



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:18 AM UTC

PDB ID : 1BYU / pdb_00001byu
Title : CANINE GDP-RAN
Authors : Stewart, M.; Kent, H.M.; Mccoy, A.J.
Deposited on : 1998-10-18
Resolution : 2.15 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)
Xtriage (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

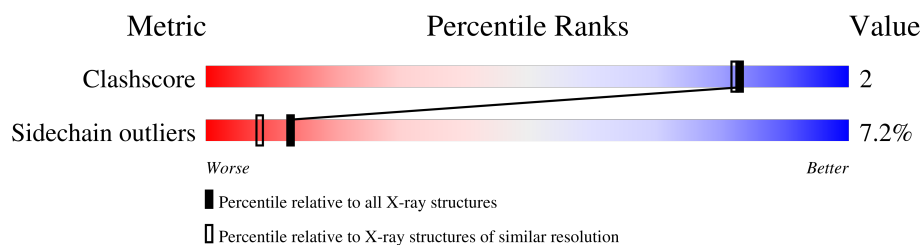
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2159 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)

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	216	
1	B	216	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3594 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 PROTEIN (GTP-BINDING PROTEIN RAN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	4	0	0
			1623	1050	280	287	6			
1	B	215	Total	C	N	O	S	5	0	0
			1716	1104	294	312	6			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 4 is water.

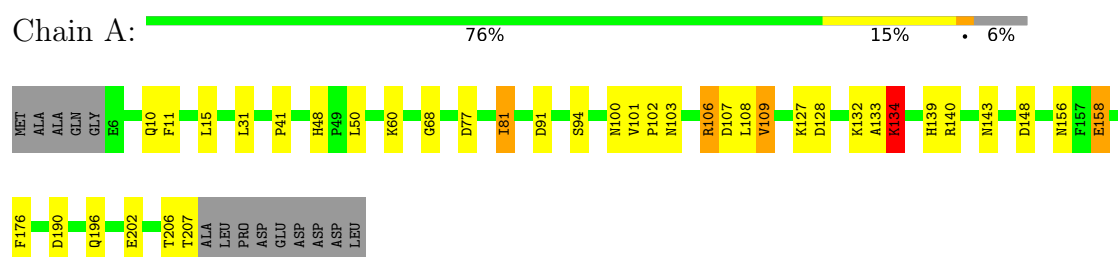
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	100	Total	O	0	0
			100	100		
4	B	97	Total	O	0	0
			97	97		

3 Residue-property plots [i](#)

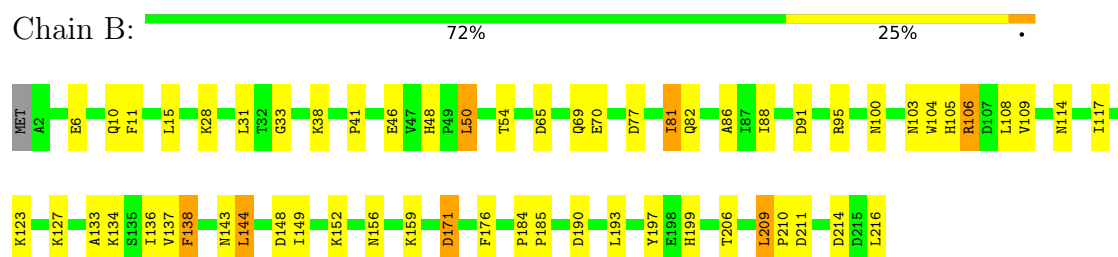
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: PROTEIN (GTP-BINDING PROTEIN RAN)



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	60.79Å 60.43Å 61.20Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	6.00 – 2.15	Depositor
% Data completeness (in resolution range)	94.7 (6.00-2.15)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.176 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3594	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.74	0/1664	1.83	30/2256 (1.3%)
1	B	0.75	0/1758	1.82	47/2384 (2.0%)
All	All	0.74	0/3422	1.82	77/4640 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	4
All	All	0	5

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ASN	CA-C-N	11.86	129.82	120.33
1	B	100	ASN	C-N-CA	11.86	129.82	120.33
1	A	148	ASP	CA-CB-CG	10.55	123.15	112.60
1	A	91	ASP	CA-CB-CG	9.20	121.80	112.60
1	A	100	ASN	CA-C-N	8.53	127.16	120.33
1	A	100	ASN	C-N-CA	8.53	127.16	120.33
1	B	41	PRO	N-CA-CB	8.33	112.35	103.52
1	B	214	ASP	CA-CB-CG	7.72	120.32	112.60
1	B	138	PHE	CA-CB-CG	7.53	121.33	113.80
1	B	91	ASP	CA-CB-CG	7.34	119.94	112.60
1	A	41	PRO	N-CA-CB	7.00	111.03	103.33
1	B	70	GLU	CA-C-N	6.82	130.11	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	GLU	C-N-CA	6.82	130.11	120.28
1	B	77	ASP	CA-C-N	6.79	128.62	120.14
1	B	77	ASP	C-N-CA	6.79	128.62	120.14
1	B	48	HIS	CA-CB-CG	6.74	120.54	113.80
1	A	107	ASP	CA-CB-CG	6.72	119.32	112.60
1	B	114	ASN	CA-CB-CG	6.71	119.31	112.60
1	B	69	GLN	CA-CB-CG	6.62	127.33	114.10
1	B	190	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	77	ASP	CA-C-N	6.22	127.92	120.14
1	A	77	ASP	C-N-CA	6.22	127.92	120.14
1	A	133	ALA	CA-C-N	6.20	128.87	120.38
1	A	133	ALA	C-N-CA	6.20	128.87	120.38
1	B	148	ASP	CA-C-O	-6.04	114.98	121.56
1	B	11	PHE	CA-CB-CG	5.95	119.75	113.80
1	B	171	ASP	O-C-N	-5.76	116.66	121.44
1	B	133	ALA	N-CA-C	5.73	118.26	111.33
1	B	105	HIS	CA-C-N	5.68	127.89	120.28
1	B	105	HIS	C-N-CA	5.68	127.89	120.28
1	A	11	PHE	CA-CB-CG	5.66	119.46	113.80
1	A	81	ILE	N-CA-CB	5.61	117.65	110.13
1	A	94	SER	CA-C-N	5.60	127.79	120.28
1	A	94	SER	C-N-CA	5.60	127.79	120.28
1	B	65	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	128	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	176	PHE	CA-CB-CG	5.54	119.34	113.80
1	B	31	LEU	N-CA-C	5.54	117.40	111.36
1	B	137	VAL	N-CA-C	5.54	120.85	109.34
1	B	50	LEU	CA-C-O	-5.50	114.69	120.58
1	B	199	HIS	CA-C-N	5.47	127.61	120.28
1	B	199	HIS	C-N-CA	5.47	127.61	120.28
1	B	197	TYR	CA-C-N	5.46	127.59	120.28
1	B	197	TYR	C-N-CA	5.46	127.59	120.28
1	B	81	ILE	N-CA-C	5.45	116.72	109.37
1	A	190	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	156	ASN	CA-CB-CG	5.42	118.02	112.60
1	B	136	ILE	O-C-N	-5.41	115.68	121.80
1	A	176	PHE	CA-CB-CG	5.41	119.21	113.80
1	B	33	GLY	CA-C-N	5.37	127.92	120.29
1	B	33	GLY	C-N-CA	5.37	127.92	120.29
1	A	108	LEU	CA-C-N	5.35	127.30	120.56
1	A	108	LEU	C-N-CA	5.35	127.30	120.56
1	B	156	ASN	CA-C-N	5.35	127.76	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	ASN	C-N-CA	5.35	127.76	120.54
1	B	69	GLN	CA-C-N	5.34	129.63	120.72
1	B	69	GLN	C-N-CA	5.34	129.63	120.72
1	B	152	LYS	N-CA-C	5.31	117.81	111.71
1	A	134	LYS	O-C-N	-5.25	116.56	122.12
1	B	104	TRP	CA-C-N	5.23	127.24	120.44
1	B	104	TRP	C-N-CA	5.23	127.24	120.44
1	A	133	ALA	N-CA-C	5.22	117.37	111.11
1	B	28	LYS	N-CA-C	5.21	119.26	113.01
1	A	31	LEU	N-CA-C	5.21	116.64	111.07
1	B	95	ARG	N-CA-C	5.20	117.69	111.71
1	A	101	VAL	O-C-N	-5.16	117.12	120.42
1	B	133	ALA	CA-C-N	5.13	127.16	120.28
1	B	133	ALA	C-N-CA	5.13	127.16	120.28
1	A	139	HIS	CA-C-N	5.11	128.08	120.31
1	A	139	HIS	C-N-CA	5.11	128.08	120.31
1	B	127	LYS	N-CA-C	5.11	116.54	111.07
1	A	102	PRO	CA-C-N	5.09	128.05	120.31
1	A	102	PRO	C-N-CA	5.09	128.05	120.31
1	B	114	ASN	N-CA-C	5.06	119.09	111.81
1	A	48	HIS	CA-CB-CG	5.03	118.83	113.80
1	A	127	LYS	N-CA-C	5.02	116.44	111.07
1	B	86	ALA	N-CA-C	5.00	116.44	108.79

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	68	GLY	Mainchain
1	B	10	GLN	Mainchain
1	B	123	LYS	Mainchain
1	B	171	ASP	Mainchain
1	B	54	THR	Mainchain

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	1623	0	1632	8	1
1	B	1716	0	1708	8	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	12	0	0
3	B	28	0	12	0	0
4	A	100	0	0	0	0
4	B	97	0	0	0	0
All	All	3594	0	3364	16	1

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 2.

All (16) 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:B:206:THR:HA	1:B:209:LEU:HD22	1.68	0.73
1:A:132:LYS:HB3	1:A:134:LYS:HE3	1.80	0.62
1:A:103:ASN:HB3	1:A:106:ARG:HH11	1.75	0.52
1:A:206:THR:O	1:A:207:THR:HB	2.13	0.47
1:A:10:GLN:HG2	1:A:60:LYS:HD2	1.98	0.46
1:A:134:LYS:H	1:A:134:LYS:CE	2.30	0.45
1:B:209:LEU:HB3	1:B:210:PRO:HD2	1.99	0.44
1:B:81:ILE:O	1:B:82:GLN:HB2	2.18	0.43
1:A:103:ASN:O	1:A:106:ARG:HD3	2.19	0.43
1:B:117:ILE:HB	1:B:144:LEU:HD12	2.00	0.42
1:B:88:ILE:HD11	1:B:108:LEU:HD12	2.02	0.42
1:B:106:ARG:HA	1:B:109:VAL:HG12	2.02	0.42
1:B:103:ASN:HB3	1:B:106:ARG:HH11	1.84	0.41
1:A:134:LYS:H	1:A:134:LYS:HE2	1.85	0.41
1:A:158:GLU:H	1:A:158:GLU:HG3	1.61	0.41
1:B:184:PRO:HA	1:B:185:PRO:HD3	1.95	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:CG1	1:B:6:GLU:OE2[1_556]	1.64	0.56

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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 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	175/186 (94%)	164 (94%)	11 (6%)	16	11
1	B	184/186 (99%)	169 (92%)	15 (8%)	10	6
All	All	359/372 (96%)	333 (93%)	26 (7%)	13	8

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	50	LEU
1	A	81	ILE
1	A	106	ARG
1	A	109	VAL
1	A	134	LYS
1	A	140	ARG
1	A	143	ASN
1	A	158	GLU
1	A	196	GLN
1	A	202	GLU
1	B	15	LEU
1	B	38	LYS
1	B	46	GLU
1	B	50	LEU
1	B	106	ARG
1	B	134	LYS
1	B	138	PHE
1	B	143	ASN
1	B	144	LEU
1	B	149	ILE

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Mol	Chain	Res	Type
1	B	159	LYS
1	B	193	LEU
1	B	209	LEU
1	B	211	ASP
1	B	216	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	62	ASN
1	A	103	ASN
1	A	199	HIS
1	B	10	GLN
1	B	62	ASN
1	B	82	GLN
1	B	103	ASN
1	B	143	ASN

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GDP	A	220	2	29,30,30	0.84	0	45,47,47	1.05	3 (6%)
3	GDP	B	220	2	29,30,30	0.85	0	45,47,47	0.94	2 (4%)

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	GDP	A	220	2	-	0/16/32/32	0/3/3/3
3	GDP	B	220	2	-	0/16/32/32	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	220	GDP	O3B-PB-O3A	2.73	113.80	104.64
3	A	220	GDP	O2'-C2'-C1'	2.72	119.48	110.10
3	B	220	GDP	O2B-PB-O3A	2.31	112.38	104.64
3	A	220	GDP	O2B-PB-O3A	2.25	112.18	104.64
3	B	220	GDP	O2'-C2'-C1'	2.01	117.03	110.10

There are no chirality outliers.

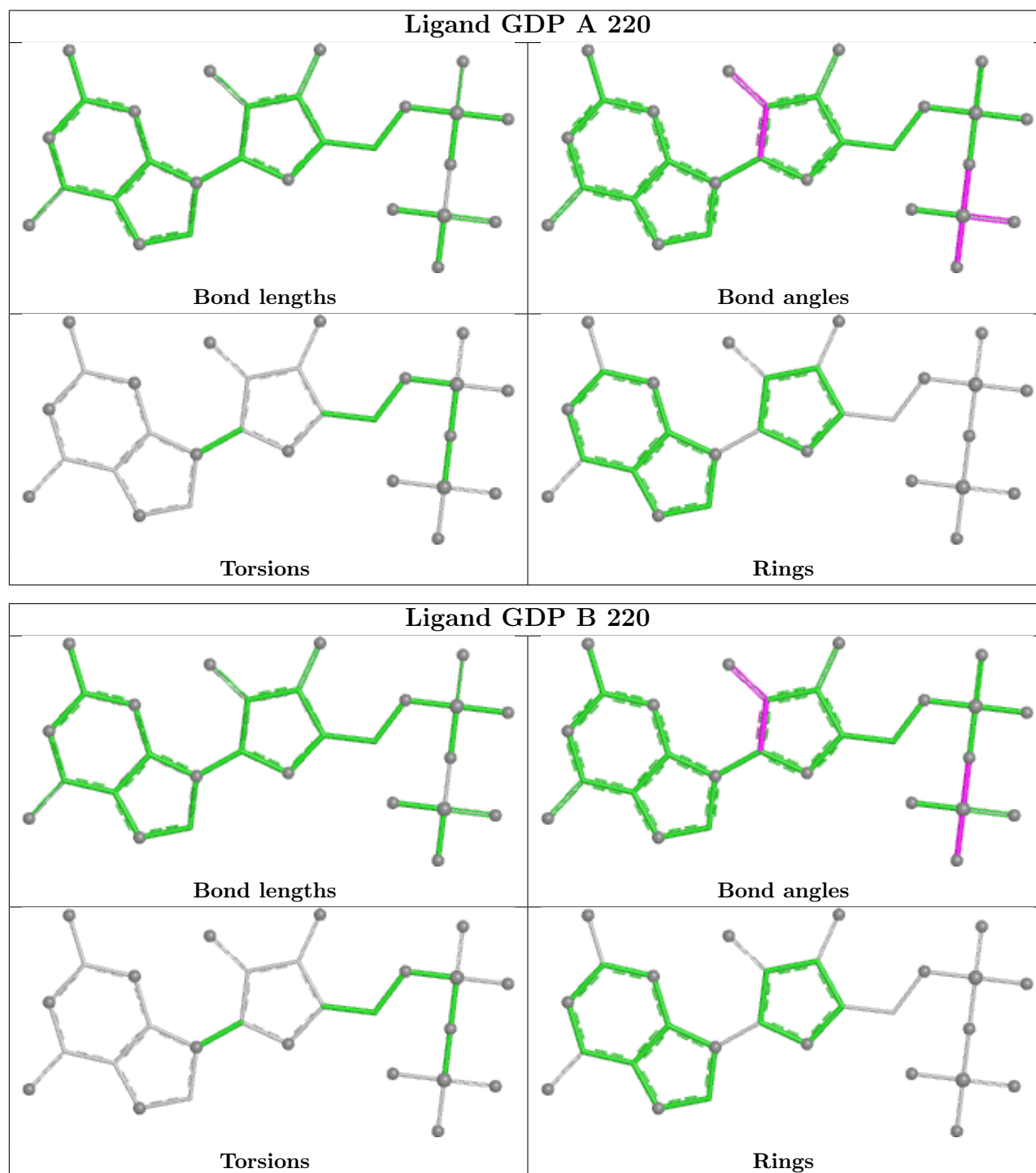
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.