



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1U2N / pdb_00001u2n
Title : Structure CBP TAZ1 Domain
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Deposited on : 2004-07-19

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 ⓘ 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
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

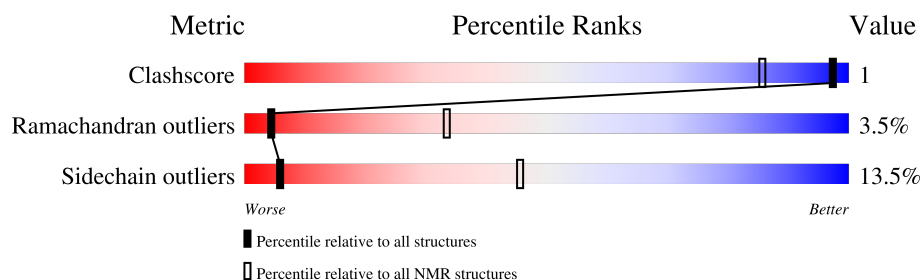
1 Overall quality at a glance

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	100	

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:347-A:372, A:381-A:432 (78)	0.70	6

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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 5, 6, 11, 12, 15, 16, 18, 20
2	2, 13, 14
3	7, 8
4	9, 10
Single-model clusters	17; 19

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1569 atoms, of which 785 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CREB binding protein.

Mol	Chain	Residues	Atoms						Trace
1	A	100	Total	C	H	N	O	S	0
			1566	472	785	162	136	11	

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

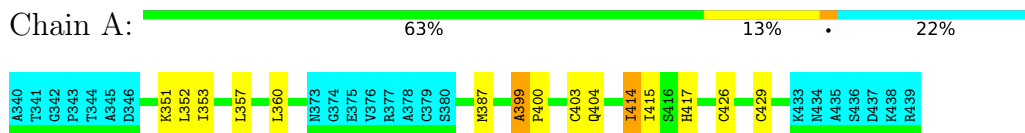
Mol	Chain	Residues	Atoms	
2	A	3	Total	Zn
			3	3

4 Residue-property plots [i](#)

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: CREB binding protein

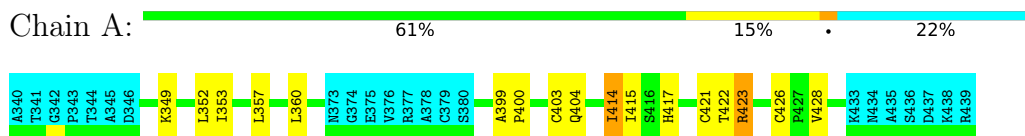


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

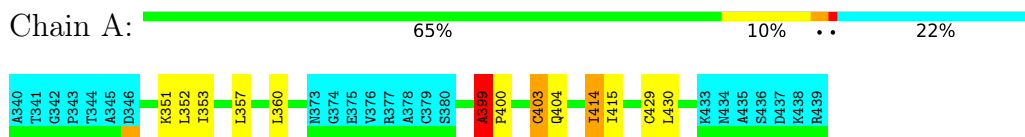
4.2.1 Score per residue for model 1

- Molecule 1: CREB binding protein



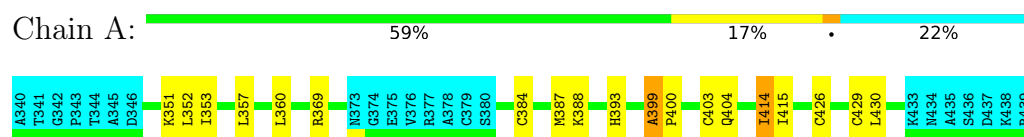
4.2.2 Score per residue for model 2

- Molecule 1: CREB binding protein



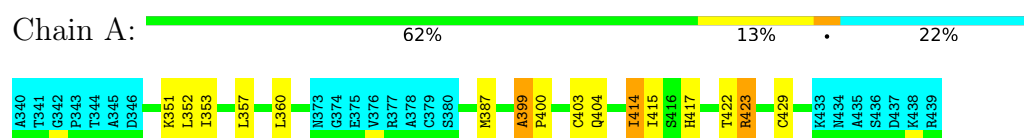
4.2.3 Score per residue for model 3

- Molecule 1: CREB binding protein



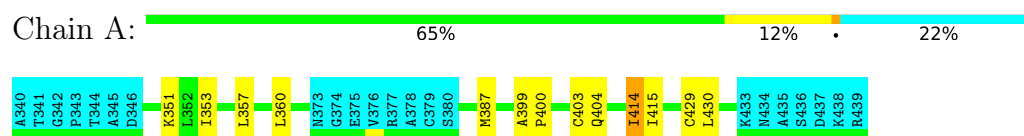
4.2.4 Score per residue for model 4

- Molecule 1: CREB binding protein



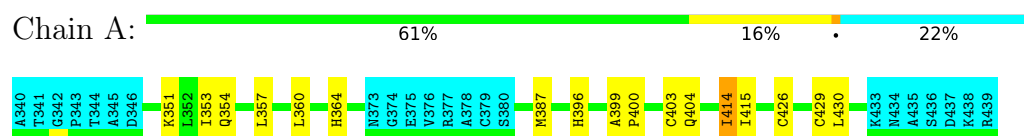
4.2.5 Score per residue for model 5

- Molecule 1: CREB binding protein



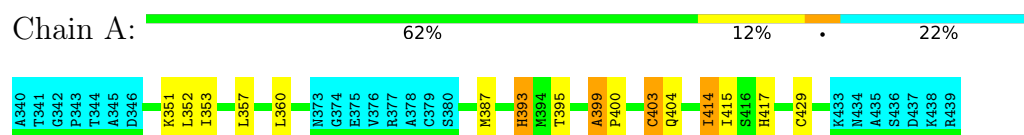
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: CREB binding protein



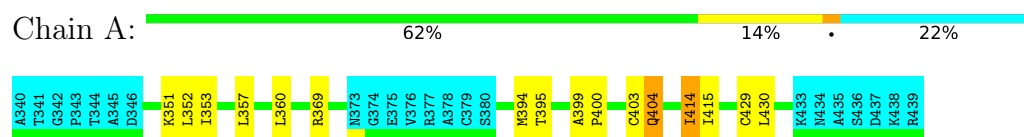
4.2.7 Score per residue for model 7

- Molecule 1: CREB binding protein



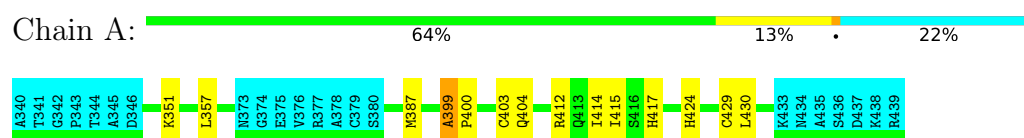
4.2.8 Score per residue for model 8

- Molecule 1: CREB binding protein



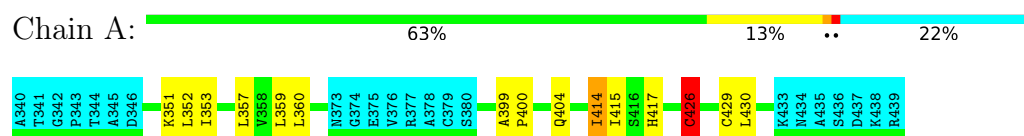
4.2.9 Score per residue for model 9

- Molecule 1: CREB binding protein



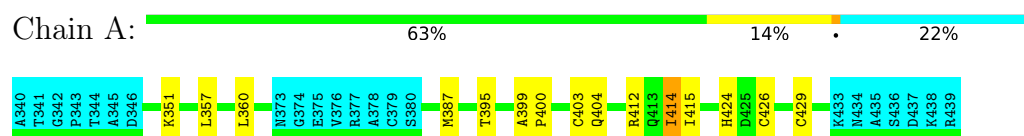
4.2.10 Score per residue for model 10

- Molecule 1: CREB binding protein



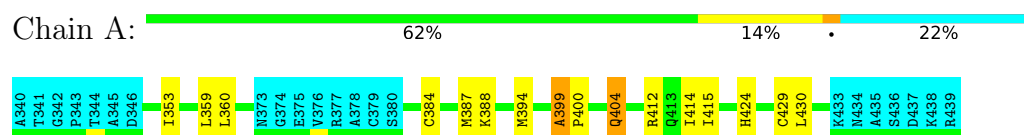
4.2.11 Score per residue for model 11

- Molecule 1: CREB binding protein



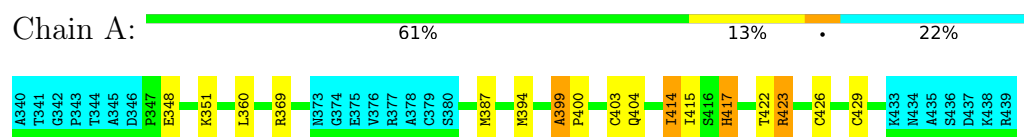
4.2.12 Score per residue for model 12

- Molecule 1: CREB binding protein



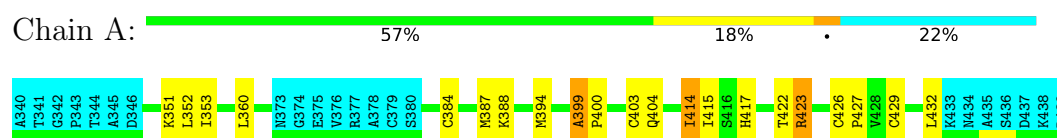
4.2.13 Score per residue for model 13

- Molecule 1: CREB binding protein



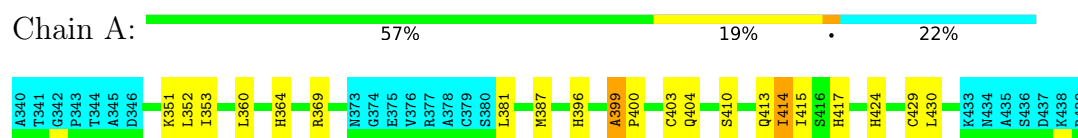
4.2.14 Score per residue for model 14

- Molecule 1: CREB binding protein



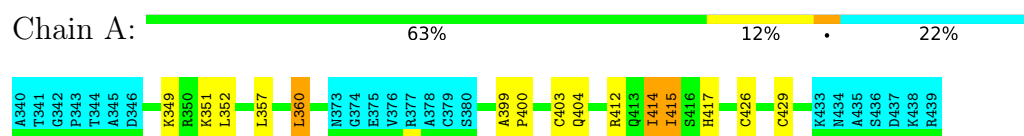
4.2.15 Score per residue for model 15

- Molecule 1: CREB binding protein



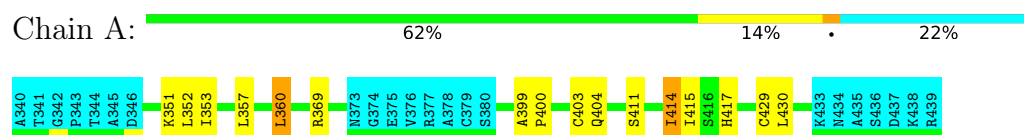
4.2.16 Score per residue for model 16

- Molecule 1: CREB binding protein



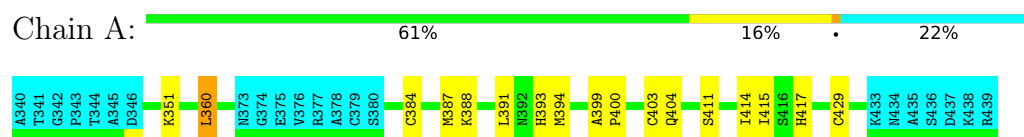
4.2.17 Score per residue for model 17

- Molecule 1: CREB binding protein



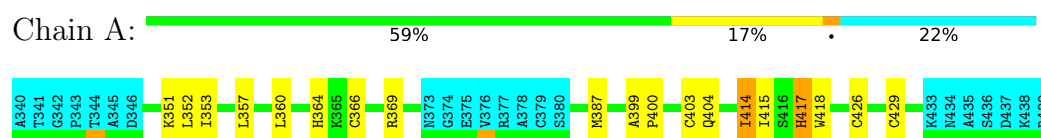
4.2.18 Score per residue for model 18

- Molecule 1: CREB binding protein



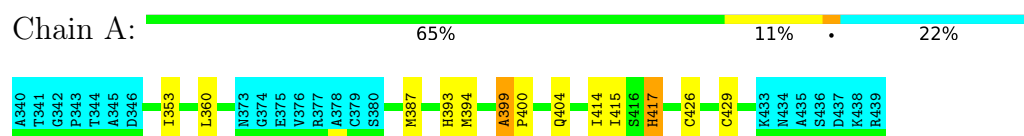
4.2.19 Score per residue for model 19

- Molecule 1: CREB binding protein



4.2.20 Score per residue for model 20

- Molecule 1: CREB binding protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics by DYANA, simulated annealing and molecular dynamics by AMBER.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
DYANA	structure solution	1.5
Amber	refinement	7

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: ZN

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	0.92±0.01	0±0/639 (0.0± 0.0%)	1.73±0.04	8±3/861 (0.9± 0.3%)
All	All	0.92	0/12780 (0.0%)	1.73	152/17220 (0.9%)

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	0.1±0.2	0.7±0.5
All	All	1	13

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	422	THR	CA-C-N	9.05	138.82	121.54	1	4
1	A	422	THR	C-N-CA	9.05	138.82	121.54	1	4
1	A	426	CYS	CB-CA-C	9.00	121.56	108.87	13	4
1	A	403	CYS	CA-C-N	8.11	137.03	121.54	7	17
1	A	403	CYS	C-N-CA	8.11	137.03	121.54	7	17
1	A	399	ALA	CA-C-N	6.89	128.45	119.84	10	20
1	A	399	ALA	C-N-CA	6.89	128.45	119.84	10	20
1	A	426	CYS	CA-C-N	6.50	126.19	119.56	13	9
1	A	426	CYS	C-N-CA	6.50	126.19	119.56	13	9
1	A	414	ILE	CA-CB-CG1	6.47	121.40	110.40	14	16
1	A	428	VAL	CA-C-N	6.14	128.43	120.44	1	1
1	A	428	VAL	C-N-CA	6.14	128.43	120.44	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	423	ARG	N-CA-C	5.95	123.48	110.80	4	4
1	A	414	ILE	N-CA-C	5.81	115.99	110.53	2	4
1	A	359	LEU	CA-C-N	5.53	127.95	120.44	12	1
1	A	359	LEU	C-N-CA	5.53	127.95	120.44	12	1
1	A	396	HIS	CA-C-N	5.38	128.87	120.75	6	2
1	A	396	HIS	C-N-CA	5.38	128.87	120.75	6	2
1	A	417	HIS	CB-CG-CD2	-5.31	124.30	131.20	20	4
1	A	393	HIS	CB-CG-CD2	-5.26	124.36	131.20	18	3
1	A	366	CYS	CB-CA-C	5.15	119.60	110.85	19	1
1	A	364	HIS	CA-C-N	5.10	127.42	120.54	15	3
1	A	364	HIS	C-N-CA	5.10	127.42	120.54	15	3
1	A	410	SER	CA-C-N	5.06	127.37	120.54	15	1
1	A	410	SER	C-N-CA	5.06	127.37	120.54	15	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	421	CYS	CA	1

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	417	HIS	Sidechain	12
1	A	393	HIS	Sidechain	1

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	625	635	632	1±1
All	All	12560	12700	12640	14

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:399:ALA:HB3	1:A:403:CYS:HB2	0.67	1.67	2	2
1:A:360:LEU:HD23	1:A:415:ILE:HD13	0.55	1.77	17	1
1:A:384:CYS:SG	1:A:388:LYS:HE3	0.48	2.48	18	4
1:A:360:LEU:HD21	1:A:411:SER:HB2	0.44	1.90	18	2
1:A:357:LEU:C	1:A:357:LEU:HD23	0.43	2.38	16	2
1:A:360:LEU:HD23	1:A:415:ILE:HG13	0.41	1.92	16	1
1:A:357:LEU:HD11	1:A:418:TRP:CE3	0.41	2.51	19	1
1:A:426:CYS:HB3	1:A:429:CYS:HB2	0.40	1.93	10	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	78/100 (78%)	69±1 (88±2%)	6±2 (8±2%)	3±1 (4±1%)	4	33
All	All	1560/2000 (78%)	1379 (88%)	126 (8%)	55 (4%)	4	33

All 6 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	400	PRO	20
1	A	404	GLN	20
1	A	399	ALA	9
1	A	423	ARG	4
1	A	424	HIS	1
1	A	427	PRO	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	71/88 (81%)	61±2 (87±2%)	10±2 (13±2%)	6	45
All	All	1420/1760 (81%)	1229 (87%)	191 (13%)	6	45

All 27 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	414	ILE	20
1	A	360	LEU	19
1	A	415	ILE	19
1	A	429	CYS	18
1	A	351	LYS	17
1	A	353	ILE	15
1	A	387	MET	14
1	A	352	LEU	12
1	A	357	LEU	11
1	A	430	LEU	10
1	A	369	ARG	6
1	A	394	MET	6
1	A	412	ARG	4
1	A	395	THR	3
1	A	424	HIS	3
1	A	349	LYS	2
1	A	404	GLN	2
1	A	421	CYS	1
1	A	354	GLN	1
1	A	393	HIS	1
1	A	359	LEU	1
1	A	426	CYS	1
1	A	348	GLU	1
1	A	432	LEU	1
1	A	381	LEU	1
1	A	413	GLN	1
1	A	391	LEU	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 [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided