.46
3:A:703:CLR:H262	3:B:703:CLR:H263	1.97	0.46
1:B:89:ASN:HA	1:B:301:ARG:HH11	1.81	0.46
1:B:144:ILE:O	1:B:147:TYR:HB2	2.16	0.46
1:B:435:PHE:CD1	3:B:708:CLR:H17	2.51	0.46
1:B:96:ILE:HB	1:B:97:PRO:HD3	1.96	0.46
1:B:230:ILE:O	1:B:462:THR:CG2	2.64	0.46
1:A:144:ILE:O	1:A:147:TYR:HB2	2.16	0.46
1:B:95:LEU:HD11	1:B:294:TYR:CZ	2.52	0.45
1:A:89:ASN:HA	1:A:301:ARG:HH11	1.81	0.45
3:A:703:CLR:C26	3:B:703:CLR:H263	2.47	0.45
3:A:707:CLR:H8	3:B:708:CLR:H8	1.97	0.45
1:A:229:ASP:OD1	1:A:229:ASP:N	2.50	0.45
1:A:145:ALA:O	1:A:148:VAL:HG22	2.17	0.45
1:A:230:ILE:O	1:A:462:THR:CG2	2.64	0.45
3:A:702:CLR:H21	1:B:553:TRP:CZ3	2.49	0.45
3:A:706:CLR:H212	3:A:707:CLR:H6	1.97	0.45
3:A:707:CLR:C21	3:B:707:CLR:C3	2.92	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:GLU:HB3	1:B:126:THR:OG1	2.17	0.45
1:B:142:ILE:HG23	1:B:427:VAL:HG22	1.98	0.45
1:A:553:TRP:CZ3	3:B:703:CLR:H21	2.49	0.45
3:B:706:CLR:H242	3:B:709:CLR:H273	1.99	0.45
1:B:145:ALA:O	1:B:148:VAL:HG22	2.17	0.45
1:A:80:TRP:NE1	1:A:384:ALA:O	2.48	0.44
3:A:706:CLR:C3	3:B:708:CLR:C21	2.93	0.44
1:B:395:ILE:HD13	1:B:405:ALA:HA	2.00	0.44
1:A:95:LEU:HD11	1:A:294:TYR:CZ	2.52	0.44
3:A:702:CLR:H112	3:B:704:CLR:H71	1.99	0.44
1:B:229:ASP:OD1	1:B:229:ASP:N	2.50	0.44
1:A:122:GLU:HB3	1:A:126:THR:OG1	2.17	0.44
1:A:395:ILE:HD13	1:A:405:ALA:HA	2.00	0.44
3:A:705:CLR:H21	3:B:701:CLR:H3	1.99	0.44
3:A:707:CLR:C14	3:B:708:CLR:H181	2.44	0.44
3:A:710:CLR:H3	3:B:706:CLR:H21	1.99	0.44
1:B:458:LEU:HA	1:B:461:ILE:HG12	1.99	0.44
1:A:246:ILE:HD13	3:A:708:CLR:H213	2.00	0.44
1:A:458:LEU:HA	1:A:461:ILE:HG12	1.99	0.43
3:A:705:CLR:H242	3:A:708:CLR:H273	1.99	0.43
1:A:572:TYR:OH	4:A:709:A1EFM:O28	2.25	0.43
3:A:702:CLR:H263	3:B:704:CLR:C26	2.48	0.43
3:B:707:CLR:H221	3:B:707:CLR:H162	1.55	0.43
1:A:100:LEU:O	1:A:104:ILE:HG12	2.19	0.43
3:A:702:CLR:H263	3:B:704:CLR:H262	1.99	0.43
3:A:707:CLR:C21	3:B:707:CLR:H12	2.30	0.43
3:A:703:CLR:H71	3:B:703:CLR:H121	2.01	0.43
1:B:156:ILE:HD13	1:B:417:LEU:HD23	2.00	0.43
3:A:703:CLR:H41	3:B:703:CLR:C1	2.48	0.43
3:A:703:CLR:H71	3:B:703:CLR:H112	2.00	0.43
1:B:242:MET:CE	3:B:709:CLR:C27	2.86	0.43
1:A:149:GLY:HA3	5:A:805:HOH:O	2.19	0.43
3:A:706:CLR:H162	3:A:706:CLR:H221	1.55	0.43
1:B:246:ILE:HD13	3:B:709:CLR:H213	2.00	0.42
1:B:258:THR:HA	2:B:702:YG7:C29	2.49	0.42
1:A:258:THR:HA	2:A:701:YG7:C29	2.49	0.42
1:B:149:GLY:HA3	5:B:805:HOH:O	2.19	0.42
1:B:100:LEU:O	1:B:104:ILE:HG12	2.19	0.42
1:A:156:ILE:HD13	1:A:417:LEU:HD23	2.01	0.42
1:A:557:VAL:HG22	3:B:703:CLR:C19	2.50	0.42
3:A:702:CLR:C19	1:B:557:VAL:HG22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASN:HA	1:B:156:ILE:HD12	2.02	0.42
1:A:435:PHE:CE2	3:A:707:CLR:H122	2.55	0.42
3:A:702:CLR:H121	3:B:704:CLR:H71	2.02	0.42
1:B:435:PHE:CE2	3:B:708:CLR:H122	2.55	0.42
1:B:75:ASP:HA	1:B:415:LEU:HD22	2.02	0.41
3:A:702:CLR:H11	3:B:704:CLR:C6	2.35	0.41
1:A:81:ARG:HA	1:A:84:TYR:CE1	2.56	0.41
3:A:707:CLR:H213	3:B:707:CLR:H3	2.02	0.41
1:B:199:HIS:O	1:B:199:HIS:ND1	2.54	0.41
3:A:707:CLR:H191	3:B:708:CLR:C6	2.50	0.41
1:A:76:LEU:HA	1:A:79:VAL:HG12	2.02	0.41
3:A:707:CLR:C6	3:B:708:CLR:H191	2.50	0.41
1:A:133:PHE:HD1	1:A:133:PHE:HA	1.78	0.41
1:A:153:ASN:HA	1:A:156:ILE:HD12	2.02	0.41
1:A:412:LEU:HD23	1:A:412:LEU:HA	1.79	0.41
3:A:710:CLR:H162	3:A:710:CLR:H221	1.89	0.41
1:B:81:ARG:HA	1:B:84:TYR:CE1	2.56	0.40
1:B:249:TYR:CZ	3:B:706:CLR:H121	2.56	0.40
1:B:412:LEU:HD23	1:B:412:LEU:HA	1.79	0.40
1:A:199:HIS:O	1:A:199:HIS:ND1	2.54	0.40
1:A:532:VAL:HA	1:A:535:VAL:HG12	2.04	0.40
1:A:361:ILE:HD13	1:A:361:ILE:HA	1.99	0.40
3:A:706:CLR:C1	3:B:708:CLR:C21	2.96	0.40

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	554/629 (88%)	542 (98%)	12 (2%)	0	100	100
1	B	554/629 (88%)	542 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1108/1258 (88%)	1084 (98%)	24 (2%)	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	466/529 (88%)	461 (99%)	5 (1%)	70	80
1	B	466/529 (88%)	461 (99%)	5 (1%)	70	80
All	All	932/1058 (88%)	922 (99%)	10 (1%)	69	80

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	THR
1	A	148	VAL
1	A	152	TYR
1	A	256	VAL
1	A	576	LYS
1	B	126	THR
1	B	148	VAL
1	B	152	TYR
1	B	256	VAL
1	B	576	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	153	ASN
1	A	170	ASN
1	A	280	HIS
1	A	337	ASN

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Mol	Chain	Res	Type
1	A	350	ASN
1	A	581	GLN
1	B	89	ASN
1	B	153	ASN
1	B	280	HIS
1	B	337	ASN
1	B	350	ASN
1	B	581	GLN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

20 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	$\# Z  > 2$
3	CLR	B	709	-	31,31,31	0.29	0	48,48,48	0.37	0
3	CLR	A	704	-	31,31,31	0.29	0	48,48,48	0.38	0
3	CLR	B	706	-	31,31,31	0.28	0	48,48,48	0.40	0
3	CLR	B	701	-	31,31,31	0.27	0	48,48,48	0.41	0
4	A1EFM	A	709	-	35,35,35	1.02	4 (11%)	38,41,41	1.01	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CLR	B	708	-	31,31,31	0.39	0	48,48,48	0.82	1 (2%)
3	CLR	A	703	-	31,31,31	0.29	0	48,48,48	0.37	0
2	YG7	A	701	-	32,37,37	2.62	10 (31%)	36,52,52	1.53	6 (16%)
3	CLR	A	708	-	31,31,31	0.29	0	48,48,48	0.37	0
3	CLR	A	710	-	31,31,31	0.27	0	48,48,48	0.41	0
4	A1EFM	B	710	-	35,35,35	1.02	4 (11%)	38,41,41	1.01	2 (5%)
3	CLR	B	707	-	31,31,31	0.28	0	48,48,48	0.40	0
3	CLR	B	703	-	31,31,31	0.27	0	48,48,48	0.47	0
3	CLR	B	704	-	31,31,31	0.29	0	48,48,48	0.37	0
3	CLR	A	702	-	31,31,31	0.27	0	48,48,48	0.46	0
2	YG7	B	702	-	32,37,37	2.62	10 (31%)	36,52,52	1.52	6 (16%)
3	CLR	A	707	-	31,31,31	0.39	0	48,48,48	0.82	1 (2%)
3	CLR	A	706	-	31,31,31	0.28	0	48,48,48	0.41	0
3	CLR	B	705	-	31,31,31	0.29	0	48,48,48	0.39	0
3	CLR	A	705	-	31,31,31	0.28	0	48,48,48	0.39	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
3	CLR	B	709	-	-	0/10/68/68	0/4/4/4
3	CLR	A	704	-	-	6/10/68/68	0/4/4/4
3	CLR	B	706	-	-	4/10/68/68	0/4/4/4
3	CLR	B	701	-	-	7/10/68/68	0/4/4/4
4	A1EFM	A	709	-	-	16/40/40/40	-
3	CLR	B	708	-	-	3/10/68/68	0/4/4/4
3	CLR	A	703	-	-	0/10/68/68	0/4/4/4
2	YG7	A	701	-	-	2/13/27/27	0/5/5/5
3	CLR	A	708	-	-	0/10/68/68	0/4/4/4
3	CLR	A	710	-	-	7/10/68/68	0/4/4/4
4	A1EFM	B	710	-	-	16/40/40/40	-
3	CLR	B	707	-	-	6/10/68/68	0/4/4/4
3	CLR	B	703	-	-	5/10/68/68	0/4/4/4
3	CLR	B	704	-	-	0/10/68/68	0/4/4/4
3	CLR	A	702	-	-	5/10/68/68	0/4/4/4
2	YG7	B	702	-	-	2/13/27/27	0/5/5/5
3	CLR	A	707	-	-	3/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLR	A	706	-	-	6/10/68/68	0/4/4/4
3	CLR	B	705	-	-	6/10/68/68	0/4/4/4
3	CLR	A	705	-	-	4/10/68/68	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	YG7	C12-N03	-8.02	1.29	1.47
2	B	702	YG7	C12-N03	-8.02	1.29	1.47
2	A	701	YG7	C32-N06	6.88	1.46	1.33
2	B	702	YG7	C32-N06	6.85	1.46	1.33
2	B	702	YG7	C08-N03	-4.05	1.35	1.46
2	A	701	YG7	C09-N03	-4.05	1.35	1.46
2	A	701	YG7	C08-N03	-4.04	1.35	1.46
2	B	702	YG7	C09-N03	-4.03	1.35	1.46
2	A	701	YG7	C30-C33	3.98	1.53	1.44
2	B	702	YG7	C30-C33	3.98	1.53	1.44
2	A	701	YG7	C15-N04	3.53	1.48	1.38
2	B	702	YG7	C15-N04	3.53	1.48	1.38
2	B	702	YG7	C29-C32	3.07	1.54	1.49
2	A	701	YG7	C29-C32	3.04	1.54	1.49
2	B	702	YG7	O02-C32	-2.71	1.19	1.24
2	A	701	YG7	O02-C32	-2.71	1.19	1.24
4	A	709	A1EFM	O13-C12	-2.61	1.40	1.46
4	B	710	A1EFM	O13-C12	-2.61	1.40	1.46
4	B	710	A1EFM	O10-C09	2.39	1.40	1.33
4	A	709	A1EFM	O10-C09	2.37	1.40	1.33
2	A	701	YG7	C21-C23	-2.34	1.38	1.43
2	B	702	YG7	C21-C23	-2.34	1.38	1.43
2	A	701	YG7	C20-C25	-2.23	1.36	1.42
2	B	702	YG7	C20-C25	-2.21	1.36	1.42
4	B	710	A1EFM	O10-C11	-2.16	1.40	1.45
4	A	709	A1EFM	O10-C11	-2.15	1.40	1.45
4	B	710	A1EFM	O13-C14	2.09	1.40	1.34
4	A	709	A1EFM	O13-C14	2.09	1.40	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	709	A1EFM	O13-C14-C15	4.03	120.19	111.50
4	B	710	A1EFM	O13-C14-C15	4.02	120.17	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	YG7	C27-C30-C33	-3.98	116.21	119.65
2	A	701	YG7	C27-C30-C33	-3.96	116.24	119.65
2	A	701	YG7	C29-C32-N06	3.92	120.13	116.25
2	B	702	YG7	C29-C32-N06	3.88	120.09	116.25
2	A	701	YG7	C26-C21-C23	-3.04	103.62	106.27
2	B	702	YG7	C26-C21-C23	-2.96	103.69	106.27
3	B	708	CLR	C17-C13-C14	2.50	103.03	100.07
3	A	707	CLR	C17-C13-C14	2.46	102.99	100.07
4	A	709	A1EFM	O10-C09-C08	2.43	119.52	111.91
4	B	710	A1EFM	O10-C09-C08	2.42	119.49	111.91
2	A	701	YG7	C31-C30-C33	2.33	123.87	119.99
2	B	702	YG7	C31-C30-C33	2.32	123.85	119.99
2	A	701	YG7	O02-C32-N06	-2.19	119.47	122.58
2	B	702	YG7	O02-C32-N06	-2.14	119.54	122.58
2	B	702	YG7	C13-C12-N03	-2.05	108.67	113.84
2	A	701	YG7	C13-C12-N03	-2.04	108.70	113.84

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	YG7	C14-C16-C17-C20
2	B	702	YG7	C14-C16-C17-C20
4	A	709	A1EFM	C25-O26-P27-O28
4	A	709	A1EFM	C25-O26-P27-O35
4	B	710	A1EFM	C25-O26-P27-O28
4	B	710	A1EFM	C25-O26-P27-O35
3	A	706	CLR	C16-C17-C20-C21
3	B	707	CLR	C16-C17-C20-C21
3	A	706	CLR	C13-C17-C20-C21
3	B	707	CLR	C13-C17-C20-C21
3	A	706	CLR	C13-C17-C20-C22
3	B	707	CLR	C13-C17-C20-C22
3	A	707	CLR	C21-C20-C22-C23
3	B	708	CLR	C21-C20-C22-C23
3	A	706	CLR	C16-C17-C20-C22
3	B	707	CLR	C16-C17-C20-C22
3	A	706	CLR	C21-C20-C22-C23
3	B	707	CLR	C21-C20-C22-C23
3	A	706	CLR	C17-C20-C22-C23
3	B	707	CLR	C17-C20-C22-C23
2	A	701	YG7	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
2	B	702	YG7	C13-C14-C16-C17
3	A	702	CLR	C21-C20-C22-C23
3	B	703	CLR	C21-C20-C22-C23
3	A	704	CLR	C17-C20-C22-C23
3	B	705	CLR	C17-C20-C22-C23
3	A	704	CLR	C21-C20-C22-C23
3	B	705	CLR	C21-C20-C22-C23
3	A	707	CLR	C17-C20-C22-C23
3	B	708	CLR	C17-C20-C22-C23
4	A	709	A1EFM	C25-O26-P27-O29
4	B	710	A1EFM	C25-O26-P27-O29
4	A	709	A1EFM	C15-C14-O13-C12
4	B	710	A1EFM	C15-C14-O13-C12
4	A	709	A1EFM	O24-C14-O13-C12
4	B	710	A1EFM	O24-C14-O13-C12
4	A	709	A1EFM	C04-C05-C06-C07
4	B	710	A1EFM	C04-C05-C06-C07
4	A	709	A1EFM	C18-C19-C20-C21
4	B	710	A1EFM	C18-C19-C20-C21
4	A	709	A1EFM	C16-C17-C18-C19
4	B	710	A1EFM	C16-C17-C18-C19
4	A	709	A1EFM	C03-C04-C05-C06
4	B	710	A1EFM	C03-C04-C05-C06
3	A	705	CLR	C13-C17-C20-C22
3	B	706	CLR	C13-C17-C20-C22
4	A	709	A1EFM	C14-C15-C16-C17
4	B	710	A1EFM	C14-C15-C16-C17
3	A	705	CLR	C16-C17-C20-C21
3	B	706	CLR	C16-C17-C20-C21
3	A	710	CLR	C13-C17-C20-C22
3	B	701	CLR	C13-C17-C20-C22
3	A	705	CLR	C13-C17-C20-C21
3	B	706	CLR	C13-C17-C20-C21
3	A	705	CLR	C16-C17-C20-C22
3	B	706	CLR	C16-C17-C20-C22
3	A	704	CLR	C16-C17-C20-C21
3	B	705	CLR	C16-C17-C20-C21
3	A	704	CLR	C13-C17-C20-C22
3	B	705	CLR	C13-C17-C20-C22
4	A	709	A1EFM	C17-C18-C19-C20
4	B	710	A1EFM	C17-C18-C19-C20
3	A	704	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
3	A	710	CLR	C16-C17-C20-C22
3	B	701	CLR	C16-C17-C20-C22
3	B	705	CLR	C16-C17-C20-C22
4	A	709	A1EFM	O10-C11-C12-C25
4	B	710	A1EFM	O10-C11-C12-C25
3	A	710	CLR	C13-C17-C20-C21
3	B	701	CLR	C13-C17-C20-C21
3	A	704	CLR	C13-C17-C20-C21
3	B	705	CLR	C13-C17-C20-C21
3	A	710	CLR	C16-C17-C20-C21
3	B	701	CLR	C16-C17-C20-C21
3	A	710	CLR	C17-C20-C22-C23
3	B	701	CLR	C17-C20-C22-C23
4	A	709	A1EFM	O32-C31-C33-O34
4	B	710	A1EFM	O32-C31-C33-O34
3	A	710	CLR	C23-C24-C25-C27
3	B	701	CLR	C23-C24-C25-C27
4	A	709	A1EFM	O10-C11-C12-O13
4	B	710	A1EFM	O10-C11-C12-O13
3	A	710	CLR	C23-C24-C25-C26
3	B	701	CLR	C23-C24-C25-C26
3	B	708	CLR	C22-C23-C24-C25
3	A	707	CLR	C22-C23-C24-C25
3	A	702	CLR	C13-C17-C20-C21
3	B	703	CLR	C13-C17-C20-C21
3	A	702	CLR	C20-C22-C23-C24
3	B	703	CLR	C20-C22-C23-C24
3	A	702	CLR	C16-C17-C20-C22
3	B	703	CLR	C16-C17-C20-C22
4	A	709	A1EFM	C30-C31-C33-O34
4	B	710	A1EFM	C30-C31-C33-O34
3	A	702	CLR	C13-C17-C20-C22
3	B	703	CLR	C13-C17-C20-C22
4	A	709	A1EFM	C30-O29-P27-O35
4	B	710	A1EFM	C30-O29-P27-O35

There are no ring outliers.

20 monomers are involved in 192 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	709	CLR	22	0
3	A	704	CLR	5	0

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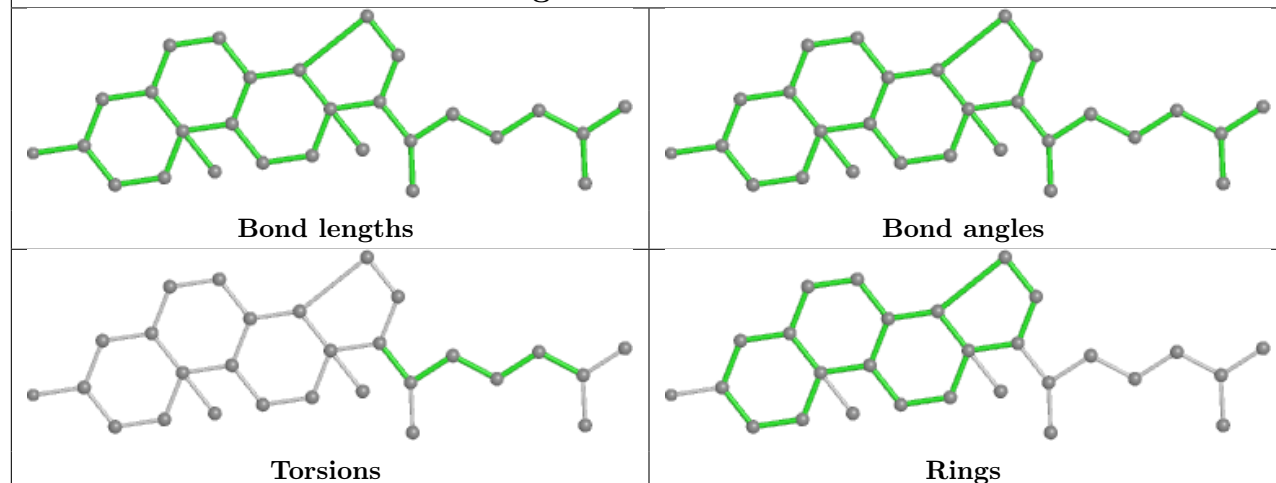


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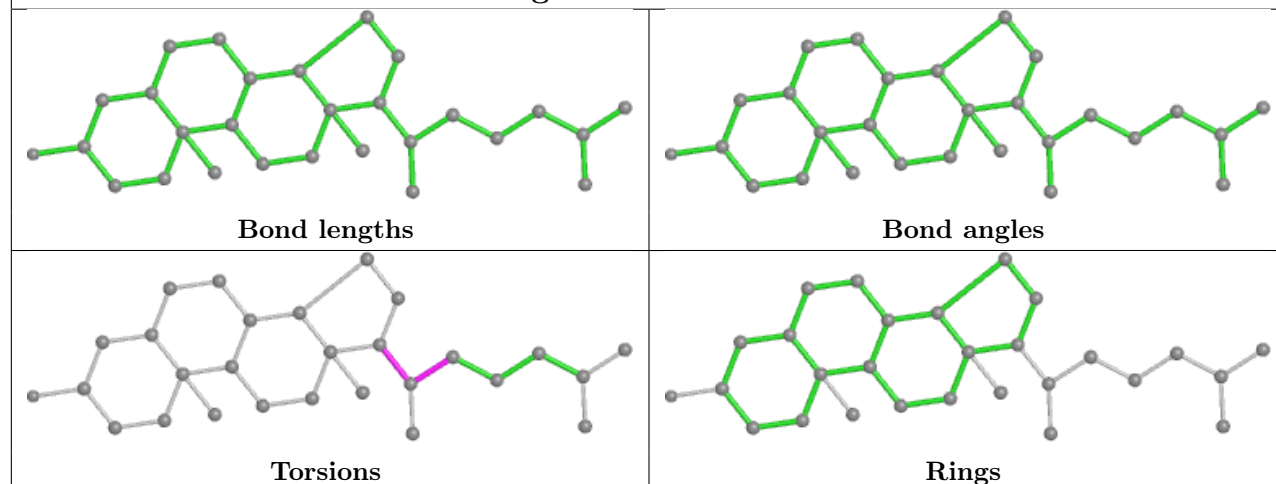
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	706	CLR	12	0
3	B	701	CLR	4	0
4	A	709	A1EFM	2	0
3	B	708	CLR	35	0
3	A	703	CLR	18	0
2	A	701	YG7	1	0
3	A	708	CLR	22	0
3	A	710	CLR	5	0
4	B	710	A1EFM	2	0
3	B	707	CLR	11	0
3	B	703	CLR	24	0
3	B	704	CLR	18	0
3	A	702	CLR	24	0
2	B	702	YG7	1	0
3	A	707	CLR	35	0
3	A	706	CLR	11	0
3	B	705	CLR	5	0
3	A	705	CLR	11	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.

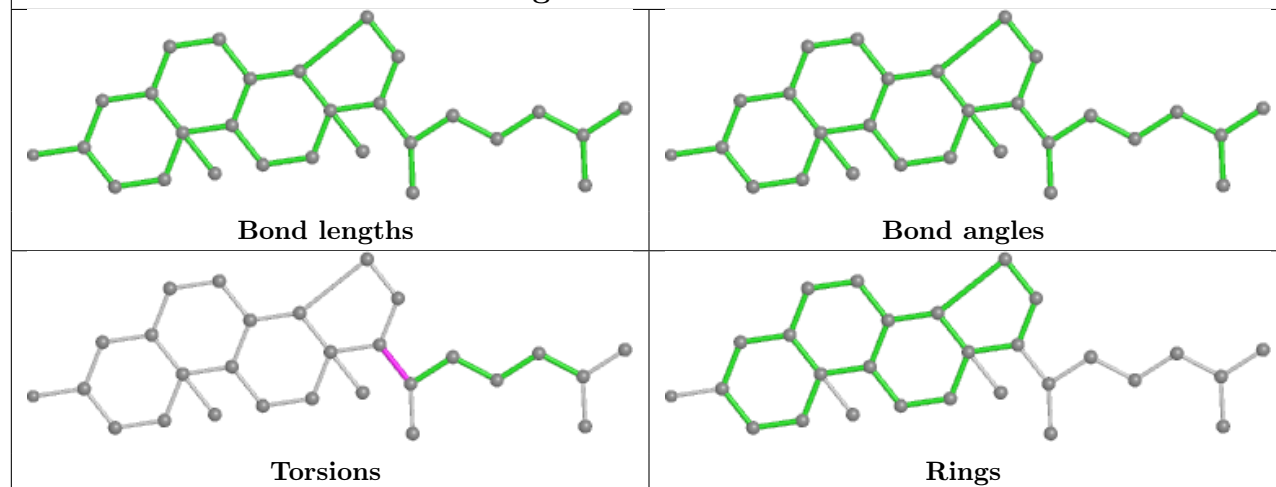
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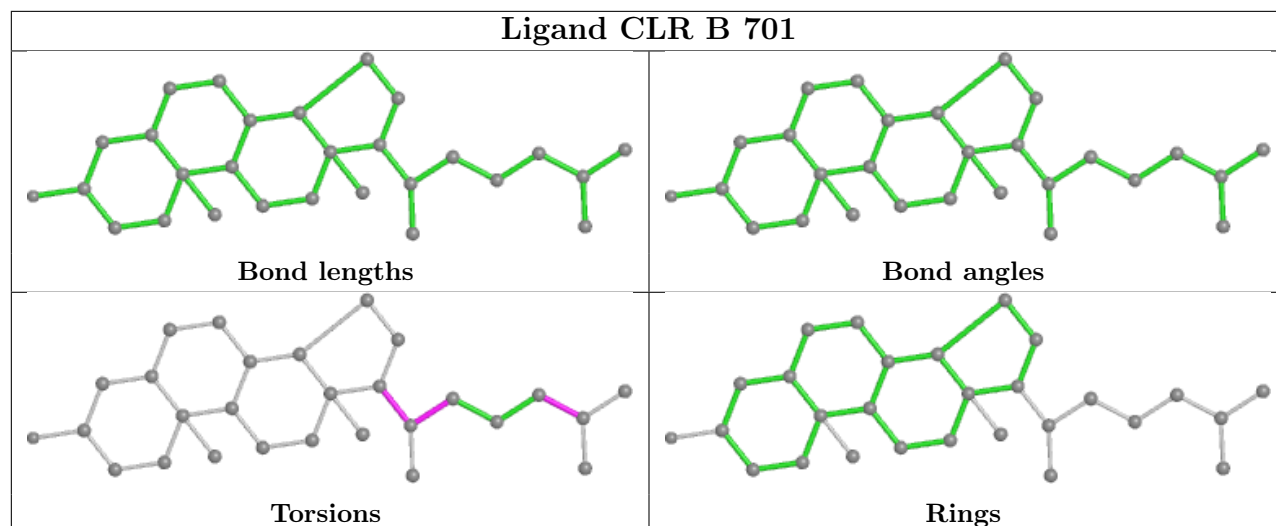
## Ligand CLR A 704



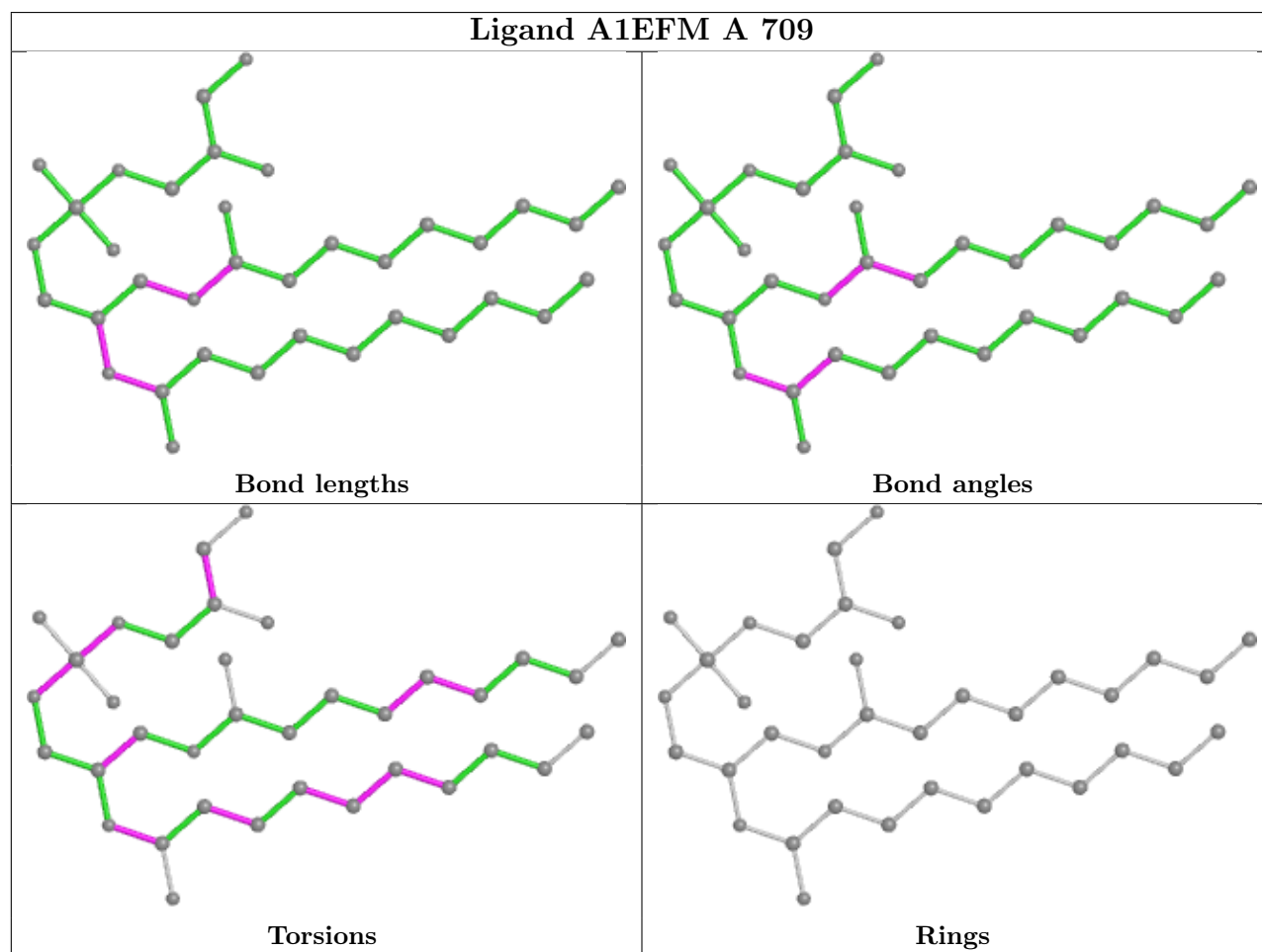
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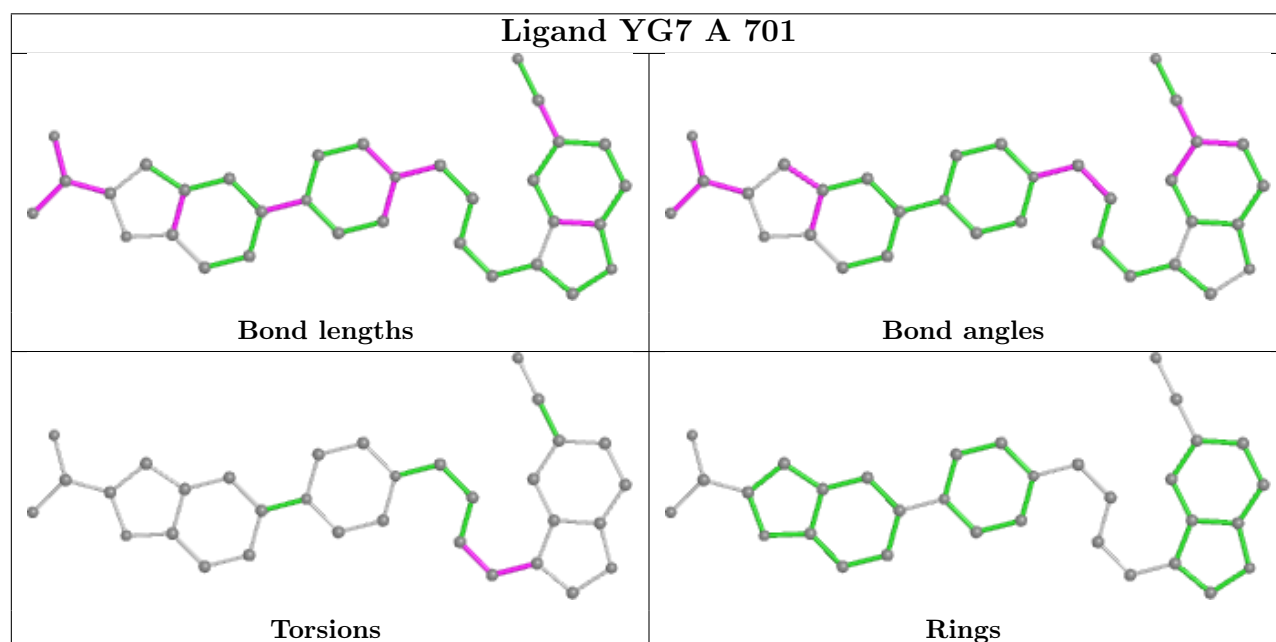
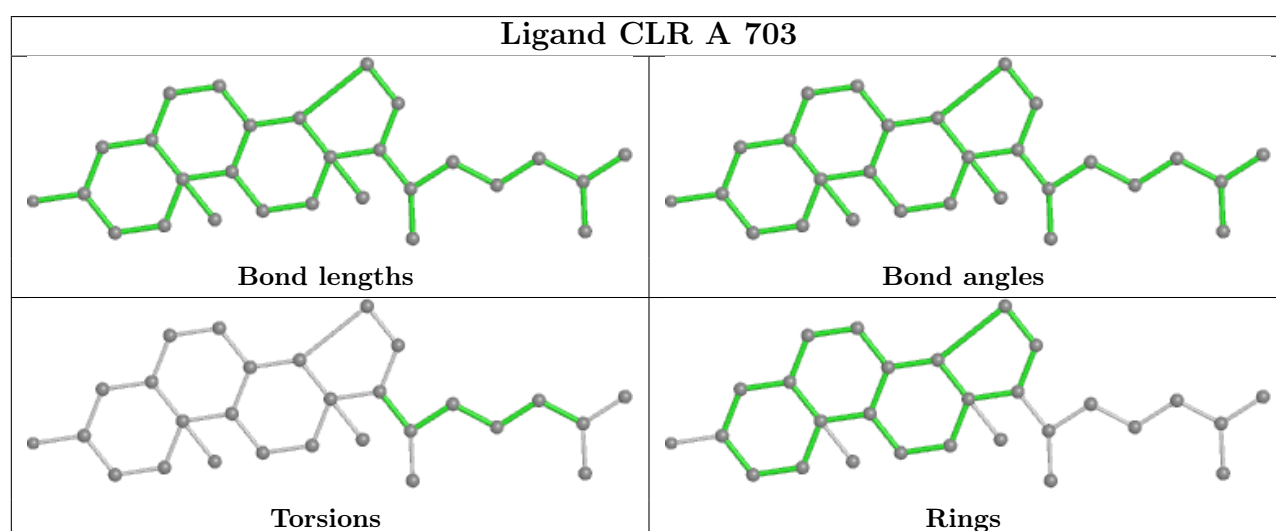
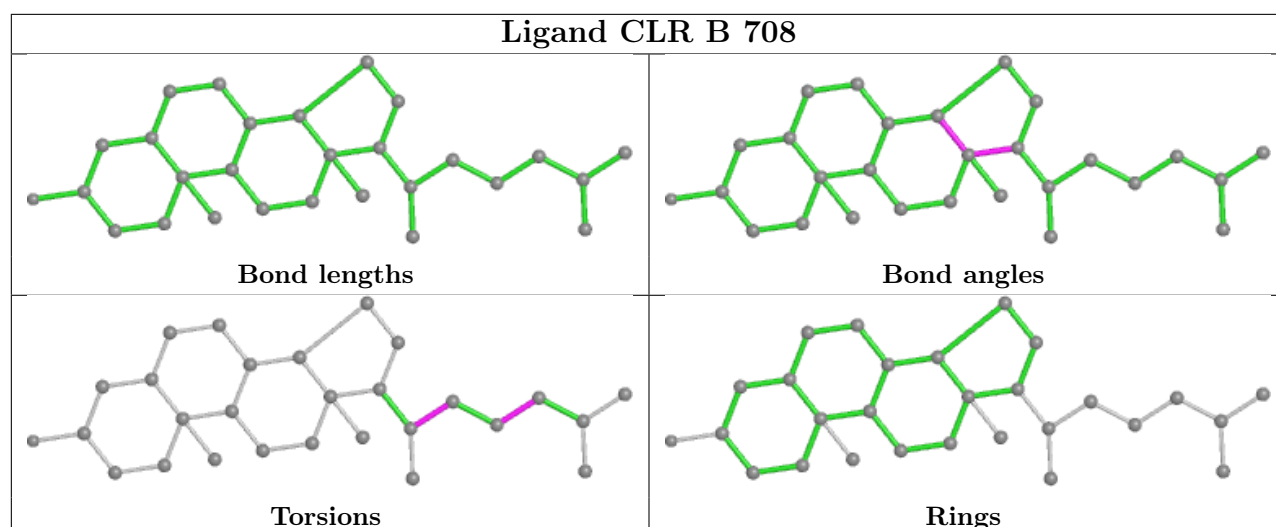


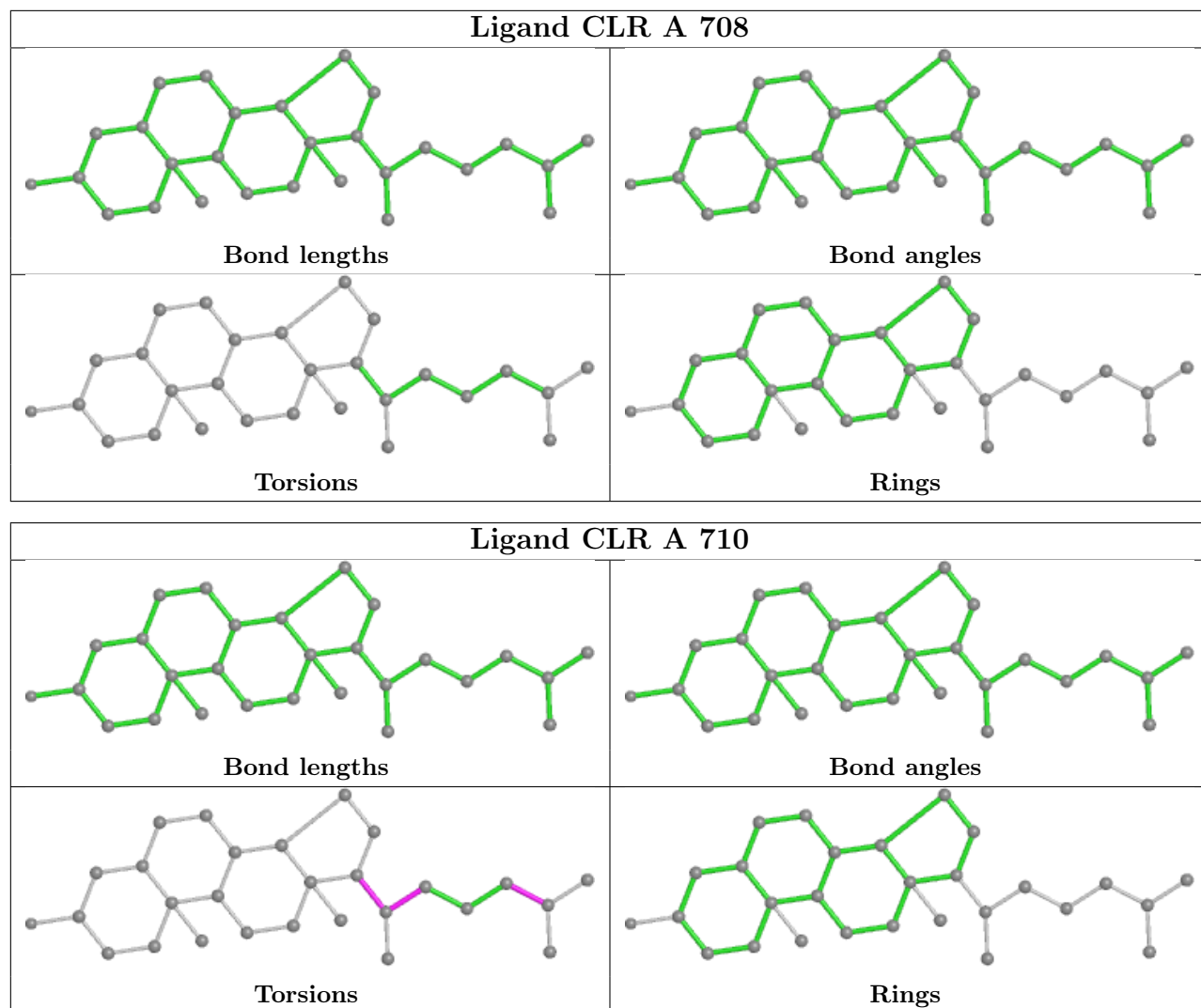
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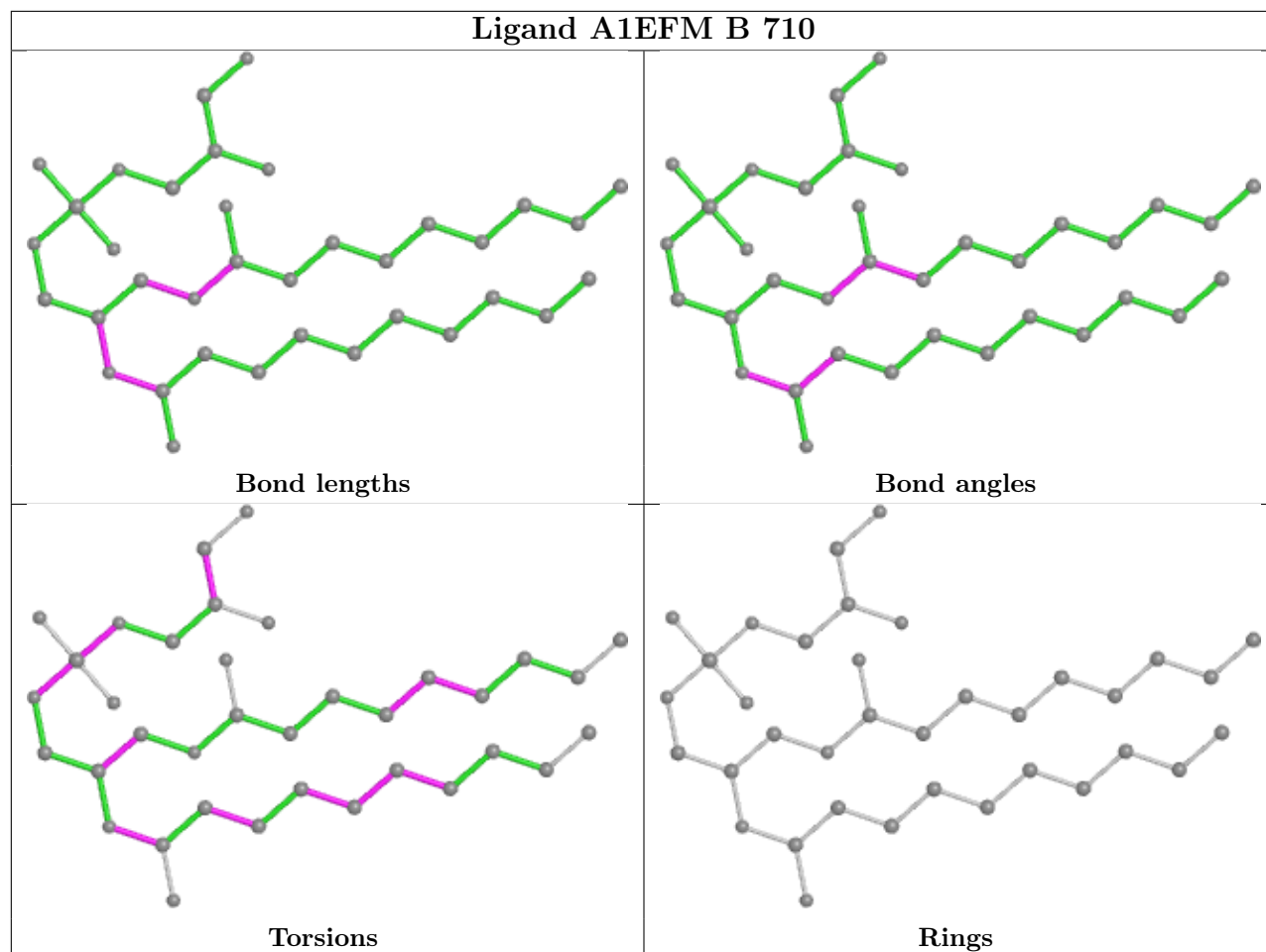
## Ligand A1EFM A 709



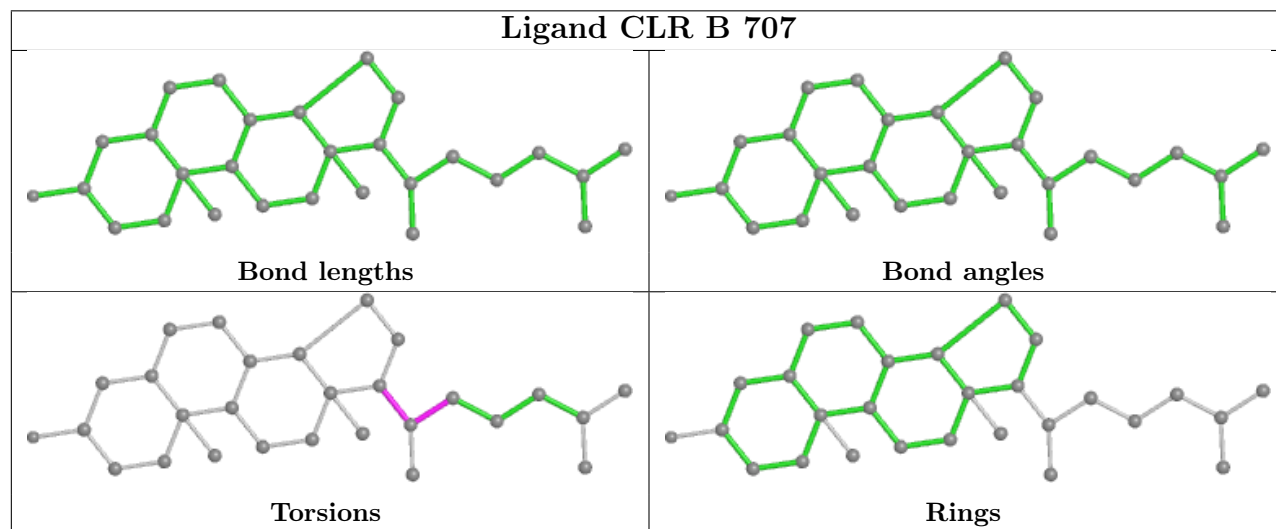


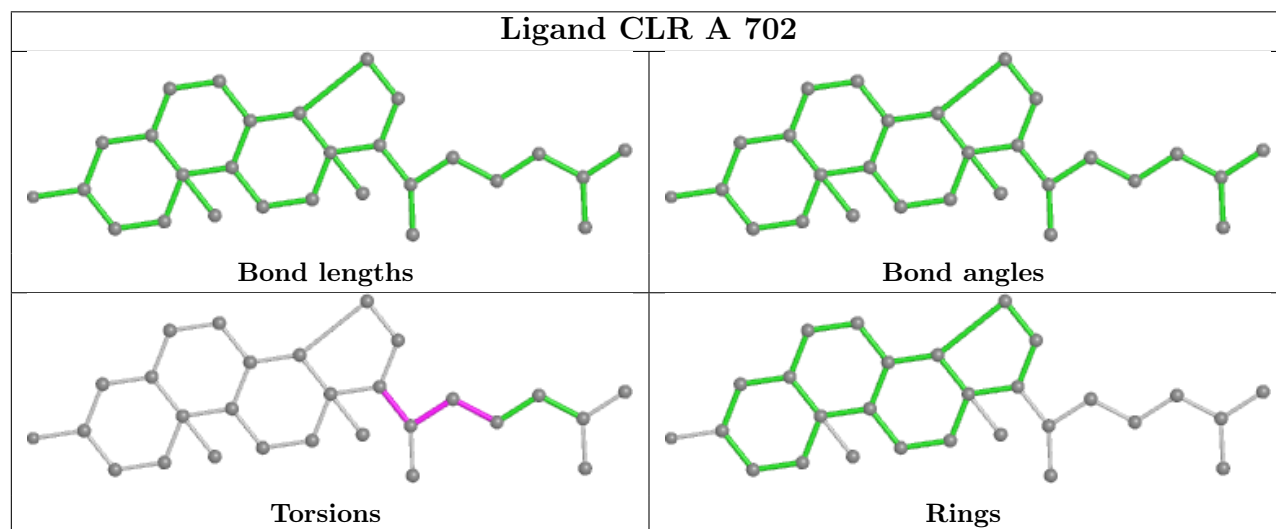
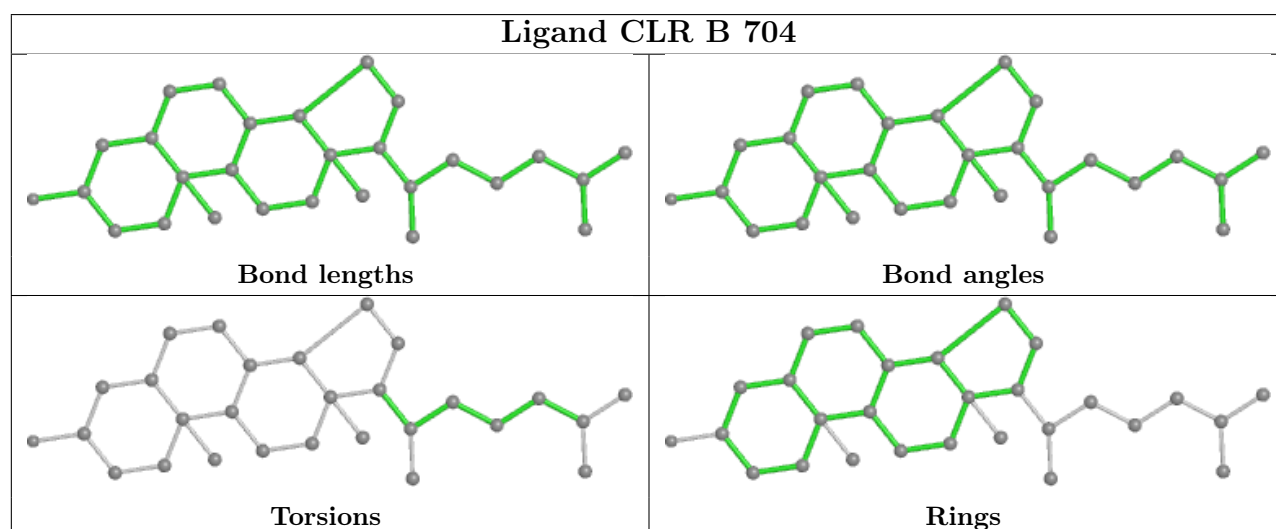
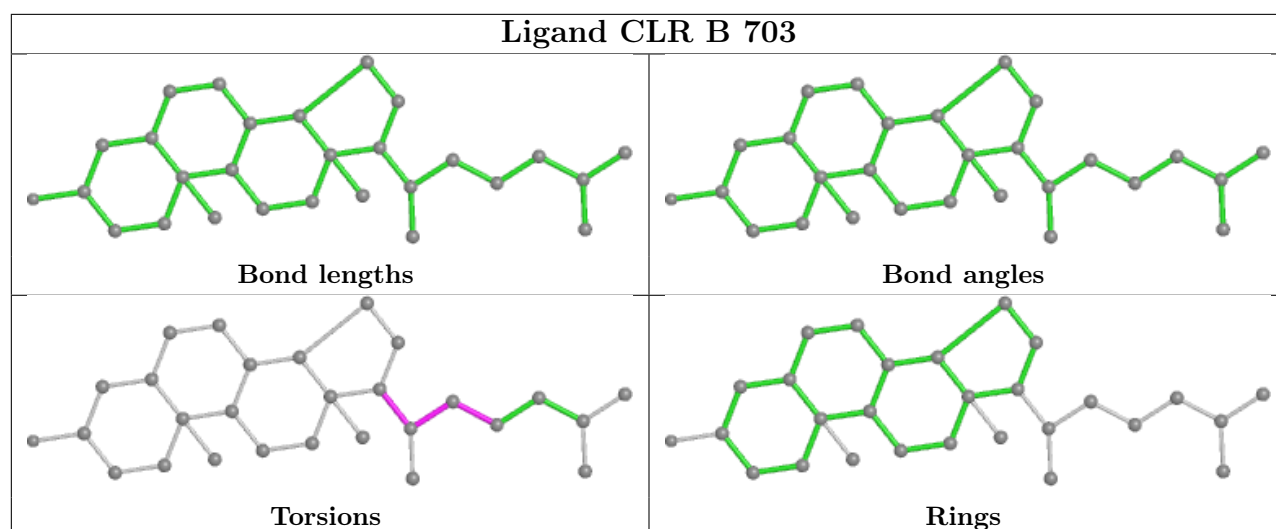


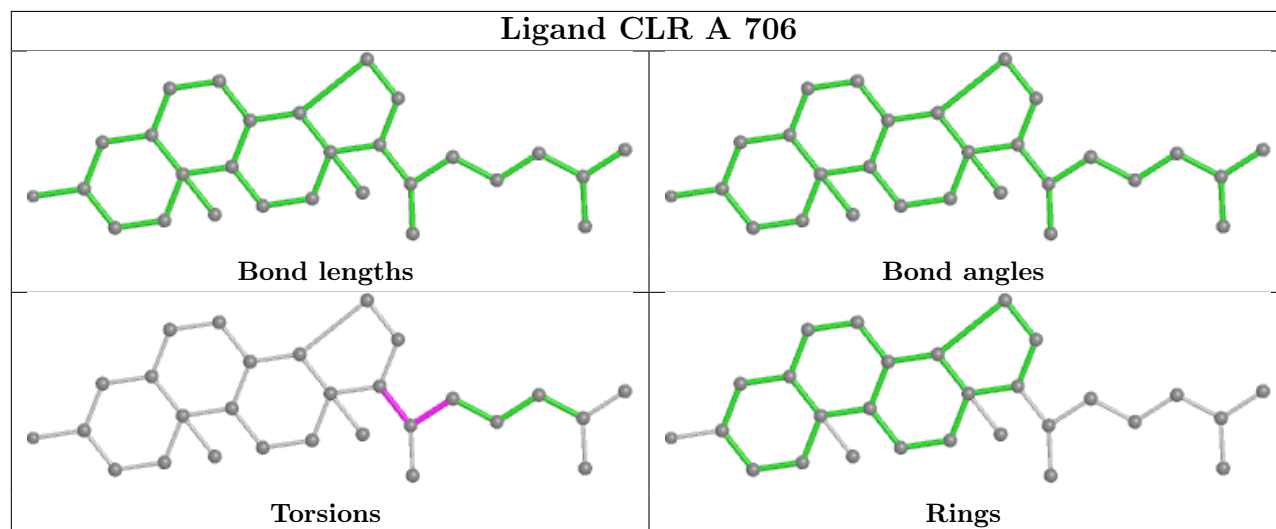
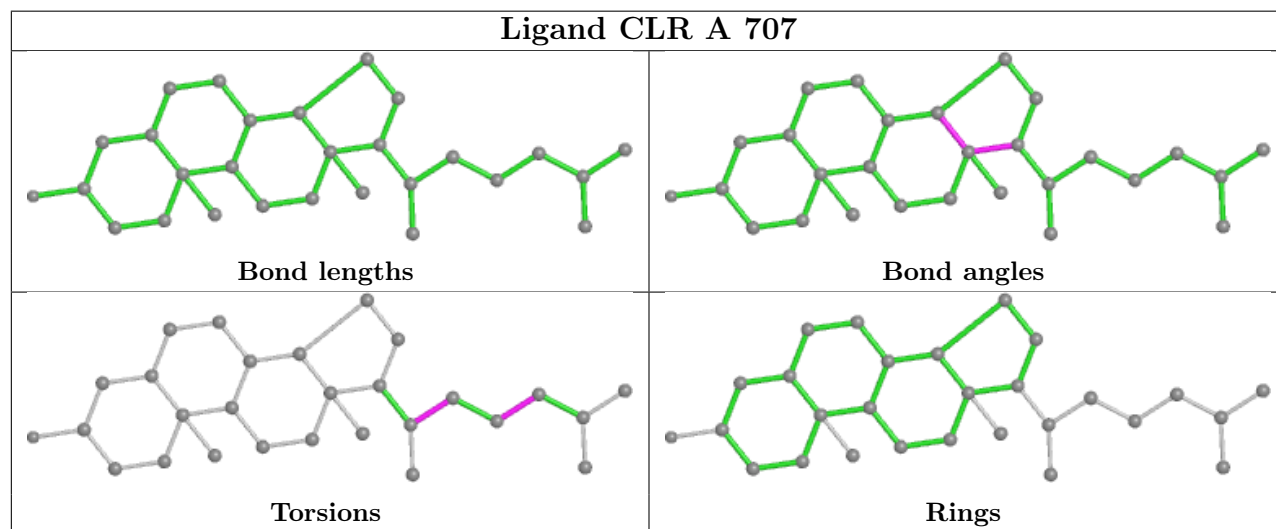
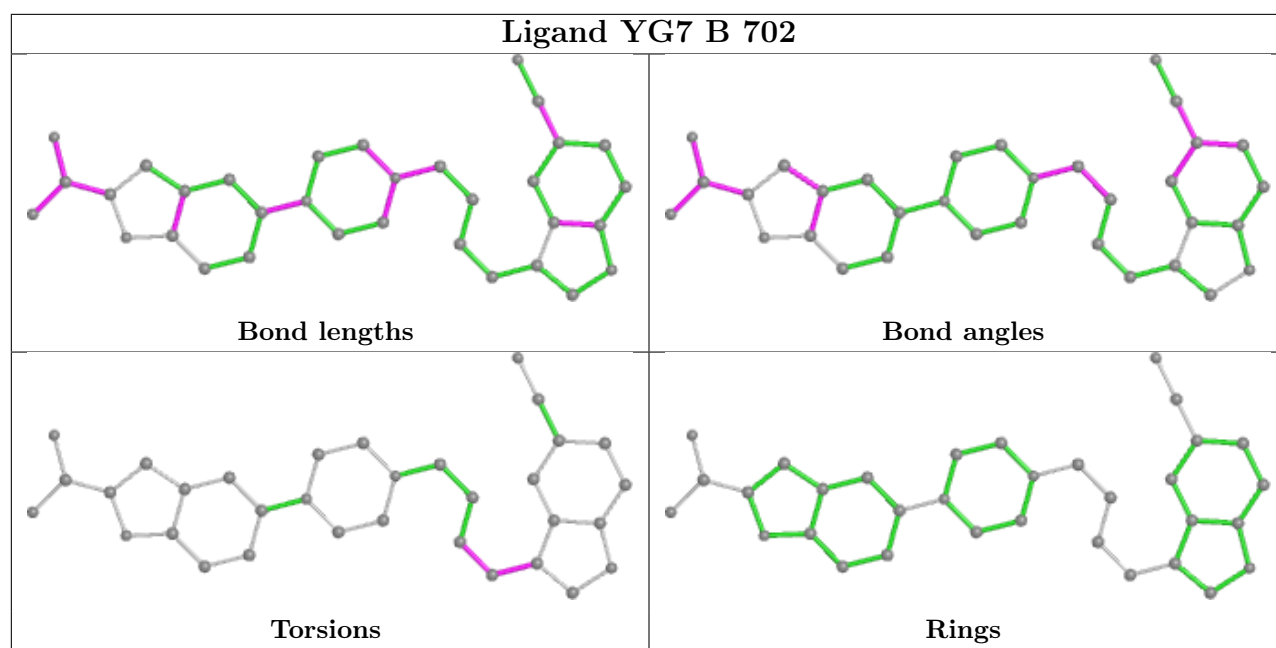
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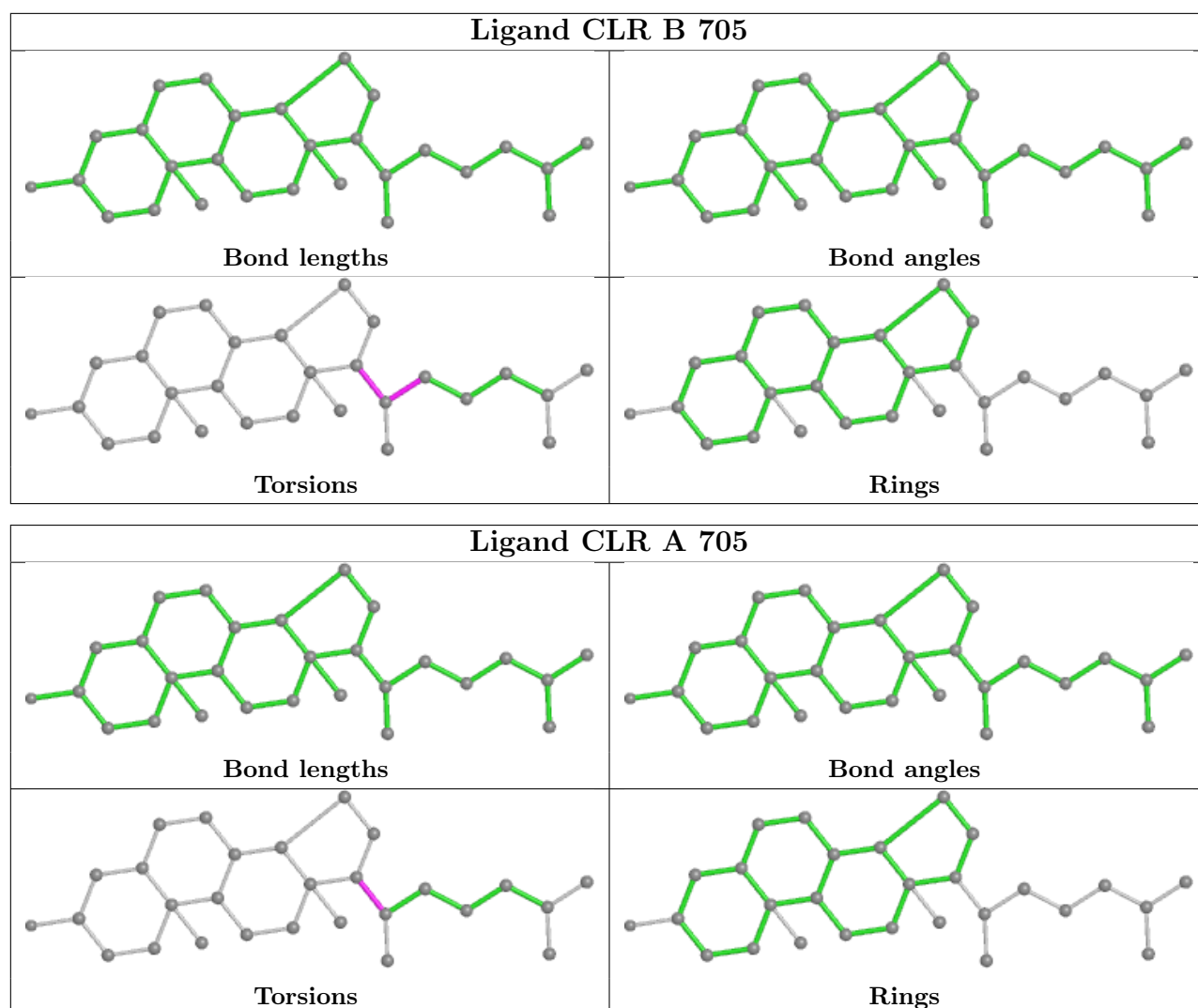
## Ligand CLR B 707











## 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.