



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:38 AM UTC

PDB ID : 1GAR / pdb_00001gar
Title : TOWARDS STRUCTURE-BASED DRUG DESIGN: CRYSTAL
STRUCTURE OF A MULTISUBSTRATE ADDUCT COMPLEX OF
GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE AT 1.96
ANGSTROMS RESOLUTION
Authors : Wilson, I.A.; Klein, C.; Chen, P.; Arevalo, J.H.
Deposited on : 1994-12-08
Resolution : 1.96 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

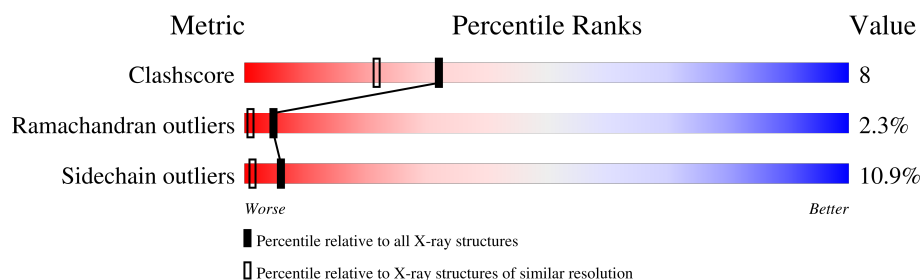
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	212	 65% 26% 5% • •
1	B	212	 61% 23% 7% • 8%

2 Entry composition [i](#)

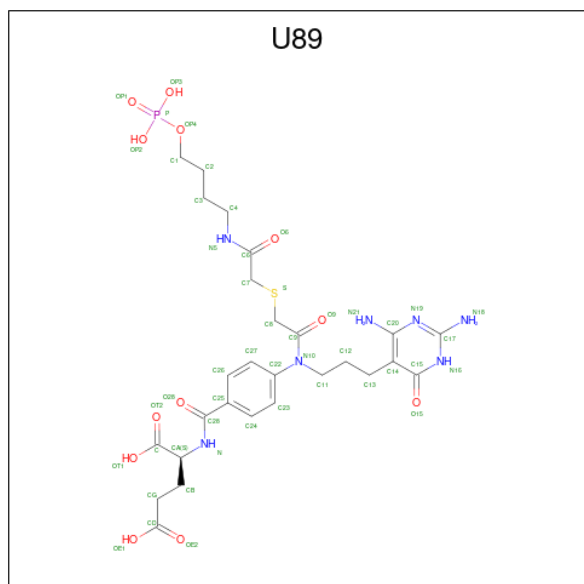
There are 3 unique types of molecules in this entry. The entry contains 3567 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	3	1
			1553	978	279	291	5			
1	B	194	Total	C	N	O	S	0	1	1
			1496	948	264	279	5			

- Molecule 2 is N-[4-[[3-(2,4-DIAMINO-1,6-DIHYDRO-6-OXO-4-PYRIMIDINYL)-PROPYL]-[2-((2-OXO-2-((4-PHOSPHORIBOXY)-BUTYL)-AMINO)-ETHYL)-THIO-ACETYL]-AMINO]BENZOYL]-1-GLUTAMIC ACID (CCD ID: U89) (formula: C₂₇H₃₈N₇O₁₂PS).



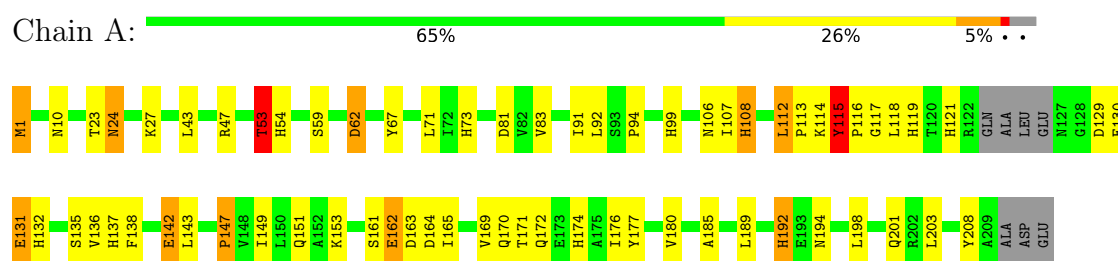
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total 163	O 163	0	0
3	B	163	Total 163	O 163	0	0

3 Residue-property plots [i](#)

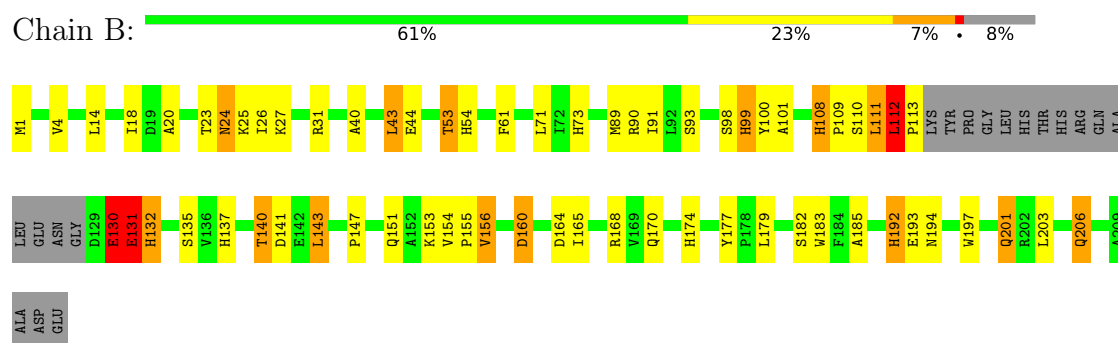
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

• Molecule 1: GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE



• Molecule 1: GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.70Å 73.30Å 35.50Å 90.00° 94.30° 90.00°	Depositor
Resolution (Å)	6.00 – 1.96	Depositor
% Data completeness (in resolution range)	71.6 (6.00-1.96)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.168 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3567	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

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: U89

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	1.10	12/1597 (0.8%)	1.70	22/2165 (1.0%)
1	B	1.09	14/1532 (0.9%)	1.84	39/2082 (1.9%)
All	All	1.09	26/3129 (0.8%)	1.77	61/4247 (1.4%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	HIS	CD2-NE2	-7.78	1.29	1.37
1	B	99	HIS	CD2-NE2	-7.24	1.29	1.37
1	A	73	HIS	CD2-NE2	-6.96	1.30	1.37
1	A	174	HIS	CD2-NE2	-6.88	1.30	1.37
1	B	112	LEU	C-N	-6.67	1.23	1.34
1	B	132	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	108[A]	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	108[B]	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	99	HIS	CD2-NE2	-6.37	1.30	1.37
1	B	99	HIS	CG-ND1	-6.34	1.31	1.38
1	A	132	HIS	CD2-NE2	-6.30	1.30	1.37
1	B	73	HIS	CD2-NE2	-6.26	1.30	1.37
1	A	121	HIS	C-N	-6.26	1.24	1.33
1	B	192	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	137	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	73	HIS	CG-ND1	-5.91	1.31	1.38
1	B	54	HIS	CD2-NE2	-5.84	1.31	1.37
1	B	108[A]	HIS	CD2-NE2	-5.74	1.31	1.37
1	B	108[B]	HIS	CD2-NE2	-5.74	1.31	1.37
1	A	192	HIS	CD2-NE2	-5.71	1.31	1.37
1	B	108[A]	HIS	CG-ND1	-5.62	1.32	1.38
1	B	108[B]	HIS	CG-ND1	-5.62	1.32	1.38
1	B	137	HIS	CD2-NE2	-5.62	1.31	1.37
1	B	174	HIS	CD2-NE2	-5.35	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	HIS	CG-ND1	-5.09	1.32	1.38
1	A	176	ILE	CA-CB	5.02	1.61	1.54

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	HIS	CA-CB-CG	9.89	123.69	113.80
1	B	130	GLU	N-CA-C	9.02	124.58	111.87
1	B	165	ILE	N-CA-C	-8.03	102.87	110.42
1	A	208	TYR	O-C-N	7.94	132.37	123.16
1	B	160	ASP	CA-CB-CG	7.23	119.83	112.60
1	A	81	ASP	N-CA-C	-7.08	104.79	113.50
1	A	194	ASN	OD1-CG-ND2	-7.08	115.52	122.60
1	B	201	GLN	OE1-CD-NE2	-7.07	115.53	122.60
1	B	192	HIS	CB-CG-CD2	-6.92	122.20	131.20
1	A	147	PRO	N-CA-C	6.87	122.07	110.95
1	B	54	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	B	160	ASP	CA-C-O	6.29	127.86	120.69
1	B	206	GLN	OE1-CD-NE2	-6.24	116.36	122.60
1	A	54	HIS	CB-CG-CD2	-6.15	123.20	131.20
1	A	10	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	A	163	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	170	GLN	OE1-CD-NE2	-6.10	116.50	122.60
1	B	26	ILE	N-CA-C	-6.07	99.01	107.80
1	B	192	HIS	CB-CG-ND1	6.04	131.76	122.70
1	B	23	THR	CA-CB-OG1	-6.02	100.57	109.60
1	A	115	TYR	N-CA-C	6.01	123.10	109.81
1	B	135	SER	CA-CB-OG	6.00	123.09	111.10
1	B	61	PHE	CA-CB-CG	-5.99	107.81	113.80
1	B	108[A]	HIS	CA-CB-CG	5.98	119.78	113.80
1	B	108[B]	HIS	CA-CB-CG	5.98	119.78	113.80
1	B	24	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	B	4	VAL	N-CA-C	-5.96	99.76	108.11
1	A	99	HIS	CB-CG-CD2	-5.92	123.50	131.20
1	A	27	LYS	N-CA-CB	-5.87	103.37	110.53
1	A	172	GLN	OE1-CD-NE2	-5.84	116.76	122.60
1	A	24	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	B	99	HIS	CB-CG-CD2	-5.78	123.68	131.20
1	A	162	GLU	CA-CB-CG	5.72	125.53	114.10
1	B	23	THR	N-CA-CB	-5.71	98.80	110.67
1	B	93	SER	CA-C-N	5.70	125.82	119.32
1	B	93	SER	C-N-CA	5.70	125.82	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	THR	N-CA-CB	-5.68	101.37	111.08
1	A	107	ILE	O-C-N	-5.62	117.24	123.20
1	B	131	GLU	CA-CB-CG	5.62	125.35	114.10
1	B	130	GLU	CA-CB-CG	5.58	125.26	114.10
1	B	89	MET	N-CA-C	5.58	119.62	113.21
1	B	160	ASP	O-C-N	5.56	129.54	123.04
1	A	83	VAL	N-CA-C	-5.55	99.55	107.77
1	B	193	GLU	N-CA-C	5.51	118.80	111.30
1	B	135	SER	O-C-N	5.50	129.84	123.41
1	B	54	HIS	CB-CG-ND1	5.35	130.72	122.70
1	A	142	GLU	N-CA-C	-5.32	100.12	108.63
1	A	54	HIS	CB-CG-ND1	5.32	130.68	122.70
1	B	183	TRP	CG-CD2-CE3	5.27	139.17	133.90
1	B	147	PRO	N-CA-C	5.26	119.34	111.14
1	B	141	ASP	N-CA-C	5.26	122.00	110.80
1	A	106	ASN	OD1-CG-ND2	-5.20	117.41	122.60
1	B	71	LEU	CA-C-N	5.14	127.22	120.60
1	B	71	LEU	C-N-CA	5.14	127.22	120.60
1	A	171	THR	N-CA-C	-5.08	105.74	111.28
1	B	140	THR	O-C-N	-5.07	116.32	123.11
1	A	114	LYS	CA-C-O	-5.05	115.24	120.70
1	A	172	GLN	CA-CB-CG	-5.03	104.04	114.10
1	B	18	ILE	N-CA-C	-5.02	105.60	110.42
1	B	53	THR	N-CA-CB	-5.02	101.92	111.00
1	B	197	TRP	CE2-CD2-CG	-5.01	101.18	107.20

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	1553	0	1498	22	0
1	B	1496	0	1471	29	0
2	A	96	0	68	4	0
2	B	96	0	68	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	163	0	0	3	0
3	B	163	0	0	4	0
All	All	3567	0	3105	51	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 8.

All (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ILE:HG13	2:A:213[A]:U89:H26	1.66	0.78
1:A:135:SER:HB3	1:A:151:GLN:HG2	1.69	0.72
1:A:115:TYR:HA	1:A:131:GLU:HB3	1.73	0.71
1:B:1:MET:HE3	1:B:185:ALA:HA	1.74	0.68
1:A:1:MET:HE3	1:A:185:ALA:HA	1.83	0.61
1:B:111:LEU:HD12	1:B:151:GLN:HB3	1.83	0.60
1:B:40:ALA:HB3	1:B:43:LEU:HD22	1.84	0.58
1:B:112:LEU:H	1:B:151:GLN:HE22	1.52	0.57
1:A:43:LEU:HD22	1:A:53:THR:HG23	1.87	0.56
1:A:108[A]:HIS:HE1	3:A:353:HOH:O	1.91	0.54
1:B:99:HIS:HD2	1:B:100:TYR:CE2	2.26	0.53
1:B:112:LEU:H	1:B:151:GLN:NE2	2.06	0.53
1:A:67:TYR:HE1	1:A:71:LEU:HD22	1.73	0.53
1:B:130:GLU:HB3	1:B:156:VAL:H	1.74	0.52
1:A:165:ILE:O	1:A:169:VAL:HG23	2.09	0.52
1:A:136:VAL:HG11	1:A:180:VAL:HG11	1.91	0.52
1:A:47:ARG:HH11	1:B:44:GLU:HB2	1.76	0.51
1:B:20:ALA:HB1	1:B:25:LYS:HE2	1.92	0.51
1:B:140:THR:HG21	1:B:194:ASN:OD1	2.10	0.51
1:B:113:PRO:N	1:B:151:GLN:HE22	2.09	0.51
1:B:160:ASP:HB2	1:B:164:ASP:HB2	1.93	0.51
1:A:161:SER:H	1:A:164:ASP:HB2	1.76	0.50
2:A:213[B]:U89:H121	2:A:213[B]:U89:O15	2.12	0.49
1:B:111:LEU:HD21	1:B:153:LYS:HA	1.94	0.49
1:B:108[A]:HIS:ND1	2:B:213[A]:U89:S	2.86	0.49
1:A:138:PHE:HB2	1:A:147:PRO:HG2	1.95	0.49
1:A:149:ILE:HD13	1:A:189:LEU:HD21	1.96	0.47
1:B:108[A]:HIS:CD2	1:B:110:SER:OG	2.67	0.47
1:A:153:LYS:H	1:A:153:LYS:HD2	1.80	0.47
1:B:108[B]:HIS:NE2	1:B:112:LEU:HD11	2.29	0.47
1:B:160:ASP:CG	1:B:168:ARG:HH22	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ASP:HB3	3:A:263:HOH:O	2.15	0.46
1:A:23:THR:HG23	3:A:344:HOH:O	2.15	0.46
1:B:155:PRO:HG2	3:B:369:HOH:O	2.15	0.46
1:A:153:LYS:HD2	1:A:153:LYS:N	2.32	0.45
1:B:91:ILE:HD11	2:B:213[A]:U89:C26	2.47	0.45
1:B:90:ARG:HA	2:B:213[A]:U89:HG1	1.99	0.44
1:B:101:ALA:HA	3:B:276:HOH:O	2.16	0.43
1:B:98:SER:HB2	3:B:324:HOH:O	2.19	0.43
1:A:91:ILE:HG13	2:A:213[A]:U89:C26	2.44	0.43
1:B:132:HIS:ND1	1:B:156:VAL:HG11	2.35	0.42
1:B:130:GLU:HA	1:B:156:VAL:HG22	2.02	0.42
1:A:47:ARG:NH1	1:B:44:GLU:HB2	2.35	0.42
1:B:27:LYS:HB3	3:B:344:HOH:O	2.20	0.42
1:B:154:VAL:HA	1:B:155:PRO:HD2	1.93	0.41
1:A:43:LEU:HD22	1:A:53:THR:CG2	2.50	0.41
1:A:129:ASP:CG	1:A:130:GLU:HG2	2.44	0.41
1:A:161:SER:O	1:A:165:ILE:HG12	2.20	0.41
1:B:179:LEU:O	1:B:182:SER:HB3	2.20	0.41
1:B:91:ILE:HD11	1:B:143:LEU:HD21	2.02	0.41
2:A:213[A]:U89:HN11	2:A:213[A]:U89:H132	1.68	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 X-ray entries followed by that with respect to entries of similar resolution.

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	204/212 (96%)	186 (91%)	10 (5%)	8 (4%)	2	0
1	B	191/212 (90%)	176 (92%)	14 (7%)	1 (0%)	24	16
All	All	395/424 (93%)	362 (92%)	24 (6%)	9 (2%)	5	1

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	PRO
1	A	115	TYR
1	A	116	PRO
1	A	118	LEU
1	B	131	GLU
1	A	131	GLU
1	A	117	GLY
1	A	119	HIS
1	A	112	LEU

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 X-ray entries followed by that with respect to entries of similar resolution.

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	159/171 (93%)	141 (89%)	18 (11%)	5	1
1	B	157/171 (92%)	140 (89%)	17 (11%)	6	1
All	All	316/342 (92%)	281 (89%)	35 (11%)	6	1

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	24	ASN
1	A	53	THR
1	A	59	SER
1	A	62	ASP
1	A	92	LEU
1	A	94	PRO
1	A	112	LEU
1	A	142	GLU
1	A	143	LEU
1	A	162	GLU
1	A	170[A]	GLN
1	A	170[B]	GLN
1	A	177	TYR
1	A	192	HIS

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Mol	Chain	Res	Type
1	A	198	LEU
1	A	201	GLN
1	A	203	LEU
1	B	14	LEU
1	B	24	ASN
1	B	31	ARG
1	B	43	LEU
1	B	53	THR
1	B	109	PRO
1	B	111	LEU
1	B	112	LEU
1	B	130	GLU
1	B	131	GLU
1	B	143	LEU
1	B	156	VAL
1	B	177	TYR
1	B	192	HIS
1	B	201	GLN
1	B	203	LEU
1	B	206	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	172	GLN
1	B	99	HIS
1	B	151	GLN
1	B	194	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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$
2	U89	B	213[A]	-	48,49,49	1.48	11 (22%)	63,66,66	1.65	13 (20%)
2	U89	B	213[B]	-	48,49,49	1.45	8 (16%)	63,66,66	1.66	15 (23%)
2	U89	A	213[A]	-	48,49,49	1.60	11 (22%)	63,66,66	1.70	15 (23%)
2	U89	A	213[B]	-	48,49,49	1.47	7 (14%)	63,66,66	1.96	15 (23%)

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
2	U89	B	213[A]	-	-	10/47/47/47	0/2/2/2
2	U89	B	213[B]	-	-	6/47/47/47	0/2/2/2
2	U89	A	213[A]	-	-	19/47/47/47	0/2/2/2
2	U89	A	213[B]	-	-	13/47/47/47	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	213[A]	U89	C25-C28	-4.75	1.39	1.50
2	B	213[A]	U89	C22-N10	-4.34	1.34	1.43
2	A	213[B]	U89	C25-C28	-3.85	1.41	1.50
2	B	213[B]	U89	C25-C28	-3.82	1.41	1.50
2	B	213[B]	U89	C22-N10	-3.60	1.36	1.43
2	A	213[A]	U89	C22-N10	-3.43	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	213[A]	U89	P-OP1	3.40	1.61	1.50
2	A	213[B]	U89	P-OP1	3.38	1.61	1.50
2	A	213[A]	U89	C24-C25	-3.33	1.34	1.39
2	B	213[B]	U89	P-OP1	3.31	1.60	1.50
2	A	213[A]	U89	C26-C25	-3.30	1.34	1.39
2	B	213[A]	U89	P-OP1	3.24	1.60	1.50
2	B	213[A]	U89	C25-C28	-3.21	1.43	1.50
2	A	213[B]	U89	C24-C25	-3.18	1.34	1.39
2	B	213[B]	U89	C26-C25	-3.15	1.34	1.39
2	A	213[B]	U89	C22-N10	-3.11	1.37	1.43
2	B	213[B]	U89	C15-C14	-2.81	1.40	1.44
2	A	213[B]	U89	C24-C23	-2.69	1.34	1.38
2	B	213[B]	U89	C27-C22	-2.68	1.34	1.39
2	B	213[A]	U89	C27-C22	-2.65	1.34	1.39
2	B	213[A]	U89	C15-C14	-2.60	1.40	1.44
2	B	213[A]	U89	C26-C25	-2.52	1.35	1.39
2	A	213[A]	U89	C15-C14	-2.49	1.40	1.44
2	A	213[B]	U89	OE1-CD	-2.44	1.22	1.30
2	A	213[A]	U89	OE1-CD	-2.37	1.23	1.30
2	A	213[A]	U89	C8-C9	2.28	1.55	1.51
2	A	213[B]	U89	C23-C22	-2.28	1.35	1.39
2	B	213[B]	U89	C24-C25	-2.26	1.36	1.39
2	A	213[A]	U89	C24-C23	-2.21	1.35	1.38
2	B	213[B]	U89	C27-C26	-2.20	1.35	1.38
2	B	213[A]	U89	C23-C22	-2.11	1.35	1.39
2	A	213[A]	U89	C23-C22	-2.10	1.35	1.39
2	B	213[A]	U89	C27-C26	-2.09	1.35	1.38
2	B	213[A]	U89	C24-C25	-2.09	1.36	1.39
2	B	213[A]	U89	OE1-CD	-2.07	1.24	1.30
2	A	213[A]	U89	OT1-C	-2.04	1.24	1.30
2	B	213[A]	U89	C8-C9	2.04	1.54	1.51

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	213[A]	U89	C-CA-N	5.91	124.28	110.57
2	A	213[A]	U89	CG-CB-CA	-5.00	103.94	113.16
2	A	213[B]	U89	C-CA-N	4.91	121.95	110.57
2	B	213[B]	U89	C-CA-N	4.85	121.81	110.57
2	A	213[B]	U89	C13-C14-C20	-4.84	116.77	124.39
2	A	213[B]	U89	C13-C14-C15	4.52	122.70	116.64
2	A	213[B]	U89	C8-S-C7	-4.39	90.57	100.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	213[B]	U89	C14-C15-N16	-4.37	112.39	115.70
2	A	213[B]	U89	CG-CB-CA	-4.28	105.26	113.16
2	A	213[A]	U89	C11-N10-C22	-3.92	110.17	117.16
2	A	213[B]	U89	C8-C9-N10	3.89	123.37	117.24
2	A	213[A]	U89	C8-C9-N10	3.79	123.22	117.24
2	A	213[A]	U89	C-CA-N	3.71	119.18	110.57
2	A	213[A]	U89	C13-C14-C20	-3.69	118.59	124.39
2	A	213[A]	U89	C11-C12-C13	3.53	120.93	111.97
2	A	213[B]	U89	O9-C9-C8	-3.49	114.23	121.19
2	B	213[A]	U89	CG-CB-CA	-3.33	107.03	113.16
2	B	213[B]	U89	CB-CA-N	-3.28	104.41	110.91
2	B	213[B]	U89	C15-C14-C20	3.20	122.25	117.67
2	B	213[A]	U89	C8-C9-N10	3.19	122.27	117.24
2	A	213[B]	U89	C11-N10-C22	-3.10	111.63	117.16
2	B	213[A]	U89	CB-CA-N	-3.01	104.94	110.91
2	A	213[B]	U89	C27-C22-N10	2.86	124.29	120.18
2	B	213[A]	U89	C14-C15-N16	-2.82	113.56	115.70
2	A	213[A]	U89	C13-C14-C15	2.81	120.41	116.64
2	B	213[A]	U89	C17-N19-C20	2.77	119.54	113.79
2	A	213[B]	U89	CB-CA-N	-2.77	105.42	110.91
2	B	213[B]	U89	O9-C9-N10	-2.76	117.86	121.70
2	B	213[A]	U89	OT1-C-CA	2.75	122.81	113.51
2	B	213[A]	U89	C13-C14-C20	-2.73	120.09	124.39
2	B	213[A]	U89	C15-C14-C20	2.70	121.53	117.67
2	B	213[B]	U89	C25-C28-N	-2.64	112.15	117.04
2	A	213[B]	U89	C17-N19-C20	2.62	119.21	113.79
2	A	213[A]	U89	CB-CA-N	-2.54	105.88	110.91
2	B	213[A]	U89	O9-C9-N10	-2.53	118.18	121.70
2	A	213[B]	U89	OP3-P-OP2	2.52	117.26	107.80
2	B	213[B]	U89	C11-C12-C13	2.52	118.35	111.97
2	A	213[B]	U89	O15-C15-C14	2.48	127.62	124.56
2	A	213[A]	U89	OP3-P-OP2	2.47	117.08	107.80
2	B	213[B]	U89	C23-C22-N10	2.46	123.72	120.18
2	B	213[B]	U89	C8-C9-N10	2.45	121.11	117.24
2	B	213[A]	U89	CA-N-C28	2.45	127.43	121.56
2	A	213[B]	U89	C11-C12-C13	2.44	118.15	111.97
2	A	213[A]	U89	C25-C28-N	-2.35	112.68	117.04
2	A	213[A]	U89	C9-C8-S	2.35	121.22	113.81
2	B	213[B]	U89	CA-N-C28	2.33	127.15	121.56
2	A	213[A]	U89	C15-C14-C20	2.32	121.00	117.67
2	B	213[A]	U89	OP3-P-OP2	2.30	116.42	107.80
2	B	213[B]	U89	C13-C14-C20	-2.26	120.83	124.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	213[A]	U89	C14-C15-N16	-2.26	113.99	115.70
2	B	213[A]	U89	OT2-C-CA	-2.25	114.98	122.26
2	B	213[B]	U89	OP3-P-OP2	2.24	116.21	107.80
2	B	213[B]	U89	OT1-C-CA	2.24	121.08	113.51
2	A	213[A]	U89	C17-N19-C20	2.22	118.39	113.79
2	A	213[B]	U89	C14-C15-N16	-2.21	114.02	115.70
2	B	213[B]	U89	CG-CB-CA	-2.19	109.12	113.16
2	A	213[A]	U89	O9-C9-C8	-2.07	117.07	121.19
2	B	213[B]	U89	C17-N19-C20	2.04	118.02	113.79

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	213[A]	U89	C8-C9-N10-C22
2	A	213[A]	U89	O9-C9-N10-C22
2	A	213[A]	U89	C12-C11-N10-C22
2	A	213[B]	U89	C6-C7-S-C8
2	A	213[B]	U89	C12-C11-N10-C9
2	A	213[B]	U89	C12-C13-C14-C15
2	A	213[B]	U89	C12-C13-C14-C20
2	B	213[A]	U89	C6-C7-S-C8
2	B	213[B]	U89	C6-C7-S-C8
2	B	213[B]	U89	C1-OP4-P-OP3
2	A	213[A]	U89	C26-C25-C28-O28
2	A	213[A]	U89	C24-C25-C28-O28
2	A	213[A]	U89	C24-C25-C28-N
2	A	213[A]	U89	C26-C25-C28-N
2	A	213[A]	U89	C23-C22-N10-C9
2	B	213[A]	U89	C-CA-CB-CG
2	B	213[A]	U89	OT2-C-CA-N
2	A	213[A]	U89	C27-C22-N10-C9
2	B	213[A]	U89	OP4-C1-C2-C3
2	B	213[A]	U89	OT1-C-CA-N
2	A	213[B]	U89	C11-C12-C13-C14
2	B	213[A]	U89	OT1-C-CA-CB
2	A	213[B]	U89	C9-C8-S-C7
2	A	213[A]	U89	C12-C11-N10-C9
2	B	213[A]	U89	OT2-C-CA-CB
2	B	213[B]	U89	OT2-C-CA-CB
2	B	213[B]	U89	OT1-C-CA-CB
2	B	213[A]	U89	C2-C3-C4-N5

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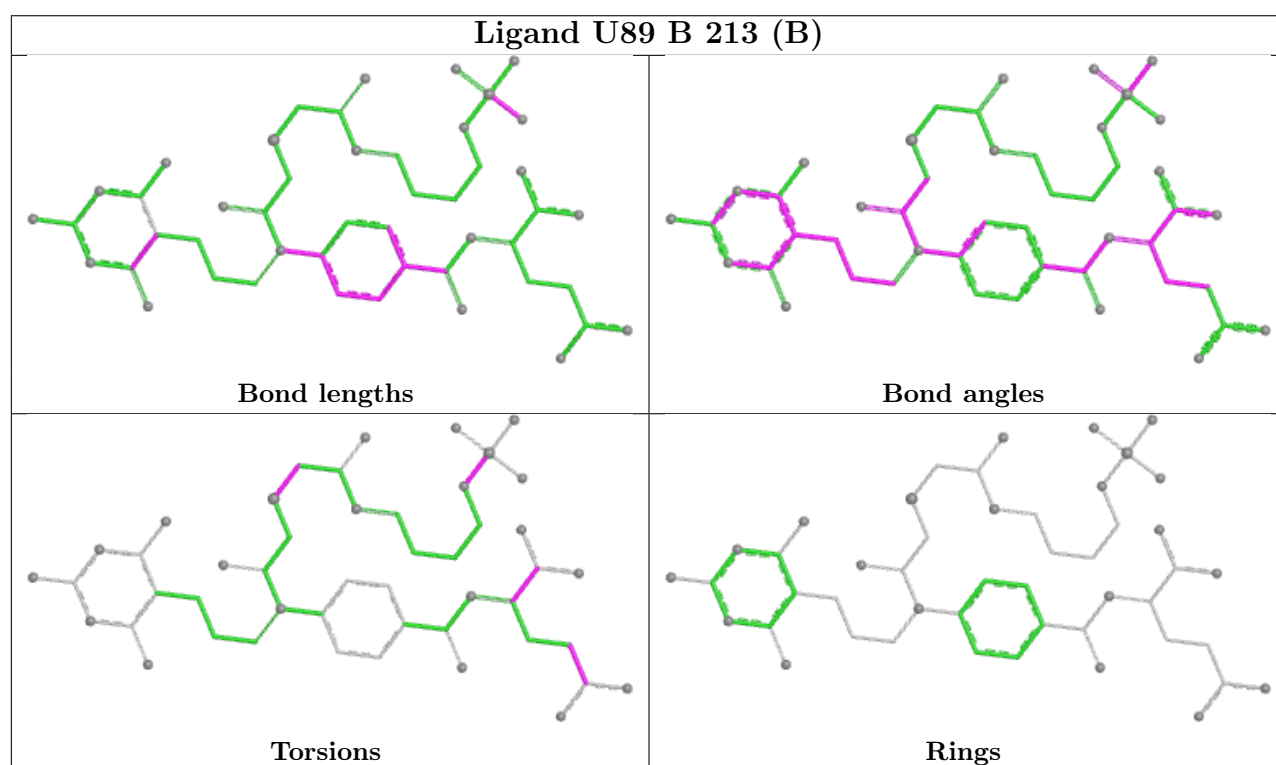
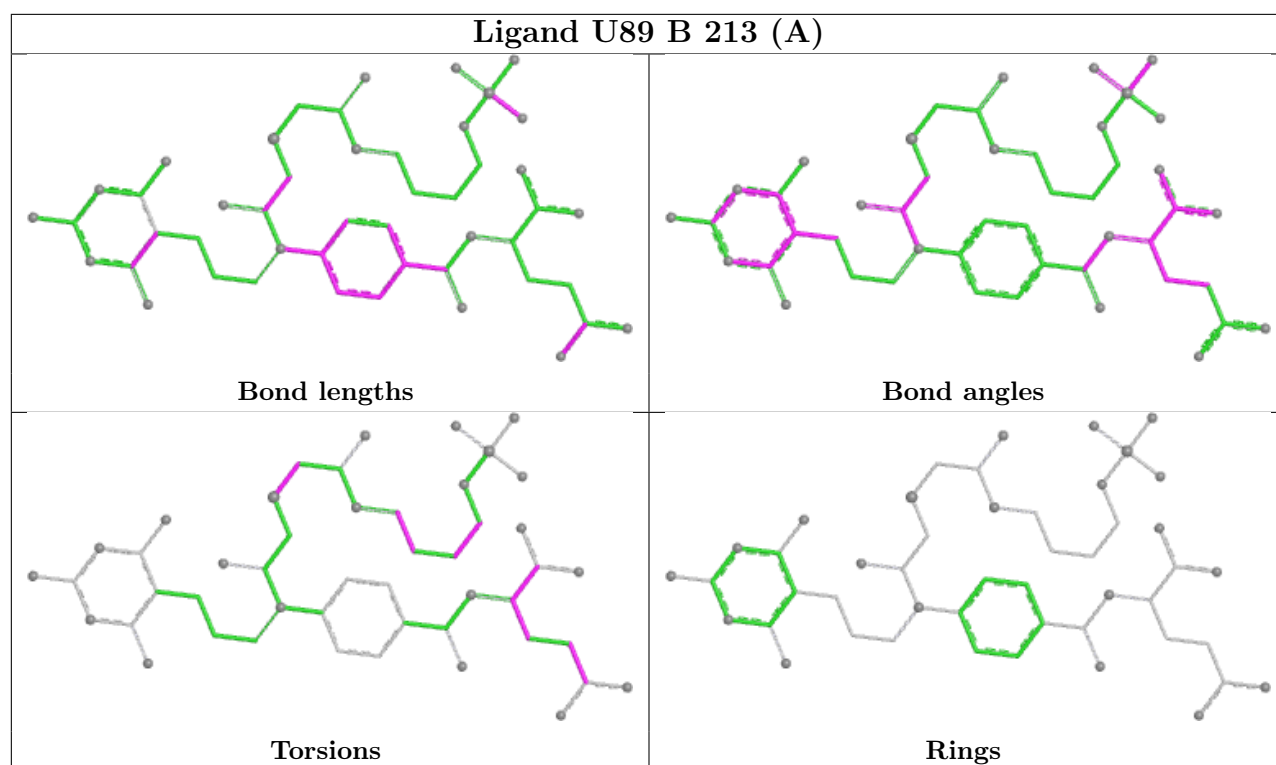
Mol	Chain	Res	Type	Atoms
2	A	213[A]	U89	S-C8-C9-N10
2	A	213[B]	U89	OT1-C-CA-CB
2	A	213[B]	U89	OT2-C-CA-CB
2	A	213[B]	U89	C12-C11-N10-C22
2	B	213[A]	U89	OE1-CD-CG-CB
2	A	213[A]	U89	OE2-CD-CG-CB
2	B	213[A]	U89	OE2-CD-CG-CB
2	A	213[A]	U89	N10-C11-C12-C13
2	A	213[A]	U89	C12-C13-C14-C15
2	A	213[A]	U89	OE1-CD-CG-CB
2	A	213[B]	U89	OE2-CD-CG-CB
2	A	213[A]	U89	C6-C7-S-C8
2	A	213[A]	U89	OT1-C-CA-CB
2	A	213[A]	U89	OT2-C-CA-CB
2	A	213[B]	U89	OE1-CD-CG-CB
2	B	213[B]	U89	OE1-CD-CG-CB
2	B	213[B]	U89	OE2-CD-CG-CB
2	A	213[B]	U89	C23-C22-N10-C11
2	A	213[A]	U89	OP4-C1-C2-C3
2	A	213[B]	U89	S-C8-C9-O9

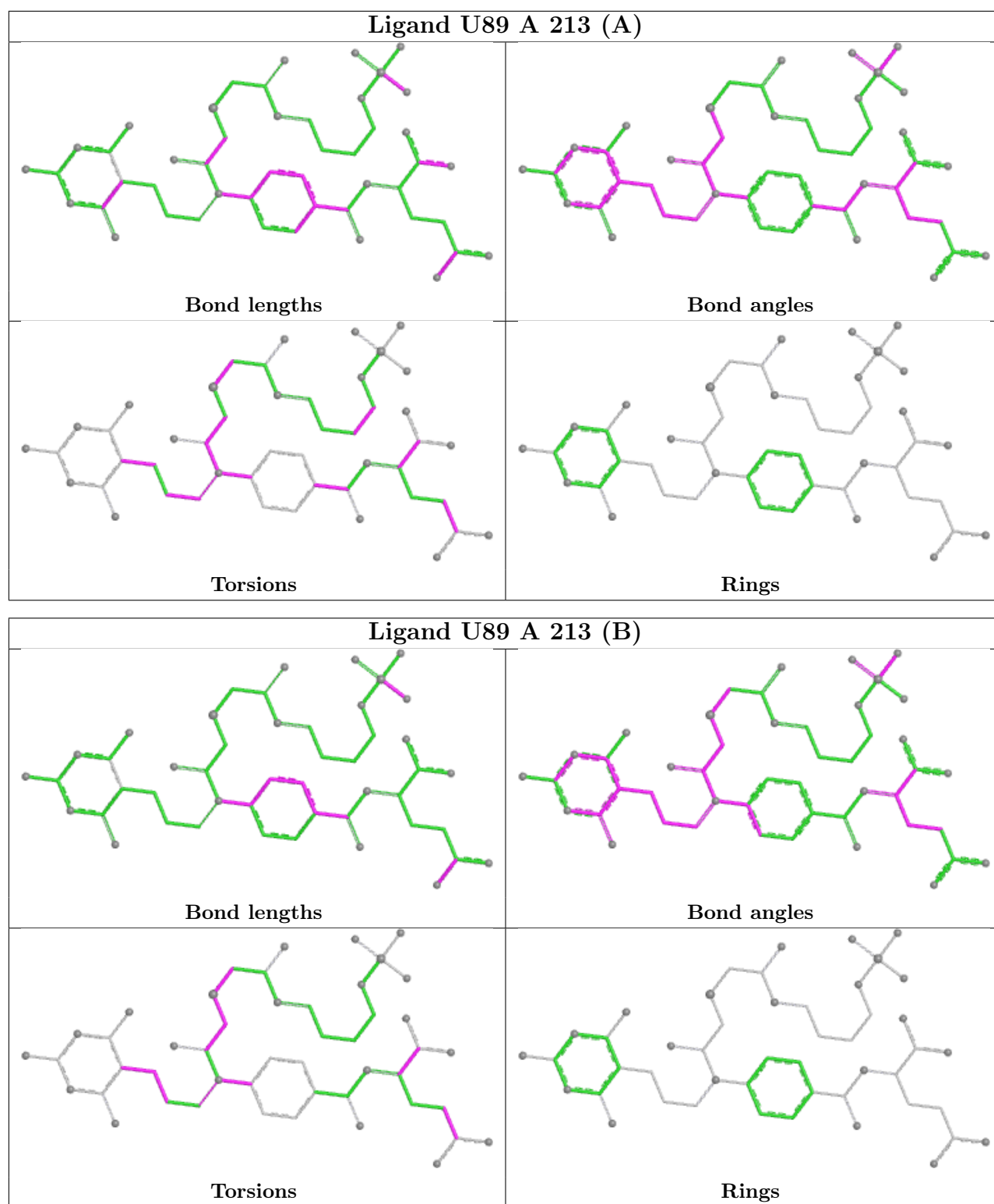
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	213[A]	U89	3	0
2	A	213[A]	U89	3	0
2	A	213[B]	U89	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.