



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 02:26 PM UTC

PDB ID : 1XWN / pdb_00001xwn
Title : solution structure of cyclophilin like 1(PPIL1) and insights into its interaction with SKIP
Authors : Xu, C.; Xu, Y.; Tang, Y.; Wu, J.; Shi, Y.; Huang, Q.; Zhang, Q.
Deposited on : 2004-11-01

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

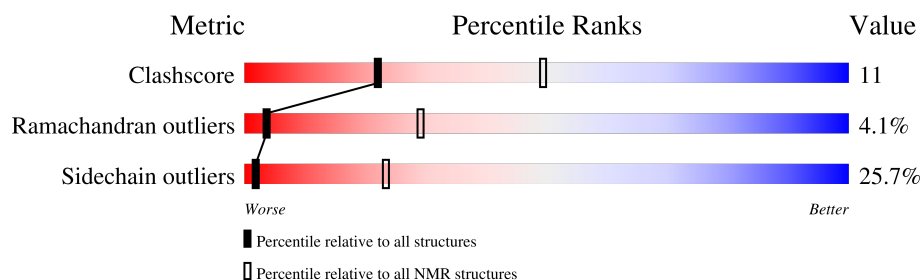
1 Overall quality at a glance

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	174	

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:12-A:65, A:75-A:166 (146)	1.08	7

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 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2548 atoms, of which 1265 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase like 1.

Mol	Chain	Residues	Atoms						Trace
1	A	166	Total	C	H	N	O	S	0
			2548	818	1265	222	235	8	

There are 8 discrepancies between the modelled and reference sequences:

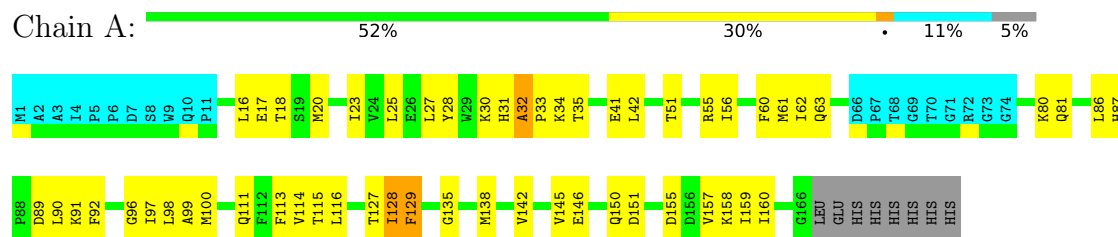
Chain	Residue	Modelled	Actual	Comment	Reference
A	167	LEU	-	expression tag	UNP Q9Y3C6
A	168	GLU	-	expression tag	UNP Q9Y3C6
A	169	HIS	-	expression tag	UNP Q9Y3C6
A	170	HIS	-	expression tag	UNP Q9Y3C6
A	171	HIS	-	expression tag	UNP Q9Y3C6
A	172	HIS	-	expression tag	UNP Q9Y3C6
A	173	HIS	-	expression tag	UNP Q9Y3C6
A	174	HIS	-	expression tag	UNP Q9Y3C6

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: Peptidyl-prolyl cis-trans isomerase like 1

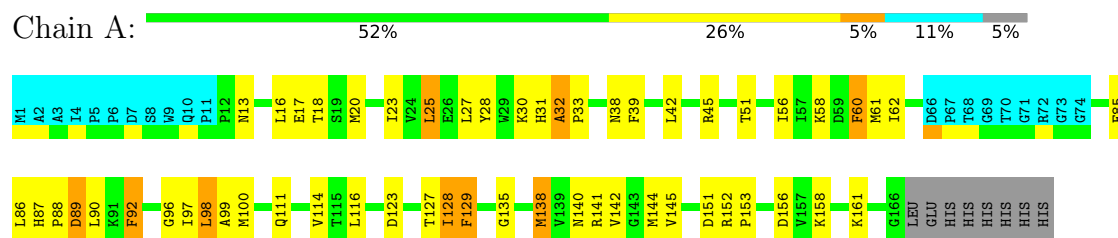


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

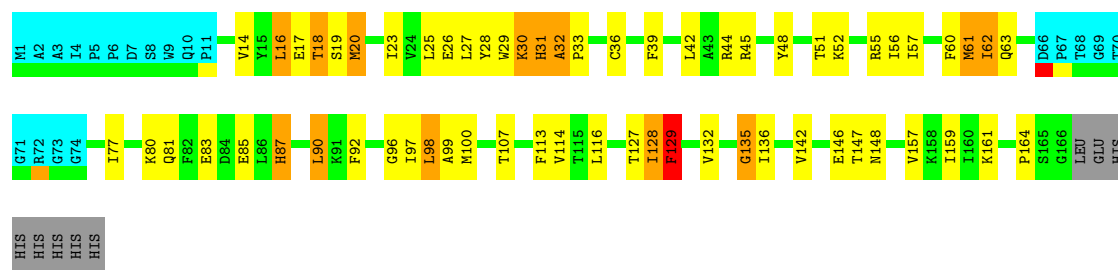
- Molecule 1: Peptidyl-prolyl cis-trans isomerase like 1



4.2.2 Score per residue for model 2

- Molecule 1: Peptidyl-prolyl cis-trans isomerase like 1

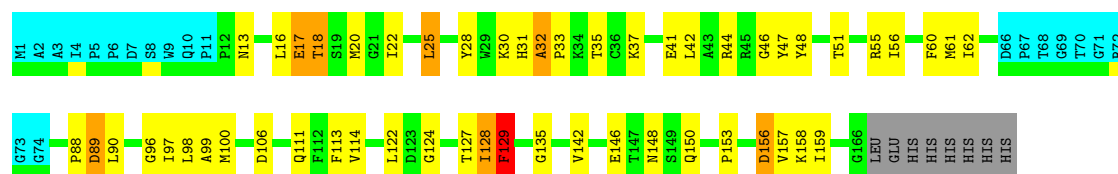




4.2.3 Score per residue for model 3

- Molecule 1: Peptidyl-prolyl cis-trans isomerase like 1

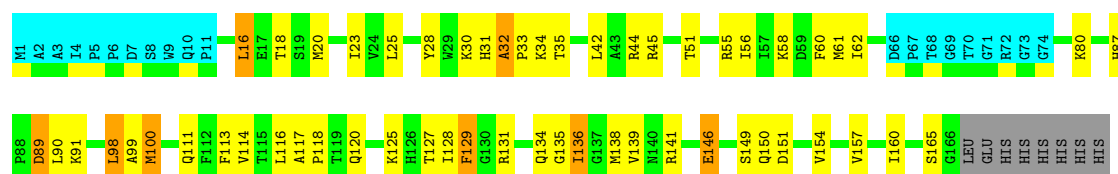
Chain A: 53% 26% 11% 5%



4.2.4 Score per residue for model 4

- Molecule 1: Peptidyl-prolyl cis-trans isomerase like 1

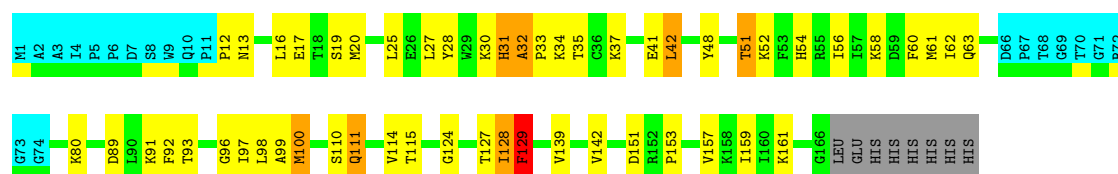
Chain A: 52% 28% 5% 11% 5%

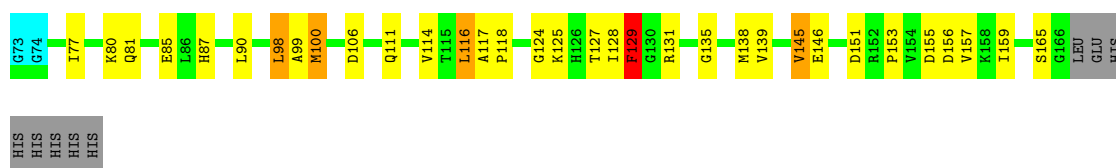


4.2.5 Score per residue for model 5

- Molecule 1: Peptidyl-prolyl cis-trans isomerase like 1

Chain A: 53% 26% 11% 5%

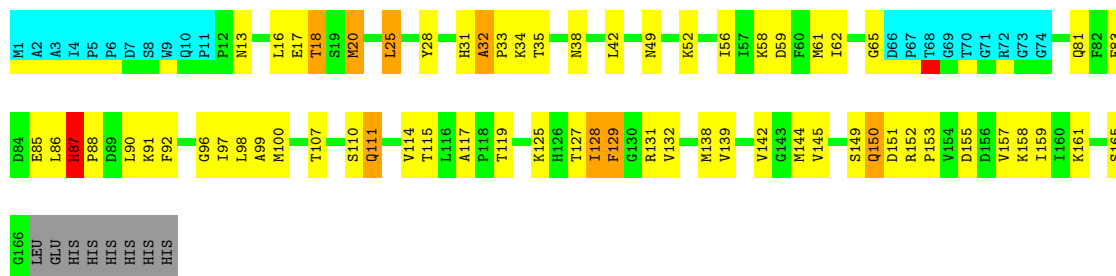




4.2.10 Score per residue for model 10

- Molecule 1: Peptidyl-prolyl cis-trans isomerase like 1

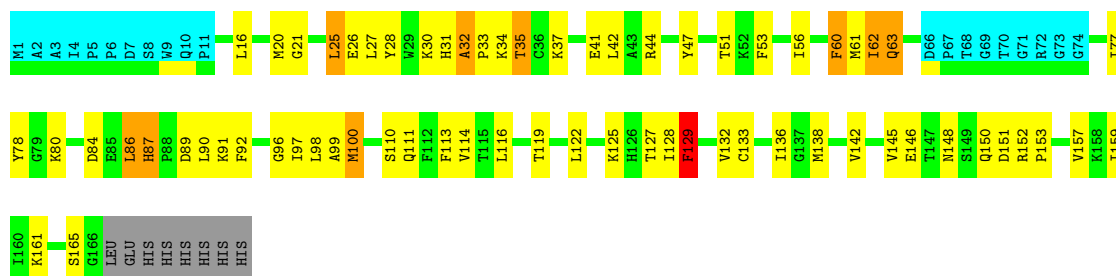
Chain A: 47% 32% 5% • 11% 5%



4.2.11 Score per residue for model 11

- Molecule 1: Peptidyl-prolyl cis-trans isomerase like 1

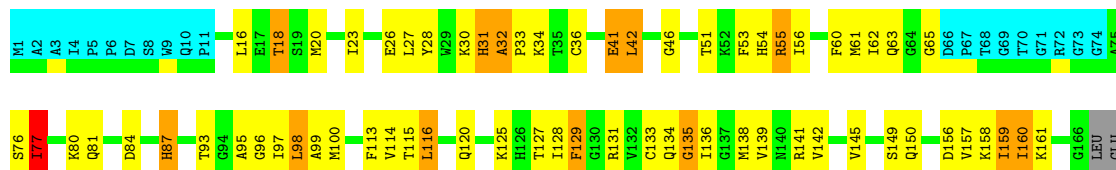
Chain A: 45% 33% 5% • 11% 5%



4.2.12 Score per residue for model 12

- Molecule 1: Peptidyl-prolyl cis-trans isomerase like 1

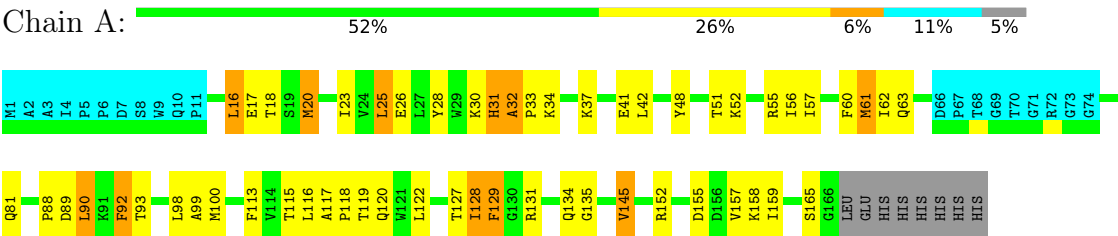
Chain A: 46% 30% 7% • 11% 5%



HIS

4.2.20 Score per residue for model 20

- Molecule 1: Peptidyl-prolyl cis-trans isomerase like 1



5 Refinement protocol and experimental data overview

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

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
CNS	refinement	1.1

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	1143	1135	1131	26±4
All	All	22860	22700	22620	522

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:ILE:HG23	1:A:62:ILE:HG22	0.86	1.48	13	4
1:A:90:LEU:HD22	1:A:128:ILE:HG21	0.85	1.47	4	6
1:A:90:LEU:HG	1:A:128:ILE:HG21	0.79	1.53	11	2
1:A:90:LEU:HB3	1:A:128:ILE:HD13	0.75	1.59	1	3
1:A:20:MET:HB2	1:A:157:VAL:HG13	0.75	1.58	18	10
1:A:98:LEU:HD13	1:A:114:VAL:HG22	0.74	1.59	14	1
1:A:119:THR:HG22	1:A:121:TRP:CZ2	0.73	2.19	7	2
1:A:56:ILE:HD13	1:A:153:PRO:HG3	0.73	1.60	19	1
1:A:28:TYR:O	1:A:32:ALA:HB3	0.72	1.84	5	20
1:A:20:MET:HB2	1:A:157:VAL:HG23	0.72	1.61	4	5
1:A:81:GLN:CB	1:A:107:THR:HG23	0.72	2.15	18	2
1:A:99:ALA:HB3	1:A:113:PHE:CE1	0.70	2.22	2	11
1:A:56:ILE:HD12	1:A:153:PRO:HB3	0.70	1.63	1	1
1:A:56:ILE:HG23	1:A:62:ILE:HG12	0.69	1.64	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:VAL:CG1	1:A:139:VAL:HG11	0.69	2.16	17	2
1:A:141:ARG:O	1:A:145:VAL:HG13	0.69	1.87	1	2
1:A:25:LEU:HD12	1:A:132:VAL:HG12	0.68	1.64	17	1
1:A:99:ALA:HB3	1:A:113:PHE:CZ	0.68	2.23	20	11
1:A:53:PHE:HB3	1:A:56:ILE:HD11	0.67	1.67	13	5
1:A:20:MET:HG2	1:A:142:VAL:HG22	0.67	1.66	6	3
1:A:32:ALA:N	1:A:33:PRO:CD	0.67	2.58	1	20
1:A:20:MET:HE3	1:A:141:ARG:CD	0.67	2.20	13	1
1:A:99:ALA:HB1	1:A:127:THR:O	0.66	1.90	12	20
1:A:56:ILE:HD12	1:A:153:PRO:HG2	0.66	1.66	11	1
1:A:16:LEU:HD12	1:A:25:LEU:CD1	0.65	2.22	20	3
1:A:51:THR:HB	1:A:159:ILE:HD12	0.65	1.67	5	3
1:A:18:THR:CG2	1:A:159:ILE:HG23	0.65	2.21	3	1
1:A:77:ILE:HD12	1:A:78:TYR:N	0.65	2.06	11	1
1:A:31:HIS:NE2	1:A:90:LEU:HD11	0.64	2.06	9	1
1:A:138:MET:O	1:A:142:VAL:HG23	0.64	1.93	16	5
1:A:25:LEU:HD22	1:A:98:LEU:HD22	0.64	1.69	10	4
1:A:23:ILE:HG23	1:A:138:MET:HE3	0.63	1.70	8	1
1:A:20:MET:CB	1:A:157:VAL:HG13	0.63	2.24	18	7
1:A:81:GLN:HG2	1:A:107:THR:HG23	0.63	1.70	10	1
1:A:35:THR:HG21	1:A:100:MET:HG3	0.62	1.71	13	5
1:A:16:LEU:HD12	1:A:25:LEU:HD21	0.62	1.71	7	1
1:A:81:GLN:HB3	1:A:107:THR:HG23	0.62	1.70	18	2
1:A:20:MET:HB3	1:A:157:VAL:HG13	0.62	1.69	19	2
1:A:56:ILE:HD12	1:A:153:PRO:HG3	0.62	1.71	5	2
1:A:98:LEU:HG	1:A:114:VAL:HG12	0.62	1.70	9	1
1:A:27:LEU:HD12	1:A:36:CYS:SG	0.62	2.35	19	1
1:A:20:MET:HE3	1:A:141:ARG:HD2	0.61	1.71	13	1
1:A:57:ILE:HD12	1:A:61:MET:HE2	0.61	1.71	2	3
1:A:96:GLY:HA3	1:A:136:ILE:HD12	0.60	1.73	2	1
1:A:114:VAL:HG11	1:A:139:VAL:HG11	0.60	1.73	17	3
1:A:98:LEU:HD23	1:A:114:VAL:HG22	0.60	1.72	6	5
1:A:53:PHE:CD1	1:A:157:VAL:HG12	0.59	2.31	14	1
1:A:56:ILE:HG21	1:A:142:VAL:HG12	0.59	1.73	2	2
1:A:20:MET:HE2	1:A:157:VAL:HG22	0.59	1.73	13	1
1:A:21:GLY:O	1:A:138:MET:HE2	0.59	1.97	11	1
1:A:119:THR:HG22	1:A:122:LEU:HD12	0.59	1.73	11	1
1:A:56:ILE:HD13	1:A:153:PRO:HB3	0.58	1.75	9	2
1:A:56:ILE:HG23	1:A:62:ILE:HG21	0.58	1.75	11	2
1:A:51:THR:CG2	1:A:159:ILE:HD12	0.58	2.28	18	2
1:A:98:LEU:CD1	1:A:114:VAL:HG22	0.57	2.29	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:ALA:O	1:A:119:THR:HG23	0.57	1.98	17	3
1:A:146:GLU:O	1:A:154:VAL:HG23	0.57	2.00	4	1
1:A:18:THR:HG22	1:A:159:ILE:CG1	0.57	2.30	13	5
1:A:56:ILE:HA	1:A:62:ILE:HG22	0.57	1.76	16	6
1:A:16:LEU:HD12	1:A:25:LEU:HD23	0.56	1.76	15	1
1:A:55:ARG:C	1:A:56:ILE:HD12	0.56	2.24	7	2
1:A:18:THR:HG22	1:A:159:ILE:HA	0.56	1.77	9	8
1:A:20:MET:CB	1:A:157:VAL:HG23	0.56	2.31	6	4
1:A:90:LEU:HD13	1:A:128:ILE:CG1	0.56	2.30	15	1
1:A:56:ILE:HG23	1:A:62:ILE:CG2	0.56	2.30	1	4
1:A:92:PHE:CE1	1:A:99:ALA:HB2	0.56	2.36	8	2
1:A:16:LEU:HD21	1:A:48:TYR:HE2	0.55	1.60	15	1
1:A:139:VAL:O	1:A:142:VAL:HG12	0.55	2.02	5	1
1:A:56:ILE:HD13	1:A:142:VAL:CG1	0.55	2.32	15	1
1:A:93:THR:HG23	1:A:97:ILE:HD11	0.55	1.79	15	1
1:A:23:ILE:HG22	1:A:135:GLY:HA2	0.55	1.77	7	5
1:A:116:LEU:HD13	1:A:116:LEU:N	0.55	2.16	17	1
1:A:23:ILE:HG22	1:A:135:GLY:CA	0.55	2.32	14	8
1:A:20:MET:HE2	1:A:157:VAL:CG2	0.54	2.32	13	1
1:A:56:ILE:HD13	1:A:142:VAL:HG11	0.54	1.79	11	1
1:A:62:ILE:C	1:A:62:ILE:HD13	0.54	2.27	14	1
1:A:96:GLY:C	1:A:97:ILE:HD12	0.53	2.28	15	1
1:A:18:THR:HG22	1:A:159:ILE:HG23	0.53	1.79	3	1
1:A:27:LEU:HD23	1:A:36:CYS:HA	0.53	1.79	12	1
1:A:128:ILE:HG22	1:A:129:PHE:H	0.52	1.63	15	5
1:A:57:ILE:CD1	1:A:61:MET:HE2	0.52	2.34	13	1
1:A:90:LEU:CG	1:A:128:ILE:HG21	0.52	2.30	11	2
1:A:145:VAL:O	1:A:145:VAL:HG22	0.52	2.04	9	2
1:A:146:GLU:O	1:A:154:VAL:HG12	0.52	2.05	6	1
1:A:98:LEU:HD12	1:A:129:PHE:HE2	0.52	1.65	15	1
1:A:56:ILE:HG23	1:A:62:ILE:CG1	0.52	2.34	14	1
1:A:48:TYR:O	1:A:51:THR:HG22	0.51	2.05	6	2
1:A:25:LEU:HD22	1:A:25:LEU:N	0.51	2.19	16	3
1:A:61:MET:HE3	1:A:61:MET:O	0.51	2.05	16	1
1:A:51:THR:HG23	1:A:159:ILE:HD12	0.51	1.80	20	2
1:A:90:LEU:CD2	1:A:128:ILE:HG21	0.51	2.36	18	1
1:A:23:ILE:HD12	1:A:25:LEU:HD11	0.51	1.82	19	1
1:A:85:GLU:O	1:A:127:THR:HG21	0.51	2.04	13	1
1:A:142:VAL:O	1:A:145:VAL:HG22	0.51	2.06	1	2
1:A:114:VAL:HG21	1:A:139:VAL:HG11	0.51	1.83	9	2
1:A:22:ILE:C	1:A:22:ILE:HD13	0.51	2.31	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:MET:HE1	1:A:63:GLN:OE1	0.51	2.05	11	2
1:A:39:PHE:HA	1:A:42:LEU:HD12	0.51	1.81	17	1
1:A:90:LEU:HD22	1:A:128:ILE:HG13	0.51	1.83	18	1
1:A:96:GLY:CA	1:A:136:ILE:HD13	0.51	2.36	12	1
1:A:31:HIS:C	1:A:33:PRO:HD2	0.50	2.31	17	20
1:A:62:ILE:HD12	1:A:142:VAL:HG11	0.50	1.82	5	1
1:A:25:LEU:HG	1:A:98:LEU:HD11	0.50	1.83	6	1
1:A:96:GLY:O	1:A:97:ILE:HD13	0.50	2.06	5	12
1:A:116:LEU:N	1:A:116:LEU:HD22	0.50	2.22	9	1
1:A:25:LEU:CD1	1:A:132:VAL:HG12	0.50	2.36	17	1
1:A:20:MET:HG3	1:A:138:MET:HE2	0.50	1.81	4	2
1:A:20:MET:HG3	1:A:157:VAL:HG22	0.50	1.84	16	1
1:A:92:PHE:CE1	1:A:128:ILE:HD12	0.50	2.41	5	1
1:A:41:GLU:HB3	1:A:77:ILE:HD13	0.50	1.83	12	1
1:A:27:LEU:HD11	1:A:129:PHE:CD1	0.49	2.42	19	2
1:A:93:THR:OG1	1:A:97:ILE:HD11	0.49	2.06	5	1
1:A:117:ALA:HB1	1:A:118:PRO:HD2	0.49	1.84	4	5
1:A:76:SER:HB2	1:A:77:ILE:HD12	0.49	1.85	8	1
1:A:132:VAL:O	1:A:132:VAL:HG23	0.49	2.07	17	2
1:A:132:VAL:HG13	1:A:132:VAL:O	0.49	2.08	2	2
1:A:98:LEU:CD2	1:A:114:VAL:HG22	0.49	2.38	18	4
1:A:51:THR:HG21	1:A:65:GLY:O	0.49	2.08	12	1
1:A:90:LEU:HD13	1:A:128:ILE:HG22	0.49	1.84	2	1
1:A:14:VAL:HG22	1:A:27:LEU:HD11	0.49	1.84	8	1
1:A:116:LEU:HD12	1:A:116:LEU:C	0.48	2.33	4	3
1:A:57:ILE:N	1:A:57:ILE:HD12	0.48	2.23	17	1
1:A:14:VAL:HG13	1:A:164:PRO:HA	0.48	1.85	2	1
1:A:16:LEU:HD12	1:A:25:LEU:CD2	0.48	2.37	15	1
1:A:81:GLN:HB2	1:A:107:THR:HG23	0.48	1.83	18	1
1:A:119:THR:HB	1:A:122:LEU:HD12	0.48	1.86	19	1
1:A:160:ILE:N	1:A:160:ILE:HD13	0.48	2.24	7	3
1:A:97:ILE:HD12	1:A:131:ARG:HH11	0.48	1.69	17	1
1:A:116:LEU:HD22	1:A:140:ASN:HA	0.48	1.85	13	1
1:A:98:LEU:HD22	1:A:129:PHE:CE2	0.48	2.44	16	3
1:A:122:LEU:C	1:A:122:LEU:HD12	0.48	2.34	18	4
1:A:41:GLU:HB3	1:A:77:ILE:HG21	0.48	1.85	17	1
1:A:97:ILE:O	1:A:114:VAL:HG23	0.47	2.09	1	1
1:A:61:MET:HE1	1:A:63:GLN:HG3	0.47	1.84	2	1
1:A:20:MET:CG	1:A:138:MET:HE2	0.47	2.39	4	1
1:A:98:LEU:HD23	1:A:129:PHE:CZ	0.47	2.44	3	2
1:A:98:LEU:HD12	1:A:131:ARG:N	0.47	2.24	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:ILE:HD12	1:A:153:PRO:CG	0.47	2.38	15	1
1:A:51:THR:OG1	1:A:159:ILE:HD12	0.47	2.10	16	1
1:A:98:LEU:HD21	1:A:114:VAL:HG22	0.47	1.85	18	1
1:A:27:LEU:HD21	1:A:129:PHE:CE1	0.46	2.45	19	2
1:A:25:LEU:HD22	1:A:98:LEU:HD11	0.46	1.86	5	1
1:A:16:LEU:HD21	1:A:48:TYR:CE2	0.46	2.44	2	1
1:A:27:LEU:HD13	1:A:36:CYS:SG	0.46	2.50	2	1
1:A:136:ILE:O	1:A:136:ILE:HD13	0.46	2.09	8	1
1:A:62:ILE:HD11	1:A:139:VAL:HG13	0.46	1.85	12	2
1:A:16:LEU:HD12	1:A:25:LEU:HD13	0.46	1.86	3	2
1:A:42:LEU:HD22	1:A:48:TYR:CE1	0.46	2.45	5	1
1:A:114:VAL:CB	1:A:139:VAL:HG11	0.46	2.40	17	2
1:A:85:GLU:O	1:A:127:THR:HG23	0.46	2.10	17	1
1:A:95:ALA:HB1	1:A:116:LEU:O	0.46	2.10	12	1
1:A:57:ILE:HD13	1:A:61:MET:HE2	0.46	1.87	13	1
1:A:103:ALA:HB3	1:A:107:THR:O	0.46	2.10	19	1
1:A:90:LEU:CB	1:A:128:ILE:HD13	0.46	2.41	11	3
1:A:138:MET:O	1:A:138:MET:HE3	0.46	2.10	18	2
1:A:25:LEU:HB3	1:A:132:VAL:HG12	0.46	1.87	7	1
1:A:14:VAL:HG21	1:A:27:LEU:CD1	0.46	2.41	16	1
1:A:41:GLU:CB	1:A:77:ILE:HD13	0.46	2.41	16	1
1:A:55:ARG:O	1:A:56:ILE:HD13	0.45	2.12	13	3
1:A:96:GLY:O	1:A:132:VAL:HG22	0.45	2.11	17	1
1:A:27:LEU:HD11	1:A:129:PHE:CE1	0.45	2.46	18	1
1:A:57:ILE:HD12	1:A:61:MET:CE	0.45	2.41	16	1
1:A:157:VAL:HG13	1:A:157:VAL:O	0.45	2.11	10	2
1:A:98:LEU:HD12	1:A:114:VAL:HG22	0.45	1.88	10	2
1:A:23:ILE:CG2	1:A:138:MET:HE3	0.45	2.39	8	1
1:A:98:LEU:HD12	1:A:132:VAL:HG13	0.45	1.88	7	1
1:A:160:ILE:H	1:A:160:ILE:HD13	0.45	1.72	19	1
1:A:16:LEU:HD12	1:A:25:LEU:HD12	0.45	1.89	4	1
1:A:135:GLY:O	1:A:139:VAL:HG23	0.44	2.13	9	1
1:A:142:VAL:O	1:A:145:VAL:HG12	0.44	2.11	14	2
1:A:160:ILE:HD13	1:A:160:ILE:N	0.44	2.27	19	1
1:A:25:LEU:HD12	1:A:27:LEU:HD21	0.44	1.88	11	1
1:A:57:ILE:CD1	1:A:61:MET:HE3	0.44	2.42	14	1
1:A:89:ASP:O	1:A:90:LEU:HD12	0.44	2.13	20	1
1:A:114:VAL:HB	1:A:139:VAL:HG11	0.44	1.89	14	2
1:A:96:GLY:C	1:A:132:VAL:HG12	0.44	2.37	10	2
1:A:89:ASP:HB3	1:A:90:LEU:HD12	0.44	1.89	4	1
1:A:25:LEU:HD13	1:A:98:LEU:CD1	0.44	2.42	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:HIS:HB2	1:A:90:LEU:HD12	0.44	1.89	9	1
1:A:62:ILE:O	1:A:62:ILE:HG23	0.44	2.12	17	2
1:A:20:MET:HE1	1:A:155:ASP:OD2	0.43	2.13	6	1
1:A:32:ALA:N	1:A:33:PRO:HD3	0.43	2.28	15	3
1:A:142:VAL:HG13	1:A:157:VAL:HG21	0.43	1.89	14	1
1:A:61:MET:HA	1:A:116:LEU:HD23	0.43	1.89	6	1
1:A:76:SER:C	1:A:77:ILE:HD12	0.43	2.38	8	1
1:A:26:GLU:C	1:A:27:LEU:HD22	0.43	2.37	9	1
1:A:136:ILE:C	1:A:136:ILE:HD13	0.43	2.38	4	1
1:A:23:ILE:HG22	1:A:135:GLY:O	0.43	2.12	16	1
1:A:61:MET:HE1	1:A:63:GLN:HE21	0.43	1.72	8	1
1:A:77:ILE:HD11	1:A:78:TYR:CZ	0.43	2.48	18	1
1:A:136:ILE:HD13	1:A:136:ILE:O	0.43	2.13	4	1
1:A:20:MET:CG	1:A:142:VAL:HG22	0.43	2.44	3	1
1:A:20:MET:SD	1:A:157:VAL:HG22	0.43	2.53	15	2
1:A:25:LEU:HD12	1:A:25:LEU:N	0.43	2.29	2	1
1:A:87:HIS:CB	1:A:88:PRO:CD	0.43	2.96	18	2
1:A:20:MET:CE	1:A:157:VAL:HG22	0.42	2.43	13	1
1:A:53:PHE:CE1	1:A:159:ILE:HD11	0.42	2.49	16	1
1:A:115:THR:HG22	1:A:117:ALA:O	0.42	2.14	19	1
1:A:90:LEU:N	1:A:90:LEU:HD12	0.42	2.29	10	1
1:A:45:ARG:HD2	1:A:77:ILE:HG22	0.42	1.90	2	1
1:A:100:MET:HE3	1:A:111:GLN:O	0.42	2.13	5	1
1:A:53:PHE:CD1	1:A:62:ILE:HG22	0.42	2.49	9	1
1:A:154:VAL:O	1:A:154:VAL:HG22	0.42	2.14	14	1
1:A:17:GLU:HG2	1:A:22:ILE:HD12	0.42	1.90	3	1
1:A:119:THR:CB	1:A:122:LEU:HD12	0.42	2.43	20	1
1:A:56:ILE:HG12	1:A:62:ILE:HG23	0.42	1.89	3	2
1:A:100:MET:N	1:A:127:THR:O	0.42	2.53	11	2
1:A:136:ILE:HD13	1:A:136:ILE:C	0.42	2.39	8	1
1:A:158:LYS:HG2	1:A:159:ILE:N	0.42	2.29	3	1
1:A:42:LEU:HD11	1:A:76:SER:HB2	0.42	1.91	12	1
1:A:86:LEU:HA	1:A:127:THR:HG23	0.42	1.91	1	2
1:A:29:TRP:CE3	1:A:30:LYS:CD	0.42	3.03	2	1
1:A:97:ILE:HD12	1:A:97:ILE:N	0.42	2.30	15	1
1:A:28:TYR:HB2	1:A:32:ALA:HB3	0.41	1.92	2	2
1:A:42:LEU:HD13	1:A:110:SER:OG	0.41	2.15	5	1
1:A:23:ILE:HG22	1:A:135:GLY:HA3	0.41	1.90	15	1
1:A:23:ILE:N	1:A:23:ILE:HD13	0.41	2.31	18	1
1:A:56:ILE:HD13	1:A:153:PRO:CB	0.41	2.44	9	1
1:A:82:PHE:CD2	1:A:108:ASN:HB2	0.41	2.51	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ILE:HD13	1:A:23:ILE:N	0.41	2.30	9	1
1:A:89:ASP:C	1:A:90:LEU:HD12	0.41	2.41	4	1
1:A:42:LEU:HD22	1:A:48:TYR:CZ	0.41	2.50	5	1
1:A:98:LEU:HB3	1:A:129:PHE:CE2	0.41	2.50	5	1
1:A:86:LEU:N	1:A:86:LEU:HD22	0.41	2.31	14	1
1:A:56:ILE:HG12	1:A:142:VAL:HG12	0.41	1.91	19	1
1:A:146:GLU:O	1:A:154:VAL:HG22	0.41	2.15	19	1
1:A:92:PHE:CE2	1:A:128:ILE:HD12	0.41	2.51	20	1
1:A:18:THR:HG23	1:A:21:GLY:O	0.41	2.16	16	1
1:A:92:PHE:CD1	1:A:92:PHE:N	0.41	2.87	1	1
1:A:96:GLY:CA	1:A:136:ILE:HD12	0.41	2.45	2	2
1:A:61:MET:HE1	1:A:63:GLN:NE2	0.41	2.30	20	1
1:A:98:LEU:HD12	1:A:131:ARG:C	0.41	2.40	12	1
1:A:114:VAL:O	1:A:114:VAL:HG23	0.40	2.16	9	1
1:A:115:THR:HG21	1:A:119:THR:OG1	0.40	2.16	13	1
1:A:99:ALA:HA	1:A:128:ILE:HA	0.40	1.93	13	1
1:A:98:LEU:HD22	1:A:129:PHE:HE2	0.40	1.74	16	1
1:A:153:PRO:CB	1:A:157:VAL:HG23	0.40	2.46	3	1
1:A:138:MET:O	1:A:141:ARG:HG3	0.40	2.17	7	1
1:A:32:ALA:N	1:A:33:PRO:HD2	0.40	2.30	17	1
1:A:129:PHE:CD1	1:A:129:PHE:C	0.40	2.99	7	1
1:A:65:GLY:HA3	1:A:111:GLN:HB3	0.40	1.93	10	1
1:A:13:ASN:HA	1:A:25:LEU:O	0.40	2.17	15	1
1:A:25:LEU:CD1	1:A:98:LEU:HD23	0.40	2.47	15	1
1:A:98:LEU:HD12	1:A:129:PHE:CE2	0.40	2.50	15	1
1:A:157:VAL:O	1:A:157:VAL:HG13	0.40	2.17	17	1
1:A:61:MET:SD	1:A:113:PHE:CD2	0.40	3.15	19	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	145/174 (83%)	118±2 (82±2%)	21±2 (14±2%)	6±1 (4±1%)	4	29
All	All	2900/3480 (83%)	2365 (82%)	415 (14%)	120 (4%)	4	29

All 27 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	ALA	20
1	A	129	PHE	20
1	A	60	PHE	15
1	A	151	ASP	9
1	A	87	HIS	9
1	A	150	GLN	6
1	A	123	ASP	5
1	A	124	GLY	5
1	A	88	PRO	4
1	A	135	GLY	3
1	A	46	GLY	3
1	A	89	ASP	2
1	A	81	GLN	2
1	A	156	ASP	2
1	A	145	VAL	2
1	A	53	PHE	2
1	A	106	ASP	1
1	A	109	GLY	1
1	A	58	LYS	1
1	A	165	SER	1
1	A	86	LEU	1
1	A	77	ILE	1
1	A	93	THR	1
1	A	84	ASP	1
1	A	90	LEU	1
1	A	91	LYS	1
1	A	110	SER	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	120/142 (85%)	89±4 (74±3%)	31±4 (26±3%)	2	23
All	All	2400/2840 (85%)	1784 (74%)	616 (26%)	2	23

All 87 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	100	MET	20
1	A	42	LEU	19
1	A	30	LYS	17
1	A	16	LEU	16
1	A	129	PHE	16
1	A	61	MET	15
1	A	128	ILE	15
1	A	17	GLU	14
1	A	18	THR	14
1	A	34	LYS	14
1	A	80	LYS	13
1	A	87	HIS	12
1	A	158	LYS	12
1	A	41	GLU	12
1	A	91	LYS	11
1	A	115	THR	11
1	A	155	ASP	11
1	A	25	LEU	10
1	A	58	LYS	9
1	A	89	ASP	9
1	A	111	GLN	9
1	A	152	ARG	9
1	A	161	LYS	9
1	A	31	HIS	9
1	A	116	LEU	9
1	A	146	GLU	9
1	A	149	SER	9
1	A	98	LEU	8
1	A	52	LYS	8
1	A	35	THR	8
1	A	37	LYS	8
1	A	86	LEU	8
1	A	20	MET	7
1	A	92	PHE	7
1	A	138	MET	7
1	A	148	ASN	7
1	A	125	LYS	7
1	A	131	ARG	7
1	A	134	GLN	7
1	A	160	ILE	7
1	A	165	SER	7
1	A	63	GLN	7

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Mol	Chain	Res	Type	Models (Total)
1	A	145	VAL	7
1	A	13	ASN	6
1	A	45	ARG	6
1	A	51	THR	6
1	A	60	PHE	6
1	A	85	GLU	6
1	A	156	ASP	6
1	A	44	ARG	6
1	A	90	LEU	6
1	A	47	TYR	6
1	A	55	ARG	6
1	A	59	ASP	6
1	A	81	GLN	6
1	A	27	LEU	5
1	A	19	SER	5
1	A	26	GLU	5
1	A	62	ILE	5
1	A	150	GLN	5
1	A	107	THR	4
1	A	48	TYR	4
1	A	120	GLN	4
1	A	141	ARG	4
1	A	151	ASP	4
1	A	84	ASP	4
1	A	110	SER	4
1	A	133	CYS	4
1	A	39	PHE	3
1	A	144	MET	3
1	A	83	GLU	3
1	A	106	ASP	3
1	A	38	ASN	2
1	A	140	ASN	2
1	A	147	THR	2
1	A	122	LEU	2
1	A	136	ILE	2
1	A	54	HIS	2
1	A	76	SER	2
1	A	77	ILE	2
1	A	49	ASN	2
1	A	93	THR	2
1	A	22	ILE	1
1	A	159	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	119	THR	1
1	A	23	ILE	1
1	A	163	TYR	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