



Full wwPDB EM Validation Report ⓘ

Oct 16, 2024 – 12:33 AM JST

PDB ID : 8JD1
EMDB ID : EMD-36172
Title : Cryo-EM structure of mGlu2-mGlu3 heterodimer in Rco state
Authors : Wang, X.; Wang, M.; Xu, T.; Feng, Y.; Han, S.; Lin, S.; Zhao, Q.; Wu, B.
Deposited on : 2023-05-12
Resolution : 3.70 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

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>.

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 : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

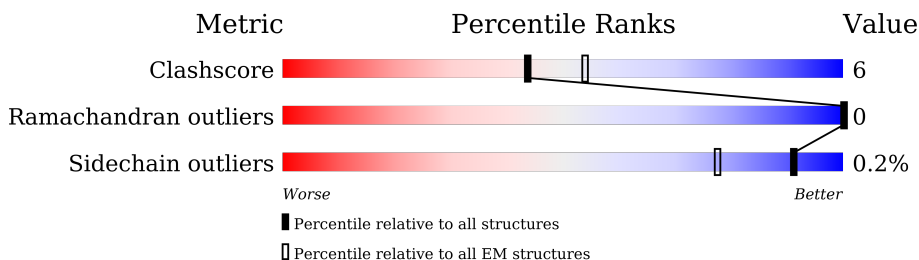
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	2	993	
2	3	993	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10766 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Metabotropic glutamate receptor 2,Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	750	Total	C	N	O	S	0	0
			5121	3233	907	950	31		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	9	ASP	-	expression tag	UNP Q14416
2	10	TYR	-	expression tag	UNP Q14416
2	11	LYS	-	expression tag	UNP Q14416
2	12	ASP	-	expression tag	UNP Q14416
2	13	ASP	-	expression tag	UNP Q14416
2	14	ASP	-	expression tag	UNP Q14416
2	15	ASP	-	expression tag	UNP Q14416
2	16	GLY	-	expression tag	UNP Q14416
2	17	ALA	-	expression tag	UNP Q14416
2	18	PRO	-	expression tag	UNP Q14416
2	873	LEU	-	linker	UNP Q14416
2	874	GLU	-	linker	UNP Q14416
2	875	VAL	-	linker	UNP Q14416
2	876	LEU	-	linker	UNP Q14416
2	877	PHE	-	linker	UNP Q14416
2	878	GLN	-	linker	UNP Q14416
2	879	GLY	-	linker	UNP Q14416
2	880	PRO	-	linker	UNP Q14416
2	988	PHE	-	expression tag	UNP P62942
2	989	ALA	-	expression tag	UNP P62942
2	990	ALA	-	expression tag	UNP P62942
2	991	ALA	-	expression tag	UNP P62942
2	992	HIS	-	expression tag	UNP P62942
2	993	HIS	-	expression tag	UNP P62942
2	994	HIS	-	expression tag	UNP P62942
2	995	HIS	-	expression tag	UNP P62942
2	996	HIS	-	expression tag	UNP P62942

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Chain	Residue	Modelled	Actual	Comment	Reference
2	997	HIS	-	expression tag	UNP P62942
2	998	HIS	-	expression tag	UNP P62942
2	999	HIS	-	expression tag	UNP P62942
2	1000	HIS	-	expression tag	UNP P62942
2	1001	HIS	-	expression tag	UNP P62942

- Molecule 2 is a protein called Metabotropic glutamate receptor 3, Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	756	Total	C	N	O	S	0	0
			5429	3444	928	1022	35		

There are 41 discrepancies between the modelled and reference sequences:

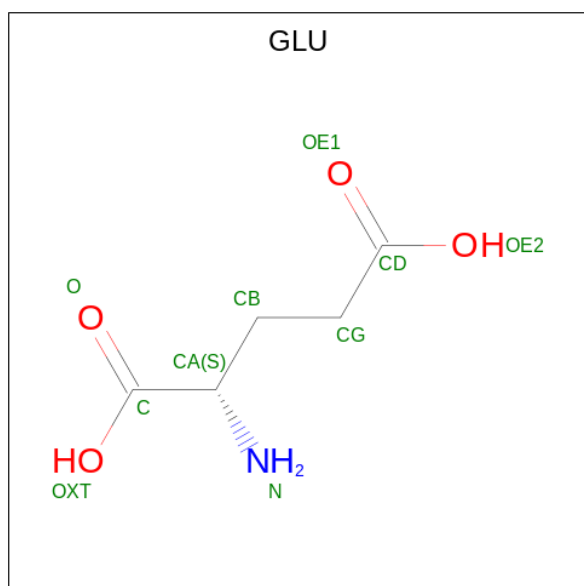
Chain	Residue	Modelled	Actual	Comment	Reference
3	-8	ASP	-	expression tag	UNP Q14832
3	-7	TYR	-	expression tag	UNP Q14832
3	-6	LYS	-	expression tag	UNP Q14832
3	-5	ASP	-	expression tag	UNP Q14832
3	-4	ASP	-	expression tag	UNP Q14832
3	-3	ASP	-	expression tag	UNP Q14832
3	-2	ASP	-	expression tag	UNP Q14832
3	-1	LYS	-	expression tag	UNP Q14832
3	0	GLY	-	expression tag	UNP Q14832
3	1	ALA	-	expression tag	UNP Q14832
3	2	PRO	-	expression tag	UNP Q14832
3	3	TRP	-	expression tag	UNP Q14832
3	4	SER	-	expression tag	UNP Q14832
3	5	HIS	-	expression tag	UNP Q14832
3	6	PRO	-	expression tag	UNP Q14832
3	7	GLN	-	expression tag	UNP Q14832
3	8	PHE	-	expression tag	UNP Q14832
3	9	GLU	-	expression tag	UNP Q14832
3	10	LYS	-	expression tag	UNP Q14832
3	11	GLY	-	expression tag	UNP Q14832
3	12	SER	-	expression tag	UNP Q14832
3	13	GLY	-	expression tag	UNP Q14832
3	14	SER	-	expression tag	UNP Q14832
3	15	TRP	-	expression tag	UNP Q14832
3	16	SER	-	expression tag	UNP Q14832
3	17	HIS	-	expression tag	UNP Q14832

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Chain	Residue	Modelled	Actual	Comment	Reference
3	18	PRO	-	expression tag	UNP Q14832
3	19	GLN	-	expression tag	UNP Q14832
3	20	PHE	-	expression tag	UNP Q14832
3	21	GLU	-	expression tag	UNP Q14832
3	22	LYS	-	expression tag	UNP Q14832
3	880	LEU	-	linker	UNP Q14832
3	881	GLU	-	linker	UNP Q14832
3	882	VAL	-	linker	UNP Q14832
3	883	LEU	-	linker	UNP Q14832
3	884	PHE	-	linker	UNP Q14832
3	885	GLN	-	linker	UNP Q14832
3	886	GLY	-	linker	UNP Q14832
3	887	PRO	-	linker	UNP Q14832
3	983	GLU	-	expression tag	UNP A0A8V8TRG9
3	984	PHE	-	expression tag	UNP A0A8V8TRG9

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).

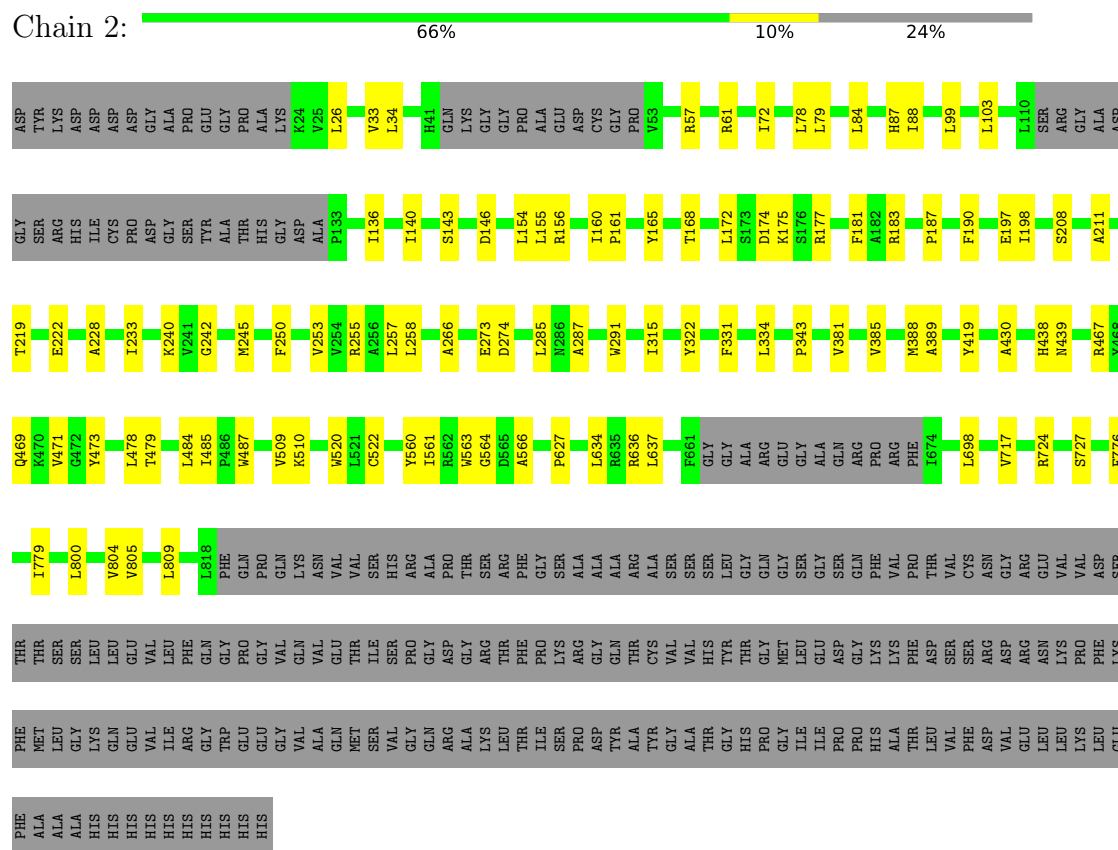


Mol	Chain	Residues	Atoms			AltConf
4	3	1	Total	C	O	0
			28	27	1	
4	3	1	Total	C	O	0
			28	27	1	
4	3	1	Total	C	O	0
			28	27	1	
4	3	1	Total	C	O	0
			28	27	1	
4	3	1	Total	C	O	0
			28	27	1	
4	3	1	Total	C	O	0
			28	27	1	

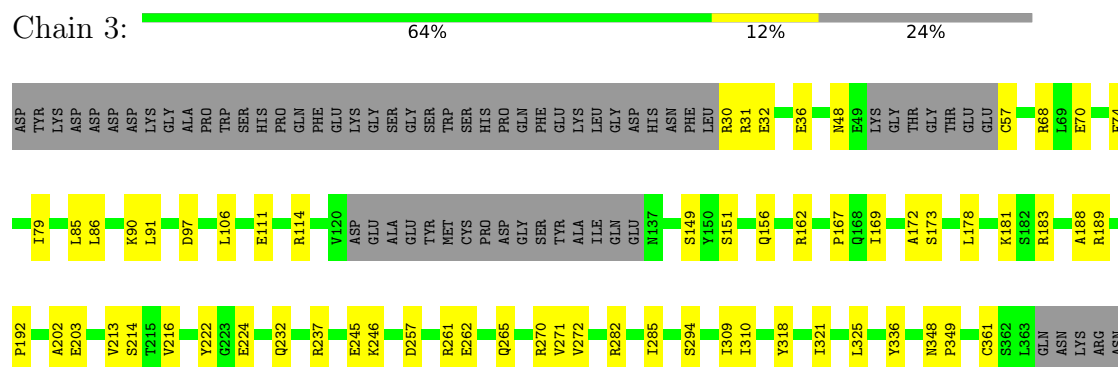
3 Residue-property plots [i](#)

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

- Molecule 1: Metabotropic glutamate receptor 2, Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 2: Metabotropic glutamate receptor 3, Serine/threonine-protein kinase mTOR



GLY	ARG	LEU	PHE	LEU	ASP	GLN	GLY	PRO	ALA	ALA	ILE	LEU	GLN	TRP	HIS	CYS	GLY	ARG	GLY	GLY	GLY	ASN	VAL	LYS	ASP	LEU	TYR	HIS	VAL	TYR	GLN	ALA	TRP	ASP	LEU	TYR	TYR	HIS	VAL	PHE	ARG	GLY	ILE	SER	LYS	GLN	PHE
L565	T792	Q799	A820	P830	GLN	LYS	ASN	VAL	VAL	THR	HIS	ARG	LEU	HIS	LEU	ASN	ILE	ARG	PHE	SER	VAL	THR	GLY	THR	GLY	VAL	LYS	ASN	THR	THR	LYS	GLY	GLY	MET	PHE	GLU	VAL	VAL	GLY	THR	THR	THR	THR	THR	THR	THR	THR
R370	C373	Y384	E385	Q386	K389	A401	K406	R407	Q408	K417	D426	L430	R465	N470	N473	W486	L490	M521	Q522	P523	G524	D525	W529	I530	C531	P536	Y537	E538	Y539	F544	T545	G546	D548	C549	G550	S551	Q552	W553	W554								
L565	I583	G587	Y626	T629	S637	P638	V639	I640	R645	W664	CYS	ILE	ALA	ARG	PHE	ILE	ASP	GLY	VAL	LYS	ASN	GLY	ALA	GLN	ARG	PRO	K681	S684	P685	V698	V701	S704	I708	A711	Y717	R723	V726	I727	L728	S740	F770						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252188	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.24	0/5231	0.47	0/7170
2	3	0.24	0/5541	0.45	0/7569
All	All	0.24	0/10772	0.46	0/14739

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	5121	0	4443	55	0
2	3	5429	0	4874	70	0
3	2	10	0	5	1	0
3	3	10	0	5	1	0
4	3	196	0	322	6	0
All	All	10766	0	9649	128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:704:SER:HB3	2:3:708:ILE:HD12	1.72	0.70
1:2:242:GLY:H	1:2:245:MET:HE1	1.57	0.69
1:2:155:LEU:HD12	1:2:160:ILE:HB	1.78	0.66
2:3:536:PRO:O	2:3:723:ARG:NH2	2.29	0.66
2:3:552:GLY:HA2	2:3:726:VAL:HG21	1.81	0.63
2:3:70:GLU:OE2	2:3:348:ASN:ND2	2.31	0.62
1:2:168:THR:HG1	3:2:1101:GLU:N	1.97	0.62
1:2:175:LYS:NZ	1:2:181:PHE:O	2.33	0.62
2:3:85:LEU:HD21	2:3:401:ALA:HB1	1.83	0.60
2:3:48:ASN:ND2	2:3:97:ASP:OD2	2.35	0.60
1:2:471:VAL:HG22	1:2:484:LEU:HD22	1.84	0.59
4:3:1004:CLR:H273	4:3:1006:CLR:H211	1.85	0.58
2:3:192:PRO:HD3	2:3:465:ARG:HH21	1.68	0.58
2:3:111:GLU:OE2	2:3:114:ARG:NH2	2.37	0.58
2:3:224:GLU:HB3	2:3:246:LYS:HZ3	1.69	0.58
2:3:408:GLN:NE2	2:3:417:LYS:O	2.37	0.57
1:2:156:ARG:NH1	1:2:177:ARG:O	2.37	0.57
2:3:270:ARG:NH2	2:3:294:SER:O	2.38	0.57
2:3:172:ALA:O	3:3:1001:GLU:N	2.37	0.57
2:3:162:ARG:NH1	2:3:183:ARG:O	2.38	0.57
2:3:538:GLU:OE2	2:3:723:ARG:NH2	2.38	0.57
1:2:509:VAL:HG23	1:2:520:TRP:HZ3	1.71	0.55
2:3:203:GLU:OE1	2:3:486:TRP:NE1	2.32	0.55
2:3:257:ASP:OD2	2:3:261:ARG:NH1	2.39	0.55
2:3:384:TYR:OH	2:3:386:GLN:OE1	2.23	0.55
2:3:68:ARG:NH1	2:3:149:SER:OG	2.40	0.55
2:3:213:VAL:HG12	2:3:271:VAL:HG13	1.90	0.54
1:2:228:ALA:HB1	1:2:233:ILE:HB	1.89	0.54
2:3:792:THR:OG1	2:3:799:GLN:O	2.25	0.54
2:3:31:ARG:NH2	2:3:349:PRO:O	2.41	0.54
2:3:86:LEU:HD23	2:3:91:LEU:HD11	1.90	0.54
2:3:626:TYR:O	2:3:629:THR:OG1	2.23	0.53
2:3:321:ILE:HD13	2:3:470:ASN:HD22	1.73	0.53
1:2:255:ARG:HA	1:2:258:LEU:HG	1.90	0.53
1:2:34:LEU:O	1:2:87:HIS:N	2.41	0.53
1:2:776:PHE:HA	1:2:779:ILE:HD12	1.89	0.52
1:2:724:ARG:HA	1:2:727:SER:HB3	1.90	0.52
1:2:26:LEU:HD12	1:2:343:PRO:HD3	1.91	0.52
2:3:637:SER:HB2	2:3:640:ILE:HG13	1.91	0.52
2:3:36:GLU:O	2:3:90:LYS:NZ	2.43	0.52
2:3:645:ARG:NH2	2:3:740:SER:OG	2.39	0.51
2:3:639:VAL:HG23	4:3:1004:CLR:H71	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:33:VAL:HG13	1:2:136:ILE:HG12	1.92	0.51
2:3:717:TYR:HA	2:3:728:LEU:HA	1.92	0.51
2:3:770:PHE:HB3	2:3:820:ALA:HB1	1.93	0.50
2:3:169:ILE:HG22	2:3:188:ALA:HB3	1.92	0.50
1:2:561:ILE:HB	1:2:563:TRP:HE3	1.76	0.50
1:2:636:ARG:NH1	1:2:727:SER:OG	2.45	0.49
2:3:214:SER:HB2	2:3:272:VAL:HG12	1.95	0.49
1:2:250:PHE:HA	1:2:253:VAL:HG12	1.93	0.49
1:2:187:PRO:HD2	1:2:190:PHE:CE2	2.48	0.49
2:3:48:ASN:HB3	2:3:57:CYS:HB2	1.95	0.49
2:3:282:ARG:HA	2:3:309:ILE:HG23	1.94	0.49
1:2:197:GLU:HB3	1:2:478:LEU:HD22	1.94	0.48
1:2:140:ILE:HD13	1:2:385:VAL:HG12	1.95	0.48
2:3:79:ILE:HD12	2:3:85:LEU:HD22	1.96	0.48
2:3:711:ALA:HB3	4:3:1004:CLR:H21	1.96	0.47
2:3:551:SER:HA	2:3:723:ARG:HG2	1.97	0.47
2:3:224:GLU:OE1	2:3:246:LYS:NZ	2.48	0.47
1:2:99:LEU:HD13	1:2:154:LEU:HD22	1.96	0.47
1:2:560:TYR:N	1:2:717:VAL:O	2.45	0.47
2:3:285:ILE:HG21	2:3:310:ILE:HG22	1.97	0.47
1:2:322:TYR:OH	1:2:438:HIS:ND1	2.36	0.47
1:2:198:ILE:HD13	1:2:315:ILE:HG21	1.96	0.47
4:3:1002:CLR:H241	4:3:1003:CLR:H272	1.97	0.47
1:2:208:SER:HB3	1:2:257:LEU:HD12	1.97	0.47
2:3:325:LEU:HD13	2:3:389:LYS:HE3	1.97	0.47
2:3:704:SER:O	2:3:708:ILE:N	2.45	0.46
1:2:285:LEU:HD22	1:2:287:ALA:HB2	1.98	0.46
2:3:151:SER:HB2	2:3:222:TYR:HB2	1.96	0.46
2:3:523:PRO:HG2	2:3:525:ASP:OD1	2.14	0.46
1:2:473:TYR:O	1:2:479:THR:OG1	2.33	0.46
2:3:361:CYS:HB3	2:3:373:CYS:HB3	1.94	0.46
2:3:181:LYS:HA	2:3:181:LYS:HD3	1.73	0.46
2:3:684:SER:OG	2:3:685:PRO:HD3	2.16	0.46
1:2:78:LEU:HD21	1:2:389:ALA:HB1	1.98	0.46
1:2:172:LEU:HB2	1:2:183:ARG:HH21	1.80	0.46
2:3:30:ARG:NH2	2:3:32:GLU:OE1	2.39	0.45
2:3:202:ALA:HB1	2:3:237:ARG:HD2	1.97	0.45
1:2:219:THR:O	1:2:222:GLU:HG3	2.16	0.45
2:3:232:GLN:CD	2:3:232:GLN:H	2.19	0.45
2:3:178:LEU:HB2	2:3:189:ARG:HH12	1.82	0.45
1:2:430:ALA:HB2	1:2:439:ASN:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:246:LYS:HE3	2:3:246:LYS:HB3	1.80	0.44
2:3:554:TRP:HB2	2:3:565:LEU:HB3	1.99	0.44
2:3:521:MET:HA	2:3:544:PHE:HB2	1.99	0.44
1:2:26:LEU:HB3	1:2:88:ILE:HB	2.00	0.44
1:2:510:LYS:H	1:2:522:CYS:HA	1.82	0.44
1:2:146:ASP:OD1	1:2:146:ASP:N	2.51	0.43
1:2:564:GLY:O	1:2:566:ALA:N	2.50	0.43
1:2:72:ILE:HD11	1:2:78:LEU:HD13	1.99	0.43
2:3:167:PRO:HG2	2:3:430:LEU:HD22	2.01	0.43
2:3:318:TYR:HE1	2:3:473:ASN:HB3	1.84	0.43
2:3:203:GLU:HB3	2:3:490:LEU:HD11	2.01	0.43
2:3:539:TYR:HD1	2:3:549:CYS:HB3	1.84	0.43
1:2:561:ILE:HD12	1:2:627:PRO:HD2	2.00	0.42
2:3:529:TRP:HZ3	2:3:531:CYS:HB2	1.83	0.42
1:2:161:PRO:HB3	1:2:419:TYR:HB2	2.01	0.42
2:3:106:LEU:HG	2:3:156:GLN:HB3	2.01	0.42
1:2:211:ALA:HB3	1:2:240:LYS:HD3	2.00	0.42
2:3:173:SER:O	2:3:173:SER:OG	2.37	0.42
1:2:143:SER:HB3	1:2:165:TYR:OH	2.19	0.42
2:3:216:VAL:HG12	2:3:245:GLU:HB2	2.01	0.42
2:3:262:GLU:O	2:3:265:GLN:HG2	2.20	0.42
1:2:61:ARG:HG2	1:2:381:VAL:HG21	2.01	0.42
2:3:545:THR:OG1	2:3:547:MET:SD	2.64	0.42
2:3:698:VAL:HA	2:3:701:VAL:HG22	2.02	0.42
1:2:485:ILE:HG22	1:2:487:TRP:H	1.83	0.42
1:2:103:LEU:HD23	1:2:103:LEU:HA	1.89	0.41
4:3:1005:CLR:H222	4:3:1005:CLR:H162	1.40	0.41
1:2:57:ARG:O	1:2:61:ARG:HD2	2.21	0.41
2:3:74:PHE:HB2	2:3:336:TYR:CD2	2.55	0.41
1:2:34:LEU:HD11	1:2:388:MET:HG2	2.02	0.41
1:2:800:LEU:O	1:2:804:VAL:N	2.43	0.41
1:2:174:ASP:OD1	1:2:174:ASP:N	2.48	0.41
1:2:273:GLU:HG2	1:2:274:ASP:N	2.36	0.41
1:2:266:ALA:HB3	1:2:291:TRP:CD1	2.55	0.41
1:2:634:LEU:HA	1:2:637:LEU:HB2	2.03	0.41
1:2:698:LEU:HD11	4:3:1004:CLR:H152	2.01	0.41
2:3:426:ASP:OD1	2:3:426:ASP:N	2.54	0.41
1:2:467:ARG:NH2	1:2:469:GLN:OE1	2.53	0.41
2:3:285:ILE:HD13	2:3:285:ILE:HA	1.95	0.41
2:3:406:LYS:HE3	2:3:406:LYS:HB2	1.95	0.41
1:2:331:PHE:HA	1:2:334:LEU:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:79:LEU:HD12	1:2:84:LEU:HD11	2.04	0.40
2:3:68:ARG:HH21	2:3:389:LYS:HB2	1.86	0.40
2:3:583:ILE:O	2:3:587:GLY:N	2.42	0.40
1:2:805:VAL:O	1:2:809:LEU:N	2.54	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	2	742/993 (75%)	693 (93%)	49 (7%)	0	100	100
2	3	746/993 (75%)	694 (93%)	52 (7%)	0	100	100
All	All	1488/1986 (75%)	1387 (93%)	101 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	429/813 (53%)	429 (100%)	0	100	100
2	3	510/867 (59%)	510 (100%)	0	100	100
All	All	939/1680 (56%)	939 (100%)	0	91	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	$\# Z > 2$
4	CLR	3	1004	-	31,31,31	0.28	0	48,48,48	0.39	0
4	CLR	3	1002	-	31,31,31	0.28	0	48,48,48	0.37	0
4	CLR	3	1005	-	31,31,31	0.29	0	48,48,48	0.35	0
4	CLR	3	1007	-	31,31,31	0.29	0	48,48,48	0.38	0
3	GLU	2	1101	-	8,9,9	1.01	0	10,11,11	1.23	0
4	CLR	3	1003	-	31,31,31	0.28	0	48,48,48	0.38	0
3	GLU	3	1001	-	8,9,9	1.05	0	10,11,11	1.43	3 (30%)
4	CLR	3	1006	-	31,31,31	0.27	0	48,48,48	0.37	0
4	CLR	3	1008	-	31,31,31	0.27	0	48,48,48	0.38	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
4	CLR	3	1004	-	-	6/10/68/68	0/4/4/4
4	CLR	3	1002	-	-	1/10/68/68	0/4/4/4
4	CLR	3	1005	-	-	6/10/68/68	0/4/4/4
4	CLR	3	1007	-	-	0/10/68/68	0/4/4/4
3	GLU	2	1101	-	-	8/9/9/9	-
4	CLR	3	1003	-	-	3/10/68/68	0/4/4/4
3	GLU	3	1001	-	-	6/9/9/9	-
4	CLR	3	1006	-	-	0/10/68/68	0/4/4/4
4	CLR	3	1008	-	-	3/10/68/68	0/4/4/4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	1001	GLU	OXT-C-CA	2.10	120.54	113.38
3	3	1001	GLU	OE2-CD-CG	2.10	120.76	114.03
3	3	1001	GLU	OXT-C-O	-2.08	119.37	124.09

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	2	1101	GLU	N-CA-CB-CG
3	2	1101	GLU	C-CA-CB-CG
3	3	1001	GLU	N-CA-CB-CG
3	3	1001	GLU	C-CA-CB-CG
4	3	1005	CLR	C16-C17-C20-C21
4	3	1005	CLR	C13-C17-C20-C21
4	3	1005	CLR	C13-C17-C20-C22
3	3	1001	GLU	OXT-C-CA-N
4	3	1005	CLR	C16-C17-C20-C22
3	2	1101	GLU	OXT-C-CA-N
4	3	1004	CLR	C17-C20-C22-C23
4	3	1005	CLR	C17-C20-C22-C23
4	3	1004	CLR	C21-C20-C22-C23
4	3	1008	CLR	C17-C20-C22-C23
4	3	1005	CLR	C21-C20-C22-C23
4	3	1003	CLR	C20-C22-C23-C24

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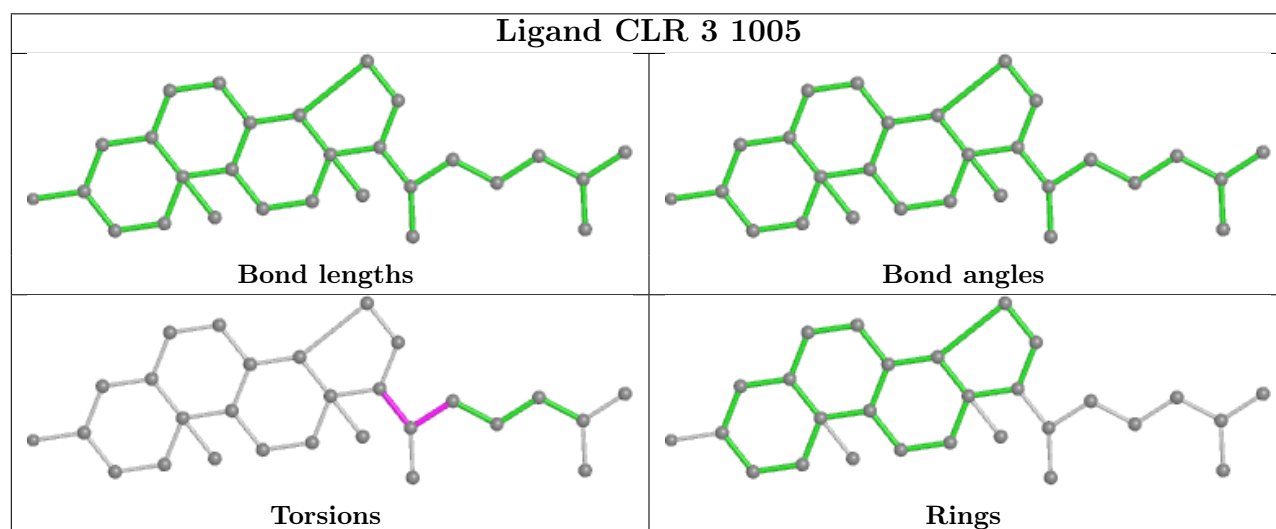
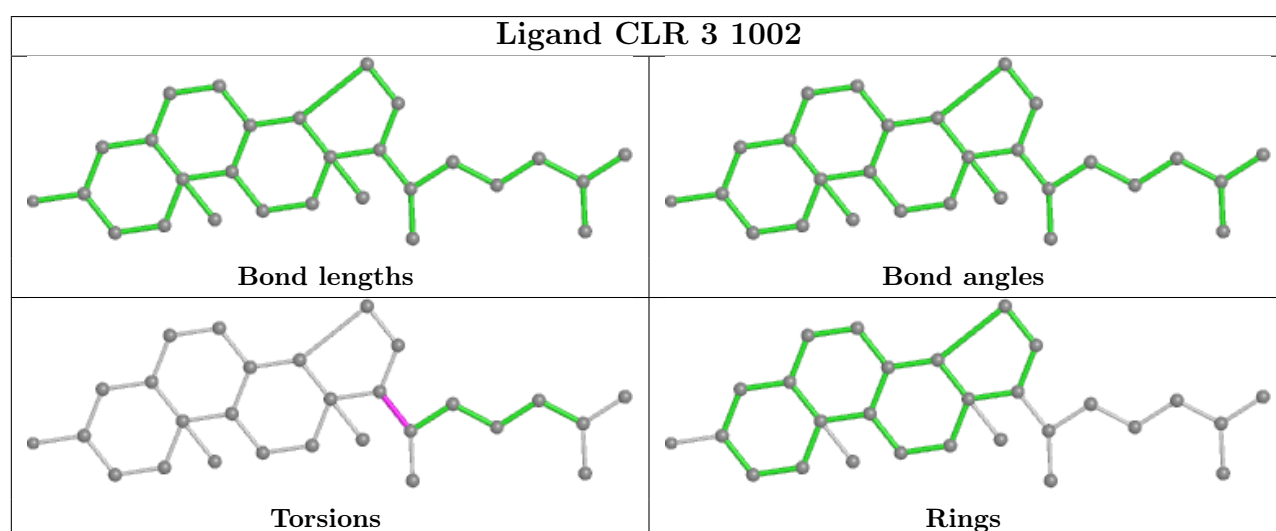
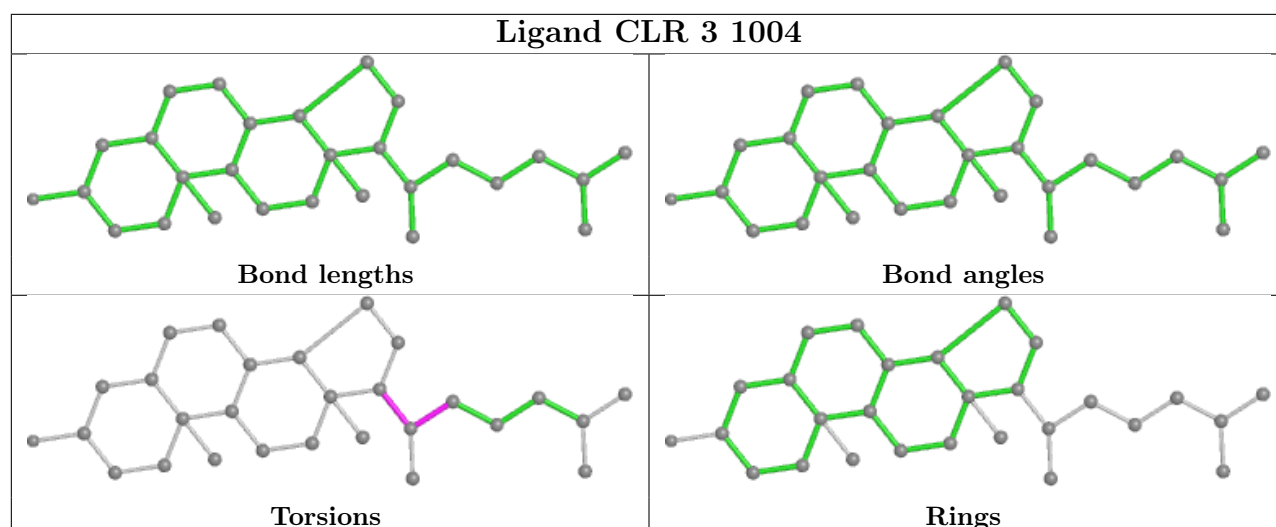
Mol	Chain	Res	Type	Atoms
4	3	1003	CLR	C22-C23-C24-C25
3	2	1101	GLU	OXT-C-CA-CB
3	3	1001	GLU	OXT-C-CA-CB
4	3	1008	CLR	C21-C20-C22-C23
3	2	1101	GLU	O-C-CA-CB
3	3	1001	GLU	O-C-CA-CB
3	2	1101	GLU	O-C-CA-N
3	3	1001	GLU	O-C-CA-N
4	3	1004	CLR	C16-C17-C20-C22
4	3	1004	CLR	C13-C17-C20-C22
4	3	1004	CLR	C16-C17-C20-C21
4	3	1004	CLR	C13-C17-C20-C21
4	3	1002	CLR	C16-C17-C20-C22
4	3	1003	CLR	C16-C17-C20-C22
3	2	1101	GLU	CA-CB-CG-CD
3	2	1101	GLU	OE2-CD-CG-CB
4	3	1008	CLR	C16-C17-C20-C22

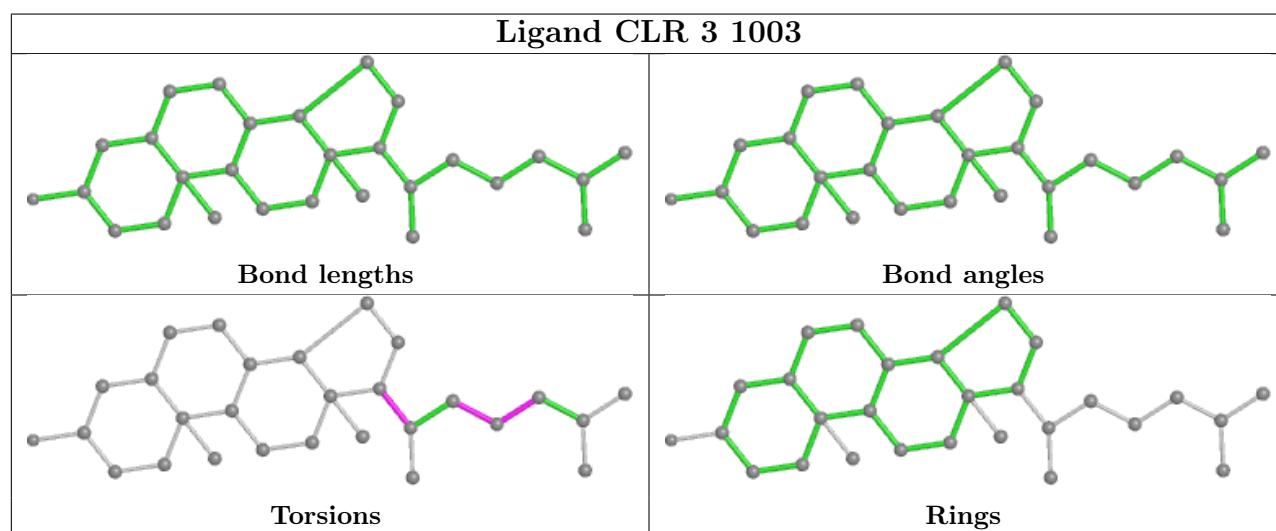
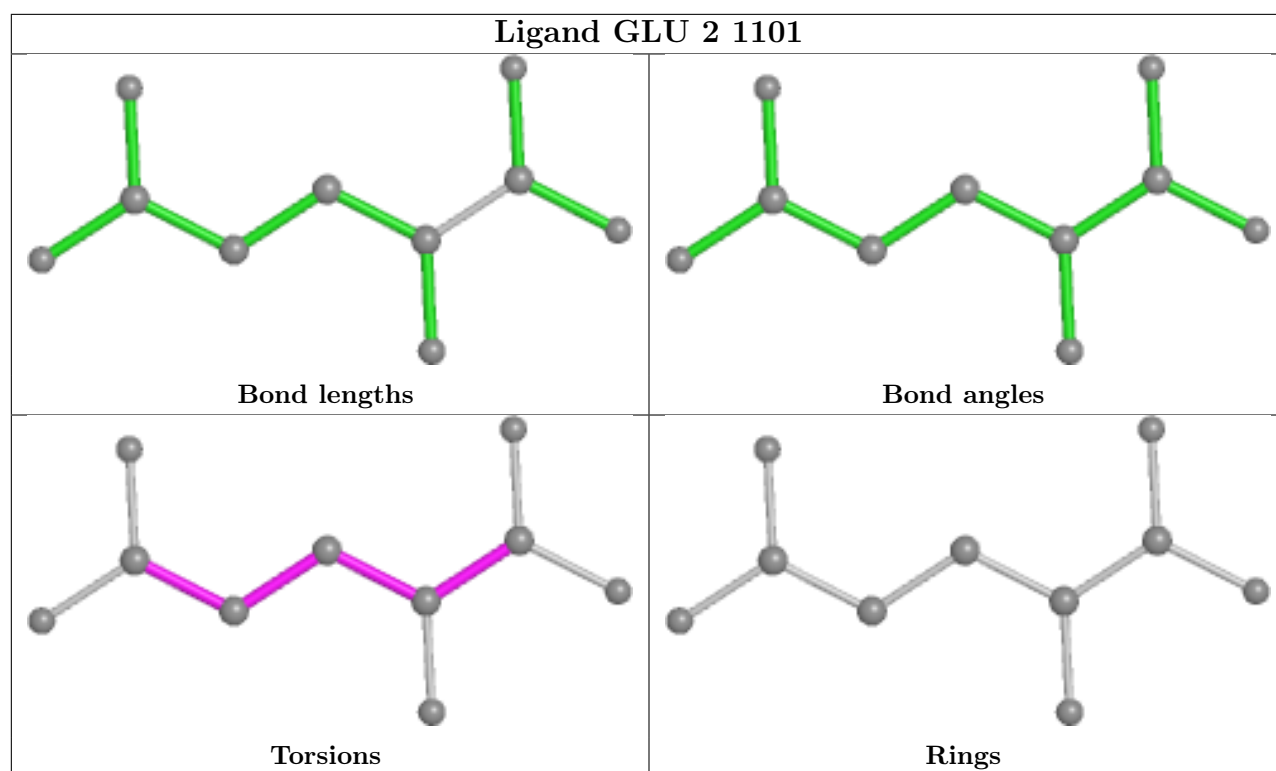
There are no ring outliers.

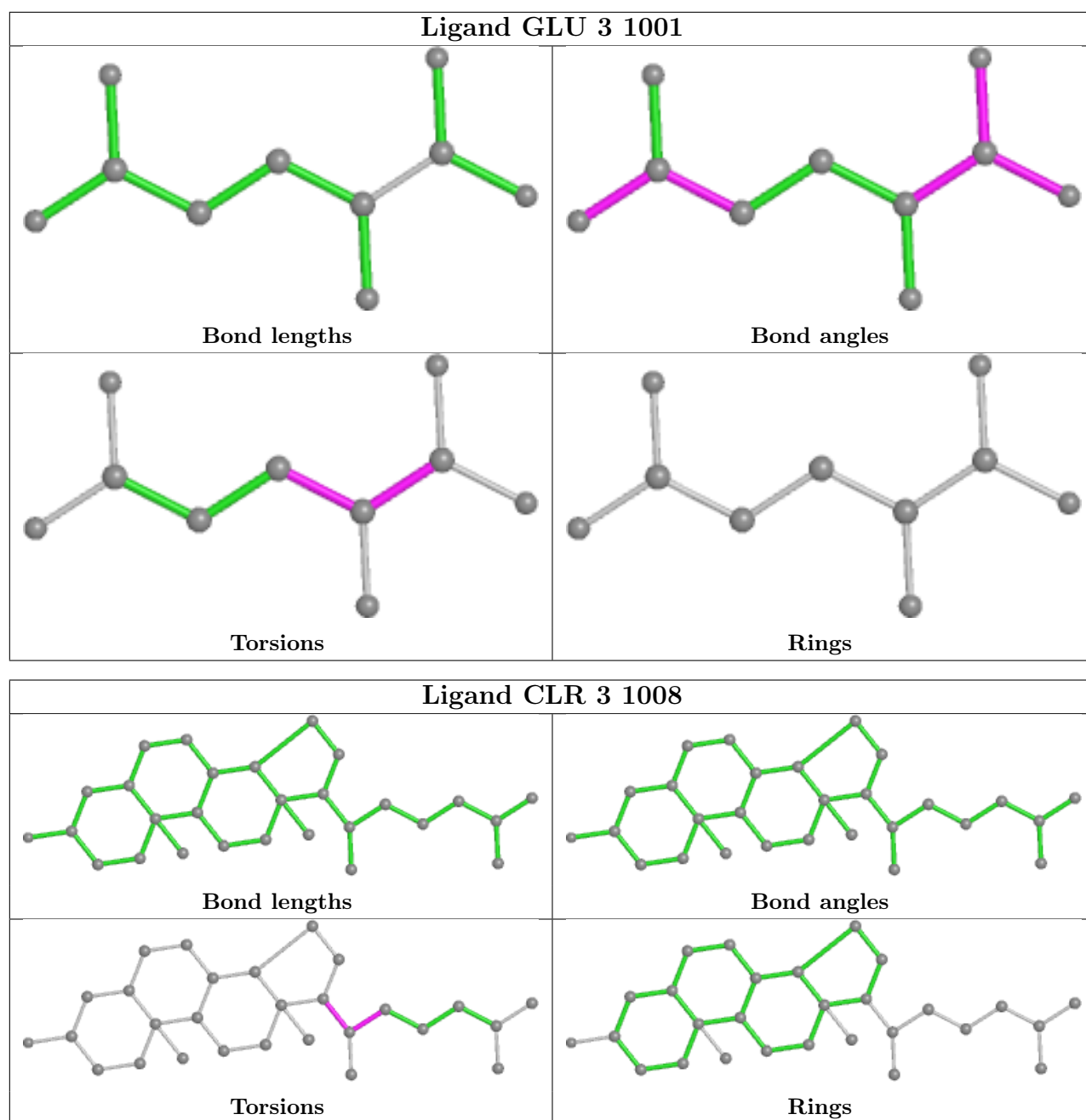
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	3	1004	CLR	4	0
4	3	1002	CLR	1	0
4	3	1005	CLR	1	0
3	2	1101	GLU	1	0
4	3	1003	CLR	1	0
3	3	1001	GLU	1	0
4	3	1006	CLR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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.