



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 03:36 AM UTC

PDB ID : 1Q27 / pdb_00001q27
Title : NMR Solution Structure of DR0079: An hypothetical Nudix protein from D. radiodurans
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Deposited on : 2003-07-23

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

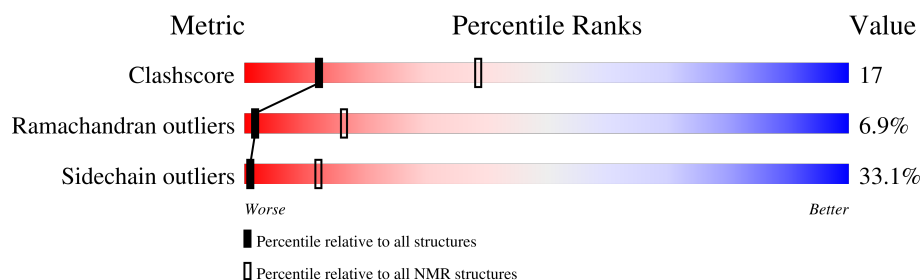
1 Overall quality at a glance

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	171	39% 48% • 10%

2 Ensemble composition and analysis

This entry contains 10 models. Model 6 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:7-A:53, A:62-A:168 (154)	1.67	6

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 6, 8, 9, 10
2	4, 5, 7
3	1, 3

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2683 atoms, of which 1324 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative Nudix hydrolase DR0079.

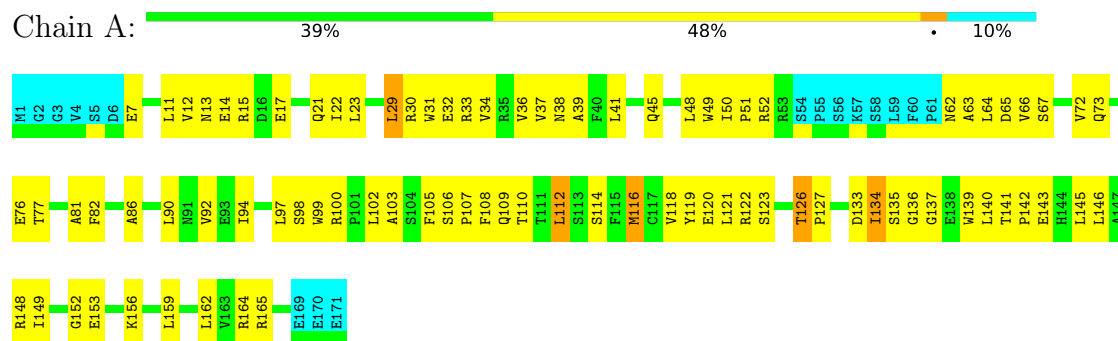
Mol	Chain	Residues	Atoms						Trace
1	A	171	Total	C	H	N	O	S	0
			2683	847	1324	245	263	4	

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: Putative Nudix hydrolase DR0079

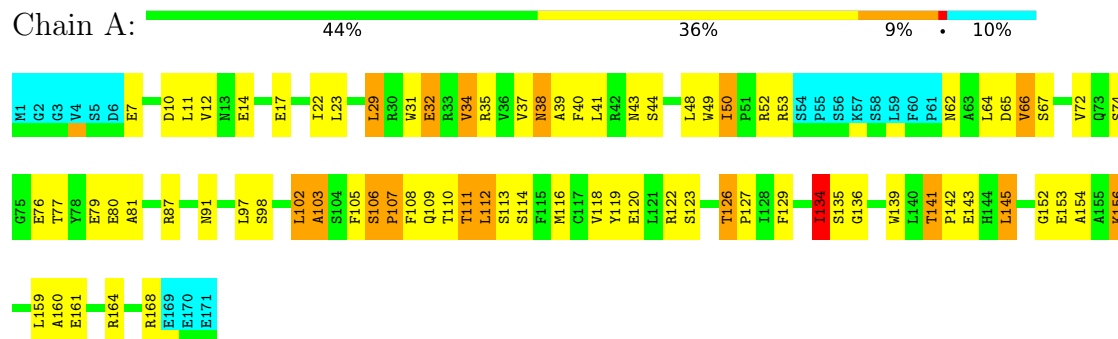


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

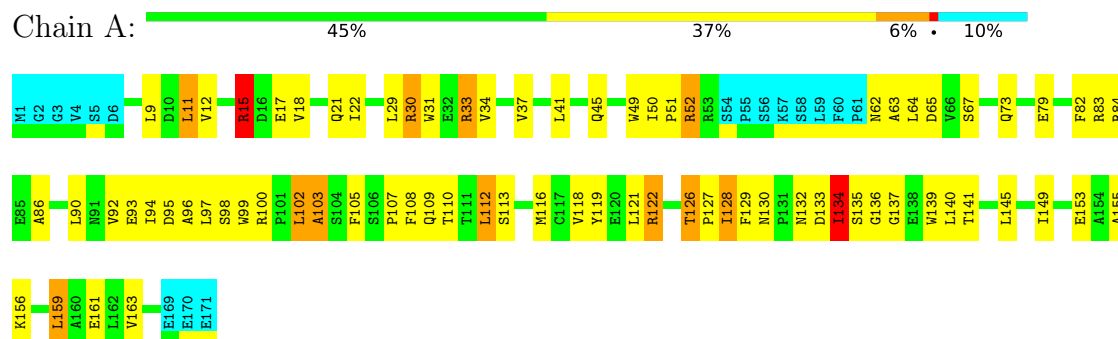
4.2.1 Score per residue for model 1

- Molecule 1: Putative Nudix hydrolase DR0079



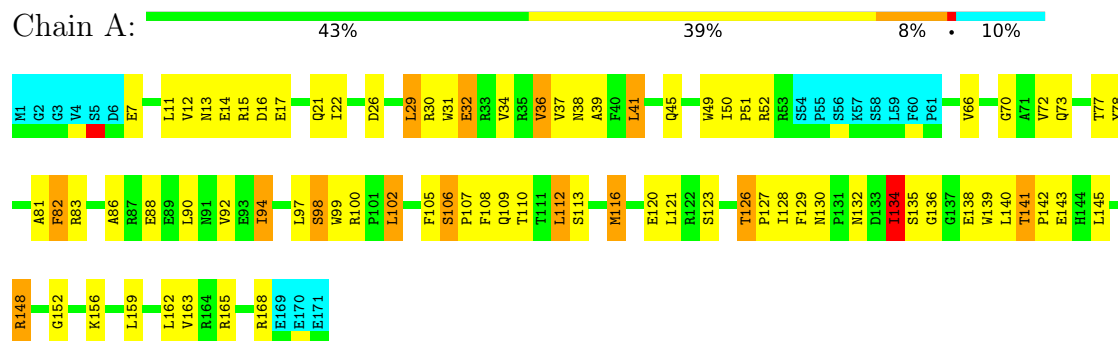
4.2.2 Score per residue for model 2

- Molecule 1: Putative Nudix hydrolase DR0079



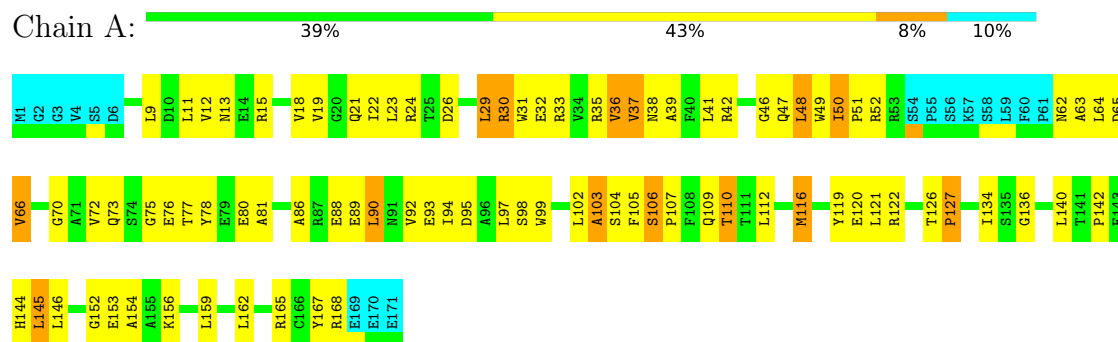
4.2.3 Score per residue for model 3

- Molecule 1: Putative Nudix hydrolase DR0079



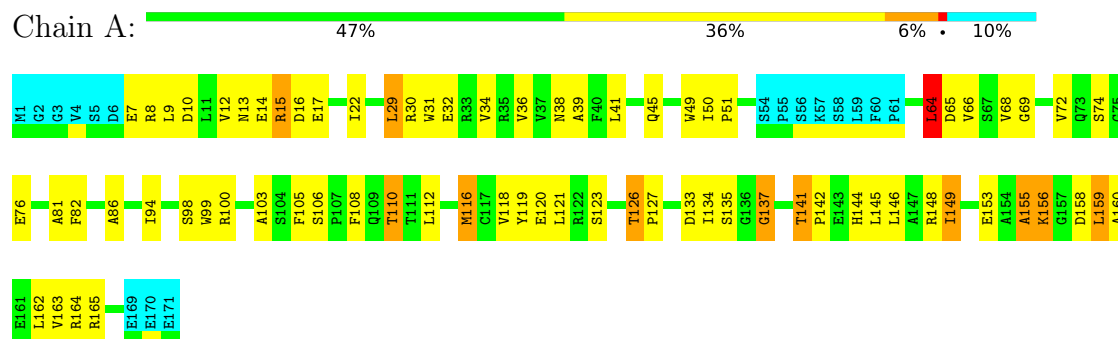
4.2.4 Score per residue for model 4

- Molecule 1: Putative Nudix hydrolase DR0079



4.2.5 Score per residue for model 5

- Molecule 1: Putative Nudix hydrolase DR0079



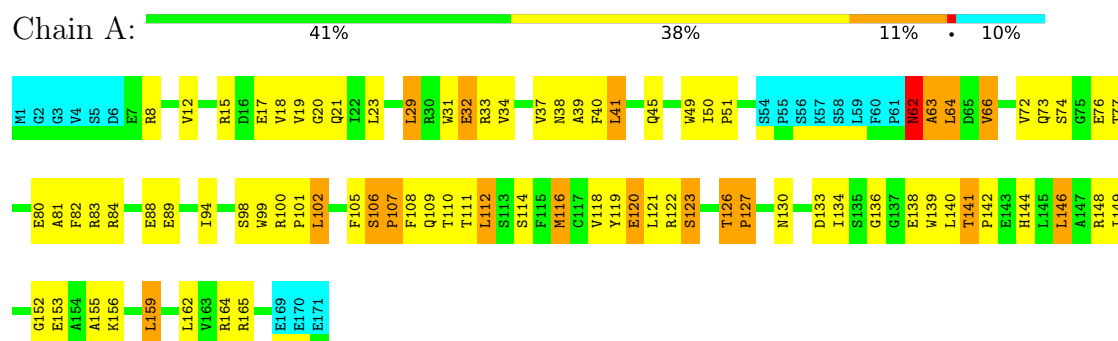
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Putative Nudix hydrolase DR0079



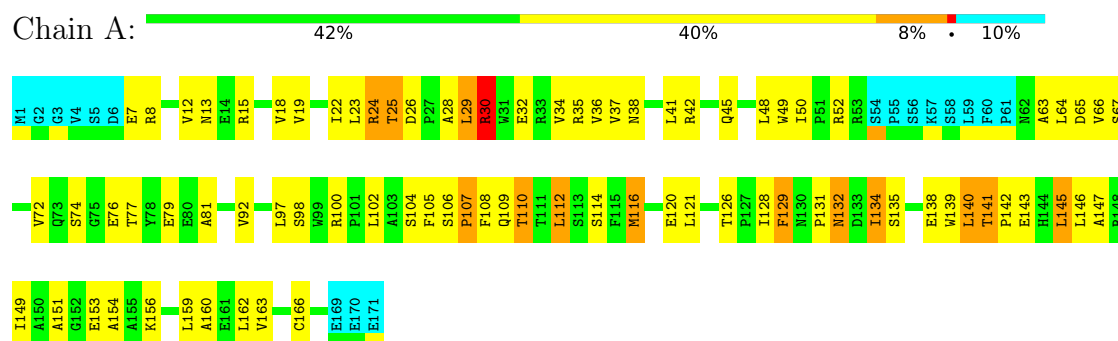
4.2.7 Score per residue for model 7

- Molecule 1: Putative Nudix hydrolase DR0079



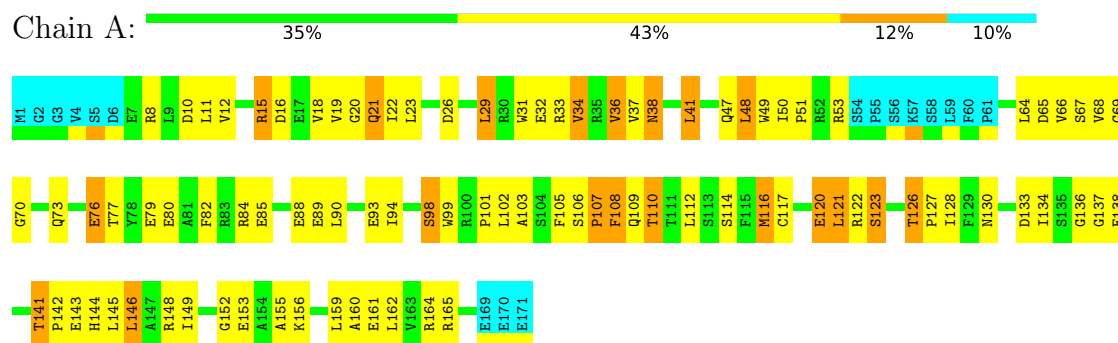
4.2.8 Score per residue for model 8

- Molecule 1: Putative Nudix hydrolase DR0079



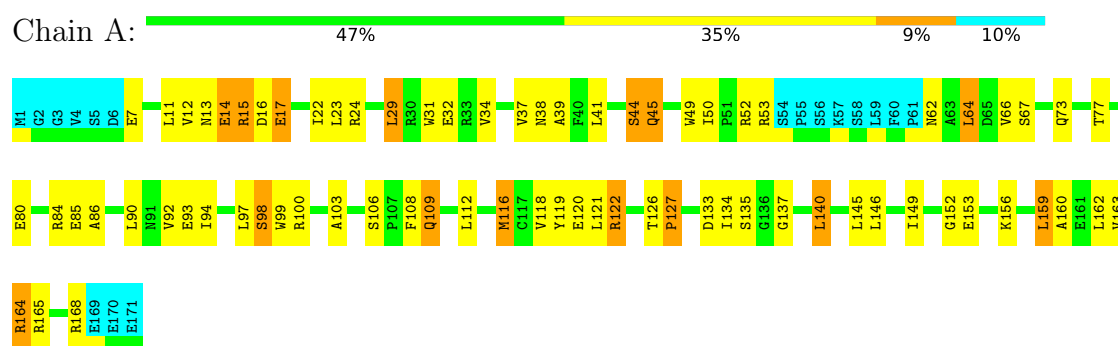
4.2.9 Score per residue for model 9

- Molecule 1: Putative Nudix hydrolase DR0079



4.2.10 Score per residue for model 10

- Molecule 1: Putative Nudix hydrolase DR0079



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 225 calculated structures, 10 were deposited, based on the following criterion: *ten best structures, in terms of total and NOE energies*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
CNS	structure solution	1.1
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	1234	1209	1208	41±4
All	All	12340	12090	12080	414

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:146:LEU:HD13	1:A:149:ILE:HD11	0.92	1.40	10	3
1:A:22:ILE:HG23	1:A:28:ALA:HB3	0.91	1.41	8	1
1:A:92:VAL:HG23	1:A:97:LEU:HD23	0.85	1.48	3	2
1:A:29:LEU:HD13	1:A:31:TRP:CD1	0.84	2.06	10	3
1:A:72:VAL:HG22	1:A:81:ALA:CB	0.83	2.03	3	2
1:A:41:LEU:HD11	1:A:121:LEU:HD23	0.82	1.48	9	1
1:A:40:PHE:CD1	1:A:50:ILE:HD11	0.82	2.10	6	1
1:A:50:ILE:HD12	1:A:145:LEU:HD11	0.80	1.54	4	1
1:A:140:LEU:HD22	1:A:148:ARG:NH1	0.79	1.92	3	1
1:A:86:ALA:HB1	1:A:92:VAL:CG1	0.78	2.09	3	1
1:A:86:ALA:HB1	1:A:92:VAL:HG13	0.78	1.54	3	2
1:A:38:ASN:ND2	1:A:66:VAL:HG21	0.78	1.94	8	1
1:A:105:PHE:CG	1:A:110:THR:HG21	0.77	2.13	1	1
1:A:97:LEU:HD13	1:A:122:ARG:O	0.77	1.79	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:VAL:HG23	1:A:17:GLU:C	0.76	2.05	10	6
1:A:112:LEU:HD22	1:A:116:MET:HE2	0.76	1.57	3	2
1:A:126:THR:HG23	1:A:139:TRP:CZ2	0.75	2.17	1	6
1:A:31:TRP:CE3	1:A:34:VAL:HG21	0.75	2.15	2	5
1:A:48:LEU:HD13	1:A:145:LEU:HD22	0.75	1.59	1	1
1:A:29:LEU:HD13	1:A:31:TRP:CG	0.74	2.16	9	2
1:A:126:THR:HG22	1:A:127:PRO:HD2	0.73	1.60	3	8
1:A:105:PHE:CB	1:A:110:THR:HG21	0.73	2.13	4	1
1:A:149:ILE:HD12	1:A:160:ALA:HB1	0.72	1.61	9	2
1:A:112:LEU:HD23	1:A:116:MET:HE3	0.71	1.60	10	2
1:A:72:VAL:HG22	1:A:81:ALA:HB2	0.71	1.62	3	1
1:A:72:VAL:HG13	1:A:81:ALA:HB2	0.71	1.62	1	2
1:A:134:ILE:HD13	1:A:136:GLY:N	0.71	2.00	1	3
1:A:41:LEU:CD1	1:A:121:LEU:HD23	0.71	2.16	9	1
1:A:105:PHE:CD1	1:A:118:VAL:HG21	0.70	2.20	1	1
1:A:38:ASN:ND2	1:A:116:MET:HE3	0.70	2.01	5	2
1:A:11:LEU:HD11	1:A:22:ILE:HD11	0.70	1.62	4	1
1:A:62:ASN:O	1:A:154:ALA:HB3	0.70	1.87	1	2
1:A:64:LEU:HD13	1:A:155:ALA:HB2	0.70	1.63	2	2
1:A:64:LEU:HD11	1:A:149:ILE:HG22	0.69	1.63	6	1
1:A:159:LEU:O	1:A:163:VAL:HG23	0.68	1.87	10	4
1:A:50:ILE:HB	1:A:145:LEU:HD11	0.68	1.65	6	2
1:A:50:ILE:HD12	1:A:145:LEU:CD1	0.68	2.17	4	1
1:A:103:ALA:HB3	1:A:118:VAL:HB	0.68	1.64	5	2
1:A:105:PHE:HB3	1:A:110:THR:HG22	0.67	1.64	3	1
1:A:86:ALA:CB	1:A:94:ILE:HG23	0.67	2.20	5	4
1:A:112:LEU:HD22	1:A:116:MET:HG3	0.67	1.65	6	1
1:A:29:LEU:HD12	1:A:34:VAL:CG1	0.67	2.20	8	1
1:A:52:ARG:HB2	1:A:140:LEU:HD11	0.66	1.68	4	1
1:A:48:LEU:HD12	1:A:50:ILE:HD11	0.66	1.67	4	1
1:A:38:ASN:CG	1:A:66:VAL:HG21	0.66	2.16	5	2
1:A:112:LEU:CD2	1:A:116:MET:HE2	0.66	2.19	3	2
1:A:107:PRO:HD2	1:A:110:THR:HG22	0.66	1.68	7	1
1:A:112:LEU:HD23	1:A:116:MET:CG	0.65	2.20	5	1
1:A:38:ASN:OD1	1:A:66:VAL:HG11	0.65	1.91	4	1
1:A:111:THR:HG21	1:A:159:LEU:HD21	0.65	1.68	7	1
1:A:82:PHE:CZ	1:A:121:LEU:HD11	0.64	2.27	3	1
1:A:12:VAL:HG12	1:A:18:VAL:HA	0.64	1.69	8	4
1:A:82:PHE:CD2	1:A:94:ILE:HG21	0.64	2.26	9	2
1:A:134:ILE:O	1:A:134:ILE:HG22	0.64	1.91	4	2
1:A:22:ILE:HG21	1:A:29:LEU:HB3	0.64	1.69	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ASN:ND2	1:A:66:VAL:HG11	0.64	2.08	9	1
1:A:38:ASN:OD1	1:A:66:VAL:HG21	0.63	1.94	5	1
1:A:38:ASN:OD1	1:A:116:MET:HE3	0.63	1.93	7	2
1:A:36:VAL:HG12	1:A:70:GLY:O	0.63	1.93	9	3
1:A:102:LEU:HD12	1:A:120:GLU:HB2	0.63	1.68	3	1
1:A:105:PHE:HB3	1:A:110:THR:HG21	0.63	1.68	8	3
1:A:29:LEU:CD1	1:A:34:VAL:HG11	0.63	2.24	8	1
1:A:149:ILE:HG22	1:A:155:ALA:CB	0.62	2.24	2	1
1:A:48:LEU:HD23	1:A:142:PRO:HG3	0.62	1.71	4	1
1:A:141:THR:HG22	1:A:142:PRO:HD2	0.62	1.69	8	5
1:A:146:LEU:HD12	1:A:164:ARG:HG3	0.62	1.71	10	1
1:A:105:PHE:CD1	1:A:110:THR:HG21	0.61	2.31	1	1
1:A:126:THR:HG23	1:A:139:TRP:CH2	0.61	2.30	2	6
1:A:110:THR:HB	1:A:112:LEU:HD12	0.61	1.72	6	1
1:A:38:ASN:HB2	1:A:66:VAL:HG21	0.61	1.71	10	3
1:A:29:LEU:HD12	1:A:34:VAL:HG11	0.61	1.70	8	1
1:A:29:LEU:HD11	1:A:31:TRP:CD1	0.61	2.30	7	4
1:A:134:ILE:O	1:A:134:ILE:HG23	0.61	1.96	1	4
1:A:64:LEU:HD13	1:A:149:ILE:HG22	0.61	1.72	8	2
1:A:23:LEU:O	1:A:29:LEU:HD23	0.60	1.96	9	1
1:A:146:LEU:HD21	1:A:164:ARG:HB3	0.60	1.72	9	1
1:A:99:TRP:HB3	1:A:121:LEU:HD12	0.60	1.72	9	2
1:A:22:ILE:CG2	1:A:29:LEU:HD23	0.60	2.26	5	2
1:A:102:LEU:HD12	1:A:120:GLU:HG3	0.60	1.71	9	1
1:A:105:PHE:HB3	1:A:112:LEU:HD21	0.60	1.73	1	1
1:A:112:LEU:HD23	1:A:116:MET:HG3	0.59	1.74	5	1
1:A:41:LEU:HD12	1:A:49:TRP:CZ3	0.59	2.33	5	1
1:A:48:LEU:CD1	1:A:145:LEU:HD22	0.59	2.27	1	1
1:A:39:ALA:HB1	1:A:119:TYR:O	0.59	1.98	10	5
1:A:37:VAL:HG22	1:A:78:TYR:CD2	0.59	2.33	4	2
1:A:102:LEU:O	1:A:102:LEU:HD23	0.59	1.98	9	1
1:A:38:ASN:CB	1:A:66:VAL:HG21	0.59	2.28	6	1
1:A:38:ASN:HB3	1:A:66:VAL:HG11	0.58	1.75	7	3
1:A:94:ILE:HD12	1:A:99:TRP:CZ2	0.58	2.33	10	1
1:A:41:LEU:HD11	1:A:123:SER:CB	0.58	2.28	7	1
1:A:64:LEU:HD13	1:A:64:LEU:N	0.58	2.13	10	1
1:A:86:ALA:HB1	1:A:92:VAL:HG23	0.58	1.75	6	1
1:A:102:LEU:O	1:A:103:ALA:HB2	0.57	1.99	6	4
1:A:40:PHE:CE1	1:A:66:VAL:HG12	0.57	2.34	1	1
1:A:12:VAL:HG12	1:A:18:VAL:HG22	0.57	1.76	9	3
1:A:82:PHE:CE2	1:A:121:LEU:HD11	0.57	2.35	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:THR:HG23	1:A:139:TRP:HZ2	0.56	1.57	1	2
1:A:72:VAL:HG22	1:A:81:ALA:HB3	0.56	1.75	3	1
1:A:31:TRP:CD1	1:A:34:VAL:HG11	0.56	2.36	10	2
1:A:49:TRP:C	1:A:49:TRP:CD1	0.55	2.83	5	5
1:A:13:ASN:ND2	1:A:19:VAL:HG12	0.55	2.16	8	1
1:A:149:ILE:CD1	1:A:160:ALA:HB1	0.55	2.30	9	1
1:A:37:VAL:HG11	1:A:82:PHE:HB2	0.55	1.78	7	1
1:A:22:ILE:HG21	1:A:29:LEU:HD23	0.55	1.78	3	1
1:A:50:ILE:HG23	1:A:51:PRO:HD2	0.55	1.78	9	2
1:A:92:VAL:HG22	1:A:94:ILE:H	0.55	1.61	2	1
1:A:38:ASN:HD21	1:A:118:VAL:HG22	0.55	1.62	6	1
1:A:134:ILE:HD13	1:A:136:GLY:H	0.55	1.60	1	3
1:A:41:LEU:HD12	1:A:49:TRP:HZ3	0.55	1.60	5	1
1:A:149:ILE:HD12	1:A:160:ALA:CB	0.55	2.32	10	2
1:A:41:LEU:HD11	1:A:121:LEU:CD2	0.54	2.30	9	1
1:A:72:VAL:HG12	1:A:81:ALA:HB2	0.54	1.77	4	2
1:A:112:LEU:HD22	1:A:116:MET:CG	0.54	2.31	6	1
1:A:22:ILE:HG23	1:A:29:LEU:HB3	0.54	1.78	10	1
1:A:41:LEU:HD13	1:A:123:SER:OG	0.54	2.02	5	1
1:A:38:ASN:HB3	1:A:66:VAL:HG21	0.53	1.79	3	1
1:A:48:LEU:HG	1:A:145:LEU:HD22	0.53	1.79	9	1
1:A:63:ALA:H	1:A:154:ALA:HB3	0.53	1.63	6	1
1:A:102:LEU:HD12	1:A:120:GLU:CG	0.53	2.34	9	1
1:A:64:LEU:CD1	1:A:149:ILE:HG22	0.53	2.33	6	2
1:A:29:LEU:HD22	1:A:31:TRP:CE2	0.53	2.39	9	1
1:A:112:LEU:CD2	1:A:116:MET:HE3	0.53	2.34	9	1
1:A:52:ARG:HG2	1:A:140:LEU:HD11	0.53	1.80	3	1
1:A:63:ALA:HB1	1:A:111:THR:HB	0.52	1.80	6	1
1:A:41:LEU:HD22	1:A:121:LEU:HB2	0.52	1.81	3	1
1:A:107:PRO:CG	1:A:110:THR:HG23	0.52	2.34	6	1
1:A:133:ASP:HB3	1:A:134:ILE:HD12	0.52	1.81	7	1
1:A:86:ALA:HB1	1:A:92:VAL:HB	0.52	1.81	10	1
1:A:62:ASN:O	1:A:63:ALA:HB3	0.52	2.05	7	2
1:A:12:VAL:CG1	1:A:18:VAL:HG22	0.52	2.35	4	2
1:A:49:TRP:O	1:A:50:ILE:HD13	0.51	2.05	10	3
1:A:39:ALA:N	1:A:66:VAL:HG11	0.51	2.20	3	1
1:A:30:ARG:O	1:A:34:VAL:HG13	0.51	2.05	8	2
1:A:29:LEU:HD21	1:A:31:TRP:NE1	0.51	2.20	6	2
1:A:149:ILE:HG22	1:A:155:ALA:HB2	0.51	1.82	2	1
1:A:12:VAL:HG12	1:A:18:VAL:CA	0.51	2.35	4	3
1:A:50:ILE:HG22	1:A:51:PRO:HD2	0.51	1.81	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:LEU:HD12	1:A:122:ARG:O	0.50	2.06	2	1
1:A:38:ASN:ND2	1:A:118:VAL:HG22	0.50	2.20	6	1
1:A:49:TRP:CD1	1:A:49:TRP:C	0.50	2.90	8	5
1:A:131:PRO:O	1:A:132:ASN:CB	0.50	2.60	8	1
1:A:29:LEU:CD1	1:A:31:TRP:CD1	0.49	2.95	3	4
1:A:112:LEU:H	1:A:112:LEU:HD13	0.49	1.67	2	1
1:A:105:PHE:CD2	1:A:112:LEU:HD11	0.49	2.41	3	2
1:A:64:LEU:HD13	1:A:149:ILE:CG2	0.49	2.37	7	1
1:A:39:ALA:HB1	1:A:121:LEU:HD13	0.49	1.83	7	1
1:A:126:THR:CG2	1:A:127:PRO:HD2	0.49	2.38	2	1
1:A:82:PHE:CE2	1:A:94:ILE:HG21	0.49	2.43	7	1
1:A:63:ALA:HB2	1:A:154:ALA:O	0.49	2.08	4	2
1:A:156:LYS:HA	1:A:160:ALA:HB2	0.48	1.83	1	1
1:A:41:LEU:C	1:A:41:LEU:HD23	0.48	2.32	2	1
1:A:112:LEU:HG	1:A:116:MET:HE2	0.48	1.83	5	1
1:A:86:ALA:HB2	1:A:94:ILE:HG23	0.48	1.85	5	1
1:A:49:TRP:O	1:A:50:ILE:HD12	0.48	2.09	6	2
1:A:12:VAL:HG11	1:A:15:ARG:O	0.48	2.08	2	1
1:A:92:VAL:HB	1:A:97:LEU:HD23	0.48	1.85	8	1
1:A:134:ILE:O	1:A:134:ILE:CG2	0.48	2.61	4	3
1:A:102:LEU:HD13	1:A:120:GLU:OE1	0.48	2.09	4	1
1:A:140:LEU:HD23	1:A:140:LEU:N	0.48	2.24	10	3
1:A:106:SER:N	1:A:107:PRO:HD2	0.48	2.24	1	1
1:A:38:ASN:CG	1:A:66:VAL:HG11	0.47	2.34	9	1
1:A:102:LEU:O	1:A:103:ALA:CB	0.47	2.62	6	2
1:A:39:ALA:HB1	1:A:121:LEU:CD1	0.47	2.40	3	1
1:A:49:TRP:C	1:A:50:ILE:CG1	0.47	2.88	4	2
1:A:48:LEU:HD13	1:A:145:LEU:CD2	0.47	2.38	1	1
1:A:126:THR:OG1	1:A:127:PRO:HD2	0.47	2.10	4	1
1:A:159:LEU:O	1:A:163:VAL:HG22	0.47	2.09	5	1
1:A:64:LEU:HD13	1:A:64:LEU:H	0.47	1.69	10	1
1:A:106:SER:N	1:A:107:PRO:CD	0.47	2.78	6	1
1:A:112:LEU:HD22	1:A:116:MET:CE	0.47	2.37	3	1
1:A:72:VAL:HG13	1:A:81:ALA:CB	0.46	2.39	1	1
1:A:42:ARG:HG3	1:A:48:LEU:HD22	0.46	1.88	4	1
1:A:112:LEU:HD12	1:A:112:LEU:H	0.46	1.71	10	2
1:A:29:LEU:HD22	1:A:31:TRP:NE1	0.46	2.26	10	1
1:A:106:SER:CB	1:A:115:PHE:CD2	0.46	2.98	6	1
1:A:13:ASN:OD1	1:A:19:VAL:HG11	0.46	2.11	4	1
1:A:50:ILE:HG21	1:A:64:LEU:HD23	0.46	1.88	8	2
1:A:64:LEU:HD22	1:A:64:LEU:O	0.46	2.11	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:ILE:CG2	1:A:51:PRO:HD2	0.46	2.40	2	3
1:A:128:ILE:HG22	1:A:129:PHE:N	0.45	2.26	8	2
1:A:112:LEU:HD23	1:A:116:MET:HG2	0.45	1.87	5	1
1:A:92:VAL:HG12	1:A:94:ILE:H	0.45	1.71	10	1
1:A:106:SER:O	1:A:110:THR:HG23	0.45	2.12	3	1
1:A:31:TRP:CE3	1:A:34:VAL:CG2	0.45	2.99	5	1
1:A:41:LEU:HD11	1:A:123:SER:HB3	0.45	1.89	6	1
1:A:39:ALA:HB2	1:A:119:TYR:HB2	0.45	1.89	10	1
1:A:29:LEU:HD12	1:A:29:LEU:O	0.45	2.12	1	1
1:A:118:VAL:HG13	1:A:118:VAL:O	0.45	2.12	7	1
1:A:29:LEU:HD21	1:A:31:TRP:HE1	0.45	1.71	6	1
1:A:134:ILE:HD13	1:A:136:GLY:CA	0.45	2.42	1	2
1:A:105:PHE:CD2	1:A:118:VAL:HG21	0.45	2.46	2	1
1:A:99:TRP:CB	1:A:121:LEU:HB3	0.44	2.42	5	1
1:A:12:VAL:HG23	1:A:17:GLU:N	0.44	2.28	7	1
1:A:39:ALA:CB	1:A:121:LEU:HD13	0.44	2.42	3	1
1:A:111:THR:HG21	1:A:159:LEU:CD2	0.44	2.38	7	1
1:A:119:TYR:CD1	1:A:119:TYR:N	0.44	2.86	4	1
1:A:89:GLU:O	1:A:90:LEU:HD12	0.44	2.13	4	1
1:A:106:SER:N	1:A:107:PRO:HD3	0.44	2.28	7	2
1:A:97:LEU:O	1:A:98:SER:CB	0.44	2.66	10	1
1:A:94:ILE:HB	1:A:99:TRP:NE1	0.43	2.28	2	1
1:A:134:ILE:HD12	1:A:134:ILE:N	0.43	2.28	8	1
1:A:106:SER:CB	1:A:107:PRO:CD	0.43	2.96	4	1
1:A:76:GLU:O	1:A:77:THR:HG23	0.43	2.12	6	1
1:A:19:VAL:HG23	1:A:20:GLY:N	0.43	2.28	7	2
1:A:18:VAL:HG11	1:A:21:GLN:NE2	0.43	2.28	9	1
1:A:112:LEU:HD13	1:A:116:MET:CG	0.43	2.43	4	1
1:A:141:THR:HG22	1:A:142:PRO:CD	0.43	2.43	1	1
1:A:49:TRP:C	1:A:50:ILE:HD12	0.43	2.38	1	1
1:A:128:ILE:HG22	1:A:129:PHE:H	0.43	1.74	2	1
1:A:39:ALA:O	1:A:66:VAL:HG12	0.43	2.13	3	1
1:A:105:PHE:CB	1:A:112:LEU:HD11	0.43	2.44	7	1
1:A:96:ALA:C	1:A:97:LEU:HD22	0.43	2.39	2	1
1:A:13:ASN:ND2	1:A:17:GLU:CB	0.43	2.82	3	1
1:A:102:LEU:HD13	1:A:120:GLU:OE2	0.43	2.13	8	1
1:A:39:ALA:HB2	1:A:82:PHE:CE1	0.42	2.49	5	1
1:A:112:LEU:HD12	1:A:112:LEU:N	0.42	2.29	5	1
1:A:163:VAL:HG23	1:A:164:ARG:N	0.42	2.29	5	1
1:A:44:SER:O	1:A:45:GLN:HB2	0.42	2.13	10	1
1:A:121:LEU:HD23	1:A:122:ARG:N	0.42	2.29	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:TRP:CE2	1:A:126:THR:O	0.42	2.71	4	1
1:A:112:LEU:N	1:A:112:LEU:CD1	0.42	2.82	5	1
1:A:106:SER:O	1:A:107:PRO:C	0.42	2.62	1	1
1:A:112:LEU:C	1:A:112:LEU:CD2	0.42	2.93	2	1
1:A:12:VAL:CG2	1:A:17:GLU:N	0.42	2.83	1	3
1:A:51:PRO:CA	1:A:137:GLY:HA3	0.42	2.44	2	2
1:A:50:ILE:HG21	1:A:145:LEU:HD21	0.42	1.91	6	1
1:A:146:LEU:HD11	1:A:167:TYR:CB	0.42	2.44	4	1
1:A:30:ARG:O	1:A:32:GLU:N	0.42	2.52	5	1
1:A:86:ALA:O	1:A:92:VAL:HG12	0.42	2.14	3	1
1:A:149:ILE:HG22	1:A:155:ALA:HB3	0.42	1.90	7	1
1:A:149:ILE:HD13	1:A:160:ALA:HA	0.42	1.92	8	1
1:A:41:LEU:HD23	1:A:123:SER:HB3	0.42	1.92	9	1
1:A:49:TRP:CZ2	1:A:127:PRO:HD3	0.42	2.50	2	2
1:A:22:ILE:HG23	1:A:29:LEU:CB	0.42	2.45	9	1
1:A:92:VAL:CG2	1:A:97:LEU:HD23	0.42	2.45	2	1
1:A:68:VAL:HG12	1:A:69:GLY:N	0.42	2.30	9	3
1:A:82:PHE:HD2	1:A:94:ILE:HD13	0.42	1.75	5	1
1:A:36:VAL:O	1:A:116:MET:CB	0.42	2.68	6	1
1:A:49:TRP:O	1:A:50:ILE:CG1	0.42	2.68	6	1
1:A:97:LEU:HD22	1:A:122:ARG:O	0.42	2.13	10	1
1:A:111:THR:CG2	1:A:159:LEU:HD21	0.41	2.41	7	1
1:A:94:ILE:O	1:A:99:TRP:CD1	0.41	2.74	3	2
1:A:24:ARG:HD2	1:A:25:THR:HG23	0.41	1.91	8	1
1:A:34:VAL:HG12	1:A:35:ARG:H	0.41	1.75	1	1
1:A:37:VAL:CG1	1:A:119:TYR:CE2	0.41	3.03	7	1
1:A:49:TRP:O	1:A:50:ILE:HG13	0.41	2.15	7	1
1:A:72:VAL:HA	1:A:81:ALA:HB2	0.41	1.93	8	1
1:A:11:LEU:HD13	1:A:22:ILE:CG1	0.41	2.45	2	1
1:A:12:VAL:HG12	1:A:18:VAL:CG2	0.41	2.45	4	1
1:A:92:VAL:O	1:A:93:GLU:CG	0.41	2.69	4	1
1:A:141:THR:HG23	1:A:143:GLU:HG3	0.41	1.91	6	1
1:A:99:TRP:CZ3	1:A:119:TYR:HB2	0.41	2.51	2	1
1:A:40:PHE:CE2	1:A:66:VAL:HG13	0.41	2.50	7	1
1:A:49:TRP:O	1:A:50:ILE:CD1	0.41	2.69	8	1
1:A:12:VAL:HG21	1:A:15:ARG:C	0.41	2.41	10	1
1:A:93:GLU:O	1:A:94:ILE:CG1	0.41	2.69	10	1
1:A:49:TRP:C	1:A:50:ILE:HG13	0.41	2.40	2	2
1:A:147:ALA:O	1:A:151:ALA:HB2	0.41	2.16	8	1
1:A:64:LEU:HD12	1:A:155:ALA:HB2	0.41	1.93	9	1
1:A:155:ALA:O	1:A:156:LYS:O	0.40	2.39	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:PRO:O	1:A:108:PHE:CD2	0.40	2.74	9	1
1:A:96:ALA:O	1:A:97:LEU:HD22	0.40	2.17	2	1
1:A:29:LEU:O	1:A:30:ARG:C	0.40	2.64	4	1
1:A:102:LEU:HD23	1:A:120:GLU:HG3	0.40	1.92	7	1
1:A:52:ARG:HG3	1:A:140:LEU:HD11	0.40	1.94	2	1
1:A:34:VAL:HG12	1:A:35:ARG:N	0.40	2.32	6	1
1:A:13:ASN:OD1	1:A:14:GLU:N	0.40	2.55	10	1
1:A:141:THR:HG22	1:A:142:PRO:HD3	0.40	1.93	1	1
1:A:112:LEU:H	1:A:112:LEU:HD12	0.40	1.77	3	1
1:A:29:LEU:HD13	1:A:31:TRP:CB	0.40	2.47	9	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	154/171 (90%)	116±4 (75±2%)	28±3 (18±2%)	11±3 (7±2%)	2	16
All	All	1540/1710 (90%)	1158 (75%)	276 (18%)	106 (7%)	2	16

All 40 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	98	SER	9
1	A	156	LYS	8
1	A	107	PRO	7
1	A	108	PHE	7
1	A	152	GLY	7
1	A	15	ARG	6
1	A	103	ALA	5
1	A	14	GLU	4
1	A	32	GLU	4
1	A	137	GLY	4
1	A	134	ILE	3
1	A	30	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	127	PRO	3
1	A	136	GLY	3
1	A	7	GLU	2
1	A	76	GLU	2
1	A	106	SER	2
1	A	129	PHE	2
1	A	13	ASN	2
1	A	62	ASN	2
1	A	101	PRO	2
1	A	66	VAL	1
1	A	111	THR	1
1	A	33	ARG	1
1	A	94	ILE	1
1	A	46	GLY	1
1	A	75	GLY	1
1	A	64	LEU	1
1	A	74	SER	1
1	A	155	ALA	1
1	A	91	ASN	1
1	A	112	LEU	1
1	A	114	SER	1
1	A	18	VAL	1
1	A	63	ALA	1
1	A	132	ASN	1
1	A	34	VAL	1
1	A	110	THR	1
1	A	45	GLN	1
1	A	109	GLN	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	130/145 (90%)	87±7 (67±5%)	43±7 (33±5%)	1	12
All	All	1300/1450 (90%)	870 (67%)	430 (33%)	1	12

All 102 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	116	MET	10
1	A	29	LEU	9
1	A	109	GLN	9
1	A	153	GLU	9
1	A	77	THR	8
1	A	141	THR	8
1	A	145	LEU	8
1	A	159	LEU	8
1	A	32	GLU	7
1	A	41	LEU	7
1	A	65	ASP	7
1	A	126	THR	7
1	A	134	ILE	7
1	A	135	SER	7
1	A	100	ARG	7
1	A	162	LEU	7
1	A	23	LEU	6
1	A	37	VAL	6
1	A	64	LEU	6
1	A	67	SER	6
1	A	112	LEU	6
1	A	15	ARG	6
1	A	73	GLN	6
1	A	90	LEU	6
1	A	110	THR	6
1	A	165	ARG	6
1	A	76	GLU	6
1	A	11	LEU	5
1	A	52	ARG	5
1	A	79	GLU	5
1	A	80	GLU	5
1	A	114	SER	5
1	A	120	GLU	5
1	A	143	GLU	5
1	A	21	GLN	5
1	A	33	ARG	5
1	A	45	GLN	5
1	A	84	ARG	5
1	A	122	ARG	5
1	A	130	ASN	5
1	A	133	ASP	5
1	A	16	ASP	5
1	A	36	VAL	5

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Mol	Chain	Res	Type	Models (Total)
1	A	106	SER	5
1	A	148	ARG	5
1	A	144	HIS	5
1	A	53	ARG	4
1	A	102	LEU	4
1	A	113	SER	4
1	A	123	SER	4
1	A	161	GLU	4
1	A	168	ARG	4
1	A	9	LEU	4
1	A	7	GLU	4
1	A	26	ASP	4
1	A	88	GLU	4
1	A	98	SER	4
1	A	138	GLU	4
1	A	24	ARG	4
1	A	48	LEU	4
1	A	8	ARG	4
1	A	121	LEU	4
1	A	140	LEU	4
1	A	10	ASP	3
1	A	50	ILE	3
1	A	74	SER	3
1	A	164	ARG	3
1	A	83	ARG	3
1	A	93	GLU	3
1	A	95	ASP	3
1	A	132	ASN	3
1	A	104	SER	3
1	A	108	PHE	3
1	A	146	LEU	3
1	A	38	ASN	2
1	A	44	SER	2
1	A	87	ARG	2
1	A	156	LYS	2
1	A	17	GLU	2
1	A	82	PHE	2
1	A	128	ILE	2
1	A	30	ARG	2
1	A	35	ARG	2
1	A	47	GLN	2
1	A	66	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	42	ARG	2
1	A	166	CYS	2
1	A	89	GLU	2
1	A	85	GLU	2
1	A	22	ILE	1
1	A	34	VAL	1
1	A	43	ASN	1
1	A	91	ASN	1
1	A	111	THR	1
1	A	149	ILE	1
1	A	158	ASP	1
1	A	92	VAL	1
1	A	62	ASN	1
1	A	25	THR	1
1	A	105	PHE	1
1	A	117	CYS	1
1	A	14	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

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