WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB NMR Structure Validation Summary Report (i)

Apr 21, 2024 – 04:06 AM EDT

PDB ID : 2L65

Title : HADDOCK calculated model of the complex of the resistance protein CalC and Calicheamicin-Gamma

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Deposited on : 2010-11-15

This is a wwPDB NMR 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
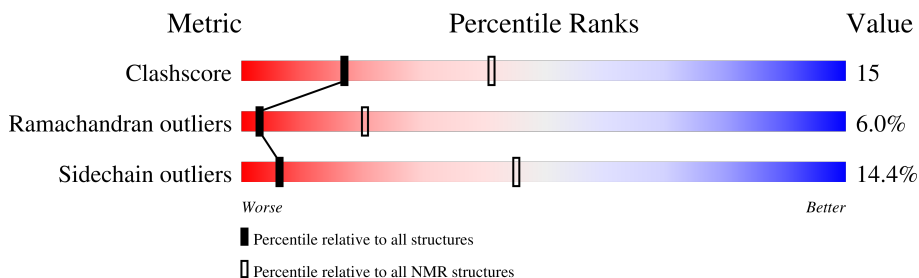http://www.wwpdb.org/validation/2017/FAQs#types.

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1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	Percentile Ranks	Value
Clashscore		15
Ramachandran outliers		6.0%
Sidechain outliers		14.4%

Worse *Better*

▮ Percentile relative to all structures
⫿ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	155	81% 17% •
2	B	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	B	EMP	2	1	-

2   Ensemble composition and analysis ⓘ

This entry contains 4 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:155 (155)	0.44	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4

wwPDB NMR Structure Validation Summary Report

3 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 1658 atoms, of which 307 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CalC.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	155	1566	802	299	228	235	2	0

- Molecule 2 is an oligosaccharide called 2,4-dideoxy-4-(ethylamino)-3-O-methyl-alpha-L-threo-pentopyranose-(1-2)-4-amino-4,6-dideoxy-beta-D-glucopyranose.
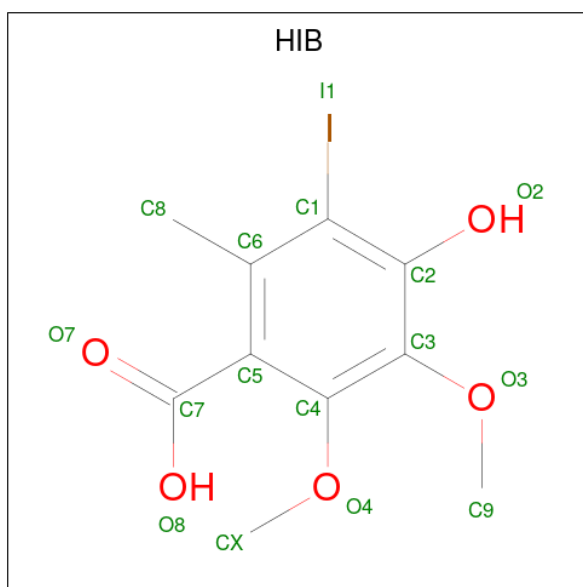
Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	2	25	14	3	2	6	0

- Molecule 3 is 2,6-dideoxy-4-thio-beta-D-allopyranose (three-letter code: DSR) (formula: $C_6H_{12}O_3S$).
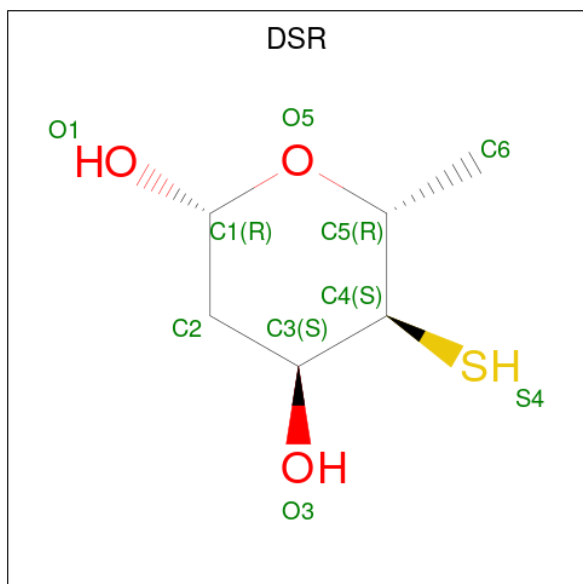
Mol	Chain	Residues	Atoms					
			Total	C	H	O	S	
3	A	1	11	6	1	3	1	

- Molecule 4 is 4-HYDROXY-5-IODO-2,3-DIMETHOXY-6-METHYLBENZOIC ACID (three-letter code: HIB) (formula: $C_{10}H_{11}IO_5$).

HIB

Mol	Chain	Residues	Atoms			
			Total	C	I	O
4	A	1	14	10	1	3

- Molecule 5 is 3-O-methyl-alpha-L-rhamnopyranose (three-letter code: MRP) (formula: $C_7H_{14}O_5$).

MRP
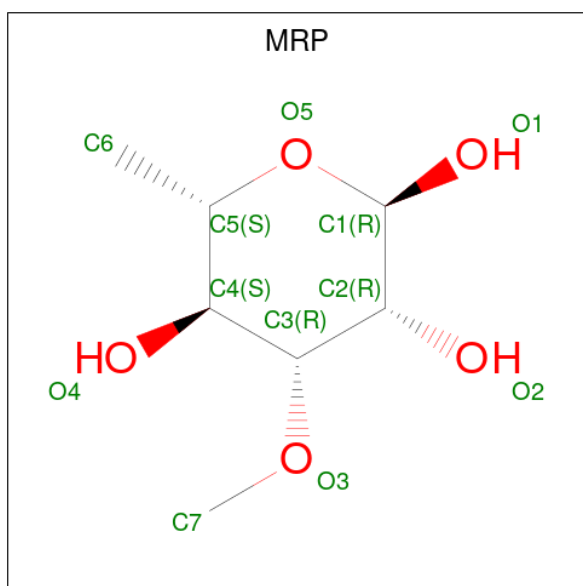
Mol	Chain	Residues	Atoms			
			Total	C	H	O
5	A	1	14	7	2	5

- Molecule 6 is [1,8-DIHYDROXY-11-OXO-13-(2-METHYLTRITHIO-ETHYLIDENE)-B ICYCLO[7.3.1]TRIDECA-4,9-DIENE-2,6-DIYN-10-YL]-CARBAMIC ACID METHYL

ESTER (three-letter code: MTC) (formula: $C_{18}H_{17}NO_4S_3$).
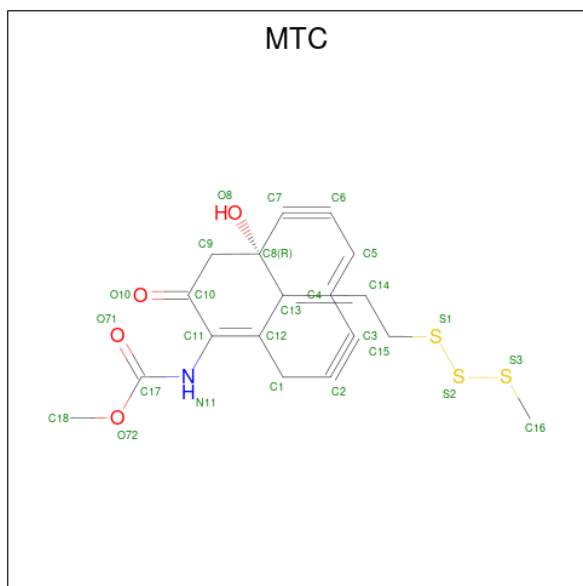
Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
6	A	1	28	18	2	1	4	3

4 Residue-property plots ⓘ

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: CalC
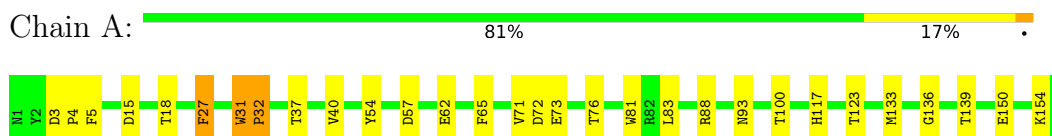
Chain A:

• Molecule 2: 2,4-dideoxy-4-(ethylamino)-3-O-methyl-alpha-L-threo-pentopyranose-(1-2)-4-amino -4,6-dideoxy-beta-D-glucopyranose

Chain B:
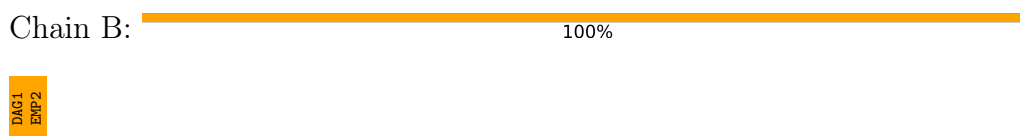
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

• Molecule 1: CalC
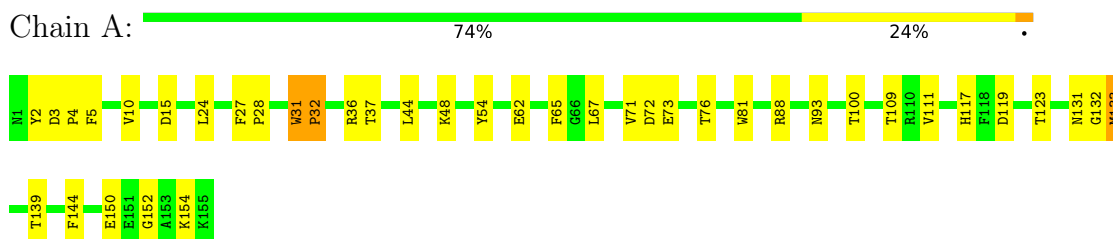
Chain A:

• Molecule 2: 2,4-dideoxy-4-(ethylamino)-3-O-methyl-alpha-L-threo-pentopyranose-(1-2)-4-amino -4,6-dideoxy-beta-D-glucopyranose

Chain B:

DAG1
EMP2

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing.*

Of the 200 calculated structures, 4 were deposited, based on the following criterion: *structures with the least restraint violations.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
HADDOCK	structure solution	2.1
HADDOCK	refinement	2.1

No chemical shift data was provided.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EMP, DSR, MTC, HIB, MRP, DAG

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1267	299	1225	18±6
2	B	22	3	26	10±1
3	A	10	1	10	7±1
4	A	14	0	9	13±2
5	A	12	2	13	8±5
6	A	26	2	17	8±1
All	All	5404	1228	5200	163

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 15.

5 of 142 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:65:PHE:CE1	5:A:637:MRP:H61	1.60	1.28	3	1
3:A:635:DSR:S4	4:A:636:HIB:C7	1.46	2.03	3	1
4:A:631:HIB:C2	5:A:632:MRP:O1	1.46	1.63	2	1
3:A:640:DSR:S4	4:A:641:HIB:C7	1.45	2.03	4	1
3:A:630:DSR:S4	4:A:631:HIB:C7	1.44	2.03	2	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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 NMR 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	A	153/155 (99%)	112±3 (73±2%)	32±4 (21±2%)	9±4 (6±2%)	3	20
All	All	612/620 (99%)	449 (73%)	126 (21%)	37 (6%)	3	20

5 of 19 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	73	GLU	4
1	A	117	HIS	4
1	A	31	TRP	3
1	A	32	PRO	3
1	A	123	THR	3

6.3.2 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 PDB entries followed by that with respect to all NMR 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	A	134/134 (100%)	115±1 (86±1%)	19±1 (14±1%)	6	45
All	All	536/536 (100%)	459 (86%)	77 (14%)	6	45

5 of 43 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	15	ASP	4
1	A	37	THR	4
1	A	54	TYR	4
1	A	71	VAL	4
1	A	81	TRP	4

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	DAG	B	1	6,2,3	10,11,11	0.53±0.00	0±0 (0±0%)
2	EMP	B	2	2	11,11,12	0.52±0.00	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	DAG	B	1	6,2,3	15,16,16	0.77±0.00	1±0 (6±0%)
2	EMP	B	2	2	11,13,15	1.27±0.00	2±0 (18±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.

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DAG	B	1	6,2,3	-	-	0±0,1,1,1
2	EMP	B	2	2	-	0±0,5,16,18	0±0,1,1,1

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models Worst	Total
2	B	2	EMP	C6-N4-C4	2.65	110.66	114.57	3	4
2	B	2	EMP	C2-C3-C4	2.40	108.17	111.31	3	4
2	B	1	DAG	C6-C5-C4	2.29	109.29	114.10	3	4

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	2	EMP	C1	1

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain B

Bond lengths

Bond angles

Torsions

Rings
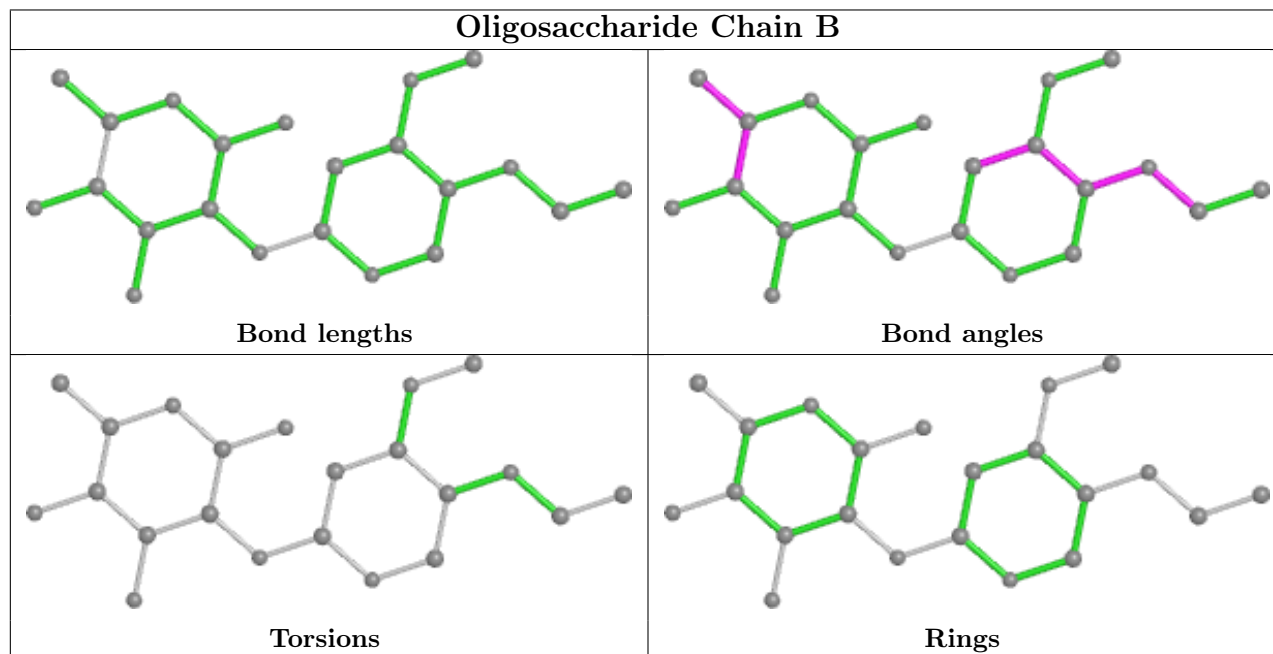
6.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	HIB	A	641	-	14,14,16	0.27±0.47	0±0 (1±3%)
4	HIB	A	631	-	14,14,16	0.27±0.46	0±0 (1±3%)
6	MTC	A	639	-	18,27,27	0.52±0.90	2±3 (8±14%)
3	DSR	A	640	-	7,10,10	0.18±0.31	0±0 (0±0%)
6	MTC	A	634	-	18,27,27	0.52±0.90	2±3 (8±14%)
5	MRP	A	642	-	12,12,12	0.13±0.23	0±0 (0±0%)
6	MTC	A	629	2	18,27,27	0.52±0.90	2±3 (8±14%)
3	DSR	A	630	-	7,10,10	0.18±0.31	0±0 (0±0%)
5	MRP	A	632	-	12,12,12	0.13±0.23	0±0 (0±0%)
5	MRP	A	637	-	12,12,12	0.13±0.23	0±0 (0±0%)
4	HIB	A	636	-	14,14,16	0.27±0.46	0±0 (1±3%)
4	HIB	A	626	5,3	14,14,16	0.27±0.46	0±0 (1±3%)
3	DSR	A	625	2,4	7,10,10	0.18±0.31	0±0 (0±0%)
3	DSR	A	635	-	7,10,10	0.18±0.31	0±0 (0±0%)
6	MTC	A	644	-	18,27,27	0.52±0.90	2±3 (8±14%)
5	MRP	A	627	4	12,12,12	0.13±0.23	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	HIB	A	641	-	17,19,23	0.52±0.89	1±2 (5±10%)
4	HIB	A	631	-	17,19,23	0.52±0.90	1±2 (5±10%)
6	MTC	A	639	-	14,36,36	0.82±1.42	2±3 (10±18%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	DSR	A	640	-	7,14,14	0.29±0.50	0±0 (3±6%)
6	MTC	A	634	-	14,36,36	0.82±1.43	2±3 (10±18%)
5	MRP	A	642	-	16,17,17	0.22±0.38	0±0 (0±0%)
6	MTC	A	629	2	14,36,36	0.82±1.43	2±3 (10±18%)
3	DSR	A	630	-	7,14,14	0.29±0.50	0±0 (3±6%)
5	MRP	A	632	-	16,17,17	0.22±0.38	0±0 (0±0%)
5	MRP	A	637	-	16,17,17	0.22±0.38	0±0 (0±0%)
4	HIB	A	636	-	17,19,23	0.52±0.90	1±2 (5±10%)
4	HIB	A	626	5,3	17,19,23	0.52±0.90	1±2 (5±10%)
3	DSR	A	625	2,4	7,14,14	0.29±0.50	0±0 (3±6%)
3	DSR	A	635	-	7,14,14	0.29±0.50	0±0 (3±6%)
6	MTC	A	644	-	14,36,36	0.82±1.42	2±3 (10±18%)
5	MRP	A	627	4	16,17,17	0.22±0.38	0±0 (0±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
6	MTC	A	629	2	-	0±0,17,46,46	0±0,1,2,2
4	HIB	A	626	5,3	-	0±0,6,6,8	0±0,1,1,1
3	DSR	A	625	2,4	-	-	0±0,1,1,1
5	MRP	A	627	4	-	0±0,2,22,22	0±0,1,1,1

5 of 28 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
6	A	634	MTC	C3-C2	4.41	1.22	1.19	2	1
6	A	644	MTC	C3-C2	4.39	1.22	1.19	4	1
6	A	639	MTC	C3-C2	4.35	1.22	1.19	3	1
6	A	629	MTC	C3-C2	4.35	1.22	1.19	1	1
6	A	634	MTC	C12-C13	4.15	1.39	1.46	2	1

5 of 44 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.
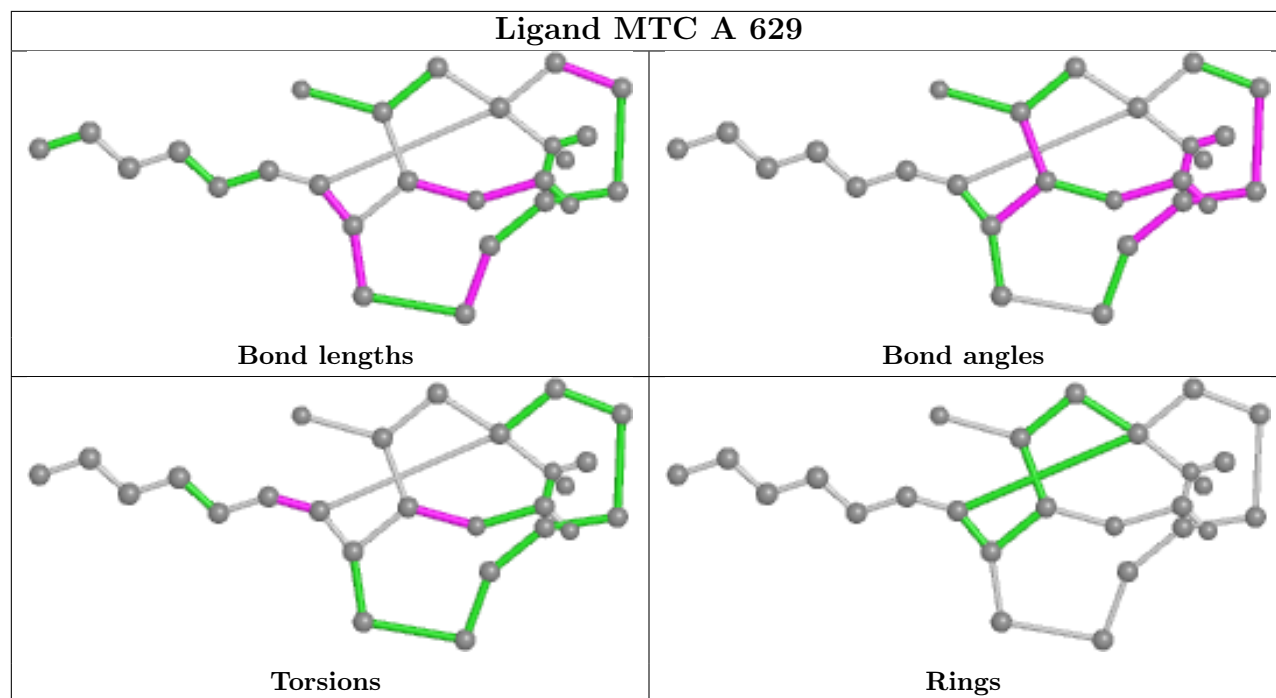
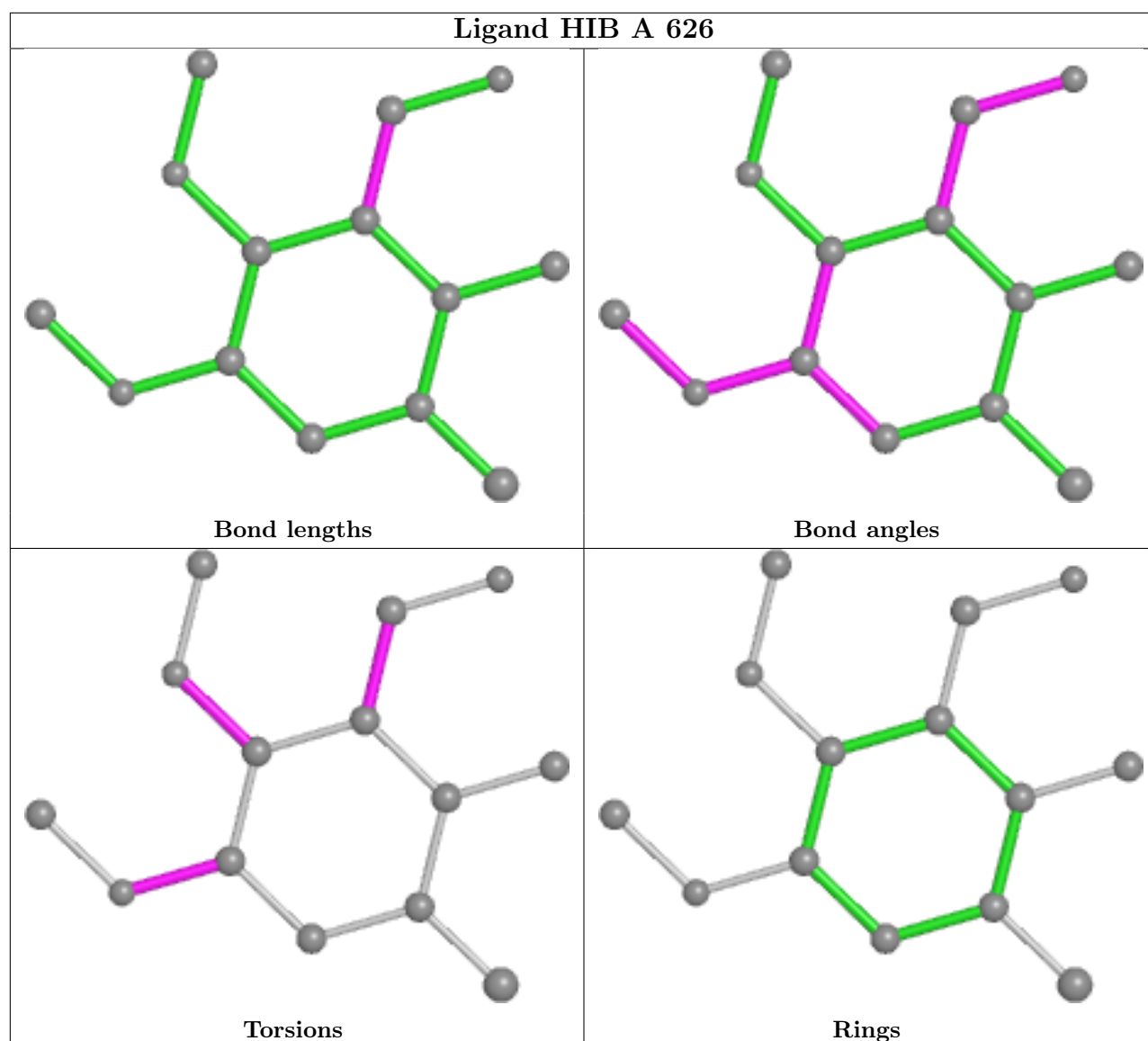| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models Worst	Total
6	A	634	MTC	O72-C17-N11	8.07	117.70	109.15	2	1
6	A	629	MTC	O72-C17-N11	8.04	117.67	109.15	1	1
6	A	639	MTC	O72-C17-N11	8.03	117.66	109.15	3	1
6	A	644	MTC	O72-C17-N11	8.02	117.65	109.15	4	1
4	A	636	HIB	C9-O3-C3	5.42	109.35	117.53	3	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 then 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 MTC A 629

Bond lengths

Bond angles

Torsions

Rings

Ligand HIB A 626

Bond lengths

Bond angles

Torsions

Rings

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

No chemical shift data were provided