



Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 03:31 AM UTC

PDB ID : 1LY7 / pdb_00001ly7
Title : The solution structure of the the c-terminal domain of frataxin, the protein responsible for friedreich ataxia
Authors : Musco, G.; Stier, G.; Kolmerer, B.; Adinolfi, S.; Martin, S.; Frenkiel, T.; Gibson, T.; Pastore, A.
Deposited on : 2002-06-07

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<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

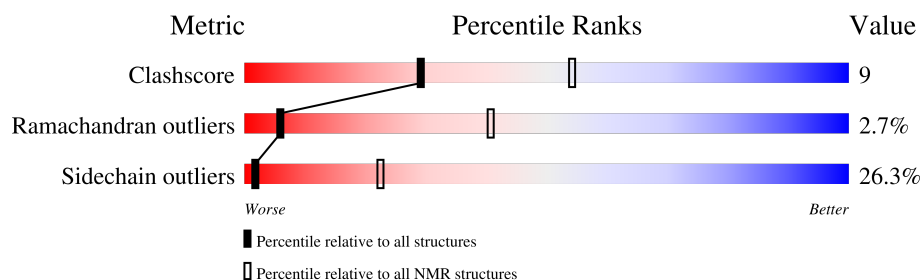
1 Overall quality at a glance

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	121	

2 Ensemble composition and analysis

This entry contains 15 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 15 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:94-A:147, A:152-A:175, A:181-A:206 (104)	0.50	15

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, 5, 9, 13, 15
2	3, 4, 10, 11, 12, 14
3	6, 7
Single-model clusters	8

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1863 atoms, of which 909 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called frataxin.

Mol	Chain	Residues	Atoms						Trace
1	A	121	Total	C	H	N	O	S	0
			1863	608	909	149	196	1	

There is a discrepancy between the modelled and reference sequences:

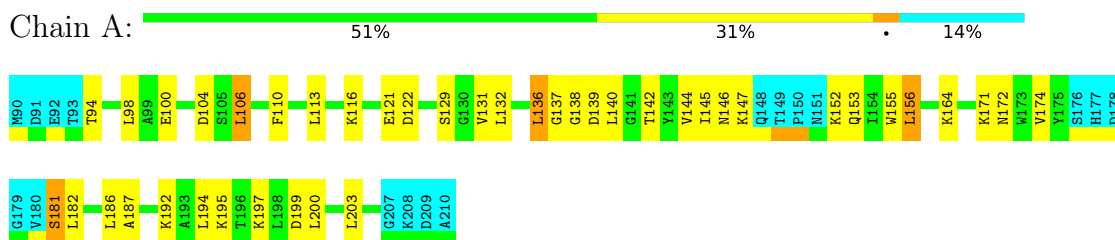
Chain	Residue	Modelled	Actual	Comment	Reference
A	90	MET	-	initiating methionine	UNP Q16595

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: frataxin

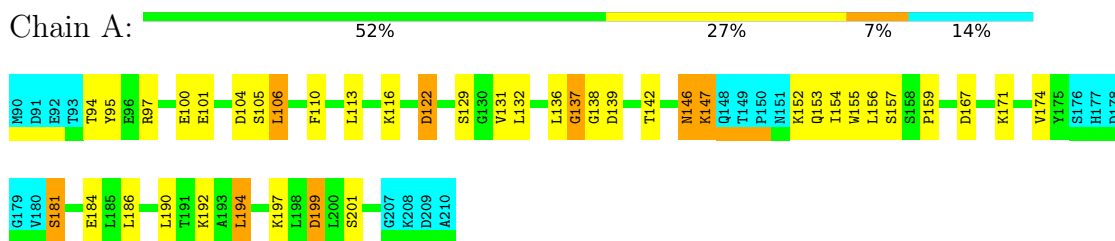


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

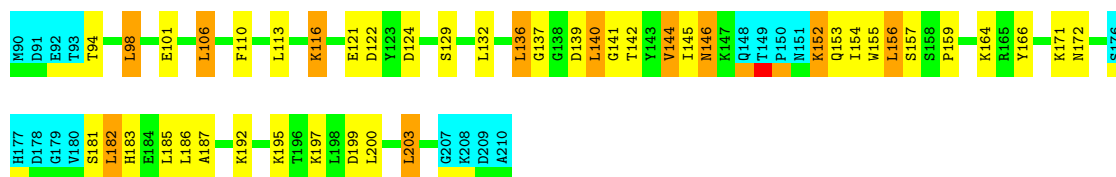
- Molecule 1: frataxin



4.2.2 Score per residue for model 2

- Molecule 1: frataxin

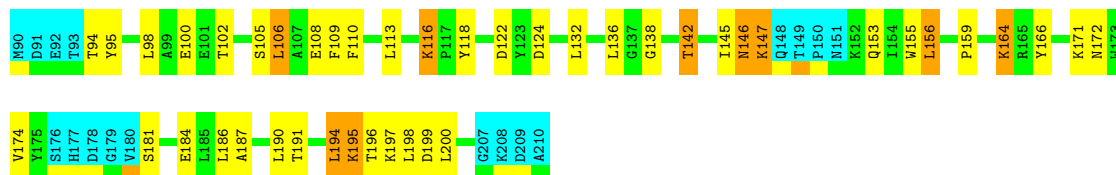




4.2.3 Score per residue for model 3

- Molecule 1: frataxin

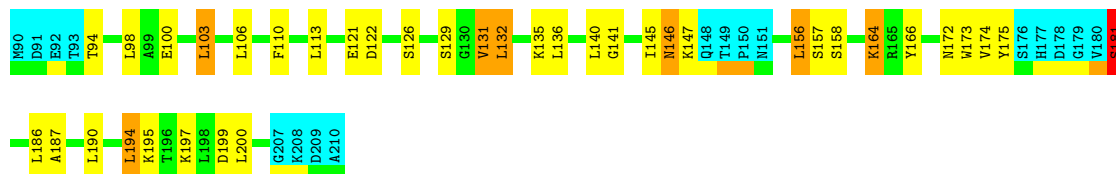
Chain A: 50% 29% 7% 14%



4.2.4 Score per residue for model 4

- Molecule 1: frataxin

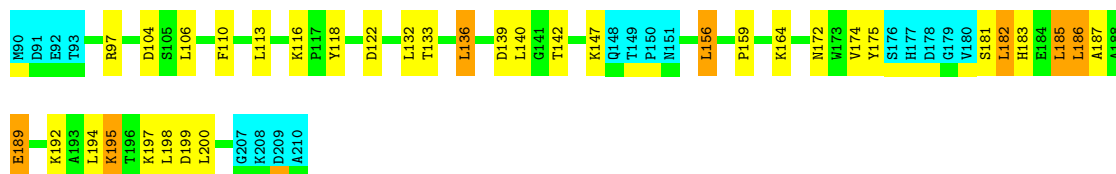
Chain A: 55% 25% 6% 14%



4.2.5 Score per residue for model 5

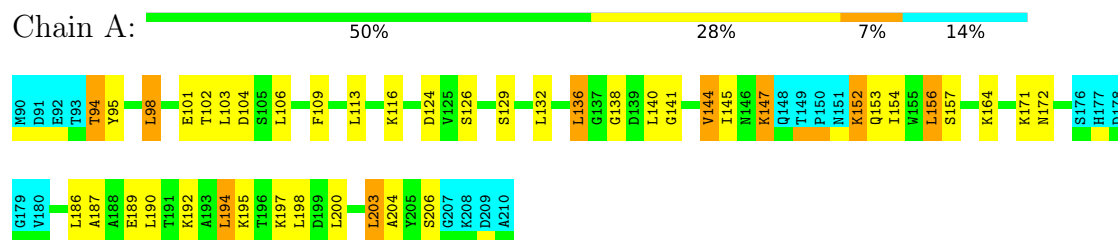
- Molecule 1: frataxin

Chain A: 57% 23% 6% 14%



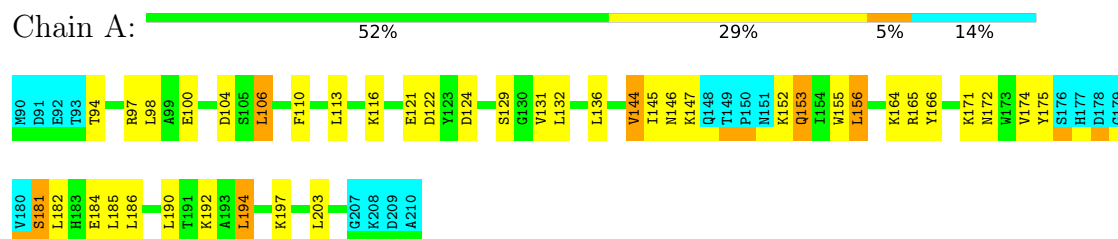
4.2.6 Score per residue for model 6

- Molecule 1: frataxin



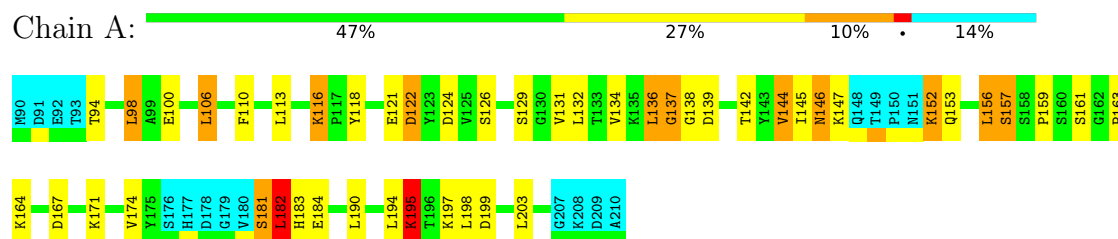
4.2.7 Score per residue for model 7

- Molecule 1: frataxin



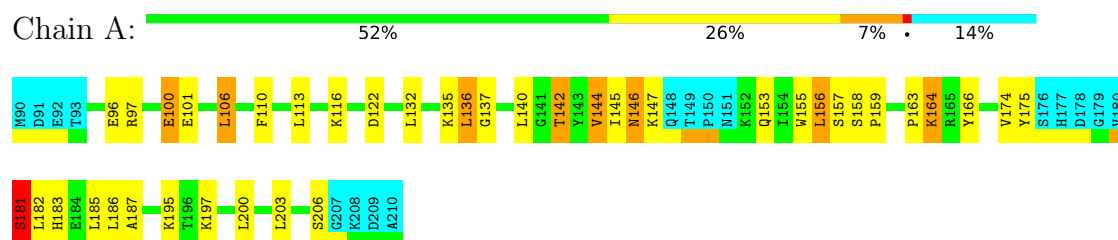
4.2.8 Score per residue for model 8

- Molecule 1: frataxin



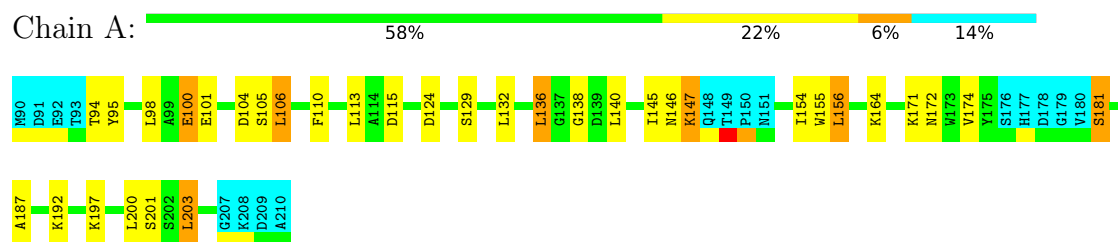
4.2.9 Score per residue for model 9

- Molecule 1: frataxin



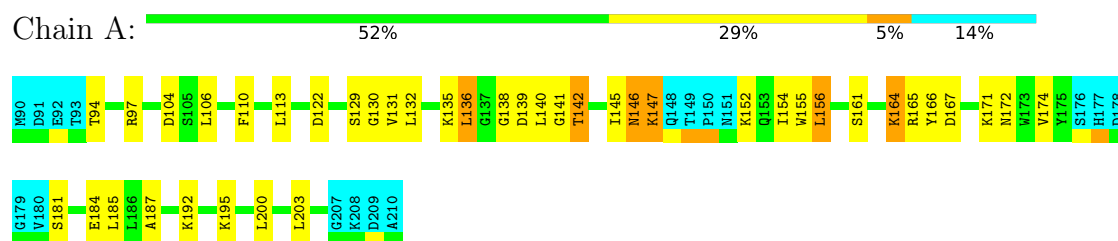
4.2.10 Score per residue for model 10

- Molecule 1: frataxin



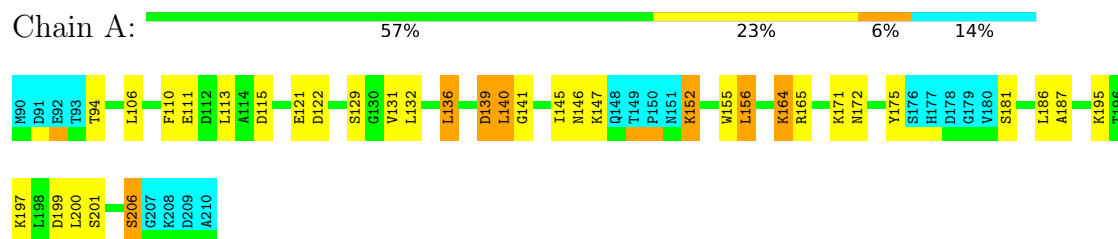
4.2.11 Score per residue for model 11

- Molecule 1: frataxin



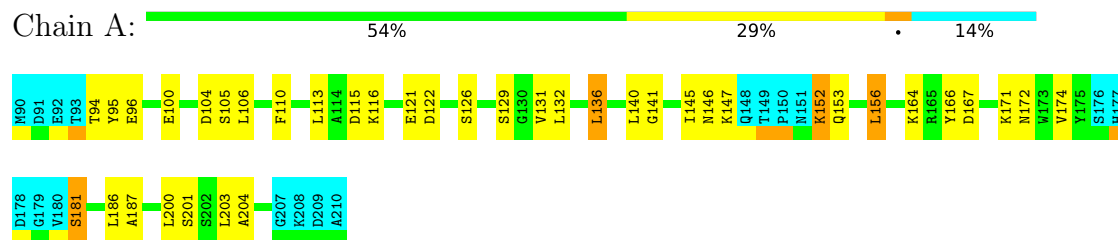
4.2.12 Score per residue for model 12

- Molecule 1: frataxin



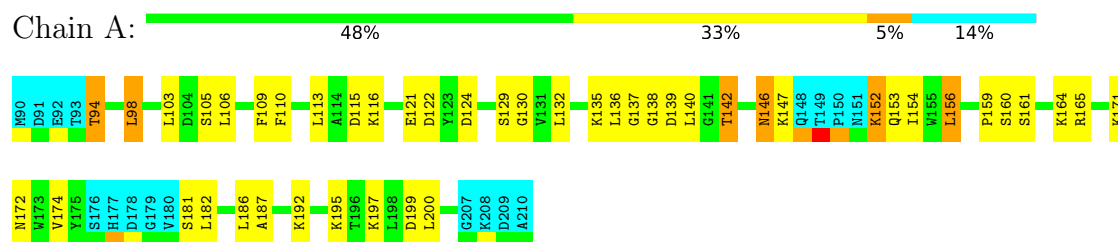
4.2.13 Score per residue for model 13

- Molecule 1: frataxin



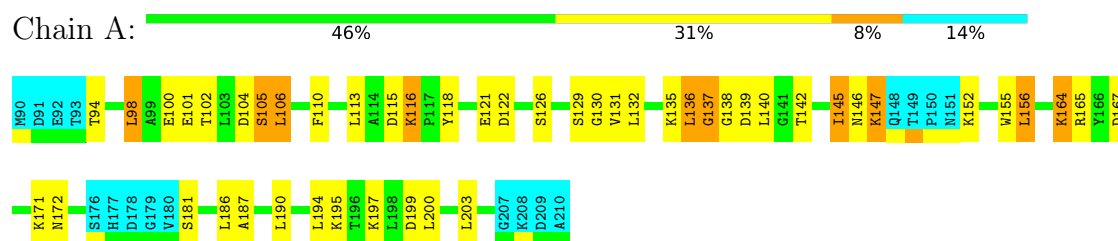
4.2.14 Score per residue for model 14

- Molecule 1: frataxin



4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: frataxin



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 15 were deposited, based on the following criterion: *structures with favorable non-bond energy*.

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

Software name	Classification	Version
ARIA	structure solution	1.0
ARIA	refinement	1.0

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	829	811	810	15±4
All	All	12435	12156	12150	228

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:LEU:HD13	1:A:140:LEU:HD23	0.80	1.53	9	9
1:A:131:VAL:HG23	1:A:146:ASN:HB3	0.74	1.57	11	6
1:A:166:TYR:HA	1:A:175:TYR:HB2	0.67	1.67	7	2
1:A:174:VAL:HG22	1:A:181:SER:HB2	0.67	1.65	7	5
1:A:156:LEU:HB3	1:A:164:LYS:HB2	0.65	1.68	12	7
1:A:94:THR:HG22	1:A:98:LEU:HD13	0.64	1.70	8	6
1:A:157:SER:HA	1:A:163:PRO:HA	0.62	1.70	8	2
1:A:110:PHE:HA	1:A:113:LEU:HD12	0.62	1.69	15	13
1:A:187:ALA:HB2	1:A:200:LEU:HB2	0.60	1.72	4	6
1:A:110:PHE:CZ	1:A:186:LEU:HD21	0.60	2.32	5	1
1:A:106:LEU:HG	1:A:203:LEU:HD21	0.59	1.72	10	4
1:A:130:GLY:HA2	1:A:147:LYS:HD3	0.59	1.73	11	2
1:A:113:LEU:HA	1:A:116:LYS:HD2	0.59	1.75	3	1
1:A:122:ASP:HB3	1:A:137:GLY:HA3	0.58	1.74	2	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:LYS:HD2	1:A:154:ILE:HG12	0.57	1.76	10	1
1:A:146:ASN:ND2	1:A:155:TRP:HB2	0.57	2.14	9	6
1:A:113:LEU:HD23	1:A:116:LYS:HE2	0.56	1.76	2	1
1:A:187:ALA:HA	1:A:200:LEU:HD13	0.56	1.77	11	9
1:A:147:LYS:HA	1:A:154:ILE:HG12	0.56	1.77	11	4
1:A:174:VAL:HG13	1:A:181:SER:N	0.55	2.17	3	2
1:A:146:ASN:HD21	1:A:155:TRP:HB2	0.54	1.63	11	2
1:A:105:SER:HB2	1:A:203:LEU:HG	0.54	1.78	15	1
1:A:136:LEU:CD2	1:A:136:LEU:N	0.54	2.70	8	1
1:A:134:VAL:HG12	1:A:136:LEU:CD2	0.54	2.32	8	1
1:A:174:VAL:HA	1:A:181:SER:HA	0.54	1.79	14	3
1:A:95:TYR:HB2	1:A:152:LYS:HD3	0.53	1.80	6	3
1:A:200:LEU:HD23	1:A:203:LEU:HD22	0.53	1.79	6	1
1:A:200:LEU:HD23	1:A:203:LEU:HD11	0.53	1.81	11	2
1:A:190:LEU:HD12	1:A:198:LEU:HD11	0.52	1.81	3	1
1:A:174:VAL:HG22	1:A:181:SER:HB3	0.52	1.80	13	5
1:A:135:LYS:HA	1:A:142:THR:HG23	0.51	1.82	15	3
1:A:145:ILE:HG13	1:A:156:LEU:HD23	0.51	1.83	4	2
1:A:113:LEU:HA	1:A:116:LYS:HD3	0.50	1.83	2	1
1:A:190:LEU:O	1:A:194:LEU:HB2	0.49	2.07	1	6
1:A:142:THR:H	1:A:159:PRO:HG3	0.49	1.67	9	7
1:A:103:LEU:HD11	1:A:147:LYS:HB3	0.49	1.85	14	2
1:A:174:VAL:HG22	1:A:181:SER:CB	0.49	2.38	7	1
1:A:103:LEU:HA	1:A:106:LEU:HB2	0.49	1.85	6	1
1:A:102:THR:O	1:A:106:LEU:HD12	0.48	2.08	15	2
1:A:131:VAL:HG12	1:A:146:ASN:HB2	0.48	1.85	4	1
1:A:153:GLN:HB3	1:A:165:ARG:HG2	0.48	1.84	7	1
1:A:130:GLY:HA3	1:A:147:LYS:HE2	0.48	1.83	15	1
1:A:190:LEU:HB2	1:A:198:LEU:HD12	0.48	1.85	6	2
1:A:145:ILE:CG1	1:A:156:LEU:HD23	0.47	2.39	11	10
1:A:106:LEU:HD11	1:A:183:HIS:CD2	0.47	2.44	9	1
1:A:136:LEU:HD12	1:A:141:GLY:C	0.47	2.35	4	6
1:A:103:LEU:N	1:A:103:LEU:HD13	0.47	2.24	4	1
1:A:194:LEU:O	1:A:195:LYS:C	0.47	2.56	8	3
1:A:106:LEU:HD22	1:A:203:LEU:HG	0.47	1.87	6	1
1:A:155:TRP:HA	1:A:164:LYS:O	0.47	2.10	12	5
1:A:194:LEU:C	1:A:195:LYS:HD2	0.46	2.36	5	1
1:A:155:TRP:NE1	1:A:165:ARG:HG3	0.46	2.25	7	1
1:A:156:LEU:O	1:A:156:LEU:HD13	0.46	2.11	2	2
1:A:182:LEU:HD23	1:A:186:LEU:HD23	0.46	1.87	2	2
1:A:166:TYR:HB3	1:A:173:TRP:HB3	0.46	1.86	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:LEU:CD1	1:A:203:LEU:HD21	0.45	2.41	6	1
1:A:109:PHE:HZ	1:A:198:LEU:HD22	0.45	1.71	3	1
1:A:118:TYR:CE2	1:A:196:THR:HG21	0.45	2.46	3	1
1:A:134:VAL:HG12	1:A:136:LEU:HD21	0.45	1.88	8	1
1:A:144:VAL:HB	1:A:157:SER:HB3	0.45	1.88	6	1
1:A:191:THR:HA	1:A:196:THR:O	0.44	2.12	3	1
1:A:134:VAL:O	1:A:136:LEU:HD23	0.44	2.11	8	1
1:A:201:SER:HA	1:A:206:SER:OG	0.44	2.12	12	1
1:A:146:ASN:OD1	1:A:155:TRP:HB2	0.44	2.13	7	1
1:A:153:GLN:HA	1:A:166:TYR:O	0.44	2.13	13	2
1:A:156:LEU:HD12	1:A:164:LYS:HG3	0.43	1.89	5	1
1:A:113:LEU:HD22	1:A:118:TYR:OH	0.43	2.12	5	2
1:A:102:THR:O	1:A:106:LEU:HD23	0.43	2.13	6	1
1:A:126:SER:O	1:A:132:LEU:HD23	0.43	2.14	4	1
1:A:183:HIS:HB3	1:A:203:LEU:HD12	0.43	1.91	9	1
1:A:174:VAL:HG13	1:A:181:SER:HA	0.43	1.90	7	1
1:A:144:VAL:C	1:A:145:ILE:HG13	0.43	2.39	6	5
1:A:109:PHE:O	1:A:113:LEU:HG	0.43	2.14	6	2
1:A:106:LEU:HD11	1:A:203:LEU:HD21	0.42	1.89	6	1
1:A:116:LYS:HB3	1:A:118:TYR:HD1	0.42	1.74	3	2
1:A:102:THR:HA	1:A:204:ALA:HB3	0.42	1.91	6	1
1:A:198:LEU:HD13	1:A:200:LEU:HD11	0.42	1.91	5	1
1:A:144:VAL:O	1:A:156:LEU:HA	0.42	2.14	7	1
1:A:156:LEU:HD22	1:A:156:LEU:C	0.42	2.40	7	2
1:A:166:TYR:OH	1:A:185:LEU:HD22	0.42	2.15	11	2
1:A:96:GLU:O	1:A:100:GLU:HB2	0.42	2.15	9	1
1:A:165:ARG:HG3	1:A:175:TYR:HE1	0.41	1.75	12	1
1:A:146:ASN:O	1:A:154:ILE:HA	0.41	2.15	14	1
1:A:154:ILE:O	1:A:166:TYR:HB2	0.41	2.15	2	1
1:A:113:LEU:HA	1:A:116:LYS:HE2	0.41	1.91	15	1
1:A:185:LEU:O	1:A:189:GLU:HB2	0.41	2.16	5	1
1:A:106:LEU:HD23	1:A:110:PHE:HE2	0.41	1.75	1	1
1:A:187:ALA:CA	1:A:200:LEU:HD13	0.41	2.46	6	3
1:A:182:LEU:O	1:A:185:LEU:HB3	0.41	2.15	5	1
1:A:95:TYR:OH	1:A:147:LYS:HB2	0.40	2.15	3	1
1:A:100:GLU:O	1:A:104:ASP:HB2	0.40	2.16	10	1
1:A:182:LEU:C	1:A:182:LEU:CD2	0.40	2.95	8	1
1:A:185:LEU:HD23	1:A:186:LEU:HD22	0.40	1.93	2	1
1:A:152:LYS:C	1:A:153:GLN:HG3	0.40	2.42	14	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	104/121 (86%)	82±2 (79±2%)	19±3 (19±3%)	3±2 (3±2%)	6	41
All	All	1560/1815 (86%)	1228 (79%)	290 (19%)	42 (3%)	6	41

All 13 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	138	GLY	8
1	A	199	ASP	7
1	A	152	LYS	5
1	A	182	LEU	4
1	A	129	SER	4
1	A	137	GLY	3
1	A	139	ASP	3
1	A	181	SER	2
1	A	140	LEU	2
1	A	187	ALA	1
1	A	153	GLN	1
1	A	195	LYS	1
1	A	204	ALA	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	90/104 (87%)	66±3 (74±3%)	24±3 (26±3%)	2	22
All	All	1350/1560 (87%)	995 (74%)	355 (26%)	2	22

All 59 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	132	LEU	15
1	A	156	LEU	15
1	A	106	LEU	14
1	A	136	LEU	14
1	A	147	LYS	13
1	A	197	LYS	13
1	A	171	LYS	12
1	A	172	ASN	12
1	A	116	LYS	11
1	A	195	LYS	11
1	A	181	SER	10
1	A	186	LEU	10
1	A	100	GLU	9
1	A	122	ASP	9
1	A	146	ASN	9
1	A	164	LYS	9
1	A	94	THR	8
1	A	129	SER	8
1	A	192	LYS	8
1	A	98	LEU	8
1	A	121	GLU	8
1	A	104	ASP	7
1	A	124	ASP	7
1	A	152	LYS	7
1	A	101	GLU	6
1	A	105	SER	6
1	A	139	ASP	6
1	A	97	ARG	5
1	A	167	ASP	5
1	A	184	GLU	5
1	A	194	LEU	5
1	A	144	VAL	5
1	A	115	ASP	5
1	A	157	SER	4
1	A	203	LEU	4
1	A	142	THR	4
1	A	126	SER	4
1	A	199	ASP	3
1	A	201	SER	3
1	A	183	HIS	3
1	A	153	GLN	3
1	A	206	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	A	161	SER	3
1	A	165	ARG	3
1	A	131	VAL	2
1	A	140	LEU	2
1	A	145	ILE	2
1	A	135	LYS	2
1	A	158	SER	2
1	A	185	LEU	2
1	A	189	GLU	2
1	A	182	LEU	2
1	A	108	GLU	1
1	A	103	LEU	1
1	A	133	THR	1
1	A	175	TYR	1
1	A	111	GLU	1
1	A	96	GLU	1
1	A	160	SER	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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided