



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 04:26 AM UTC

PDB ID : 1H9U / pdb_00001h9u
Title : The structure of the human retinoid-X-receptor beta ligand binding domain
in complex with the specific synthetic agonist LG100268
Authors : Schwabe, J.W.R.; Love, J.D.; Gooch, J.T.
Deposited on : 2001-03-21
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

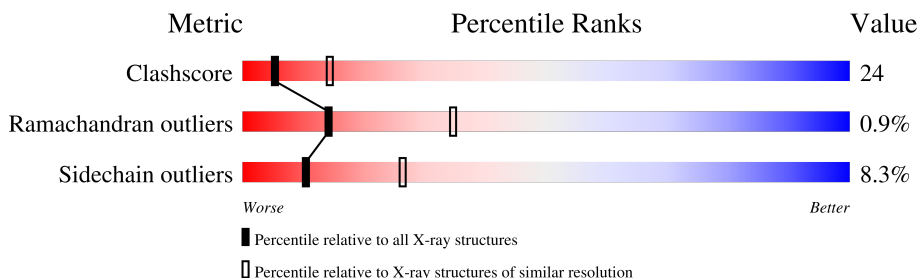
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	224	49% 36% • 10%
1	B	224	57% 29% • 10%
1	C	224	53% 32% • 10%
1	D	224	52% 34% • 10%

2 Entry composition [i](#)

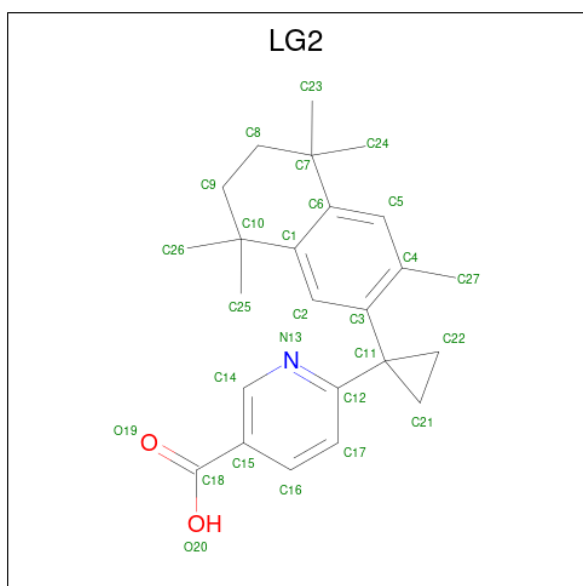
There are 5 unique types of molecules in this entry. The entry contains 6338 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RETINOID X RECEPTOR, BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1560	999	276	277	8			
1	B	201	Total	C	N	O	S	0	0	0
			1553	994	275	276	8			
1	C	201	Total	C	N	O	S	0	0	0
			1555	1001	271	275	8			
1	D	201	Total	C	N	O	S	0	0	0
			1552	996	272	276	8			

- Molecule 2 is 6-[1-(3,5,5,8,8-PENTAMETHYL-5,6,7,8-TETRAHYDRONAPHTHALEN-2-YL)CYCLOPROPYL]PYRIDINE-3-CARBOXYLIC ACID (CCD ID: LG2) (formula: C₂₄H₂₉NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	24	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			27	24	1	2		
2	C	1	Total	C	N	O	0	0
			27	24	1	2		
2	D	1	Total	C	N	O	0	0
			27	24	1	2		

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	B	1	Total	Ni	0	0
			1	1		
3	C	1	Total	Ni	0	0
			1	1		
3	D	1	Total	Ni	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

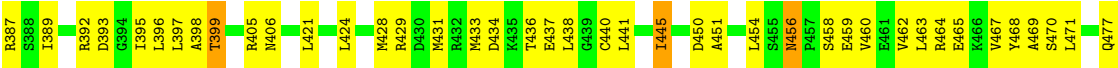
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	C	1	Total	O	0	0
			1	1		
5	D	1	Total	O	0	0
			1	1		



● Molecule 1: RETINOID X RECEPTOR, BETA



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.89Å 106.88Å 100.59Å 90.00° 122.56° 90.00°	Depositor
Resolution (Å)	38.14 – 2.70	Depositor
% Data completeness (in resolution range)	97.3 (38.14-2.70)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.273 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6338	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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: LG2, CL, NI

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	0.56	0/1589	0.99	7/2149 (0.3%)
1	B	0.55	0/1582	0.99	3/2139 (0.1%)
1	C	0.54	0/1585	1.01	11/2143 (0.5%)
1	D	0.51	0/1582	0.98	6/2138 (0.3%)
All	All	0.54	0/6338	0.99	27/8569 (0.3%)

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	469	ALA	N-CA-C	-6.20	103.83	111.40
1	B	469	ALA	N-CA-C	-6.11	103.95	111.40
1	C	469	ALA	N-CA-C	-6.08	103.98	111.40
1	C	357	ILE	CA-C-N	5.78	127.06	119.84
1	C	357	ILE	C-N-CA	5.78	127.06	119.84

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	A	1560	0	1581	89	0
1	B	1553	0	1571	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1555	0	1580	81	0
1	D	1552	0	1567	77	0
2	A	27	0	28	6	0
2	B	27	0	28	1	0
2	C	27	0	28	8	0
2	D	27	0	28	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	2	0
5	B	1	0	0	0	0
5	C	1	0	0	1	0
5	D	1	0	0	0	0
All	All	6338	0	6411	308	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 24.

The worst 5 of 308 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:C:379:LEU:HG	1:C:445:ILE:HD11	1.46	0.98
1:A:379:LEU:HG	1:A:445:ILE:HD11	1.46	0.97
1:B:389:ILE:HG23	1:B:429:ARG:HG3	1.47	0.96
1:D:299:MET:HE2	1:D:467:VAL:HG22	1.47	0.96
1:D:379:LEU:HG	1:D:445:ILE:HD11	1.47	0.96

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	197/224 (88%)	186 (94%)	9 (5%)	2 (1%)	12	32
1	B	197/224 (88%)	188 (95%)	8 (4%)	1 (0%)	24	48
1	C	197/224 (88%)	190 (96%)	5 (2%)	2 (1%)	12	32
1	D	197/224 (88%)	188 (95%)	7 (4%)	2 (1%)	12	32
All	All	788/896 (88%)	752 (95%)	29 (4%)	7 (1%)	14	35

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	PRO
1	A	521	PHE
1	B	358	PRO
1	C	358	PRO
1	D	358	PRO

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	166/191 (87%)	152 (92%)	14 (8%)	10	26
1	B	165/191 (86%)	151 (92%)	14 (8%)	10	25
1	C	166/191 (87%)	152 (92%)	14 (8%)	10	26
1	D	165/191 (86%)	152 (92%)	13 (8%)	11	28
All	All	662/764 (87%)	607 (92%)	55 (8%)	10	26

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	305	LEU
1	C	406	ASN
1	D	512	LEU

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Mol	Chain	Res	Type
1	D	421	LEU
1	C	358	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	377	ASN
1	D	506	HIS
1	B	506	HIS
1	C	377	ASN
1	C	477	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\# Z > 2$
2	LG2	B	1	-	29,30,30	2.75	10 (34%)	44,49,49	1.28	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LG2	D	1	-	29,30,30	3.01	11 (37%)	44,49,49	1.30	6 (13%)
2	LG2	C	1	-	29,30,30	2.67	11 (37%)	44,49,49	1.25	5 (11%)
2	LG2	A	1	-	29,30,30	2.42	11 (37%)	44,49,49	1.31	6 (13%)

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	LG2	B	1	-	-	2/15/39/39	0/4/4/4
2	LG2	D	1	-	-	3/15/39/39	0/4/4/4
2	LG2	C	1	-	-	2/15/39/39	0/4/4/4
2	LG2	A	1	-	-	5/15/39/39	0/4/4/4

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	LG2	C4-C3	12.00	1.50	1.41
2	B	1	LG2	C4-C3	10.36	1.49	1.41
2	C	1	LG2	C4-C3	8.73	1.48	1.41
2	A	1	LG2	C4-C3	7.50	1.47	1.41
2	C	1	LG2	C5-C6	4.64	1.46	1.39

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	LG2	C21-C11-C12	-3.43	111.89	117.30
2	B	1	LG2	C21-C11-C12	-3.01	112.56	117.30
2	A	1	LG2	C22-C11-C21	2.97	60.51	58.70
2	B	1	LG2	C14-N13-C12	2.91	120.72	117.60
2	C	1	LG2	C14-N13-C12	2.79	120.59	117.60

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	LG2	C22-C11-C12-C17
2	A	1	LG2	C21-C11-C3-C4
2	A	1	LG2	C22-C11-C3-C4

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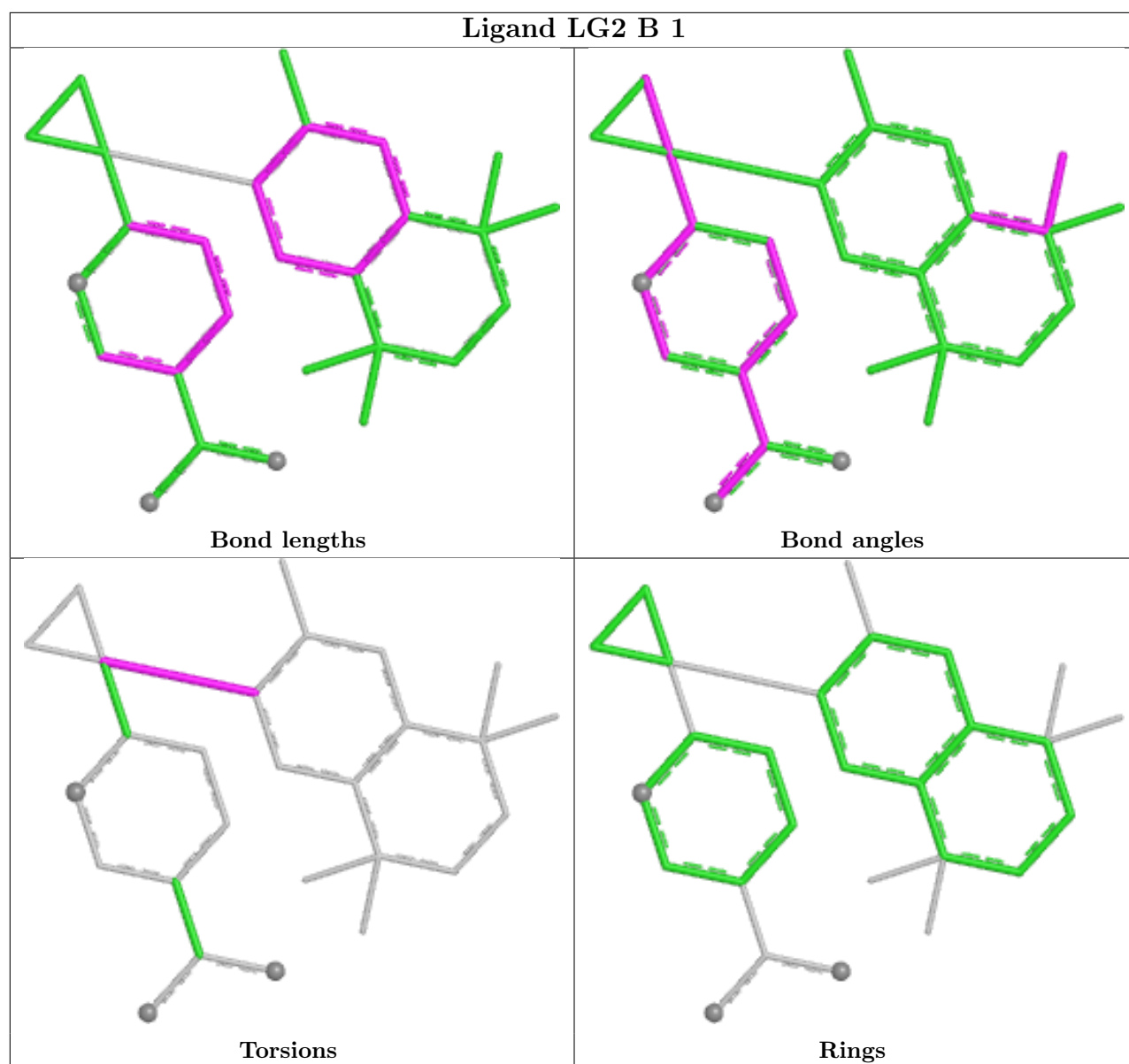
Mol	Chain	Res	Type	Atoms
2	B	1	LG2	C21-C11-C3-C4
2	B	1	LG2	C22-C11-C3-C4

There are no ring outliers.

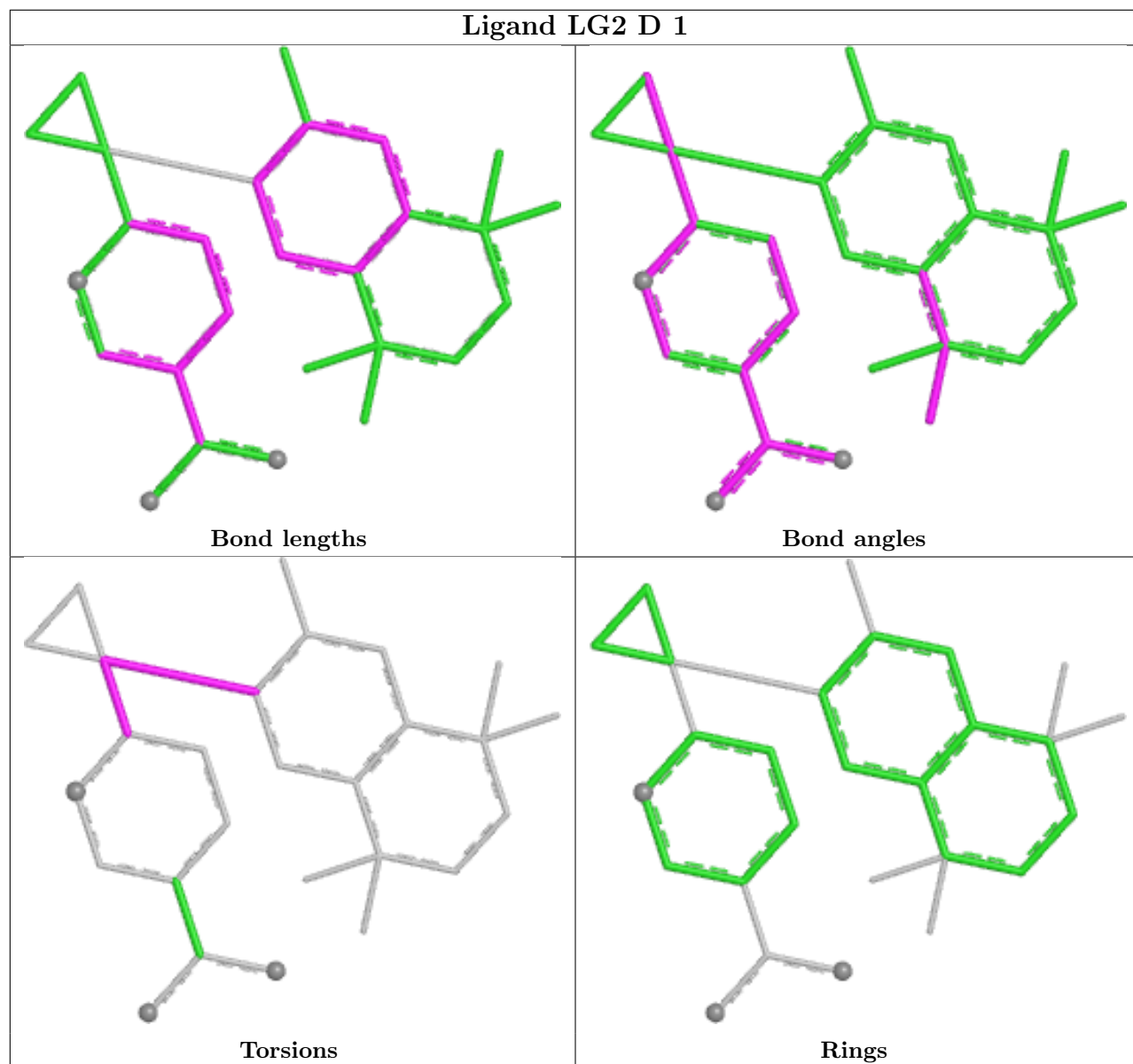
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	LG2	1	0
2	D	1	LG2	3	0
2	C	1	LG2	8	0
2	A	1	LG2	6	0

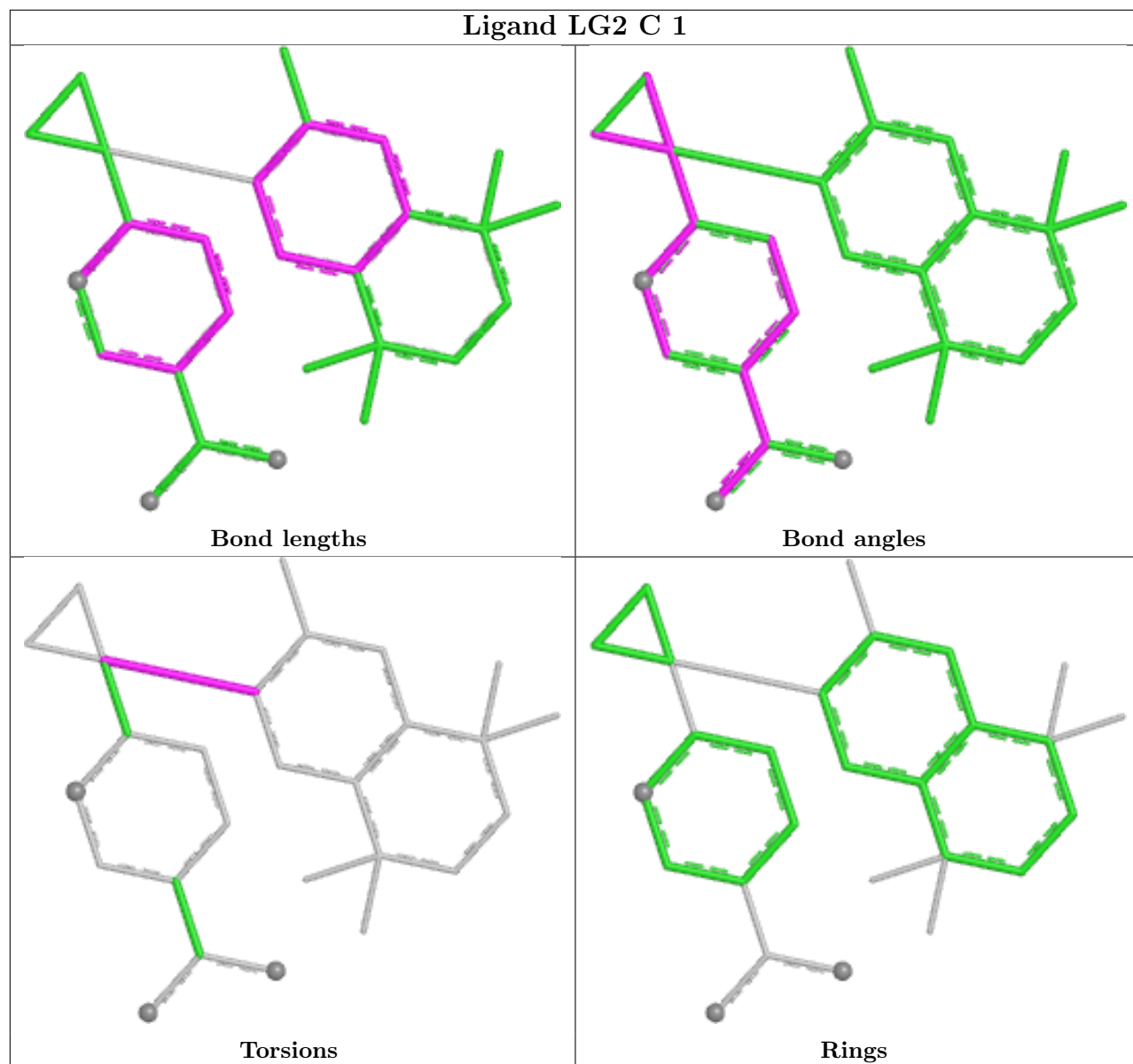
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

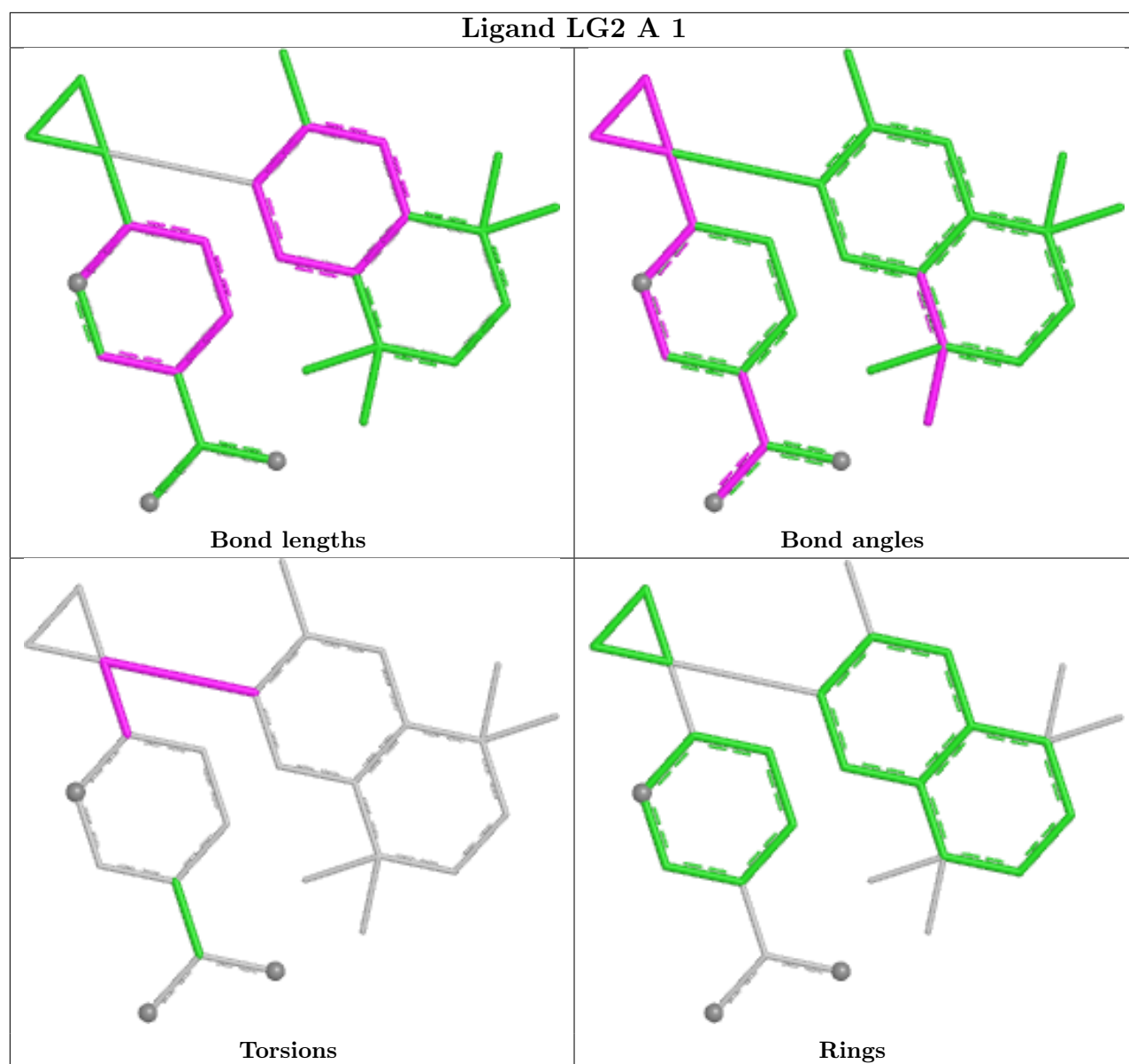


Ligand LG2 D 1



Ligand LG2 C 1





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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.