Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2026 – 07:26 PM UTC

PDB ID	:	2L61 / pdb_00002l61
Title	:	Protein and metal cluster structure of the wheat metallothionein domain g-Ec-1. The second part of the puzzle.
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Deposited on	:	2010-11-12

This is a Full wwPDB NMR 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/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.

The following versions of software and data (see references (i)) were used in the production of this report:

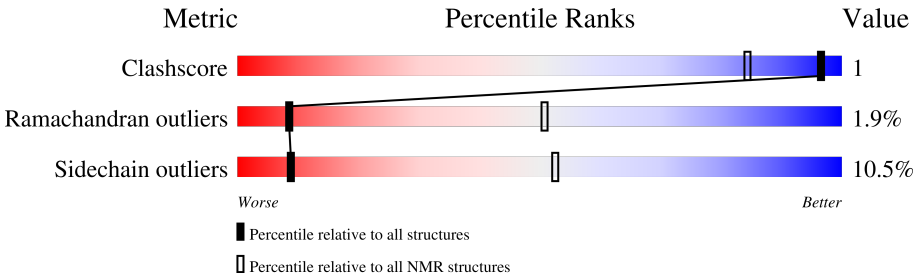
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	26	77% 23%

2 Ensemble composition and analysis (i)

This entry contains 40 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:4-A:23 (20)	1.15	11

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 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19
2	23, 24, 27, 30, 31, 32, 36, 37, 38, 39, 40
3	21, 22, 25, 26, 28, 29, 33, 34, 35
Single-model clusters	20

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 312 atoms, of which 146 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called EC protein I/II.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	26	310	91	146	33	34	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P30569
A	2	SER	-	expression tag	UNP P30569

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	
			Total	Cd
2	A	2	2	2

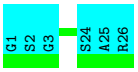
4 Residue-property plots

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: EC protein I/II

Chain A: 



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: EC protein I/II

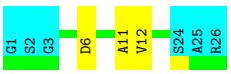
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: EC protein I/II

Chain A: 



4.2.3 Score per residue for model 3

• Molecule 1: EC protein I/II

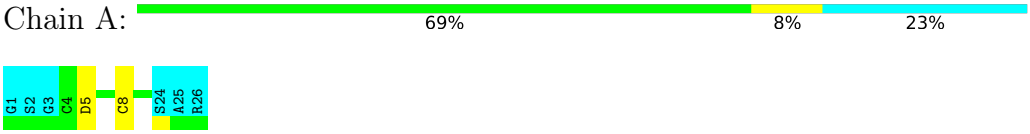
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: EC protein I/II

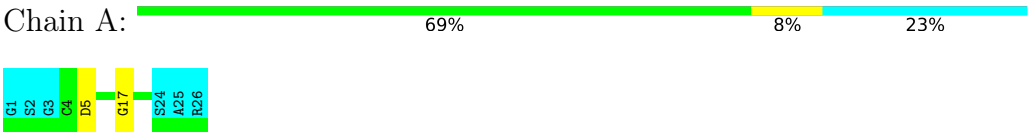
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: EC protein I/II

Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: EC protein I/II

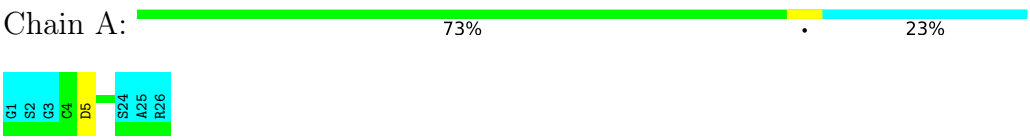
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: EC protein I/II

Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: EC protein I/II

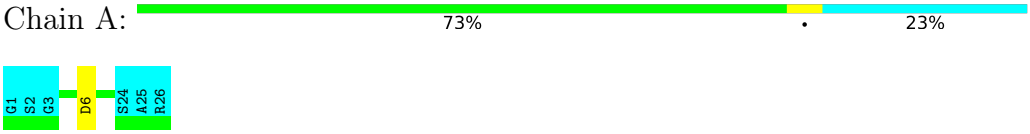
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: EC protein I/II

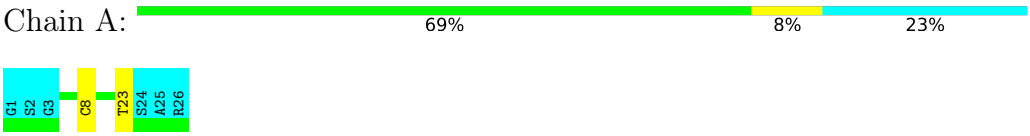
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: EC protein I/II

Chain A:



4.2.11 Score per residue for model 11 (medoid)

• Molecule 1: EC protein I/II

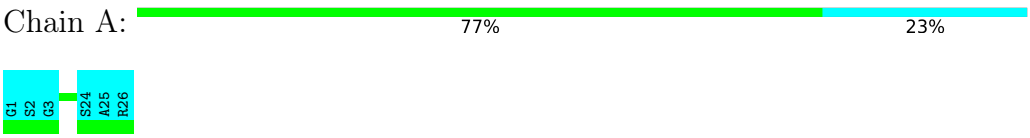
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: EC protein I/II

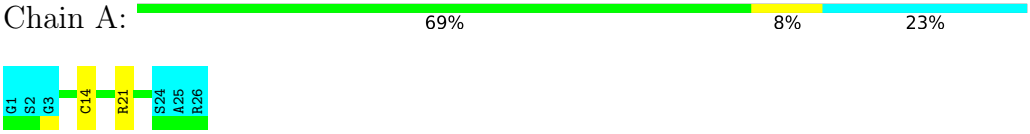
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: EC protein I/II

Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: EC protein I/II

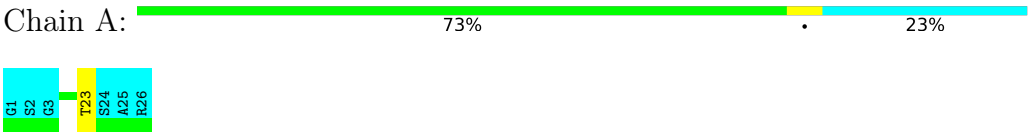
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: EC protein I/II

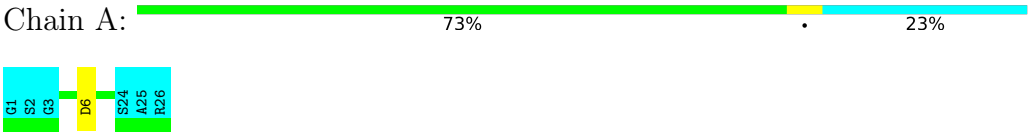
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: EC protein I/II

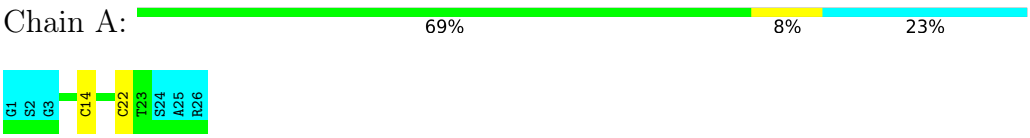
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: EC protein I/II

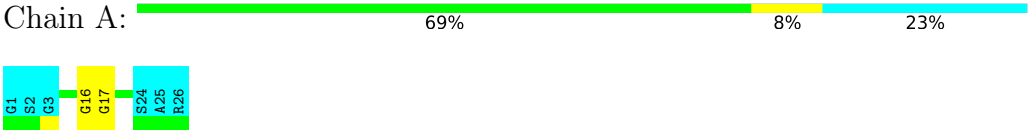
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: EC protein I/II

Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: EC protein I/II

Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: EC protein I/II

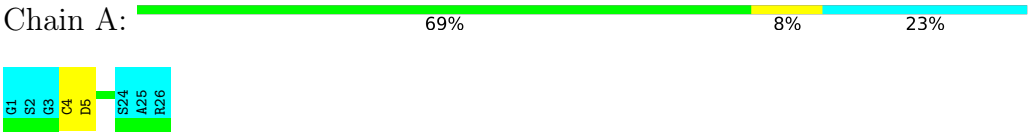
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: EC protein I/II

Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: EC protein I/II

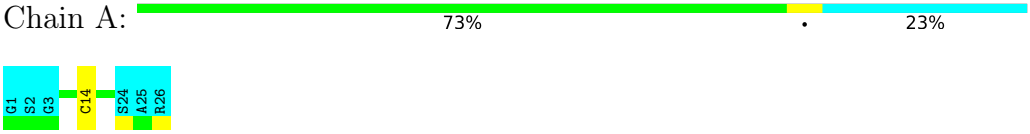
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: EC protein I/II

Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: EC protein I/II

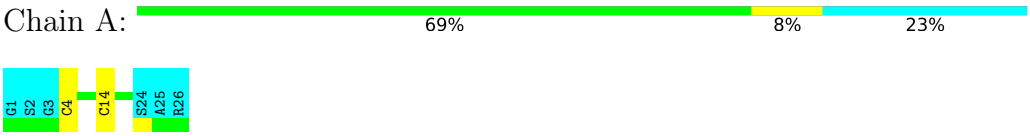
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: EC protein I/II

Chain A:



4.2.26 Score per residue for model 26

• Molecule 1: EC protein I/II

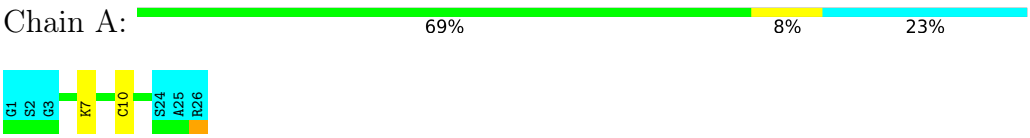
Chain A:



4.2.27 Score per residue for model 27

• Molecule 1: EC protein I/II

Chain A:



4.2.28 Score per residue for model 28

• Molecule 1: EC protein I/II

Chain A:



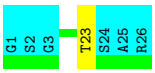


4.2.29 Score per residue for model 29

• Molecule 1: EC protein I/II

Chain A:



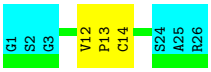


4.2.30 Score per residue for model 30

• Molecule 1: EC protein I/II

Chain A:



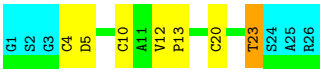


4.2.31 Score per residue for model 31

• Molecule 1: EC protein I/II

Chain A:





4.2.32 Score per residue for model 32

• Molecule 1: EC protein I/II

Chain A:

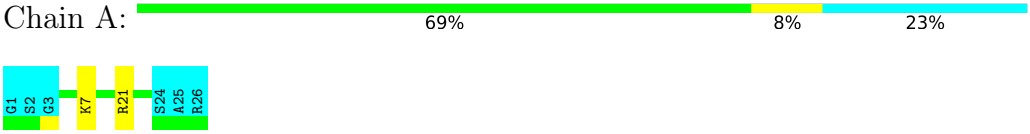




4.2.33 Score per residue for model 33

• Molecule 1: EC protein I/II

Chain A:



4.2.34 Score per residue for model 34

• Molecule 1: EC protein I/II

Chain A:



4.2.35 Score per residue for model 35

• Molecule 1: EC protein I/II

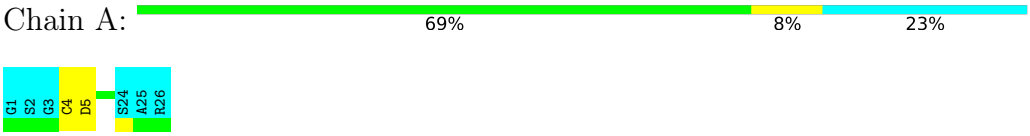
Chain A:



4.2.36 Score per residue for model 36

• Molecule 1: EC protein I/II

Chain A:



4.2.37 Score per residue for model 37

• Molecule 1: EC protein I/II

Chain A:



4.2.38 Score per residue for model 38

• Molecule 1: EC protein I/II

Chain A:



4.2.39 Score per residue for model 39

• Molecule 1: EC protein I/II

Chain A:



4.2.40 Score per residue for model 40

• Molecule 1: EC protein I/II

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 200 calculated structures, 40 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
CYANA 3.0, OPALP	refinement	
CYANA	structure solution	3.0

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

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 (average) 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	0.66±0.04	0±0/130 (0.0± 0.0%)	1.63±0.15	1±1/176 (0.7± 0.8%)
All	All	0.66	0/5200 (0.0%)	1.63	48/7040 (0.7%)

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	Planarity
1	A	0.0±0.0	0.0±0.2
All	All	0	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
1	A	20	CYS	CB-CA-C	7.09	121.24	109.89	3	1
1	A	17	GLY	CA-C-N	7.07	129.63	120.44	19	4
1	A	17	GLY	C-N-CA	7.07	129.63	120.44	19	4
1	A	11	ALA	N-CA-C	-6.93	100.72	110.50	24	5
1	A	20	CYS	CA-C-N	6.84	132.80	122.95	8	2
1	A	20	CYS	C-N-CA	6.84	132.80	122.95	8	2
1	A	5	ASP	CA-C-N	6.19	132.90	121.52	4	3
1	A	5	ASP	C-N-CA	6.19	132.90	121.52	4	3
1	A	11	ALA	CA-C-N	6.06	125.17	120.33	6	3
1	A	11	ALA	C-N-CA	6.06	125.17	120.33	6	3
1	A	23	THR	CB-CA-C	5.92	118.56	111.22	14	1
1	A	18	THR	N-CA-C	5.92	117.40	111.07	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	21	ARG	CB-CA-C	5.75	120.02	111.17	8	1
1	A	22	CYS	CA-CB-SG	5.70	127.50	114.40	40	1
1	A	13	PRO	CA-C-N	5.44	128.40	120.51	6	1
1	A	13	PRO	C-N-CA	5.44	128.40	120.51	6	1
1	A	23	THR	N-CA-C	-5.38	102.16	109.54	29	1
1	A	22	CYS	CA-C-N	5.30	127.92	120.28	39	1
1	A	22	CYS	C-N-CA	5.30	127.92	120.28	39	1
1	A	6	ASP	CA-C-N	5.28	127.62	120.38	16	1
1	A	6	ASP	C-N-CA	5.28	127.62	120.38	16	1
1	A	23	THR	CA-CB-CG2	5.24	119.42	110.50	31	1
1	A	7	LYS	N-CA-C	-5.17	107.10	113.41	34	1
1	A	21	ARG	CA-C-N	5.16	127.91	120.38	1	1
1	A	21	ARG	C-N-CA	5.16	127.91	120.38	1	1
1	A	4	CYS	CB-CA-C	-5.02	101.99	110.43	37	1
1	A	10	CYS	CB-CA-C	-5.01	101.48	109.75	27	1
1	A	12	VAL	CA-C-O	-5.01	115.34	118.69	2	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	21	ARG	Sidechain	1

6.2 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 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	128	112	112	0±0
All	All	5200	4480	4480	8

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 1.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:VAL:HA	1:A:13:PRO:C	0.45	2.37	26	7
1:A:10:CYS:HB3	1:A:14:CYS:SG	0.41	2.55	34	1

6.3 Torsion angles (i)

6.3.1 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 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	20/26 (77%)	17±2 (85±9%)	3±2 (13±8%)	0±1 (2±3%)	8	51
All	All	800/1040 (77%)	679 (85%)	106 (13%)	15 (2%)	8	51

All 5 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	17	GLY	6
1	A	16	GLY	5
1	A	23	THR	2
1	A	22	CYS	1
1	A	18	THR	1

6.3.2 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 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	15/18 (83%)	13±1 (90±7%)	2±1 (10±7%)	9	52
All	All	600/720 (83%)	537 (90%)	63 (10%)	9	52

All 13 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	4	CYS	11
1	A	14	CYS	10
1	A	6	ASP	7
1	A	23	THR	7
1	A	5	ASP	6
1	A	18	THR	4
1	A	10	CYS	4
1	A	20	CYS	3
1	A	8	CYS	3
1	A	21	ARG	3
1	A	22	CYS	2
1	A	7	LYS	2
1	A	12	VAL	1

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

There are no oligosaccharides in this entry.

6.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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