



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 04:47 AM BST

PDB ID : 2NZZ
Title : NMR structure analysis of the Penetratin conjugated Gas (374-394) peptide
Authors : D'Ursi, A.M.; Rovero, P.; Albrizio, S.; Espsito, C.; D'Errico, G.; Novellino, E.
Deposited on : 2006-11-27

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

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

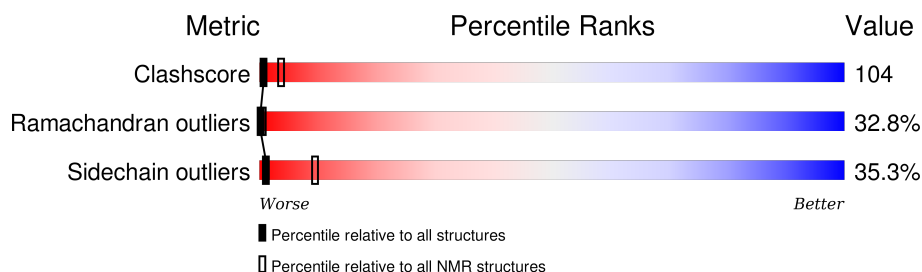
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	37	

2 Ensemble composition and analysis

This entry contains 30 models. Model 4 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:17-A:37 (21)	0.56	4

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 5 clusters and 8 single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 5, 7, 8, 11, 12, 16, 17, 21, 25, 29
2	14, 19, 26
3	13, 18
4	15, 24
5	6, 9
Single-model clusters	3; 10; 20; 22; 23; 27; 28; 30

3 Entry composition [i](#)

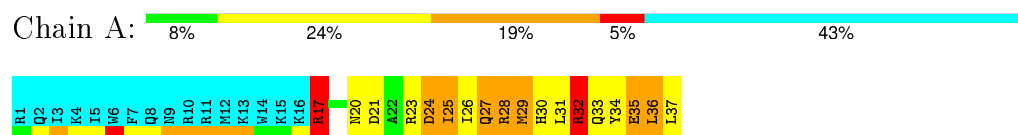
There is only 1 type of molecule in this entry. The entry contains 702 atoms, of which 356 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Penetratin conjugated Gas (374-394) peptide.

Mol	Chain	Residues	Atoms						Trace
1	A	37	Total	C	H	N	O	S	0
			702	222	356	72	50	2	

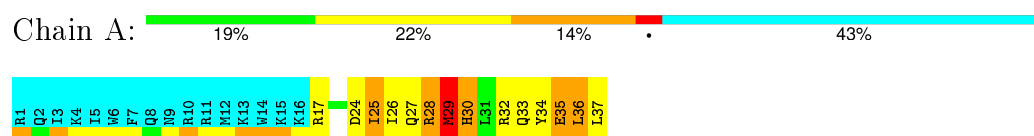
4.2.3 Score per residue for model 3

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



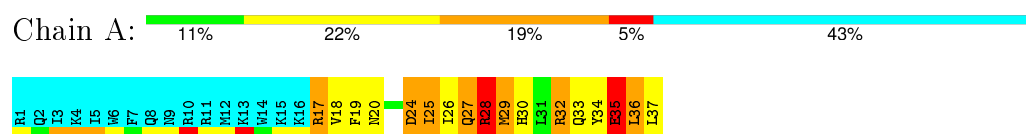
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



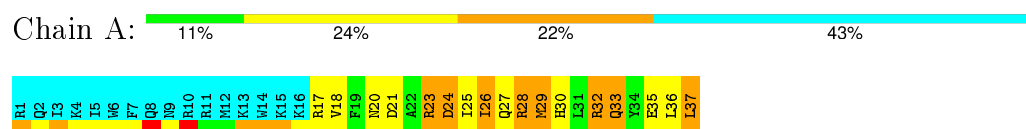
4.2.5 Score per residue for model 5

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



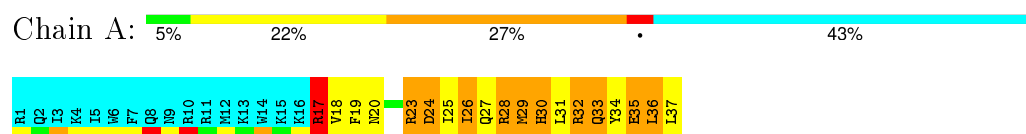
4.2.6 Score per residue for model 6

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



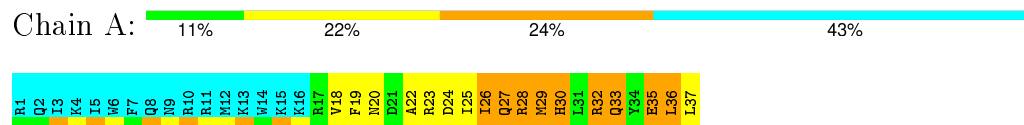
4.2.7 Score per residue for model 7

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



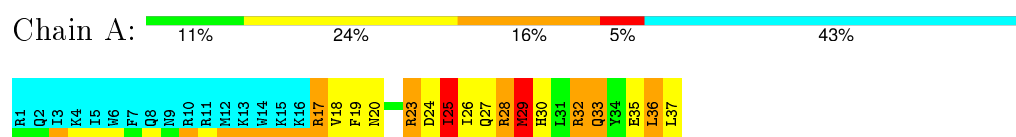
4.2.8 Score per residue for model 8

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



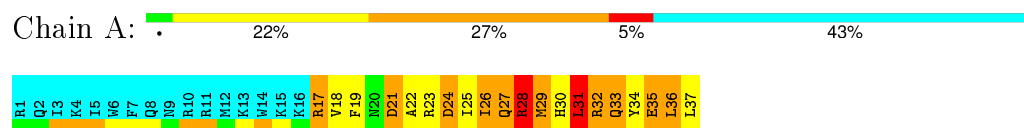
4.2.9 Score per residue for model 9

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



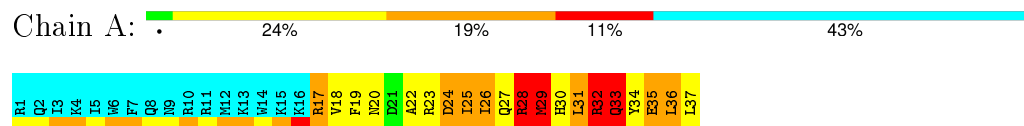
4.2.10 Score per residue for model 10

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



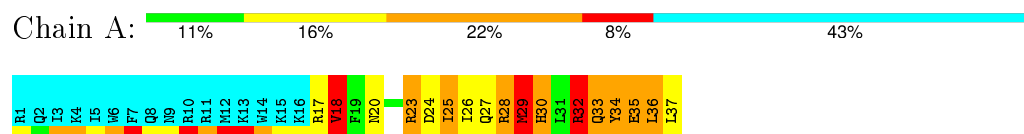
4.2.11 Score per residue for model 11

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



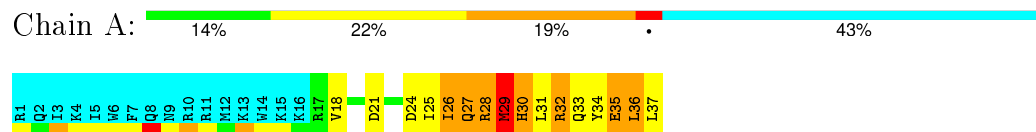
4.2.12 Score per residue for model 12

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



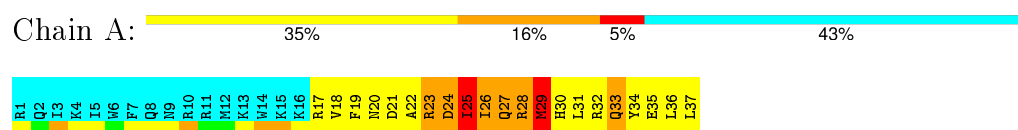
4.2.13 Score per residue for model 13

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



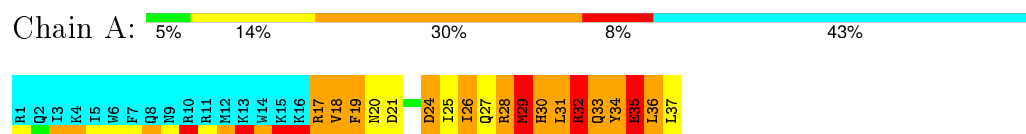
4.2.14 Score per residue for model 14

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



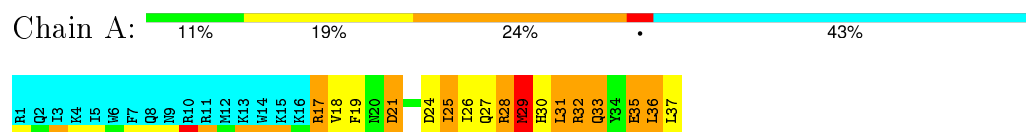
4.2.15 Score per residue for model 15

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



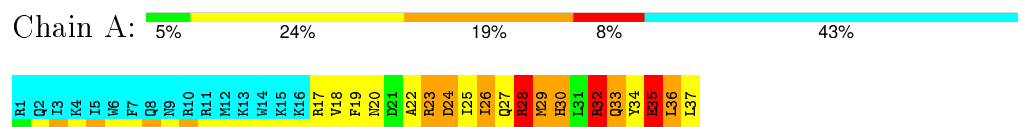
4.2.16 Score per residue for model 16

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



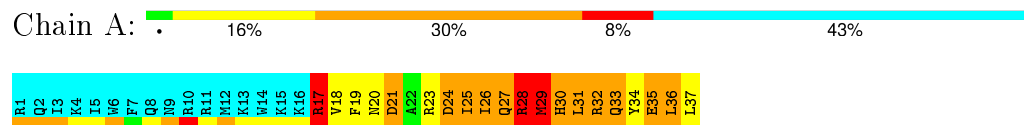
4.2.17 Score per residue for model 17

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



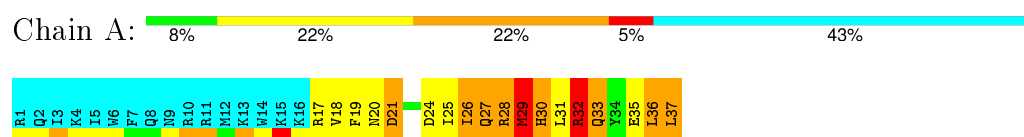
4.2.18 Score per residue for model 18

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



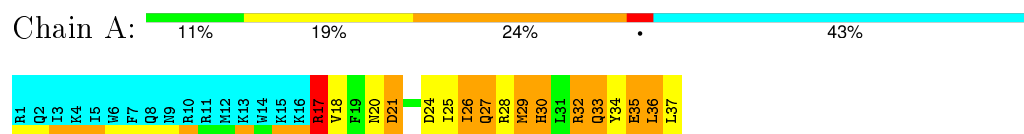
4.2.19 Score per residue for model 19

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



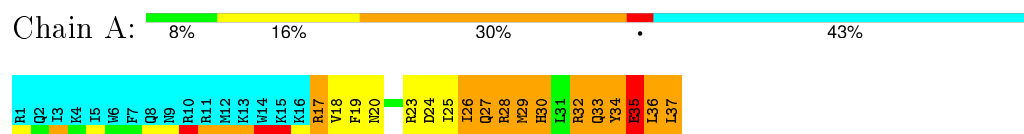
4.2.20 Score per residue for model 20

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



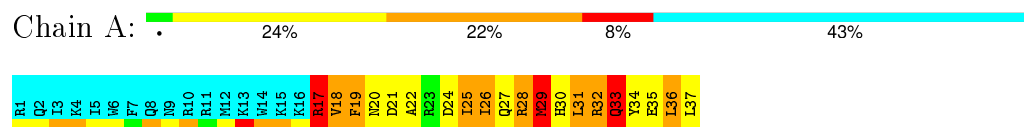
4.2.21 Score per residue for model 21

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



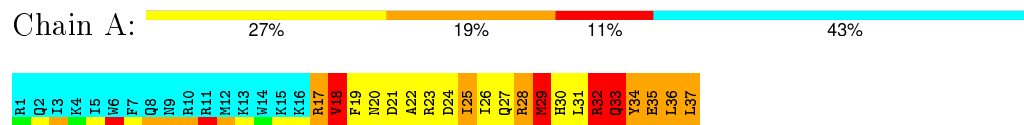
4.2.22 Score per residue for model 22

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



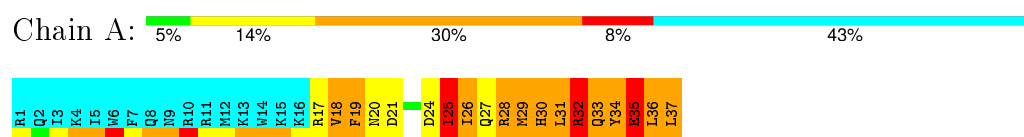
4.2.23 Score per residue for model 23

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



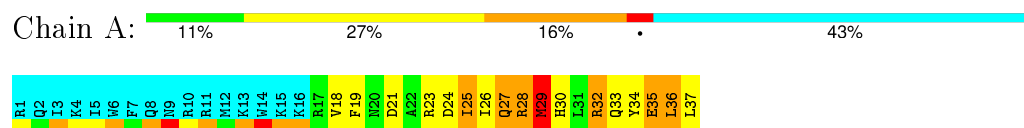
4.2.24 Score per residue for model 24

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



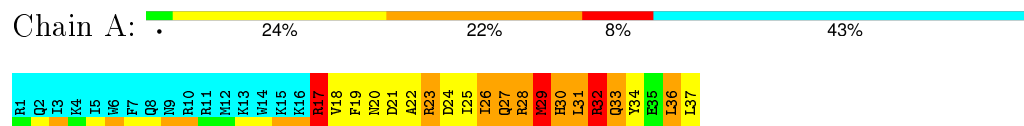
4.2.25 Score per residue for model 25

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



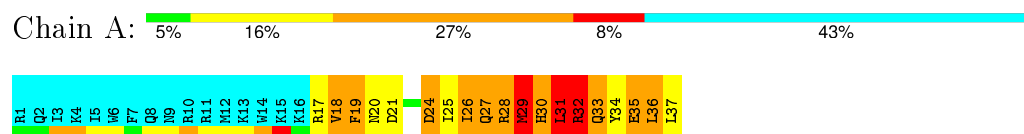
4.2.26 Score per residue for model 26

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



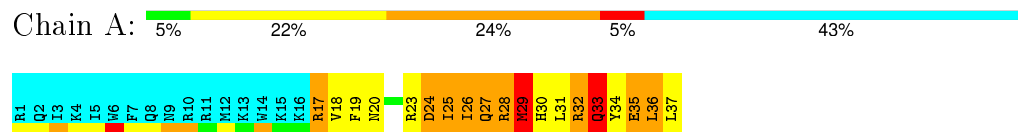
4.2.27 Score per residue for model 27

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



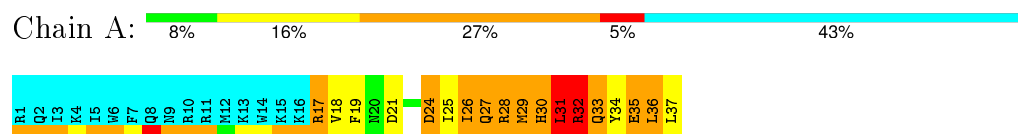
4.2.28 Score per residue for model 28

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



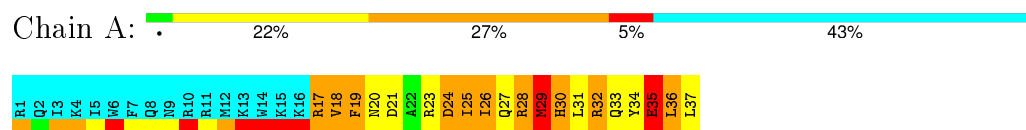
4.2.29 Score per residue for model 29

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



4.2.30 Score per residue for model 30

- Molecule 1: Penetratin conjugated Gas (374-394) peptide



5 Refinement protocol and experimental data overview ⓘ

Of the 30 calculated structures, 30 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
DYANA	refinement	1.5

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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	188	190	191	39±8
All	All	5640	5700	5730	1180

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 104.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ILE:HD13	1:A:29:MET:SD	0.95	2.02	17	10
1:A:36:LEU:O	1:A:36:LEU:HD22	0.94	1.62	9	6
1:A:36:LEU:HD22	1:A:36:LEU:O	0.93	1.62	28	4
1:A:25:ILE:O	1:A:26:ILE:HD13	0.93	1.63	16	14
1:A:28:ARG:O	1:A:30:HIS:N	0.89	2.04	28	30
1:A:26:ILE:H	1:A:30:HIS:CE1	0.87	1.86	20	1
1:A:25:ILE:HG22	1:A:26:ILE:HD12	0.86	1.47	20	10
1:A:26:ILE:O	1:A:26:ILE:HG22	0.86	1.71	29	13
1:A:24:ASP:O	1:A:25:ILE:HD13	0.85	1.71	21	18
1:A:26:ILE:HG22	1:A:26:ILE:O	0.85	1.71	21	8
1:A:25:ILE:HG22	1:A:26:ILE:HG12	0.83	1.49	12	6
1:A:30:HIS:N	1:A:30:HIS:HD1	0.83	1.71	20	1
1:A:36:LEU:HD13	1:A:37:LEU:N	0.82	1.90	5	12
1:A:25:ILE:HG22	1:A:26:ILE:CD1	0.81	2.05	20	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ALA:HB2	1:A:27:GLN:OE1	0.81	1.74	11	2
1:A:25:ILE:O	1:A:26:ILE:HD12	0.81	1.75	17	11
1:A:24:ASP:C	1:A:25:ILE:HD12	0.81	1.95	25	6
1:A:31:LEU:HD13	1:A:31:LEU:C	0.78	1.98	27	1
1:A:25:ILE:C	1:A:26:ILE:HD12	0.77	1.99	20	11
1:A:30:HIS:N	1:A:30:HIS:ND1	0.77	2.32	20	2
1:A:27:GLN:HA	1:A:30:HIS:CE1	0.77	2.15	13	13
1:A:26:ILE:CG2	1:A:26:ILE:O	0.76	2.34	17	9
1:A:33:GLN:HE21	1:A:33:GLN:N	0.75	1.79	7	7
1:A:36:LEU:HD22	1:A:37:LEU:N	0.74	1.98	3	7
1:A:27:GLN:N	1:A:30:HIS:CE1	0.74	2.56	26	8
1:A:33:GLN:N	1:A:33:GLN:HE21	0.74	1.81	9	11
1:A:30:HIS:NE2	1:A:31:LEU:HD12	0.73	1.98	16	1
1:A:26:ILE:O	1:A:26:ILE:CG2	0.73	2.36	29	9
1:A:36:LEU:C	1:A:36:LEU:HD22	0.72	2.04	18	10
1:A:36:LEU:HD22	1:A:36:LEU:C	0.72	2.03	28	10
1:A:18:VAL:O	1:A:20:ASN:N	0.72	2.22	22	5
1:A:24:ASP:CB	1:A:30:HIS:CE1	0.72	2.73	11	2
1:A:24:ASP:O	1:A:25:ILE:HD12	0.72	1.85	9	5
1:A:27:GLN:HA	1:A:30:HIS:NE2	0.72	1.99	18	13
1:A:27:GLN:CA	1:A:30:HIS:CE1	0.71	2.73	13	7
1:A:26:ILE:N	1:A:30:HIS:CE1	0.71	2.59	20	1
1:A:25:ILE:CG2	1:A:26:ILE:HD12	0.70	2.15	22	4
1:A:25:ILE:HG21	1:A:29:MET:SD	0.69	2.27	10	2
1:A:28:ARG:CG	1:A:29:MET:N	0.68	2.56	8	30
1:A:28:ARG:C	1:A:30:HIS:H	0.68	1.90	20	30
1:A:25:ILE:N	1:A:30:HIS:NE2	0.68	2.41	10	7
1:A:17:ARG:O	1:A:20:ASN:CB	0.67	2.42	22	16
1:A:25:ILE:O	1:A:26:ILE:CD1	0.67	2.43	26	22
1:A:33:GLN:O	1:A:36:LEU:HD23	0.67	1.89	14	2
1:A:28:ARG:O	1:A:31:LEU:HD22	0.67	1.89	22	4
1:A:18:VAL:HG13	1:A:27:GLN:OE1	0.66	1.91	26	1
1:A:24:ASP:HB3	1:A:30:HIS:CD2	0.65	2.26	19	8
1:A:27:GLN:CG	1:A:27:GLN:O	0.65	2.44	22	20
1:A:27:GLN:O	1:A:27:GLN:CG	0.65	2.45	8	8
1:A:26:ILE:HB	1:A:29:MET:HG3	0.64	1.68	15	6
1:A:18:VAL:O	1:A:22:ALA:HB3	0.64	1.93	23	1
1:A:36:LEU:HD13	1:A:37:LEU:H	0.64	1.52	5	8
1:A:18:VAL:O	1:A:18:VAL:HG13	0.64	1.92	30	2
1:A:33:GLN:O	1:A:34:TYR:C	0.64	2.34	23	1
1:A:31:LEU:HD22	1:A:32:ARG:N	0.64	2.07	27	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ILE:HB	1:A:29:MET:CG	0.63	2.24	7	18
1:A:24:ASP:HB2	1:A:30:HIS:CE1	0.63	2.27	26	9
1:A:25:ILE:HG22	1:A:29:MET:SD	0.63	2.33	19	2
1:A:24:ASP:CB	1:A:30:HIS:CD2	0.63	2.82	19	6
1:A:19:PHE:HA	1:A:22:ALA:HB3	0.62	1.71	8	2
1:A:33:GLN:OE1	1:A:34:TYR:CG	0.62	2.52	17	1
1:A:24:ASP:CG	1:A:30:HIS:CD2	0.62	2.72	23	1
1:A:28:ARG:NH2	1:A:34:TYR:CE2	0.62	2.68	10	1
1:A:25:ILE:HG22	1:A:26:ILE:CG1	0.61	2.24	11	1
1:A:32:ARG:C	1:A:34:TYR:H	0.61	1.97	23	2
1:A:31:LEU:HD23	1:A:33:GLN:NE2	0.61	2.10	18	3
1:A:34:TYR:CD2	1:A:34:TYR:O	0.61	2.54	2	5
1:A:21:ASP:O	1:A:30:HIS:CD2	0.60	2.54	18	1
1:A:28:ARG:C	1:A:30:HIS:N	0.60	2.55	20	30
1:A:27:GLN:HA	1:A:30:HIS:CD2	0.60	2.32	12	10
1:A:35:GLU:OE1	1:A:36:LEU:HD23	0.60	1.97	29	1
1:A:26:ILE:N	1:A:30:HIS:NE2	0.60	2.49	26	5
1:A:21:ASP:O	1:A:30:HIS:CE1	0.60	2.55	13	4
1:A:26:ILE:O	1:A:27:GLN:C	0.59	2.40	18	15
1:A:33:GLN:NE2	1:A:33:GLN:N	0.59	2.50	8	7
1:A:32:ARG:CD	1:A:32:ARG:C	0.59	2.69	19	3
1:A:34:TYR:O	1:A:34:TYR:CD2	0.59	2.56	4	3
1:A:28:ARG:O	1:A:31:LEU:N	0.59	2.31	28	7
1:A:32:ARG:C	1:A:32:ARG:CD	0.59	2.70	27	1
1:A:31:LEU:HD12	1:A:33:GLN:H	0.59	1.58	10	2
1:A:35:GLU:O	1:A:36:LEU:HD23	0.59	1.98	10	2
1:A:18:VAL:HG13	1:A:18:VAL:O	0.59	1.98	24	1
1:A:24:ASP:O	1:A:25:ILE:CD1	0.58	2.51	11	20
1:A:27:GLN:HA	1:A:30:HIS:HE2	0.58	1.58	18	12
1:A:33:GLN:N	1:A:33:GLN:NE2	0.58	2.51	2	7
1:A:28:ARG:H	1:A:30:HIS:CE1	0.58	2.17	18	2
1:A:37:LEU:C	1:A:37:LEU:HD12	0.58	2.19	19	2
1:A:17:ARG:HD2	1:A:18:VAL:HG13	0.58	1.73	5	1
1:A:24:ASP:HB3	1:A:30:HIS:CG	0.58	2.34	9	4
1:A:25:ILE:HG21	1:A:29:MET:CE	0.57	2.30	26	2
1:A:27:GLN:HA	1:A:30:HIS:HE1	0.57	1.59	26	5
1:A:28:ARG:O	1:A:29:MET:C	0.57	2.43	28	7
1:A:24:ASP:HB2	1:A:30:HIS:CD2	0.56	2.35	25	3
1:A:32:ARG:C	1:A:34:TYR:N	0.56	2.58	23	9
1:A:32:ARG:O	1:A:34:TYR:N	0.56	2.39	23	4
1:A:34:TYR:CG	1:A:34:TYR:O	0.55	2.59	12	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ARG:O	1:A:20:ASN:N	0.55	2.36	22	6
1:A:31:LEU:CD1	1:A:33:GLN:NE2	0.55	2.70	11	4
1:A:25:ILE:O	1:A:26:ILE:HG12	0.55	2.02	19	1
1:A:31:LEU:HD23	1:A:33:GLN:CD	0.55	2.22	26	3
1:A:18:VAL:HG23	1:A:27:GLN:OE1	0.55	2.01	18	3
1:A:35:GLU:O	1:A:36:LEU:CG	0.55	2.55	10	2
1:A:25:ILE:CG2	1:A:29:MET:SD	0.55	2.94	10	5
1:A:30:HIS:NE2	1:A:31:LEU:CD1	0.54	2.71	16	1
1:A:26:ILE:HB	1:A:29:MET:SD	0.54	2.42	12	9
1:A:32:ARG:HD2	1:A:32:ARG:N	0.54	2.18	26	3
1:A:25:ILE:O	1:A:26:ILE:HG13	0.54	2.03	20	4
1:A:31:LEU:CD1	1:A:31:LEU:C	0.54	2.73	27	1
1:A:17:ARG:O	1:A:19:PHE:N	0.54	2.40	24	3
1:A:27:GLN:CA	1:A:30:HIS:CD2	0.53	2.90	12	9
1:A:18:VAL:HG23	1:A:19:PHE:CD2	0.53	2.39	23	1
1:A:26:ILE:CG1	1:A:29:MET:SD	0.53	2.97	26	4
1:A:18:VAL:C	1:A:20:ASN:N	0.53	2.61	27	9
1:A:17:ARG:O	1:A:18:VAL:C	0.53	2.47	22	4
1:A:25:ILE:O	1:A:26:ILE:CG1	0.53	2.56	19	6
1:A:32:ARG:N	1:A:32:ARG:HD2	0.53	2.19	19	1
1:A:26:ILE:O	1:A:28:ARG:N	0.53	2.41	10	12
1:A:27:GLN:CA	1:A:30:HIS:NE2	0.53	2.72	12	11
1:A:22:ALA:HB2	1:A:27:GLN:CD	0.53	2.24	11	2
1:A:18:VAL:HG23	1:A:27:GLN:HE22	0.53	1.62	9	1
1:A:24:ASP:CG	1:A:30:HIS:CE1	0.52	2.83	11	1
1:A:36:LEU:O	1:A:37:LEU:C	0.52	2.47	21	22
1:A:18:VAL:CG1	1:A:18:VAL:O	0.52	2.58	30	3
1:A:31:LEU:HD23	1:A:33:GLN:HE22	0.52	1.64	18	1
1:A:24:ASP:O	1:A:25:ILE:CG1	0.52	2.58	11	2
1:A:25:ILE:HG21	1:A:29:MET:HE2	0.52	1.82	26	1
1:A:26:ILE:CD1	1:A:29:MET:SD	0.51	2.95	29	5
1:A:27:GLN:N	1:A:30:HIS:HE1	0.51	2.03	14	2
1:A:31:LEU:HD23	1:A:33:GLN:OE1	0.51	2.04	26	2
1:A:18:VAL:O	1:A:19:PHE:C	0.51	2.48	22	5
1:A:27:GLN:N	1:A:30:HIS:NE2	0.51	2.58	20	1
1:A:28:ARG:N	1:A:30:HIS:NE2	0.51	2.58	25	5
1:A:26:ILE:CG2	1:A:29:MET:HG3	0.51	2.36	9	4
1:A:33:GLN:O	1:A:35:GLU:N	0.51	2.43	23	1
1:A:34:TYR:HB2	1:A:37:LEU:HD12	0.51	1.83	26	1
1:A:23:ARG:CG	1:A:23:ARG:O	0.51	2.57	6	3
1:A:28:ARG:HG2	1:A:29:MET:N	0.51	2.21	23	30

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:TYR:CD1	1:A:34:TYR:C	0.51	2.84	1	2
1:A:32:ARG:HG2	1:A:32:ARG:O	0.50	2.07	19	2
1:A:28:ARG:O	1:A:31:LEU:CD2	0.50	2.59	22	4
1:A:32:ARG:CG	1:A:32:ARG:O	0.50	2.59	19	2
1:A:24:ASP:CB	1:A:30:HIS:CG	0.50	2.93	18	6
1:A:24:ASP:C	1:A:25:ILE:CD1	0.50	2.77	25	1
1:A:27:GLN:C	1:A:30:HIS:NE2	0.50	2.65	25	6
1:A:33:GLN:O	1:A:36:LEU:CD2	0.50	2.60	6	2
1:A:18:VAL:HG13	1:A:27:GLN:NE2	0.50	2.21	8	1
1:A:24:ASP:O	1:A:25:ILE:HG13	0.50	2.07	25	2
1:A:31:LEU:C	1:A:32:ARG:CD	0.50	2.80	3	1
1:A:36:LEU:C	1:A:36:LEU:CD2	0.50	2.80	26	7
1:A:36:LEU:CD2	1:A:36:LEU:C	0.50	2.80	30	9
1:A:33:GLN:CD	1:A:34:TYR:N	0.50	2.65	24	4
1:A:32:ARG:HD3	1:A:34:TYR:CE2	0.49	2.42	24	2
1:A:25:ILE:HG23	1:A:26:ILE:HD12	0.49	1.81	22	2
1:A:18:VAL:HG13	1:A:19:PHE:N	0.49	2.21	10	7
1:A:25:ILE:HG22	1:A:26:ILE:N	0.49	2.23	9	2
1:A:33:GLN:O	1:A:37:LEU:CD1	0.49	2.59	21	1
1:A:31:LEU:CD2	1:A:33:GLN:OE1	0.49	2.60	18	1
1:A:24:ASP:CB	1:A:30:HIS:NE2	0.49	2.76	14	2
1:A:34:TYR:CD1	1:A:34:TYR:O	0.49	2.65	24	1
1:A:23:ARG:O	1:A:23:ARG:CG	0.49	2.61	12	2
1:A:24:ASP:OD1	1:A:30:HIS:CD2	0.48	2.66	16	1
1:A:18:VAL:O	1:A:22:ALA:CB	0.48	2.60	23	2
1:A:32:ARG:O	1:A:32:ARG:CG	0.48	2.61	27	1
1:A:25:ILE:HG22	1:A:26:ILE:HD11	0.48	1.85	11	1
1:A:35:GLU:O	1:A:36:LEU:CD2	0.48	2.62	10	2
1:A:28:ARG:N	1:A:30:HIS:CD2	0.48	2.82	25	4
1:A:19:PHE:CD1	1:A:19:PHE:N	0.47	2.79	29	2
1:A:25:ILE:H	1:A:30:HIS:CD2	0.47	2.27	13	3
1:A:21:ASP:OD1	1:A:22:ALA:N	0.47	2.47	22	1
1:A:19:PHE:O	1:A:23:ARG:CG	0.47	2.61	11	1
1:A:20:ASN:O	1:A:23:ARG:CG	0.47	2.62	8	7
1:A:18:VAL:HG23	1:A:19:PHE:H	0.47	1.69	23	1
1:A:25:ILE:CG2	1:A:29:MET:CE	0.47	2.93	26	1
1:A:35:GLU:O	1:A:37:LEU:N	0.47	2.47	27	16
1:A:24:ASP:CB	1:A:30:HIS:ND1	0.47	2.77	11	1
1:A:28:ARG:NH2	1:A:34:TYR:CZ	0.47	2.82	10	1
1:A:26:ILE:C	1:A:28:ARG:N	0.47	2.68	25	1
1:A:18:VAL:C	1:A:22:ALA:HB3	0.47	2.30	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:VAL:HG23	1:A:19:PHE:N	0.47	2.25	28	3
1:A:32:ARG:O	1:A:32:ARG:HG2	0.47	2.08	27	1
1:A:34:TYR:O	1:A:34:TYR:CG	0.47	2.67	4	1
1:A:26:ILE:CG2	1:A:29:MET:SD	0.47	3.03	22	2
1:A:25:ILE:C	1:A:26:ILE:CD1	0.47	2.79	20	1
1:A:18:VAL:O	1:A:22:ALA:N	0.47	2.48	23	4
1:A:18:VAL:CG2	1:A:27:GLN:OE1	0.46	2.63	18	1
1:A:34:TYR:C	1:A:34:TYR:CD1	0.46	2.89	18	2
1:A:17:ARG:O	1:A:20:ASN:HB2	0.46	2.10	22	2
1:A:31:LEU:HD22	1:A:33:GLN:H	0.46	1.70	27	1
1:A:25:ILE:N	1:A:30:HIS:CD2	0.46	2.84	19	3
1:A:33:GLN:OE1	1:A:34:TYR:N	0.46	2.48	15	3
1:A:28:ARG:O	1:A:31:LEU:HD23	0.46	2.11	29	2
1:A:31:LEU:HG	1:A:32:ARG:N	0.46	2.26	22	4
1:A:24:ASP:HB3	1:A:30:HIS:NE2	0.46	2.26	14	3
1:A:35:GLU:C	1:A:37:LEU:N	0.46	2.69	25	20
1:A:26:ILE:O	1:A:28:ARG:HB3	0.46	2.11	18	2
1:A:18:VAL:HG12	1:A:19:PHE:N	0.46	2.26	21	1
1:A:31:LEU:HD22	1:A:33:GLN:NE2	0.46	2.26	7	1
1:A:18:VAL:HG12	1:A:27:GLN:HE22	0.46	1.70	17	1
1:A:36:LEU:N	1:A:36:LEU:HD13	0.45	2.26	3	3
1:A:26:ILE:CG1	1:A:29:MET:HG2	0.45	2.41	5	1
1:A:35:GLU:O	1:A:36:LEU:C	0.45	2.54	24	9
1:A:31:LEU:O	1:A:32:ARG:NH1	0.45	2.50	2	1
1:A:18:VAL:CG1	1:A:19:PHE:N	0.45	2.80	10	1
1:A:24:ASP:HB3	1:A:30:HIS:CB	0.45	2.41	4	10
1:A:34:TYR:N	1:A:34:TYR:CD1	0.45	2.84	23	1
1:A:25:ILE:HB	1:A:30:HIS:HB3	0.45	1.88	25	1
1:A:17:ARG:CB	1:A:21:ASP:OD1	0.45	2.65	22	1
1:A:21:ASP:OD2	1:A:30:HIS:CE1	0.44	2.70	16	1
1:A:32:ARG:NE	1:A:35:GLU:OE1	0.44	2.51	24	1
1:A:30:HIS:O	1:A:31:LEU:O	0.44	2.35	10	3
1:A:26:ILE:CB	1:A:29:MET:HG3	0.44	2.42	25	2
1:A:34:TYR:O	1:A:35:GLU:O	0.44	2.34	21	8
1:A:24:ASP:HB2	1:A:30:HIS:CG	0.44	2.46	18	1
1:A:18:VAL:HG23	1:A:27:GLN:NE2	0.44	2.27	9	1
1:A:35:GLU:O	1:A:36:LEU:CB	0.44	2.66	10	2
1:A:36:LEU:HD13	1:A:36:LEU:N	0.44	2.28	2	4
1:A:31:LEU:HD12	1:A:33:GLN:NE2	0.44	2.28	15	2
1:A:21:ASP:O	1:A:30:HIS:NE2	0.44	2.49	18	1
1:A:21:ASP:C	1:A:23:ARG:N	0.44	2.70	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ILE:HG21	1:A:29:MET:SD	0.43	2.53	9	3
1:A:25:ILE:HB	1:A:30:HIS:CD2	0.43	2.48	10	3
1:A:35:GLU:C	1:A:37:LEU:H	0.43	2.16	9	4
1:A:35:GLU:O	1:A:36:LEU:HB3	0.43	2.14	28	3
1:A:31:LEU:HD11	1:A:33:GLN:NE2	0.43	2.28	22	2
1:A:18:VAL:HG13	1:A:19:PHE:H	0.43	1.72	9	1
1:A:29:MET:C	1:A:30:HIS:HD1	0.43	2.15	20	1
1:A:28:ARG:CB	1:A:33:GLN:OE1	0.43	2.66	23	1
1:A:31:LEU:CD2	1:A:33:GLN:CD	0.43	2.87	18	1
1:A:25:ILE:HB	1:A:30:HIS:CB	0.42	2.44	23	1
1:A:25:ILE:C	1:A:26:ILE:HD13	0.42	2.34	23	1
1:A:30:HIS:CD2	1:A:30:HIS:N	0.42	2.86	27	3
1:A:21:ASP:O	1:A:24:ASP:N	0.42	2.52	23	1
1:A:26:ILE:CG2	1:A:29:MET:CG	0.42	2.97	11	1
1:A:31:LEU:C	1:A:32:ARG:HD3	0.42	2.35	3	1
1:A:25:ILE:HB	1:A:30:HIS:CE1	0.42	2.49	20	1
1:A:26:ILE:HG13	1:A:29:MET:SD	0.42	2.53	3	1
1:A:21:ASP:CB	1:A:27:GLN:CD	0.42	2.88	20	1
1:A:26:ILE:HD13	1:A:26:ILE:HA	0.42	1.73	19	1
1:A:25:ILE:C	1:A:26:ILE:HG12	0.41	2.36	14	2
1:A:30:HIS:O	1:A:32:ARG:NH1	0.41	2.49	3	1
1:A:26:ILE:CB	1:A:29:MET:SD	0.41	3.08	12	1
1:A:17:ARG:O	1:A:20:ASN:HB3	0.41	2.15	23	1
1:A:31:LEU:HD13	1:A:31:LEU:O	0.41	2.14	27	1
1:A:17:ARG:CD	1:A:18:VAL:N	0.41	2.83	22	1
1:A:27:GLN:CA	1:A:30:HIS:HE1	0.41	2.21	26	1
1:A:23:ARG:CD	1:A:23:ARG:O	0.41	2.68	6	1
1:A:30:HIS:N	1:A:30:HIS:CD2	0.41	2.89	19	1
1:A:26:ILE:HB	1:A:29:MET:HG2	0.41	1.91	8	3
1:A:27:GLN:H	1:A:30:HIS:CE1	0.41	2.30	13	2
1:A:31:LEU:HD12	1:A:33:GLN:HE21	0.41	1.76	15	1
1:A:33:GLN:OE1	1:A:34:TYR:CD2	0.41	2.73	17	1
1:A:35:GLU:OE2	1:A:36:LEU:N	0.41	2.52	15	1
1:A:36:LEU:HG	1:A:37:LEU:N	0.41	2.30	1	2
1:A:18:VAL:O	1:A:27:GLN:NE2	0.41	2.53	7	1
1:A:31:LEU:HD22	1:A:32:ARG:H	0.41	1.76	27	1
1:A:33:GLN:CD	1:A:33:GLN:C	0.41	2.77	12	1
1:A:17:ARG:HD2	1:A:18:VAL:HG23	0.41	1.91	20	1
1:A:18:VAL:O	1:A:27:GLN:OE1	0.41	2.39	10	1
1:A:37:LEU:HD12	1:A:37:LEU:C	0.40	2.36	7	1
1:A:32:ARG:HD2	1:A:33:GLN:NE2	0.40	2.32	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ALA:N	1:A:27:GLN:OE1	0.40	2.53	10	1
1:A:24:ASP:C	1:A:25:ILE:HG12	0.40	2.37	23	1
1:A:33:GLN:C	1:A:33:GLN:CD	0.40	2.79	24	1
1:A:18:VAL:O	1:A:21:ASP:OD1	0.40	2.40	26	1
1:A:23:ARG:NE	1:A:23:ARG:O	0.40	2.49	26	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	20/37 (54%)	8±2 (38±8%)	6±1 (29±6%)	7±2 (33±8%)	0	0
All	All	600/1110 (54%)	230 (38%)	173 (29%)	197 (33%)	0	0

All 14 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	32	ARG	30
1	A	29	MET	30
1	A	28	ARG	29
1	A	26	ILE	20
1	A	35	GLU	20
1	A	25	ILE	16
1	A	27	GLN	15
1	A	17	ARG	11
1	A	31	LEU	7
1	A	18	VAL	7
1	A	19	PHE	5
1	A	33	GLN	4
1	A	36	LEU	2
1	A	34	TYR	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	20/36 (56%)	13±2 (65±8%)	7±2 (35±8%)	1	9
All	All	600/1080 (56%)	388 (65%)	212 (35%)	1	9

All 17 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	33	GLN	30
1	A	32	ARG	26
1	A	36	LEU	26
1	A	29	MET	18
1	A	17	ARG	16
1	A	30	HIS	16
1	A	24	ASP	14
1	A	23	ARG	13
1	A	35	GLU	13
1	A	21	ASP	12
1	A	31	LEU	6
1	A	28	ARG	5
1	A	37	LEU	5
1	A	18	VAL	4
1	A	34	TYR	4
1	A	25	ILE	3
1	A	26	ILE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

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