



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 23, 2024 – 12:09 PM JST

PDB ID : 9JTI
Title : X-ray structure of Nelle indicator complexed with isoleucine
Authors : Samygina, V.R.; Subach, O.M.; Vlaskina, A.V.; Dronova, E.A.; Subach, F.V.
Deposited on : 2024-10-04
Resolution : 1.62 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

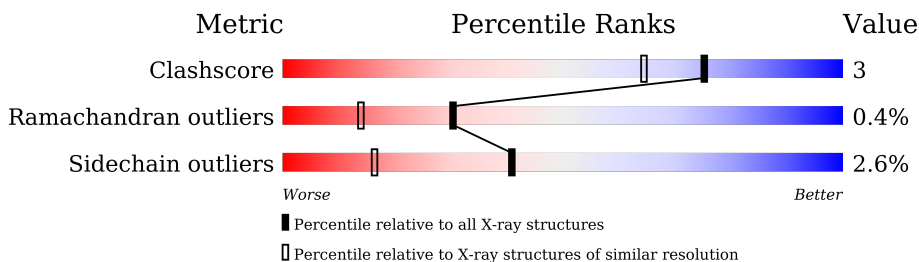
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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	180529	6617 (1.64-1.60)
Ramachandran outliers	177936	6498 (1.64-1.60)
Sidechain outliers	177891	6497 (1.64-1.60)

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	593	89% 6% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5074 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.

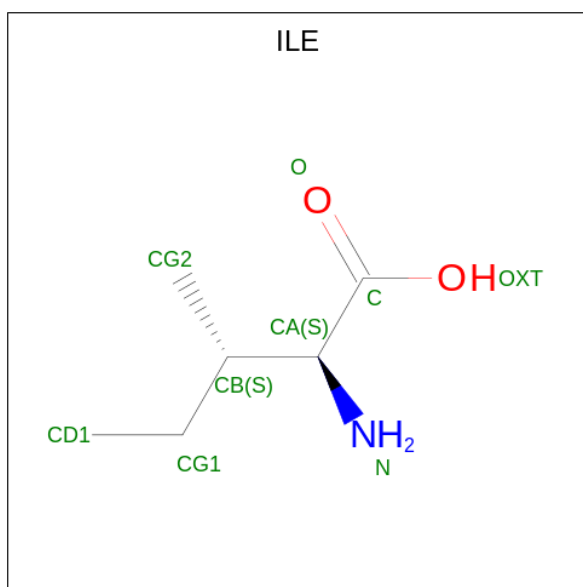
- Molecule 1 is a protein called NeIle,Leu/Ile/Val-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	571	4486	2842	768	858	18	0	14	0

There are 9 discrepancies between the modelled and reference sequences:

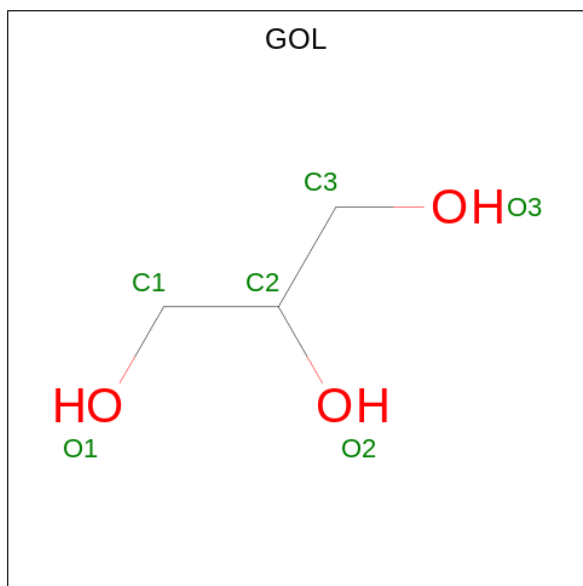
Chain	Residue	Modelled	Actual	Comment	Reference
A	267	THR	ALA	conflict	UNP P0AD96
A	287	ARG	LYS	conflict	UNP P0AD96
A	315	ARG	LYS	conflict	UNP P0AD96
A	333	ALA	THR	conflict	UNP P0AD96
A	343	ALA	GLU	conflict	UNP P0AD96
A	377	LEU	PRO	conflict	UNP P0AD96
A	411	GLY	ASP	conflict	UNP P0AD96
A	511	HIS	PRO	conflict	UNP P0AD96
A	516	VAL	ILE	conflict	UNP P0AD96

- Molecule 2 is ISOLEUCINE (three-letter code: ILE) (formula: C₆H₁₃NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	9	6	1	2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
3	A	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is water.

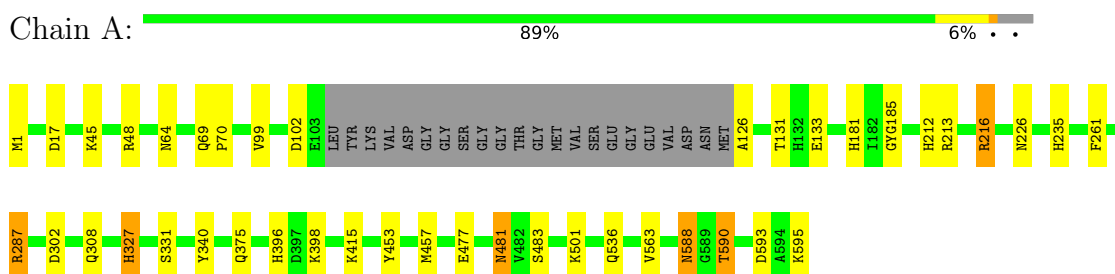
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	560	Total	O	0	0
			560	560		

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: NeIIe,Leu/Ile/Val-binding protein



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	61.10Å 69.20Å 80.50Å 90.00° 111.11° 90.00°	Depositor
Resolution (Å)	75.55 – 1.62	Depositor
% Data completeness (in resolution range)	100.0 (75.55-1.62)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.158 , 0.184	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5074	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: CR2, CL, GOL, CSX

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	0.92	0/4583	0.82	1/6200 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	453	TYR	CB-CG-CD1	5.19	124.11	121.00

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	4486	0	4384	26	0
2	A	9	0	10	0	0
3	A	18	0	24	0	0
4	A	1	0	0	0	0
5	A	560	0	0	8	0
All	All	5074	0	4418	26	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 3.

All (26) 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:261[B]:PHE:CE1	5:A:941:HOH:O	2.19	0.96
1:A:261[B]:PHE:CD1	5:A:941:HOH:O	2.33	0.81
1:A:212:HIS:HD2	1:A:226:ASN:HD21	1.31	0.77
1:A:593:ASP:HB3	5:A:993:HOH:O	1.83	0.77
1:A:48:ARG:HH12	1:A:308[B]:GLN:HE22	1.36	0.73
1:A:536:GLN:HE22	1:A:563:VAL:H	1.36	0.71
1:A:181:HIS:HD2	1:A:213:ARG:HH11	1.43	0.67
1:A:396:HIS:HD2	1:A:398:LYS:H	1.43	0.65
1:A:99:VAL:HA	5:A:1042:HOH:O	1.97	0.64
1:A:588:ASN:ND2	1:A:590[A]:THR:HB	2.19	0.57
1:A:133:GLU:OE1	1:A:235:HIS:HE1	1.88	0.55
1:A:212:HIS:HD2	1:A:226:ASN:ND2	2.01	0.55
1:A:375:GLN:HE22	1:A:477:GLU:H	1.52	0.55
1:A:302:ASP:OD2	1:A:327:HIS:HD2	1.90	0.55
1:A:131:THR:OG1	1:A:235:HIS:HD2	1.90	0.54
1:A:595:LYS:CE	1:A:595:LYS:HA	2.39	0.53
1:A:126:ALA:HB3	5:A:1051:HOH:O	2.08	0.53
1:A:181:HIS:HE1	5:A:961:HOH:O	1.92	0.51
1:A:216:ARG:HD2	5:A:1117:HOH:O	2.13	0.48
1:A:212:HIS:CD2	1:A:226:ASN:HD21	2.21	0.48
1:A:327:HIS:HE1	1:A:340:TYR:OH	1.96	0.47
1:A:588:ASN:HD21	1:A:590[A]:THR:HB	1.79	0.47
1:A:45:LYS:HB3	1:A:308[A]:GLN:HE22	1.82	0.43
1:A:69:GLN:HB2	1:A:70:PRO:HA	2.01	0.41
1:A:287:ARG:NH1	5:A:716:HOH:O	2.52	0.41
1:A:481:ASN:HD22	1:A:483:SER:H	1.69	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	577/593 (97%)	563 (98%)	12 (2%)	2 (0%)	37 20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ASP
1	A	327	HIS

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	465/468 (99%)	452 (97%)	13 (3%)	38 14

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	17	ASP
1	A	64	ASN
1	A	216	ARG
1	A	287	ARG
1	A	331	SER
1	A	415	LYS
1	A	457	MET
1	A	481	ASN
1	A	501	LYS
1	A	588	ASN
1	A	590[A]	THR
1	A	590[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS

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Mol	Chain	Res	Type
1	A	150	GLN
1	A	181	HIS
1	A	212	HIS
1	A	226	ASN
1	A	235	HIS
1	A	327	HIS
1	A	375	GLN
1	A	396	HIS
1	A	481	ASN
1	A	509	ASN
1	A	536	GLN
1	A	543	ASN
1	A	588	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](#)

2 non-standard protein/DNA/RNA residues 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$
1	CSX	A	25	1	3,6,7	0.86	0	1,6,8	0.60	0
1	CR2	A	185	1	20,20,21	3.64	5 (25%)	25,27,29	3.75	4 (16%)

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
1	CSX	A	25	1	-	0/1/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR2	A	185	1	-	0/6/25/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	CR2	CB2-CA2	14.37	1.47	1.35
1	A	185	CR2	O2-C2	3.86	1.31	1.23
1	A	185	CR2	C1-N2	3.32	1.38	1.32
1	A	185	CR2	C2-N3	-3.31	1.32	1.39
1	A	185	CR2	CA2-C2	-2.25	1.46	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	CR2	CA2-C2-N3	12.83	109.44	103.37
1	A	185	CR2	O2-C2-CA2	-8.88	125.97	130.96
1	A	185	CR2	C1-CA1-N1	-7.10	97.14	112.85
1	A	185	CR2	C2-N3-C1	-5.85	105.13	107.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is 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	ILE	A	601	-	7,8,8	0.55	0	7,10,10	0.95	0
3	GOL	A	604	-	5,5,5	0.17	0	5,5,5	0.47	0
3	GOL	A	603	-	5,5,5	0.39	0	5,5,5	0.85	0
3	GOL	A	602	-	5,5,5	0.13	0	5,5,5	0.30	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
2	ILE	A	601	-	-	0/10/10/10	-
3	GOL	A	604	-	-	2/4/4/4	-
3	GOL	A	603	-	-	0/4/4/4	-
3	GOL	A	602	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

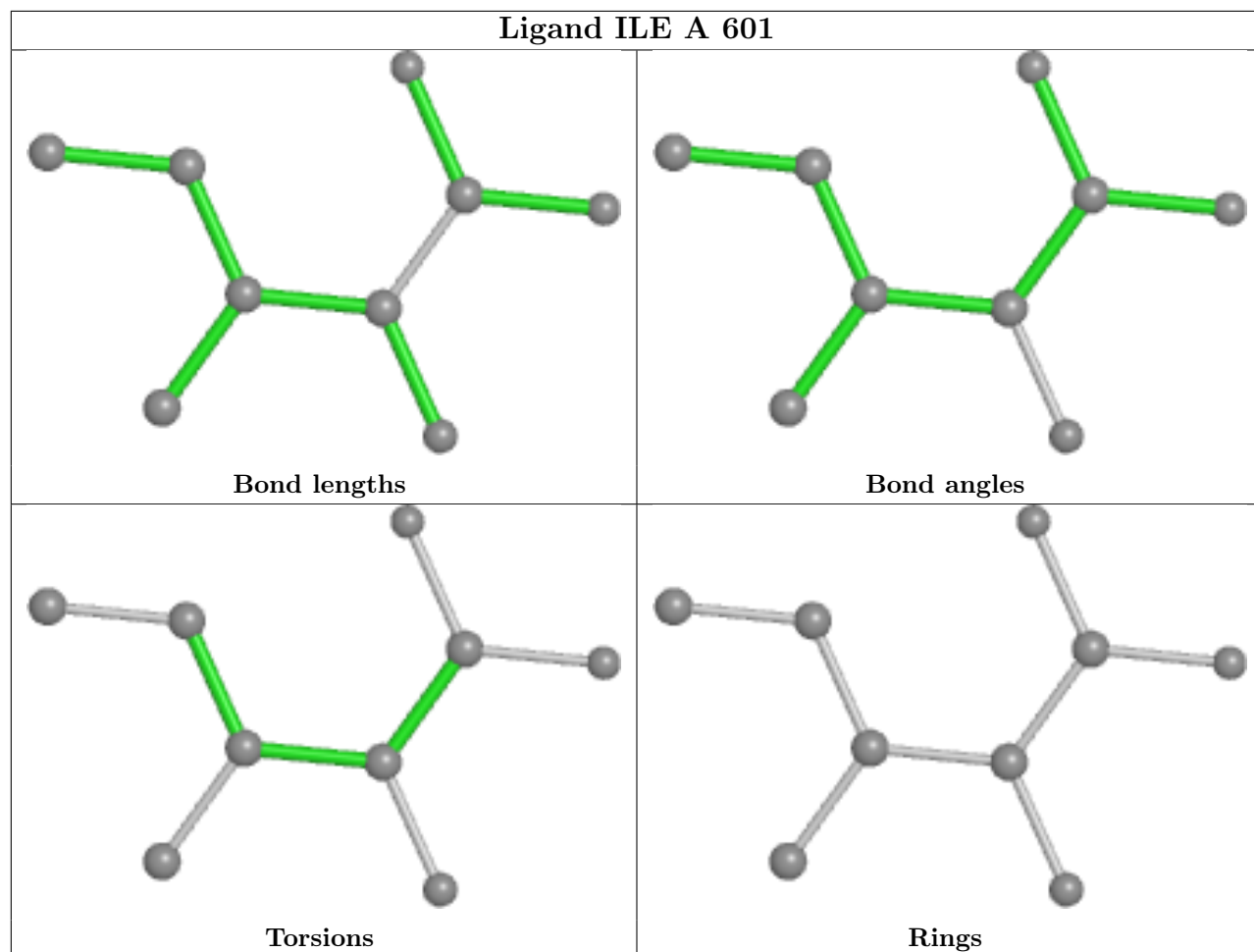
All (2) torsion outliers are listed below:

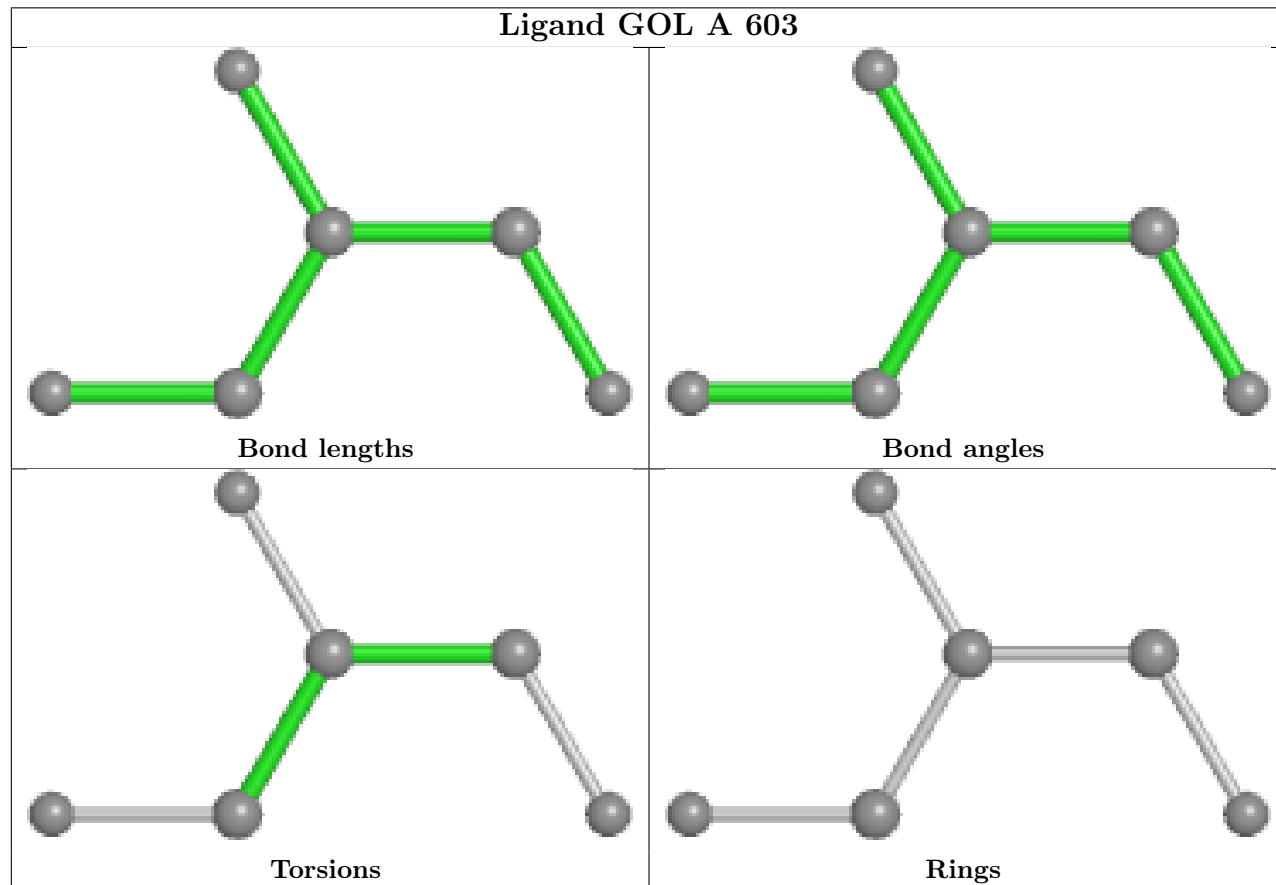
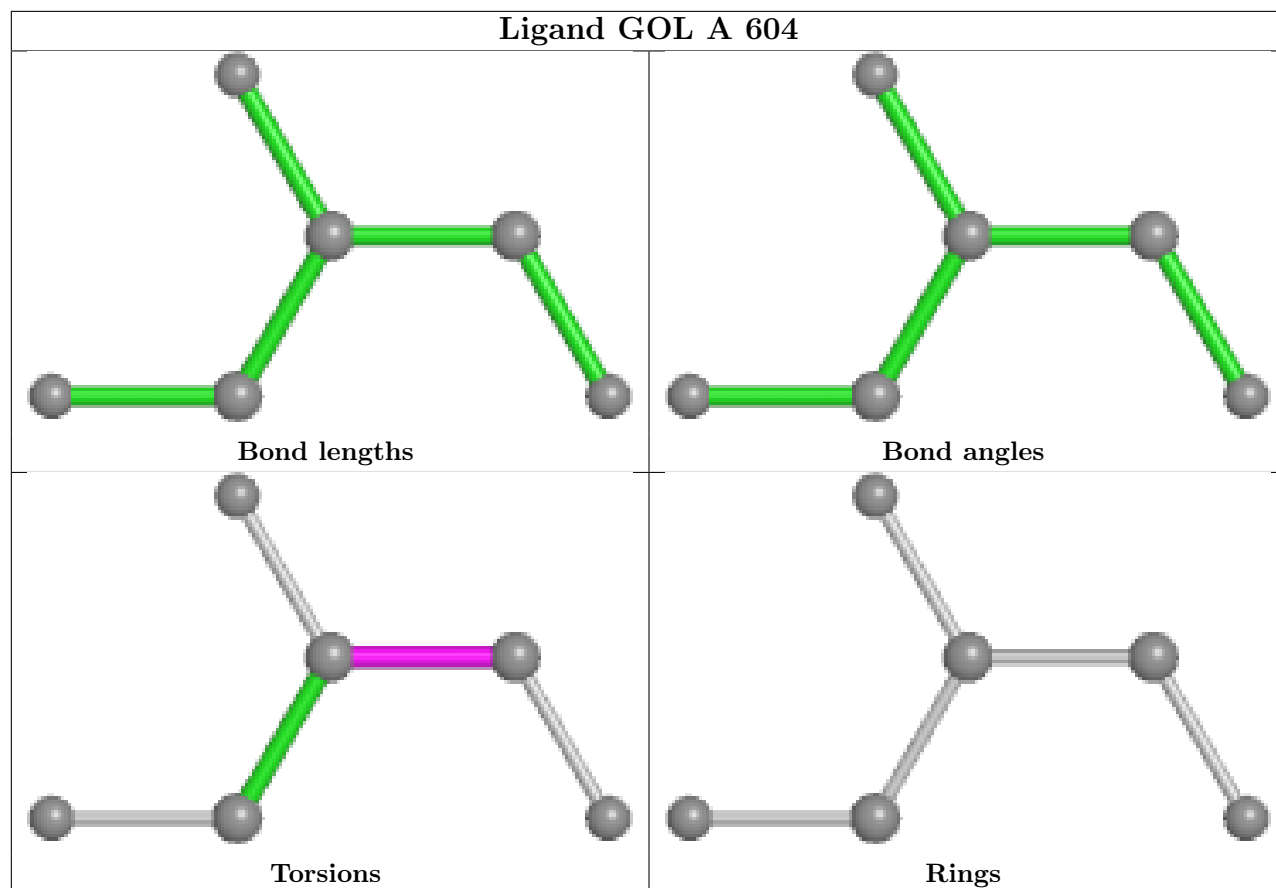
Mol	Chain	Res	Type	Atoms
3	A	604	GOL	O1-C1-C2-O2
3	A	604	GOL	O1-C1-C2-C3

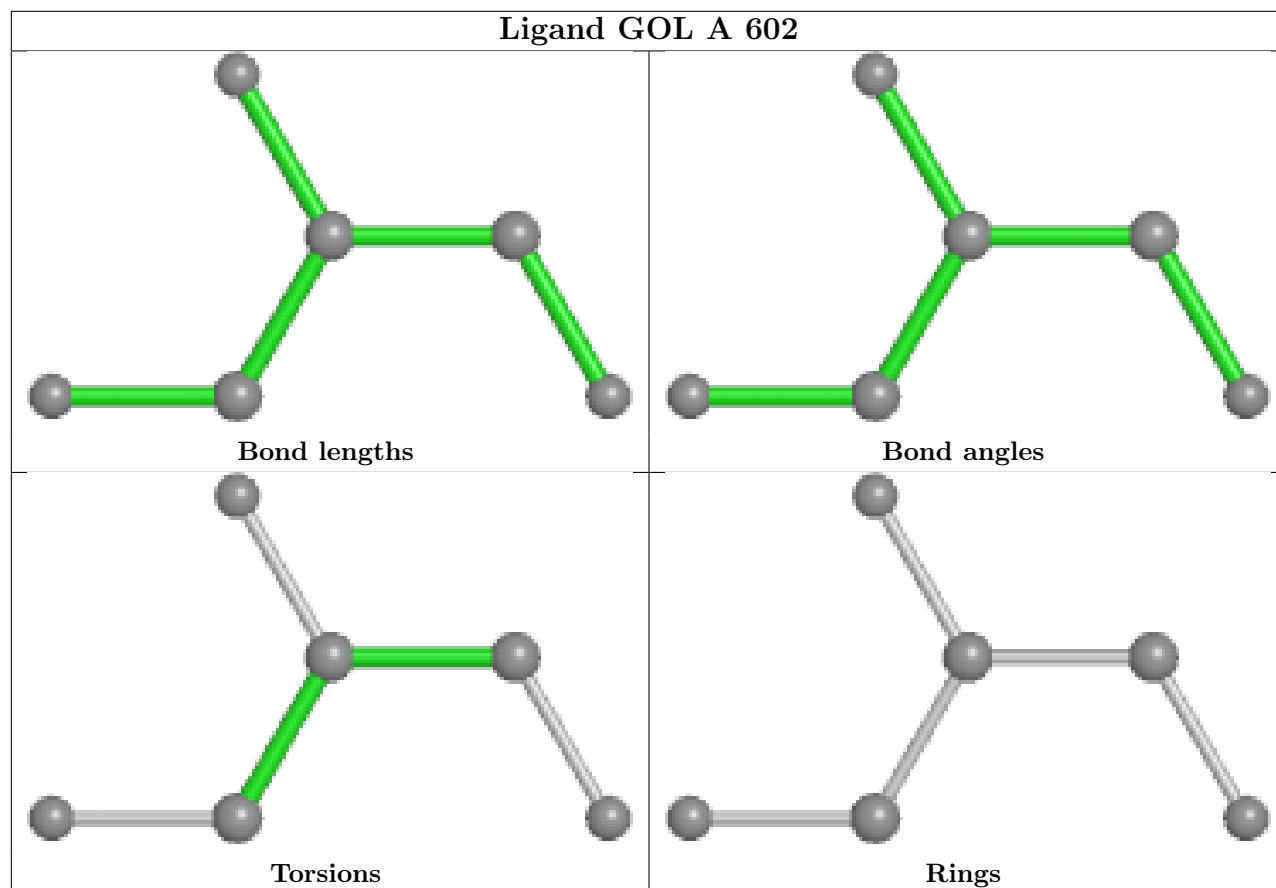
There are no ring outliers.

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 [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.