



Full wwPDB NMR Structure Validation Report ⓘ

Mar 28, 2026 – 09:50 AM UTC

PDB ID : 1TH5 / pdb_00001th5
Title : Solution structure of C-terminal domain of NifU-like protein from *Oryza sativa*
Authors : Kumeta, H.; Ogura, K.; Asayama, M.; Katoh, S.; Katoh, E.; Inagaki, F.
Deposited on : 2004-06-01

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

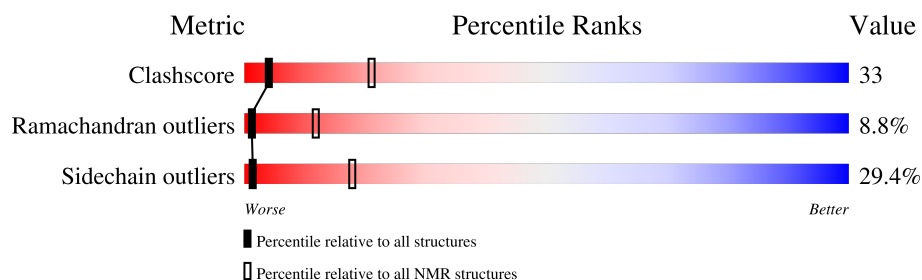
1 Overall quality at a glance

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	74	

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 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:154-A:226 (73)	0.65	5

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 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1197 atoms, of which 630 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NifU1.

Mol	Chain	Residues	Atoms						Trace
1	A	74	Total	C	H	N	O	S	0
			1197	365	630	101	99	2	

There is a discrepancy between the modelled and reference sequences:

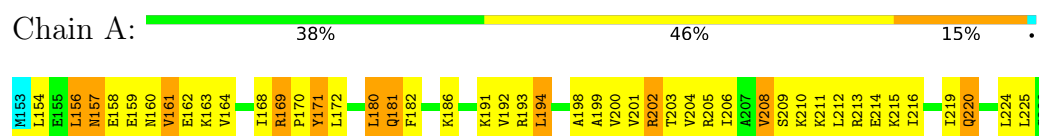
Chain	Residue	Modelled	Actual	Comment	Reference
A	153	MET	-	cloning artifact	UNP Q84LK7

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: NifU1

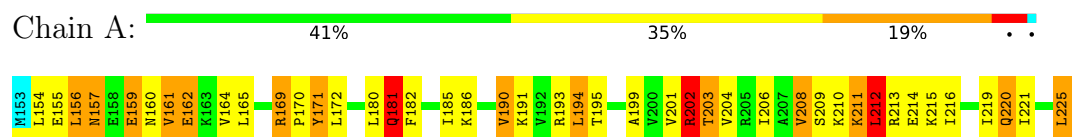


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

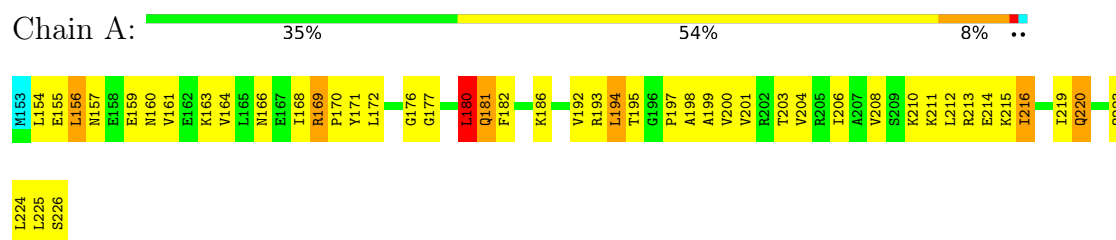
4.2.1 Score per residue for model 1

- Molecule 1: NifU1



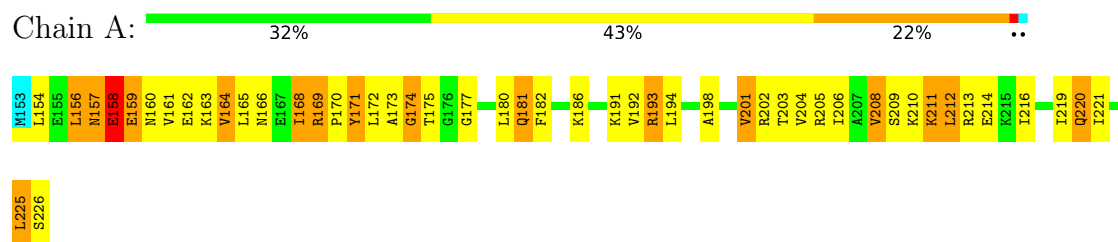
4.2.2 Score per residue for model 2

- Molecule 1: NifU1



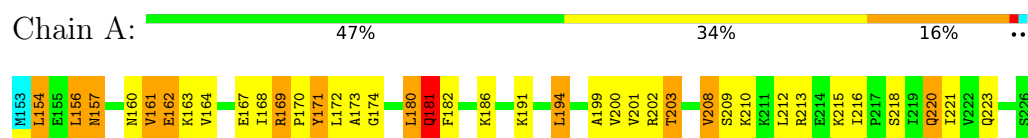
4.2.3 Score per residue for model 3

- Molecule 1: NifU1



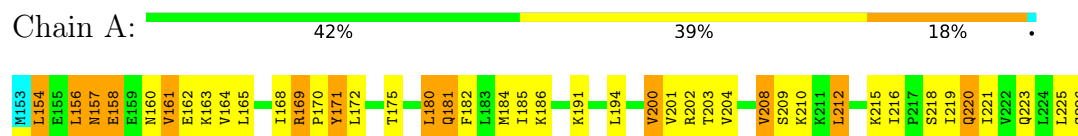
4.2.4 Score per residue for model 4

- Molecule 1: NifU1



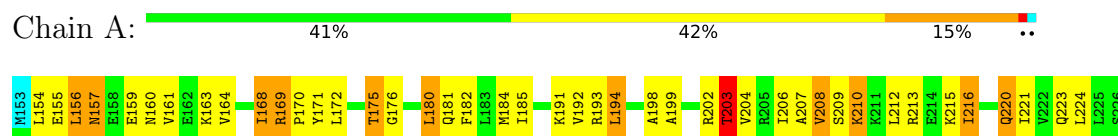
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: NifU1



4.2.6 Score per residue for model 6

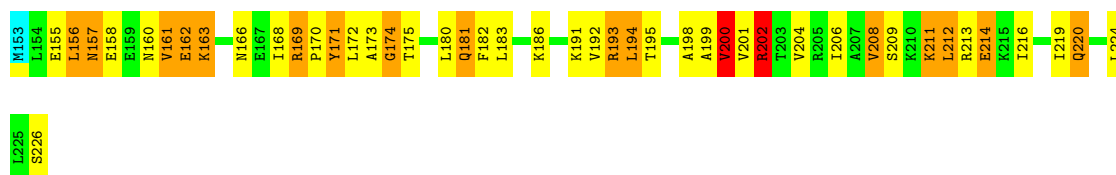
- Molecule 1: NifU1



4.2.7 Score per residue for model 7

- Molecule 1: NifU1

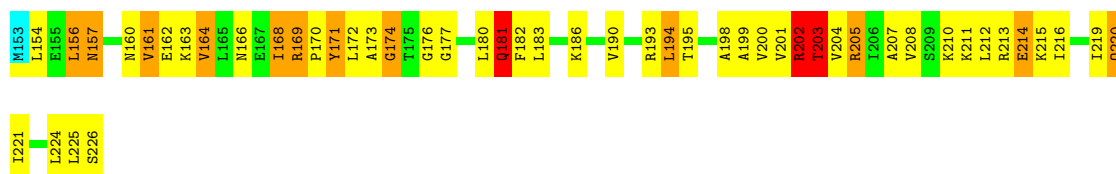




4.2.8 Score per residue for model 8

- Molecule 1: NifU1

Chain A: 31% 47% 16%



4.2.9 Score per residue for model 9

- Molecule 1: NifU1

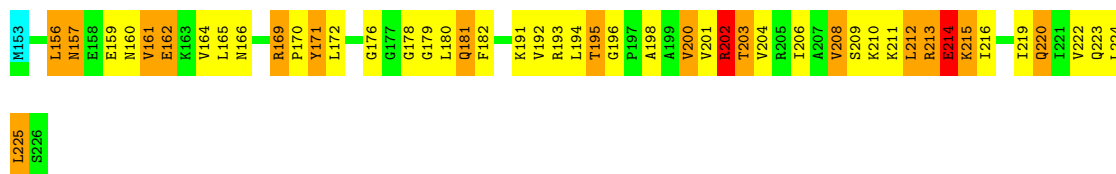
Chain A: 41% 38% 20%



4.2.10 Score per residue for model 10

- Molecule 1: NifU1

Chain A: 35% 39% 22%



4.2.11 Score per residue for model 11

- Molecule 1: NifU1

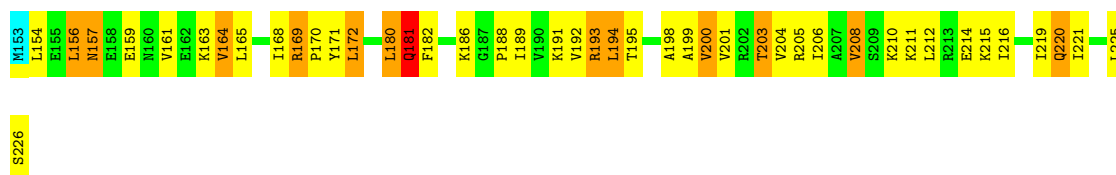
Chain A: 43% 41% 15%



4.2.12 Score per residue for model 12

- Molecule 1: NifU1

Chain A: 39% 42% 16% ..



4.2.13 Score per residue for model 13

- Molecule 1: NifU1

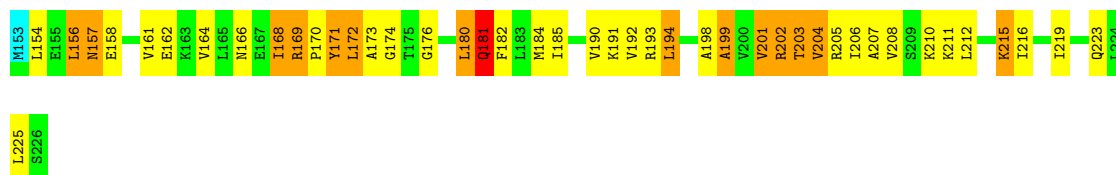
Chain A: 43% 41% 15% ..



4.2.14 Score per residue for model 14

- Molecule 1: NifU1

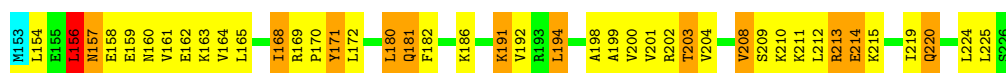
Chain A: 39% 39% 19% ..



4.2.15 Score per residue for model 15

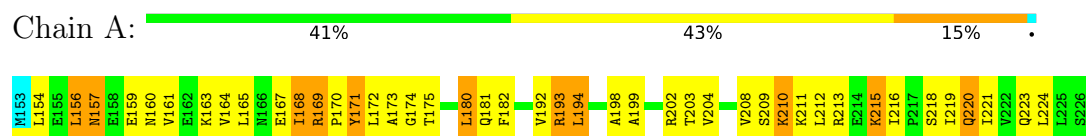
- Molecule 1: NifU1

Chain A: 42% 39% 16% ..



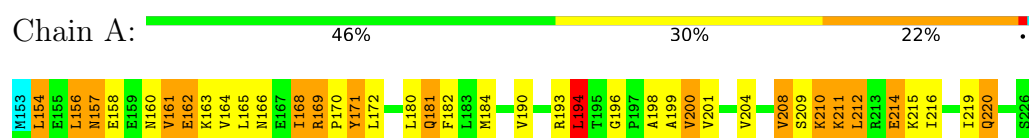
4.2.16 Score per residue for model 16

- Molecule 1: NifU1



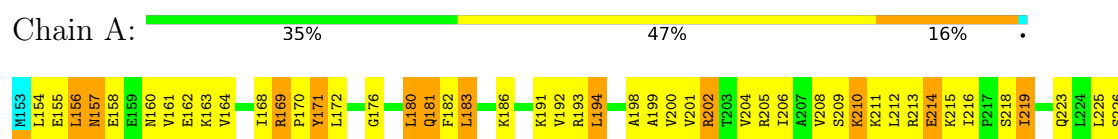
4.2.17 Score per residue for model 17

- Molecule 1: NifU1



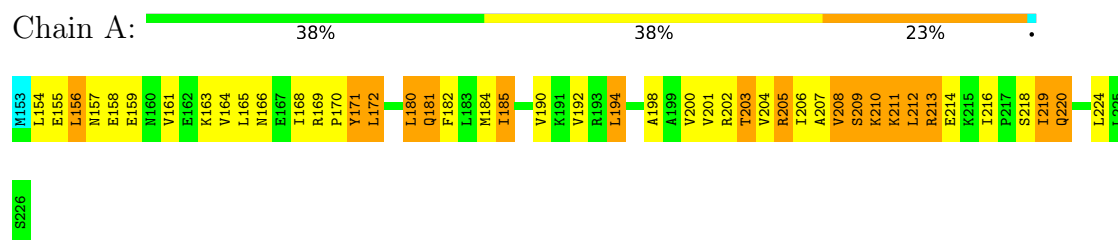
4.2.18 Score per residue for model 18

- Molecule 1: NifU1



4.2.19 Score per residue for model 19

- Molecule 1: NifU1



4.2.20 Score per residue for model 20

- Molecule 1: NifU1



M153	L154	E155	L156	N157	E158	E159	N160	V161	E162	K163	V164	I168	R169	P170	Y171	L172	A173	G176	G177	L180	Q181	F182	L183	M184	L194	T195	A199	V200	V201	R202	T203	V204	R205	I206	A207	V208	S209	K210	K211	L212	R213	E214	K215	I216	F217	S218	I219	Q220	L224	L225	S226
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5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry simulated annealing, torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	1.06
CYANA	refinement	1.06

No chemical shift data was provided.

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	559	621	621	39±5
All	All	11180	12420	12420	784

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 33.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:198:ALA:HB1	1:A:204:VAL:HG11	1.02	1.25	19	8
1:A:201:VAL:HG12	1:A:203:THR:HG22	0.84	1.49	12	2
1:A:208:VAL:HG12	1:A:212:LEU:HD11	0.84	1.48	16	5
1:A:168:ILE:HD12	1:A:208:VAL:HG13	0.84	1.48	16	2
1:A:165:LEU:HD22	1:A:180:LEU:CD1	0.83	2.04	16	1
1:A:180:LEU:HD22	1:A:180:LEU:O	0.80	1.77	20	2
1:A:161:VAL:HG11	1:A:182:PHE:CE1	0.79	2.12	5	6
1:A:164:VAL:HG11	1:A:212:LEU:HA	0.78	1.54	6	15
1:A:193:ARG:O	1:A:194:LEU:HD22	0.78	1.78	14	5
1:A:172:LEU:HD11	1:A:180:LEU:CD2	0.77	2.09	13	1
1:A:157:ASN:O	1:A:161:VAL:HG22	0.77	1.80	8	9
1:A:172:LEU:HD12	1:A:180:LEU:HD23	0.76	1.56	2	1
1:A:161:VAL:HG21	1:A:182:PHE:CZ	0.75	2.16	12	10
1:A:161:VAL:HG21	1:A:182:PHE:CE2	0.74	2.17	4	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:220:GLN:C	1:A:221:ILE:HD12	0.74	2.08	13	3
1:A:157:ASN:H	1:A:161:VAL:HG23	0.73	1.43	15	5
1:A:154:LEU:HD12	1:A:215:LYS:O	0.71	1.85	4	4
1:A:154:LEU:HD22	1:A:160:ASN:CG	0.71	2.09	15	4
1:A:198:ALA:HB1	1:A:204:VAL:HG21	0.71	1.60	8	4
1:A:169:ARG:NE	1:A:180:LEU:HD11	0.71	2.01	1	1
1:A:171:TYR:CD2	1:A:172:LEU:HD23	0.70	2.22	7	20
1:A:156:LEU:HD13	1:A:216:ILE:HD12	0.70	1.61	16	13
1:A:194:LEU:HD12	1:A:199:ALA:HA	0.69	1.62	1	10
1:A:220:GLN:HB3	1:A:221:ILE:HD12	0.69	1.65	3	4
1:A:202:ARG:O	1:A:203:THR:HG23	0.69	1.87	8	1
1:A:154:LEU:HD23	1:A:160:ASN:CG	0.68	2.13	17	3
1:A:156:LEU:HD12	1:A:161:VAL:CG2	0.68	2.18	20	2
1:A:180:LEU:C	1:A:180:LEU:HD12	0.67	2.14	10	1
1:A:157:ASN:N	1:A:161:VAL:HG23	0.67	2.05	5	5
1:A:157:ASN:HD21	1:A:160:ASN:ND2	0.66	1.88	5	2
1:A:189:ILE:HD12	1:A:221:ILE:HB	0.66	1.66	12	1
1:A:168:ILE:CD1	1:A:208:VAL:HG13	0.66	2.19	16	3
1:A:169:ARG:HG3	1:A:180:LEU:HD21	0.65	1.68	15	3
1:A:157:ASN:O	1:A:161:VAL:HG12	0.65	1.91	9	5
1:A:180:LEU:HD22	1:A:180:LEU:H	0.65	1.51	12	1
1:A:201:VAL:HG22	1:A:201:VAL:O	0.65	1.89	19	3
1:A:200:VAL:O	1:A:200:VAL:HG22	0.65	1.91	18	4
1:A:199:ALA:C	1:A:200:VAL:HG23	0.65	2.17	12	1
1:A:154:LEU:HD13	1:A:215:LYS:O	0.64	1.92	14	2
1:A:208:VAL:C	1:A:212:LEU:HD23	0.64	2.16	8	1
1:A:161:VAL:HG11	1:A:182:PHE:CZ	0.64	2.27	13	5
1:A:157:ASN:HA	1:A:185:ILE:HD13	0.63	1.71	19	3
1:A:180:LEU:N	1:A:180:LEU:HD13	0.62	2.09	12	2
1:A:156:LEU:C	1:A:157:ASN:CG	0.62	2.68	14	8
1:A:156:LEU:CD1	1:A:216:ILE:HD12	0.62	2.25	5	7
1:A:164:VAL:HG22	1:A:215:LYS:CB	0.62	2.25	20	4
1:A:165:LEU:HD22	1:A:180:LEU:HD12	0.61	1.71	16	2
1:A:208:VAL:O	1:A:212:LEU:HD23	0.61	1.96	8	1
1:A:185:ILE:HG23	1:A:190:VAL:HG22	0.61	1.73	19	1
1:A:200:VAL:O	1:A:200:VAL:HG13	0.60	1.96	5	3
1:A:202:ARG:HD3	1:A:206:ILE:HD11	0.60	1.73	18	1
1:A:183:LEU:CD1	1:A:225:LEU:HD13	0.60	2.27	18	1
1:A:157:ASN:N	1:A:157:ASN:ND2	0.60	2.48	14	4
1:A:212:LEU:HD22	1:A:212:LEU:H	0.60	1.57	7	5
1:A:208:VAL:CG1	1:A:212:LEU:HD11	0.59	2.27	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:208:VAL:HG12	1:A:212:LEU:CD1	0.59	2.26	18	4
1:A:202:ARG:C	1:A:206:ILE:HD12	0.59	2.23	18	2
1:A:154:LEU:HD22	1:A:160:ASN:ND2	0.59	2.13	8	2
1:A:161:VAL:HG21	1:A:185:ILE:HD11	0.58	1.74	14	1
1:A:171:TYR:CD2	1:A:172:LEU:CD2	0.57	2.87	7	10
1:A:168:ILE:HD13	1:A:208:VAL:HA	0.57	1.76	14	4
1:A:154:LEU:HD22	1:A:154:LEU:N	0.57	2.14	5	1
1:A:180:LEU:C	1:A:180:LEU:CD2	0.57	2.77	6	1
1:A:161:VAL:HG12	1:A:216:ILE:CD1	0.57	2.28	4	4
1:A:204:VAL:O	1:A:208:VAL:HG23	0.57	1.99	12	3
1:A:172:LEU:HD11	1:A:180:LEU:HD23	0.57	1.76	13	2
1:A:154:LEU:HD12	1:A:216:ILE:HG23	0.57	1.77	12	1
1:A:164:VAL:HG11	1:A:212:LEU:CA	0.57	2.29	14	4
1:A:161:VAL:HG12	1:A:216:ILE:HD13	0.57	1.77	4	2
1:A:164:VAL:CG1	1:A:212:LEU:HD23	0.56	2.30	12	4
1:A:183:LEU:HD12	1:A:225:LEU:HD13	0.56	1.75	18	1
1:A:171:TYR:CD1	1:A:171:TYR:O	0.56	2.59	4	16
1:A:198:ALA:HB1	1:A:204:VAL:CG1	0.56	2.21	17	1
1:A:194:LEU:HD23	1:A:224:LEU:HB3	0.56	1.76	8	3
1:A:185:ILE:HG12	1:A:190:VAL:HG23	0.56	1.76	14	1
1:A:169:ARG:HA	1:A:180:LEU:HD21	0.56	1.77	16	2
1:A:156:LEU:HD12	1:A:161:VAL:HG22	0.55	1.77	20	2
1:A:169:ARG:HD2	1:A:180:LEU:HD11	0.55	1.79	16	4
1:A:192:VAL:HG12	1:A:193:ARG:N	0.55	2.17	2	5
1:A:169:ARG:HG2	1:A:180:LEU:HD13	0.55	1.78	2	1
1:A:198:ALA:CB	1:A:204:VAL:HG11	0.55	2.23	17	3
1:A:181:GLN:CD	1:A:181:GLN:C	0.54	2.74	20	2
1:A:168:ILE:HG21	1:A:208:VAL:HA	0.54	1.79	3	3
1:A:199:ALA:O	1:A:201:VAL:HG23	0.54	2.02	15	1
1:A:172:LEU:CD1	1:A:180:LEU:CD2	0.54	2.84	13	1
1:A:208:VAL:HG12	1:A:209:SER:N	0.54	2.18	6	7
1:A:154:LEU:HD23	1:A:160:ASN:ND2	0.54	2.17	17	1
1:A:165:LEU:HD11	1:A:182:PHE:CD1	0.53	2.38	15	8
1:A:201:VAL:HG13	1:A:202:ARG:H	0.53	1.63	14	1
1:A:180:LEU:O	1:A:181:GLN:C	0.53	2.51	10	20
1:A:212:LEU:HD22	1:A:212:LEU:N	0.53	2.18	8	1
1:A:201:VAL:O	1:A:202:ARG:CB	0.53	2.57	3	4
1:A:206:ILE:HG22	1:A:210:LYS:HG3	0.53	1.79	6	1
1:A:185:ILE:CG1	1:A:190:VAL:HG23	0.53	2.34	14	1
1:A:157:ASN:O	1:A:161:VAL:HG13	0.52	2.04	4	1
1:A:156:LEU:HD12	1:A:161:VAL:CG1	0.52	2.34	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:LEU:HD23	1:A:224:LEU:HD22	0.52	1.81	15	4
1:A:154:LEU:HD13	1:A:216:ILE:HG23	0.52	1.82	2	1
1:A:199:ALA:C	1:A:200:VAL:HG12	0.52	2.30	7	1
1:A:208:VAL:O	1:A:208:VAL:HG12	0.52	2.05	8	1
1:A:169:ARG:NH2	1:A:181:GLN:NE2	0.52	2.56	9	2
1:A:188:PRO:O	1:A:189:ILE:HD13	0.52	2.05	12	1
1:A:219:ILE:CG2	1:A:220:GLN:N	0.52	2.72	1	14
1:A:157:ASN:ND2	1:A:157:ASN:N	0.52	2.57	9	2
1:A:209:SER:HA	1:A:212:LEU:HD23	0.52	1.81	3	3
1:A:201:VAL:HG12	1:A:203:THR:CG2	0.51	2.31	12	1
1:A:220:GLN:O	1:A:221:ILE:HD13	0.51	2.05	4	3
1:A:180:LEU:C	1:A:180:LEU:CD1	0.51	2.83	10	1
1:A:211:LYS:O	1:A:212:LEU:C	0.51	2.52	20	5
1:A:154:LEU:CD1	1:A:216:ILE:HG23	0.51	2.35	12	1
1:A:157:ASN:ND2	1:A:160:ASN:ND2	0.51	2.59	8	2
1:A:156:LEU:HD11	1:A:219:ILE:CG1	0.51	2.36	19	1
1:A:180:LEU:HD12	1:A:181:GLN:N	0.51	2.20	7	2
1:A:208:VAL:O	1:A:209:SER:C	0.51	2.54	10	4
1:A:203:THR:N	1:A:206:ILE:HD12	0.51	2.20	19	2
1:A:194:LEU:HD12	1:A:199:ALA:HB2	0.51	1.81	15	2
1:A:175:THR:O	1:A:175:THR:HG23	0.51	2.06	5	1
1:A:208:VAL:O	1:A:212:LEU:HD22	0.51	2.06	5	4
1:A:164:VAL:HG22	1:A:215:LYS:HB2	0.50	1.83	20	3
1:A:180:LEU:CD1	1:A:180:LEU:N	0.50	2.75	15	2
1:A:157:ASN:O	1:A:158:GLU:C	0.50	2.54	5	3
1:A:166:ASN:O	1:A:170:PRO:CG	0.50	2.59	17	9
1:A:181:GLN:O	1:A:182:PHE:C	0.50	2.55	7	10
1:A:172:LEU:CD1	1:A:180:LEU:HD23	0.50	2.37	13	1
1:A:157:ASN:O	1:A:161:VAL:N	0.50	2.45	18	8
1:A:194:LEU:CD1	1:A:198:ALA:O	0.50	2.60	12	3
1:A:165:LEU:HD22	1:A:180:LEU:HD13	0.50	1.81	16	1
1:A:211:LYS:O	1:A:214:GLU:N	0.50	2.45	17	5
1:A:156:LEU:HD12	1:A:216:ILE:HD12	0.50	1.84	18	2
1:A:160:ASN:O	1:A:162:GLU:N	0.49	2.45	8	9
1:A:198:ALA:O	1:A:199:ALA:C	0.49	2.55	14	1
1:A:208:VAL:O	1:A:212:LEU:CD2	0.49	2.60	8	3
1:A:156:LEU:HA	1:A:216:ILE:HG21	0.49	1.83	6	2
1:A:199:ALA:O	1:A:200:VAL:C	0.49	2.55	15	2
1:A:157:ASN:C	1:A:161:VAL:HG22	0.49	2.32	1	1
1:A:157:ASN:HD22	1:A:157:ASN:N	0.49	2.06	6	3
1:A:209:SER:HB3	1:A:222:VAL:HG21	0.49	1.82	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:160:ASN:O	1:A:161:VAL:C	0.49	2.55	7	13
1:A:173:ALA:O	1:A:175:THR:N	0.49	2.45	3	2
1:A:154:LEU:HD22	1:A:215:LYS:O	0.49	2.06	5	1
1:A:168:ILE:O	1:A:169:ARG:C	0.49	2.55	15	2
1:A:154:LEU:CD2	1:A:215:LYS:O	0.49	2.60	5	1
1:A:171:TYR:CE2	1:A:172:LEU:CD2	0.49	2.95	7	1
1:A:166:ASN:O	1:A:170:PRO:CD	0.49	2.60	10	3
1:A:173:ALA:O	1:A:174:GLY:C	0.49	2.56	8	6
1:A:201:VAL:HG11	1:A:204:VAL:HG23	0.49	1.85	19	2
1:A:225:LEU:O	1:A:226:SER:C	0.49	2.55	9	2
1:A:181:GLN:NE2	1:A:182:PHE:O	0.49	2.46	13	1
1:A:201:VAL:O	1:A:201:VAL:CG2	0.48	2.61	19	2
1:A:157:ASN:OD1	1:A:159:GLU:CG	0.48	2.60	6	3
1:A:198:ALA:HA	1:A:201:VAL:HG22	0.48	1.84	2	1
1:A:193:ARG:O	1:A:194:LEU:CD2	0.48	2.61	7	1
1:A:172:LEU:O	1:A:176:GLY:C	0.48	2.56	8	1
1:A:202:ARG:O	1:A:206:ILE:CG1	0.48	2.62	18	1
1:A:157:ASN:O	1:A:161:VAL:CG1	0.48	2.61	6	3
1:A:156:LEU:O	1:A:157:ASN:CB	0.48	2.61	20	1
1:A:202:ARG:O	1:A:203:THR:CB	0.48	2.62	3	5
1:A:208:VAL:O	1:A:210:LYS:N	0.48	2.46	19	2
1:A:180:LEU:O	1:A:193:ARG:CB	0.48	2.62	1	1
1:A:172:LEU:O	1:A:173:ALA:C	0.48	2.57	20	6
1:A:156:LEU:C	1:A:157:ASN:ND2	0.48	2.71	14	2
1:A:208:VAL:C	1:A:212:LEU:CD2	0.48	2.87	8	1
1:A:180:LEU:HD22	1:A:180:LEU:C	0.48	2.32	20	2
1:A:161:VAL:HG22	1:A:216:ILE:HD13	0.47	1.86	5	1
1:A:225:LEU:N	1:A:225:LEU:HD12	0.47	2.24	5	1
1:A:198:ALA:O	1:A:199:ALA:HB3	0.47	2.08	15	1
1:A:204:VAL:O	1:A:205:ARG:C	0.47	2.56	8	5
1:A:203:THR:N	1:A:206:ILE:CD1	0.47	2.78	14	1
1:A:206:ILE:HG22	1:A:210:LYS:CE	0.47	2.40	19	1
1:A:169:ARG:CB	1:A:170:PRO:CD	0.47	2.93	18	20
1:A:180:LEU:C	1:A:180:LEU:HD22	0.47	2.35	6	1
1:A:160:ASN:C	1:A:162:GLU:N	0.47	2.73	13	8
1:A:156:LEU:O	1:A:157:ASN:CG	0.47	2.58	5	4
1:A:156:LEU:CD1	1:A:161:VAL:CG2	0.47	2.93	15	1
1:A:180:LEU:O	1:A:182:PHE:N	0.47	2.48	20	3
1:A:176:GLY:O	1:A:177:GLY:C	0.46	2.58	20	1
1:A:208:VAL:C	1:A:210:LYS:N	0.46	2.71	19	7
1:A:212:LEU:O	1:A:216:ILE:CG1	0.46	2.63	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:211:LYS:O	1:A:214:GLU:CB	0.46	2.63	3	1
1:A:169:ARG:N	1:A:170:PRO:HD2	0.46	2.25	15	20
1:A:201:VAL:HG12	1:A:202:ARG:N	0.46	2.25	8	3
1:A:203:THR:O	1:A:204:VAL:C	0.46	2.57	20	3
1:A:206:ILE:HG22	1:A:210:LYS:CD	0.46	2.41	9	2
1:A:192:VAL:CG1	1:A:193:ARG:N	0.46	2.79	10	1
1:A:193:ARG:NH1	1:A:195:THR:HG21	0.46	2.26	12	1
1:A:197:PRO:O	1:A:201:VAL:HG13	0.46	2.10	2	1
1:A:225:LEU:N	1:A:225:LEU:CD2	0.46	2.77	10	2
1:A:160:ASN:O	1:A:163:LYS:N	0.46	2.48	7	1
1:A:169:ARG:CD	1:A:180:LEU:HD11	0.46	2.40	10	1
1:A:202:ARG:O	1:A:206:ILE:HD12	0.46	2.11	18	1
1:A:191:LYS:O	1:A:192:VAL:CG2	0.46	2.64	6	6
1:A:169:ARG:HG3	1:A:180:LEU:HD11	0.46	1.88	10	1
1:A:157:ASN:OD1	1:A:160:ASN:N	0.45	2.50	13	2
1:A:219:ILE:HG22	1:A:220:GLN:N	0.45	2.26	3	5
1:A:194:LEU:CD2	1:A:224:LEU:HD22	0.45	2.42	20	1
1:A:212:LEU:C	1:A:214:GLU:N	0.45	2.74	8	3
1:A:212:LEU:O	1:A:213:ARG:C	0.45	2.59	10	2
1:A:199:ALA:O	1:A:200:VAL:CB	0.45	2.64	12	1
1:A:206:ILE:HG22	1:A:210:LYS:HE2	0.45	1.88	19	1
1:A:171:TYR:CD1	1:A:171:TYR:C	0.45	2.92	10	3
1:A:201:VAL:CG1	1:A:204:VAL:HG23	0.45	2.41	19	1
1:A:164:VAL:HG12	1:A:211:LYS:HB3	0.45	1.88	19	2
1:A:162:GLU:O	1:A:166:ASN:ND2	0.45	2.50	7	1
1:A:209:SER:HA	1:A:212:LEU:HD12	0.45	1.88	16	2
1:A:161:VAL:HG22	1:A:216:ILE:CD1	0.45	2.41	5	1
1:A:214:GLU:O	1:A:215:LYS:C	0.45	2.60	10	2
1:A:199:ALA:O	1:A:200:VAL:HG23	0.44	2.12	12	1
1:A:154:LEU:HD12	1:A:215:LYS:C	0.44	2.37	2	1
1:A:190:VAL:CG2	1:A:191:LYS:N	0.44	2.79	1	1
1:A:200:VAL:HG12	1:A:200:VAL:O	0.44	2.13	17	1
1:A:180:LEU:HD22	1:A:180:LEU:N	0.44	2.23	12	1
1:A:199:ALA:C	1:A:200:VAL:CG2	0.44	2.86	12	1
1:A:213:ARG:NH2	1:A:222:VAL:HG11	0.44	2.28	13	1
1:A:161:VAL:HG21	1:A:182:PHE:CE1	0.44	2.47	17	1
1:A:173:ALA:C	1:A:175:THR:N	0.44	2.75	3	1
1:A:201:VAL:CG1	1:A:203:THR:HG22	0.44	2.32	12	1
1:A:198:ALA:O	1:A:204:VAL:HG11	0.44	2.13	7	1
1:A:191:LYS:C	1:A:192:VAL:HG23	0.44	2.38	7	6
1:A:191:LYS:C	1:A:192:VAL:CG2	0.44	2.91	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:180:LEU:O	1:A:180:LEU:CD2	0.44	2.60	20	1
1:A:169:ARG:HH21	1:A:181:GLN:NE2	0.44	2.10	9	1
1:A:203:THR:HA	1:A:206:ILE:HD12	0.43	1.89	1	1
1:A:198:ALA:CB	1:A:204:VAL:HG21	0.43	2.37	8	1
1:A:201:VAL:HG13	1:A:202:ARG:N	0.43	2.28	14	1
1:A:225:LEU:N	1:A:225:LEU:HD22	0.43	2.28	2	1
1:A:158:GLU:O	1:A:162:GLU:CG	0.43	2.67	18	2
1:A:206:ILE:O	1:A:207:ALA:C	0.43	2.62	6	2
1:A:180:LEU:N	1:A:180:LEU:CD1	0.43	2.79	12	1
1:A:161:VAL:HG11	1:A:182:PHE:CE2	0.43	2.49	17	1
1:A:206:ILE:C	1:A:208:VAL:N	0.43	2.75	12	3
1:A:157:ASN:O	1:A:159:GLU:N	0.43	2.52	3	1
1:A:204:VAL:O	1:A:207:ALA:N	0.43	2.52	14	3
1:A:172:LEU:HD23	1:A:172:LEU:N	0.43	2.29	14	3
1:A:155:GLU:H	1:A:160:ASN:ND2	0.43	2.11	20	1
1:A:204:VAL:C	1:A:206:ILE:N	0.43	2.76	19	2
1:A:218:SER:O	1:A:219:ILE:C	0.43	2.62	19	1
1:A:191:LYS:O	1:A:192:VAL:HG23	0.42	2.14	10	1
1:A:209:SER:OG	1:A:213:ARG:CZ	0.42	2.67	15	1
1:A:156:LEU:HD11	1:A:219:ILE:HG13	0.42	1.90	19	1
1:A:154:LEU:CB	1:A:216:ILE:HG22	0.42	2.43	18	1
1:A:156:LEU:HD13	1:A:219:ILE:HG12	0.42	1.91	18	1
1:A:164:VAL:HG13	1:A:215:LYS:HD3	0.42	1.90	6	1
1:A:180:LEU:C	1:A:180:LEU:HD13	0.42	2.39	20	1
1:A:195:THR:OG1	1:A:196:GLY:N	0.42	2.51	10	1
1:A:161:VAL:O	1:A:162:GLU:C	0.42	2.63	18	1
1:A:184:MET:HE3	1:A:191:LYS:CE	0.42	2.45	5	1
1:A:204:VAL:O	1:A:206:ILE:N	0.42	2.53	19	1
1:A:206:ILE:CG2	1:A:210:LYS:HE2	0.42	2.45	19	1
1:A:157:ASN:CG	1:A:159:GLU:HG2	0.42	2.39	20	2
1:A:154:LEU:CD2	1:A:160:ASN:OD1	0.42	2.68	1	1
1:A:172:LEU:O	1:A:177:GLY:N	0.41	2.53	2	3
1:A:159:GLU:CG	1:A:160:ASN:N	0.41	2.83	10	1
1:A:165:LEU:HD11	1:A:182:PHE:HD1	0.41	1.74	15	1
1:A:225:LEU:H	1:A:225:LEU:HD12	0.41	1.74	12	1
1:A:168:ILE:O	1:A:171:TYR:N	0.41	2.53	8	1
1:A:156:LEU:C	1:A:157:ASN:OD1	0.41	2.64	4	1
1:A:213:ARG:NH2	1:A:222:VAL:CG1	0.41	2.83	13	1
1:A:174:GLY:O	1:A:175:THR:C	0.41	2.63	16	1
1:A:156:LEU:HD12	1:A:161:VAL:HG12	0.41	1.92	2	1
1:A:157:ASN:O	1:A:161:VAL:CG2	0.41	2.66	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:200:VAL:C	1:A:201:VAL:CG2	0.41	2.94	4	1
1:A:180:LEU:CD1	1:A:180:LEU:H	0.41	2.28	15	1
1:A:201:VAL:O	1:A:201:VAL:HG12	0.41	2.15	1	1
1:A:169:ARG:CG	1:A:180:LEU:HD13	0.41	2.46	2	1
1:A:210:LYS:O	1:A:214:GLU:OE1	0.41	2.39	15	1
1:A:164:VAL:HG12	1:A:212:LEU:HD23	0.41	1.91	20	2
1:A:220:GLN:O	1:A:221:ILE:CD1	0.41	2.69	1	2
1:A:220:GLN:C	1:A:221:ILE:HG13	0.41	2.41	6	2
1:A:154:LEU:HD22	1:A:160:ASN:HD21	0.41	1.75	8	1
1:A:202:ARG:C	1:A:203:THR:HG22	0.40	2.41	6	1
1:A:181:GLN:C	1:A:181:GLN:NE2	0.40	2.79	5	1
1:A:191:LYS:HG2	1:A:225:LEU:HD11	0.40	1.93	18	1
1:A:180:LEU:HD22	1:A:181:GLN:N	0.40	2.31	6	1
1:A:180:LEU:O	1:A:181:GLN:O	0.40	2.40	7	1
1:A:157:ASN:ND2	1:A:160:ASN:CG	0.40	2.80	9	1
1:A:223:GLN:O	1:A:224:LEU:HD23	0.40	2.17	10	1
1:A:184:MET:C	1:A:185:ILE:HG13	0.40	2.41	13	1
1:A:155:GLU:O	1:A:156:LEU:O	0.40	2.39	19	1
1:A:179:GLY:O	1:A:193:ARG:O	0.40	2.39	10	1
1:A:154:LEU:HD12	1:A:216:ILE:CG2	0.40	2.45	12	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	72/74 (97%)	45±2 (63±3%)	21±2 (29±3%)	6±2 (9±2%)	1	12
All	All	1440/1480 (97%)	901 (63%)	413 (29%)	126 (9%)	1	12

All 28 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	156	LEU	20
1	A	208	VAL	13

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Mol	Chain	Res	Type	Models (Total)
1	A	181	GLN	12
1	A	203	THR	12
1	A	161	VAL	10
1	A	200	VAL	9
1	A	202	ARG	6
1	A	176	GLY	6
1	A	212	LEU	4
1	A	214	GLU	3
1	A	174	GLY	3
1	A	201	VAL	3
1	A	183	LEU	3
1	A	225	LEU	2
1	A	209	SER	2
1	A	178	GLY	2
1	A	199	ALA	2
1	A	204	VAL	2
1	A	157	ASN	2
1	A	194	LEU	2
1	A	180	LEU	1
1	A	158	GLU	1
1	A	175	THR	1
1	A	196	GLY	1
1	A	192	VAL	1
1	A	205	ARG	1
1	A	219	ILE	1
1	A	177	GLY	1

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	62/63 (98%)	44±2 (71±3%)	18±2 (29±3%)	1	18
All	All	1240/1260 (98%)	876 (71%)	364 (29%)	1	18

All 46 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	194	LEU	19
1	A	169	ARG	18
1	A	163	LYS	17
1	A	171	TYR	16
1	A	213	ARG	16
1	A	220	GLN	16
1	A	168	ILE	16
1	A	157	ASN	15
1	A	211	LYS	15
1	A	180	LEU	14
1	A	202	ARG	13
1	A	181	GLN	12
1	A	210	LYS	12
1	A	186	LYS	11
1	A	214	GLU	10
1	A	215	LYS	9
1	A	162	GLU	8
1	A	223	GLN	8
1	A	158	GLU	8
1	A	193	ARG	8
1	A	218	SER	7
1	A	155	GLU	6
1	A	159	GLU	6
1	A	195	THR	6
1	A	226	SER	6
1	A	205	ARG	6
1	A	203	THR	5
1	A	225	LEU	5
1	A	164	VAL	5
1	A	154	LEU	5
1	A	184	MET	5
1	A	212	LEU	4
1	A	224	LEU	4
1	A	219	ILE	4
1	A	190	VAL	3
1	A	216	ILE	3
1	A	167	GLU	3
1	A	191	LYS	3
1	A	200	VAL	3
1	A	222	VAL	3
1	A	172	LEU	3
1	A	185	ILE	2
1	A	209	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	201	VAL	2
1	A	175	THR	1
1	A	156	LEU	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 oligosaccharides 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