



## Full wwPDB EM Validation Report ⓘ

Oct 8, 2023 – 12:33 AM JST

PDB ID : 8JCU  
EMDB ID : EMD-36165  
Title : Cryo-EM structure of mGlu2-mGlu3 heterodimer in presence of LY341495  
(dimerization mode I)  
Authors : Wang, X.; Wang, M.; Xu, T.; Feng, Y.; Zhao, Q.; Wu, B.  
Deposited on : 2023-05-12  
Resolution : 2.80 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 : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

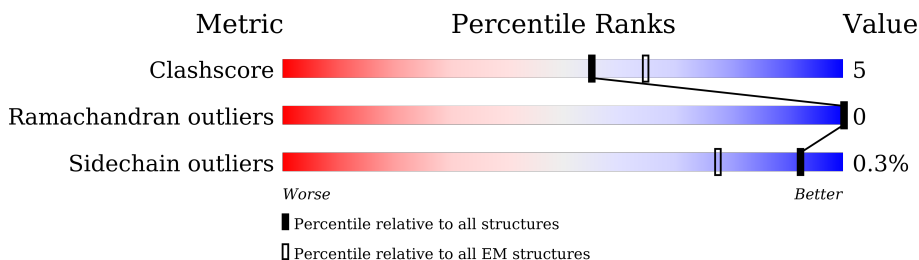
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	2	993	68% (green), 9% (yellow), 23% (grey)
2	3	993	68% (green), 9% (yellow), 23% (grey)

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 10830 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
			Total	C	N	O	S		
1	2	762	5371	3386	960	994	31	0	0

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
			Total	C	N	O	S		
2	3	765	5379	3372	951	1027	29	0	0

There are 41 discrepancies between the modelled and reference sequences:

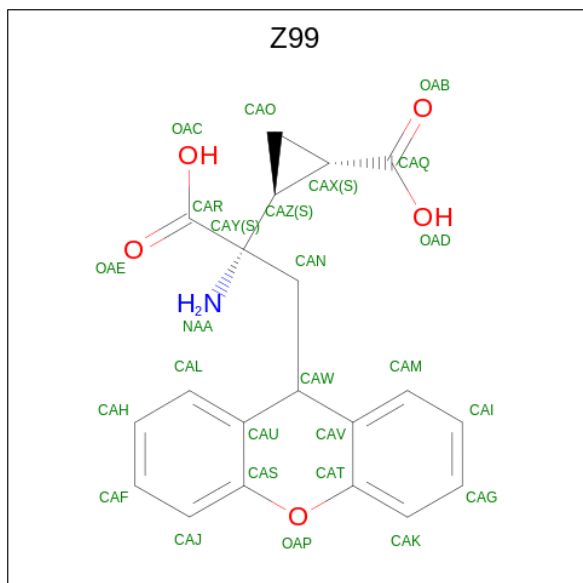
Chain	Residue	Modelled	Actual	Comment	Reference
3	-8	ASP	-	expression tag	UNP Q14832
3	-7	TYR	-	expression tag	UNP Q14832
3	-6	LYS	-	expression tag	UNP Q14832
3	-5	ASP	-	expression tag	UNP Q14832
3	-4	ASP	-	expression tag	UNP Q14832
3	-3	ASP	-	expression tag	UNP Q14832
3	-2	ASP	-	expression tag	UNP Q14832
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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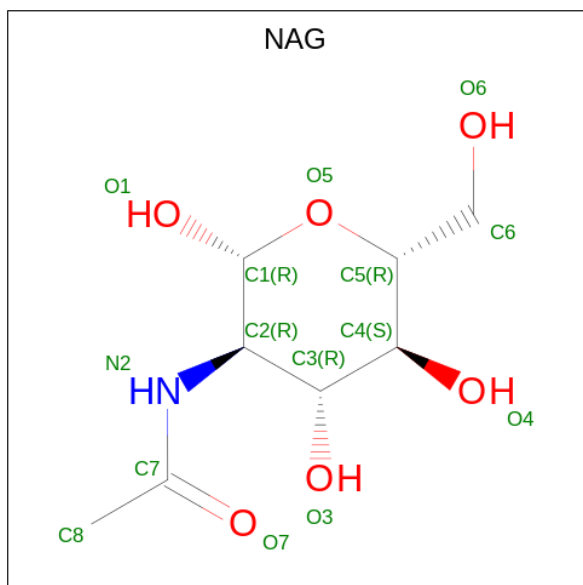
Chain	Residue	Modelled	Actual	Comment	Reference
3	18	PRO	-	expression tag	UNP Q14832
3	19	GLN	-	expression tag	UNP Q14832
3	20	PHE	-	expression tag	UNP Q14832
3	21	GLU	-	expression tag	UNP Q14832
3	22	LYS	-	expression tag	UNP Q14832
3	880	LEU	-	linker	UNP Q14832
3	881	GLU	-	linker	UNP Q14832
3	882	VAL	-	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 2-[(1S,2S)-2-carboxycyclopropyl]-3-(9H-xanthen-9-yl)-D-alanine (three-letter code: Z99) (formula: C<sub>20</sub>H<sub>19</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	2	1	Total	C	N	O	0
			26	20	1	5	
3	3	1	Total	C	N	O	0
			26	20	1	5	

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

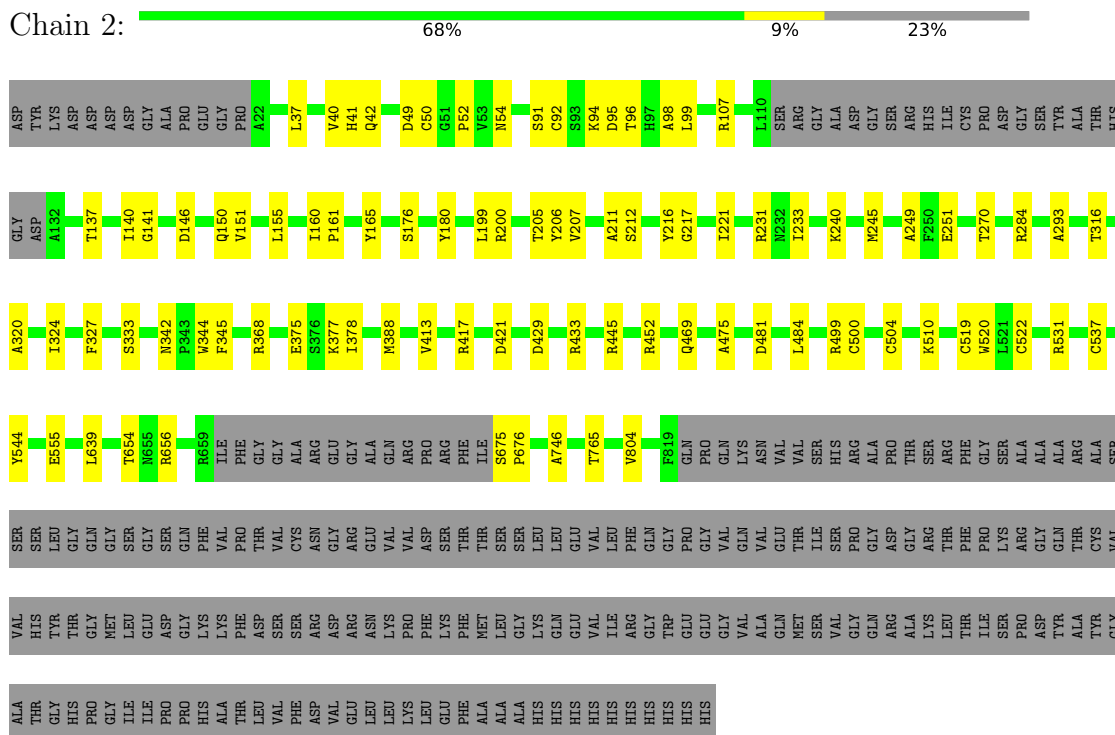


Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
4	2	1	14	8	1	5	0
4	3	1	14	8	1	5	0

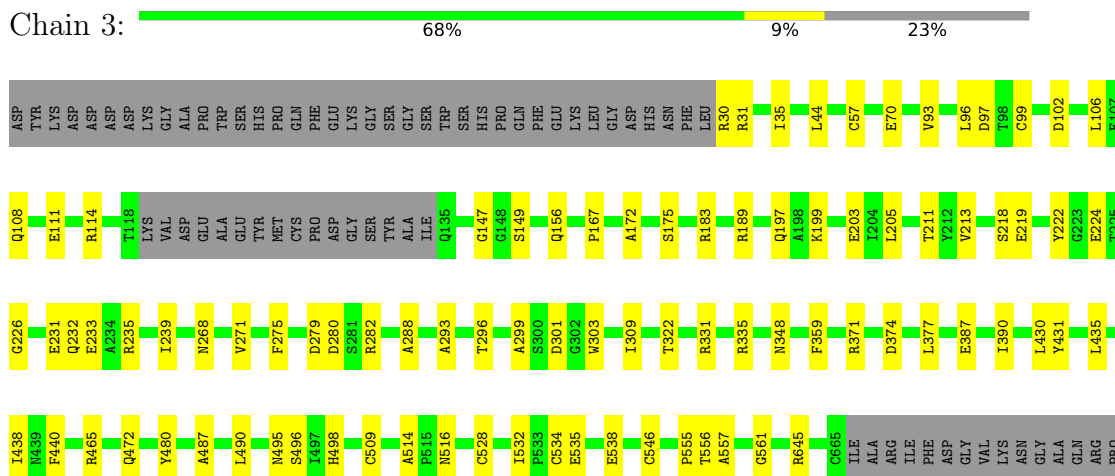
### 3 Residue-property plots

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

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



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



LYS	F662	W706	A711	P712	I826	LEU	PHE	GLN	PRO	GLN	LYS	ASN	VAL	VAL	THR	HIS	ARG	HIS	LEU	HIS	LEU	LEU	ASN	ASN	ARG	PHE	SER	VAL	VAL	GLY	THR	GLY	THR	THR	TYR	SER	GLN	SER	SER	ALA	ALA	THR	TYR	VAL	VAL	ASN	GLY	ARG	GLY	VAL	LEU	ASP	SER	THR	THR	SER
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SER	LEU	GLU	VAL	LEU	PHE	GLN	GLY	PRO	ALA	ILE	LEU	TRP	HIS	GLU	MET	TRP	HIS	GLY	GLY	GLU	GLU	GLU	ALA	SER	ARG	ARG	TYR	PHE	GLY	GLY	ARG	ASN	VAL	LEU	PRO	PRO	HIS	ALA	MET	MET	GLU	ARG	GLY	PRO	GLN	GLN	THR	LEU	LYS	GLU	THR	SER
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PHE	ASN	GLN	ALA	TYR	GLY	ARG	ASP	LEU	MET	GLU	ALA	GLN	GLU	TRP	CYS	ARG	LYS	TYR	MET	LYS	SER	GLY	ASN	VAL	LYS	ASP	LEU	THR	GLN	ALA	TRP	ASP	LEU	TYR	TYR	HIS	HIS	VAL	PHE	ARG	ARG	ILE	SER	LYS	GLN	GLU	PHE
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	512450	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: Z99, NAG

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	0/5485	0.47	0/7493
2	3	0.24	0/5479	0.46	0/7479
All	All	0.24	0/10964	0.46	0/14972

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	5371	0	4806	54	0
2	3	5379	0	4710	55	0
3	2	26	0	17	3	0
3	3	26	0	17	2	0
4	2	14	0	13	0	0
4	3	14	0	13	0	0
All	All	10830	0	9576	109	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.

All (109) 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)
2:3:555:PRO:HA	2:3:561:GLY:HA3	1.69	0.74
2:3:149:SER:HA	2:3:172:ALA:HB3	1.73	0.69
2:3:331:ARG:HH22	2:3:335:ARG:HE	1.46	0.63
1:2:49:ASP:OD1	1:2:94:LYS:NZ	2.30	0.62
2:3:374:ASP:HB3	2:3:377:LEU:HG	1.82	0.61
2:3:35:ILE:HB	2:3:93:VAL:HG22	1.82	0.60
1:2:216:TYR:HB2	3:2:1101:Z99:CAJ	2.31	0.60
2:3:211:THR:HG23	2:3:239:ILE:HA	1.85	0.58
2:3:205:LEU:HD13	2:3:213:VAL:HG11	1.86	0.58
1:2:212:SER:HB3	1:2:217:GLY:HA3	1.86	0.58
2:3:299:ALA:HB3	2:3:322:THR:HG22	1.86	0.57
1:2:375:GLU:HG3	1:2:377:LYS:H	1.70	0.56
1:2:452:ARG:HD3	1:2:475:ALA:HB2	1.86	0.56
2:3:359:PHE:O	2:3:371:ARG:NH2	2.39	0.55
2:3:97:ASP:O	2:3:108:GLN:NE2	2.27	0.55
2:3:70:GLU:OE2	2:3:348:ASN:ND2	2.39	0.55
2:3:30:ARG:HH22	2:3:111:GLU:HG3	1.72	0.54
2:3:534:CYS:SG	2:3:535:GLU:N	2.81	0.54
2:3:199:LYS:HA	2:3:233:GLU:HG2	1.91	0.53
2:3:438:ILE:HD12	2:3:440:PHE:HE1	1.74	0.53
1:2:42:GLN:HB2	1:2:52:PRO:HG2	1.91	0.53
1:2:199:LEU:HD13	1:2:207:VAL:HG11	1.91	0.53
2:3:211:THR:HA	2:3:239:ILE:HG12	1.89	0.53
1:2:176:SER:HB2	2:3:183:ARG:HH22	1.73	0.53
1:2:429:ASP:OD1	1:2:433:ARG:NH2	2.42	0.53
2:3:282:ARG:HA	2:3:309:ILE:HG23	1.91	0.53
1:2:107:ARG:HH22	2:3:114:ARG:HG2	1.73	0.52
2:3:472:GLN:HB2	2:3:498:HIS:CE1	2.44	0.52
1:2:216:TYR:HB2	3:2:1101:Z99:CAS	2.40	0.52
1:2:161:PRO:HA	1:2:180:TYR:HB3	1.91	0.52
1:2:212:SER:HB2	1:2:270:THR:HG22	1.92	0.52
1:2:146:ASP:OD1	1:2:146:ASP:N	2.43	0.52
2:3:268:ASN:ND2	2:3:509:CYS:H	2.09	0.51
1:2:417:ARG:NE	1:2:421:ASP:OD2	2.38	0.51
2:3:279:ASP:OD1	2:3:280:ASP:N	2.44	0.51
1:2:95:ASP:OD1	1:2:96:THR:N	2.44	0.51
1:2:531:ARG:HA	1:2:537:CYS:HA	1.92	0.50
1:2:320:ALA:HB3	1:2:452:ARG:HG3	1.92	0.50
1:2:469:GLN:NE2	1:2:484:LEU:HD13	2.26	0.50
1:2:500:CYS:HB3	1:2:519:CYS:HA	1.94	0.50
1:2:155:LEU:HD22	1:2:160:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:538:GLU:N	2:3:538:GLU:OE1	2.45	0.49
1:2:206:TYR:HB2	1:2:499:ARG:HA	1.94	0.49
1:2:140:ILE:HD11	1:2:388:MET:HG2	1.95	0.49
3:3:2002:Z99:HAM	3:3:2002:Z99:HANA	1.65	0.49
2:3:226:GLY:HA3	2:3:275:PHE:CZ	2.49	0.48
1:2:510:LYS:HD2	1:2:520:TRP:HE1	1.77	0.48
1:2:765:THR:HG23	1:2:804:VAL:HG22	1.94	0.48
2:3:495:ASN:OD1	2:3:496:SER:N	2.46	0.48
2:3:509:CYS:HB3	2:3:528:CYS:O	2.14	0.48
1:2:49:ASP:O	1:2:94:LYS:NZ	2.46	0.48
1:2:251:GLU:OE2	1:2:284:ARG:NH1	2.40	0.48
2:3:106:LEU:HD21	2:3:156:GLN:HB3	1.95	0.48
1:2:324:ILE:HG22	1:2:327:PHE:H	1.80	0.47
1:2:504:CYS:HB3	1:2:522:CYS:HB3	1.84	0.47
2:3:288:ALA:HB1	2:3:293:ALA:HB3	1.96	0.47
2:3:231:GLU:HB3	2:3:235:ARG:NH1	2.29	0.47
1:2:333:SER:HB2	1:2:368:ARG:HH21	1.80	0.47
1:2:654:THR:HG22	1:2:746:ALA:HB2	1.97	0.47
2:3:532:ILE:O	2:3:534:CYS:N	2.39	0.47
2:3:203:GLU:HB3	2:3:490:LEU:HD22	1.97	0.46
1:2:41:HIS:HE1	1:2:344:TRP:CD1	2.34	0.46
2:3:268:ASN:HD21	2:3:509:CYS:H	1.63	0.46
1:2:200:ARG:NH2	1:2:231:ARG:O	2.49	0.46
2:3:197:GLN:HE22	2:3:301:ASP:HB2	1.80	0.46
2:3:219:GLU:HA	2:3:224:GLU:OE2	2.16	0.46
1:2:99:LEU:HG	1:2:150:GLN:HB3	1.98	0.46
2:3:96:LEU:HD13	2:3:108:GLN:HB3	1.97	0.46
2:3:282:ARG:HG3	2:3:309:ILE:HA	1.98	0.45
1:2:95:ASP:HB2	1:2:150:GLN:HG3	1.99	0.45
2:3:514:ALA:O	2:3:516:ASN:N	2.47	0.45
2:3:218:SER:OG	2:3:280:ASP:OD2	2.31	0.45
2:3:387:GLU:HB3	2:3:390:ILE:HG12	1.98	0.45
1:2:141:GLY:HA2	1:2:165:TYR:HE2	1.81	0.45
1:2:40:VAL:O	1:2:54:ASN:N	2.43	0.44
2:3:431:TYR:HD1	2:3:435:LEU:HD23	1.82	0.44
2:3:102:ASP:HB2	2:3:156:GLN:HG3	1.99	0.44
1:2:205:THR:HA	1:2:233:ILE:HD13	2.00	0.44
2:3:556:THR:OG1	2:3:557:ALA:N	2.50	0.44
1:2:469:GLN:HE22	1:2:484:LEU:HD13	1.83	0.44
1:2:342:ASN:HB3	1:2:345:PHE:HB2	1.99	0.44
1:2:544:TYR:CG	1:2:555:GLU:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:271:VAL:HG12	2:3:296:THR:HB	2.00	0.43
1:2:245:MET:HB3	1:2:249:ALA:HB3	2.00	0.43
1:2:211:ALA:HB2	1:2:221:ILE:HG13	2.01	0.43
2:3:175:SER:O	2:3:189:ARG:NH1	2.40	0.43
2:3:534:CYS:HB2	2:3:546:CYS:HB2	1.91	0.43
2:3:57:CYS:HB3	2:3:99:CYS:HB3	1.55	0.43
1:2:91:SER:HB2	1:2:98:ALA:HB2	2.00	0.42
1:2:510:LYS:HD2	1:2:520:TRP:NE1	2.34	0.42
2:3:645:ARG:HH22	2:3:706:TRP:HB3	1.82	0.42
3:2:1101:Z99:HAM	3:2:1101:Z99:HANA	1.72	0.42
2:3:465:ARG:HH11	2:3:487:ALA:HB2	1.85	0.42
1:2:293:ALA:HB3	1:2:316:THR:HG22	2.02	0.42
2:3:303:TRP:NE1	2:3:480:TYR:OH	2.39	0.42
1:2:675:SER:HB3	1:2:676:PRO:HD3	2.02	0.42
1:2:211:ALA:HB3	1:2:240:LYS:HD3	2.01	0.41
1:2:50:CYS:HB3	1:2:92:CYS:HB3	1.54	0.41
1:2:137:THR:HG22	1:2:413:VAL:HG11	2.02	0.41
2:3:167:PRO:HG2	2:3:430:LEU:HD23	2.03	0.41
2:3:44:LEU:HB2	2:3:147:GLY:HA3	2.03	0.41
2:3:431:TYR:HA	2:3:435:LEU:HB3	2.02	0.41
2:3:711:ALA:HB3	2:3:712:PRO:HD3	2.02	0.41
1:2:375:GLU:HB3	1:2:378:ILE:HG12	2.02	0.41
2:3:222:TYR:HB2	3:3:2002:Z99:CAJ	2.50	0.40
1:2:481:ASP:OD1	1:2:481:ASP:N	2.54	0.40
2:3:232:GLN:OE1	2:3:232:GLN:N	2.47	0.40
1:2:37:LEU:HD13	1:2:151:VAL:HG21	2.03	0.40
1:2:639:LEU:HD23	1:2:639:LEU:H	1.86	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	756/993 (76%)	730 (97%)	26 (3%)	0	100	100
2	3	759/993 (76%)	723 (95%)	36 (5%)	0	100	100
All	All	1515/1986 (76%)	1453 (96%)	62 (4%)	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	473/813 (58%)	471 (100%)	2 (0%)	91	97
2	3	478/867 (55%)	477 (100%)	1 (0%)	93	98
All	All	951/1680 (57%)	948 (100%)	3 (0%)	92	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	445	ARG
1	2	656	ARG
2	3	31	ARG

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

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	Z99	2	1101	-	26,29,29	1.60	4 (15%)	36,44,44	2.13	13 (36%)
3	Z99	3	2002	-	26,29,29	1.58	4 (15%)	36,44,44	2.01	13 (36%)
4	NAG	3	2001	2	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	2	1102	1	14,14,15	0.22	0	17,19,21	0.43	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	Z99	2	1101	-	-	8/15/38/38	0/4/4/4
3	Z99	3	2002	-	-	8/15/38/38	0/4/4/4
4	NAG	3	2001	2	-	4/6/23/26	0/1/1/1
4	NAG	2	1102	1	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	1101	Z99	OAP-CAT	4.80	1.46	1.38
3	3	2002	Z99	OAP-CAT	4.53	1.45	1.38
3	2	1101	Z99	OAP-CAS	4.52	1.45	1.38
3	3	2002	Z99	OAP-CAS	4.40	1.45	1.38
3	3	2002	Z99	CAN-CAY	2.39	1.57	1.54
3	2	1101	Z99	CAN-CAY	2.27	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	2002	Z99	CAO-CAZ	2.12	1.53	1.50
3	2	1101	Z99	CAO-CAZ	2.05	1.53	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	2002	Z99	CAO-CAZ-CAY	-4.81	114.65	122.00
3	2	1101	Z99	CAO-CAZ-CAY	-4.67	114.87	122.00
3	2	1101	Z99	CAY-CAN-CAW	-4.51	109.92	117.06
3	2	1101	Z99	CAM-CAV-CAT	3.85	122.10	117.75
3	3	2002	Z99	CAM-CAV-CAT	3.75	121.98	117.75
3	3	2002	Z99	CAT-OAP-CAS	-3.60	110.69	118.58
3	3	2002	Z99	CAY-CAN-CAW	-3.55	111.44	117.06
3	2	1101	Z99	CAL-CAU-CAS	3.41	121.59	117.75
3	2	1101	Z99	CAT-OAP-CAS	-3.33	111.29	118.58
3	2	1101	Z99	OAP-CAS-CAU	-3.00	118.25	122.38
3	2	1101	Z99	OAP-CAT-CAV	-2.98	118.28	122.38
3	3	2002	Z99	CAL-CAU-CAS	2.96	121.09	117.75
3	3	2002	Z99	OAP-CAS-CAU	-2.89	118.40	122.38
3	3	2002	Z99	OAP-CAT-CAV	-2.86	118.44	122.38
3	2	1101	Z99	OAP-CAT-CAK	2.79	122.61	116.48
3	2	1101	Z99	CAO-CAX-CAQ	-2.78	114.46	119.10
3	3	2002	Z99	CAO-CAX-CAQ	-2.72	114.56	119.10
3	3	2002	Z99	OAP-CAT-CAK	2.65	122.31	116.48
3	2	1101	Z99	OAP-CAS-CAJ	2.65	122.30	116.48
3	2	1101	Z99	OAC-CAR-CAY	2.62	120.67	113.60
3	2	1101	Z99	CAT-CAV-CAW	-2.55	116.01	119.99
3	3	2002	Z99	OAP-CAS-CAJ	2.49	121.95	116.48
3	2	1101	Z99	CAS-CAU-CAW	-2.44	116.19	119.99
3	3	2002	Z99	OAC-CAR-CAY	2.27	119.74	113.60
3	3	2002	Z99	CAT-CAV-CAW	-2.21	116.54	119.99
3	3	2002	Z99	CAS-CAU-CAW	-2.19	116.57	119.99

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	2	1101	Z99	OAB-CAQ-CAX-CAO
3	2	1101	Z99	OAD-CAQ-CAX-CAO
3	2	1101	Z99	OAC-CAR-CAY-CAZ
3	2	1101	Z99	OAE-CAR-CAY-NAA
3	2	1101	Z99	OAE-CAR-CAY-CAZ

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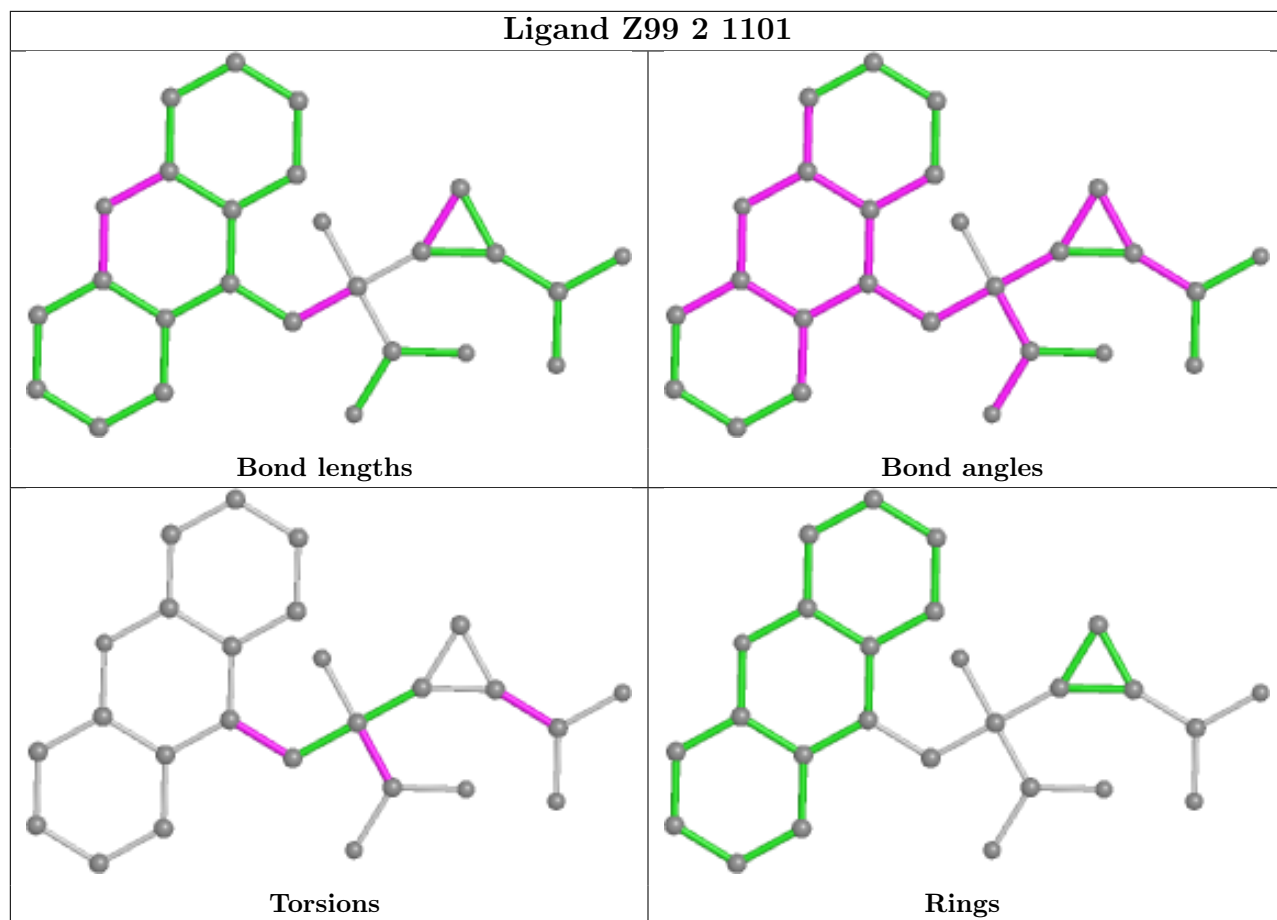
Mol	Chain	Res	Type	Atoms
3	3	2002	Z99	OAB-CAQ-CAX-CAO
3	3	2002	Z99	OAD-CAQ-CAX-CAO
3	3	2002	Z99	OAC-CAR-CAY-CAZ
3	3	2002	Z99	OAE-CAR-CAY-NAA
3	3	2002	Z99	OAE-CAR-CAY-CAZ
4	2	1102	NAG	C8-C7-N2-C2
4	2	1102	NAG	O7-C7-N2-C2
4	3	2001	NAG	C8-C7-N2-C2
4	3	2001	NAG	O7-C7-N2-C2
4	3	2001	NAG	O5-C5-C6-O6
4	3	2001	NAG	C4-C5-C6-O6
3	2	1101	Z99	CAY-CAN-CAW-CAV
3	3	2002	Z99	CAY-CAN-CAW-CAV
3	3	2002	Z99	OAB-CAQ-CAX-CAZ
3	3	2002	Z99	OAD-CAQ-CAX-CAZ
3	2	1101	Z99	OAB-CAQ-CAX-CAZ
3	2	1101	Z99	OAD-CAQ-CAX-CAZ

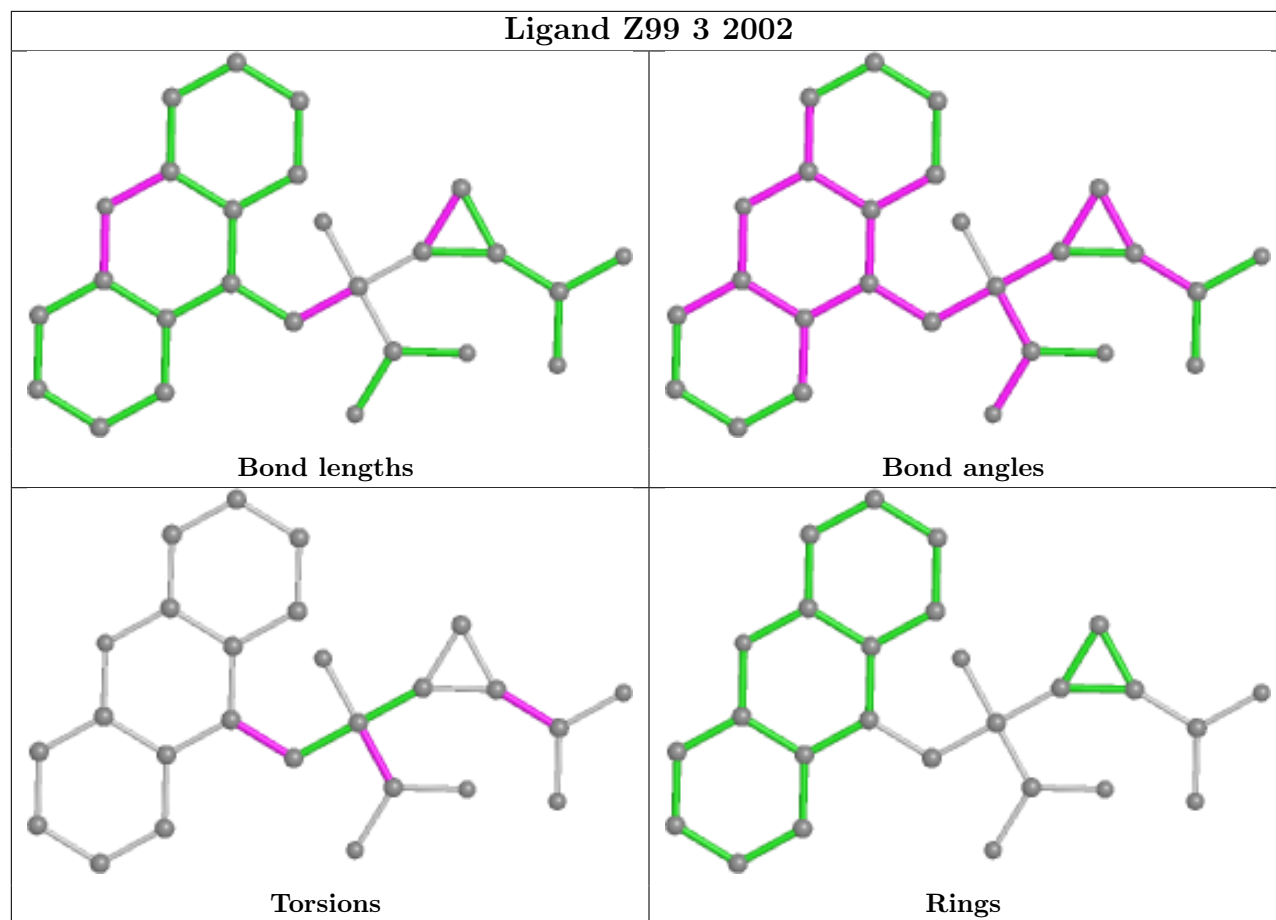
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	2	1101	Z99	3	0
3	3	2002	Z99	2	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.