



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 07:51 PM BST

PDB ID : 2EC1
Title : Solution structure of the RanBD1 domain from human Nucleoporin 50 kDa
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Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-02-09

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

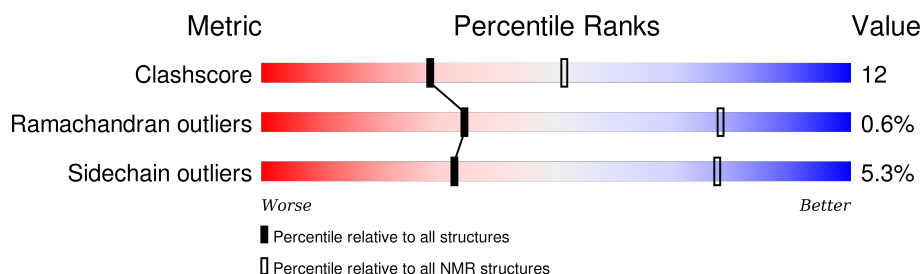
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	125	<div> <div></div> <div>70%</div> <div>17%</div> <div>8%</div> <div>6%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 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:14-A:55, A:60-A:125 (108)	0.41	1

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 and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1912 atoms, of which 980 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nucleoporin 50 kDa.

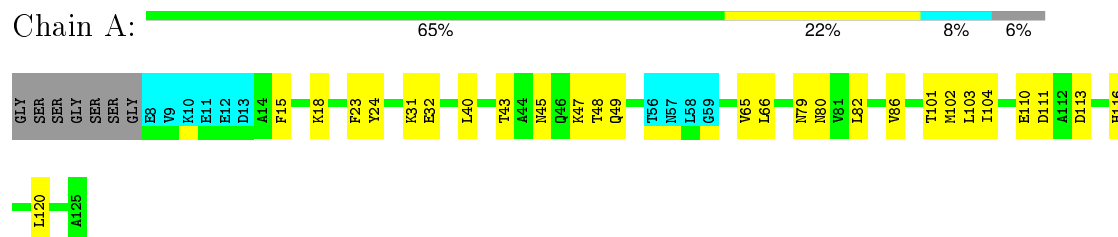
Mol	Chain	Residues	Atoms						Trace
1	A	118	Total	C	H	N	O	S	0
			1912	592	980	159	175	6	

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP Q9UKX7
A	2	SER	-	CLONING ARTIFACT	UNP Q9UKX7
A	3	SER	-	CLONING ARTIFACT	UNP Q9UKX7
A	4	GLY	-	CLONING ARTIFACT	UNP Q9UKX7
A	5	SER	-	CLONING ARTIFACT	UNP Q9UKX7
A	6	SER	-	CLONING ARTIFACT	UNP Q9UKX7
A	7	GLY	-	CLONING ARTIFACT	UNP Q9UKX7

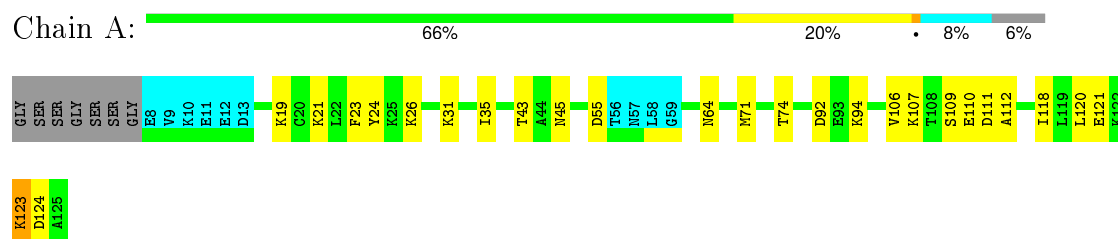
4.2.3 Score per residue for model 3

- Molecule 1: Nucleoporin 50 kDa



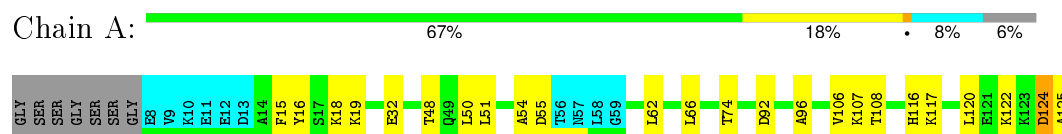
4.2.4 Score per residue for model 4

- Molecule 1: Nucleoporin 50 kDa



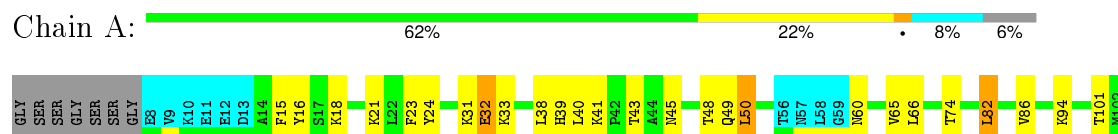
4.2.5 Score per residue for model 5

- Molecule 1: Nucleoporin 50 kDa



4.2.6 Score per residue for model 6

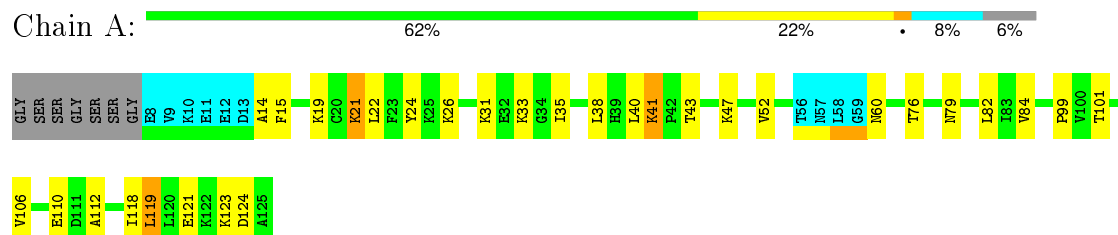
- Molecule 1: Nucleoporin 50 kDa





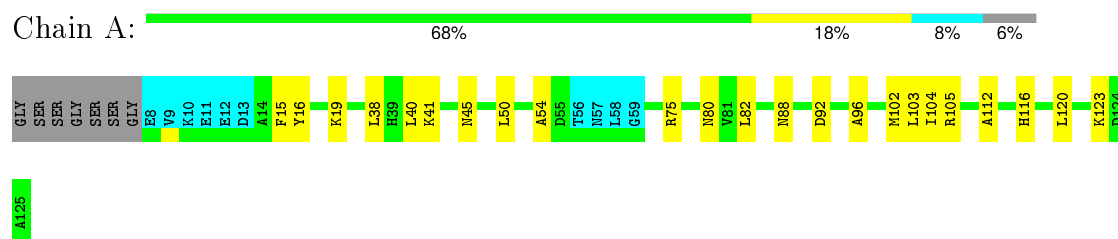
4.2.7 Score per residue for model 7

- Molecule 1: Nucleoporin 50 kDa



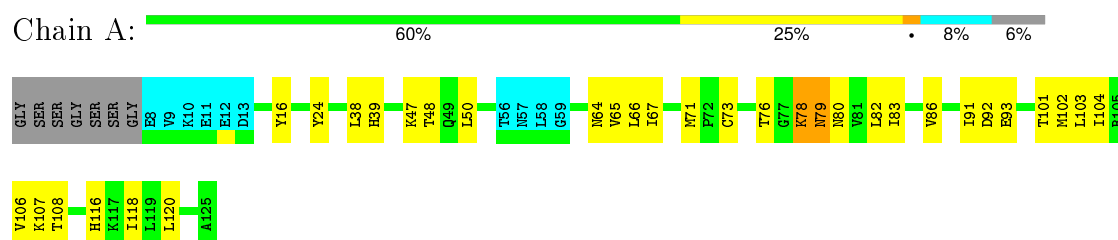
4.2.8 Score per residue for model 8

- Molecule 1: Nucleoporin 50 kDa



4.2.9 Score per residue for model 9

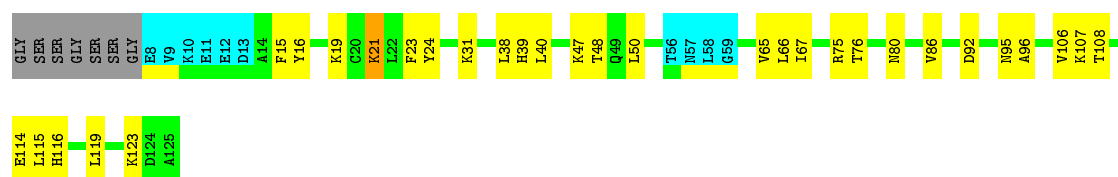
- Molecule 1: Nucleoporin 50 kDa



4.2.10 Score per residue for model 10

- Molecule 1: Nucleoporin 50 kDa

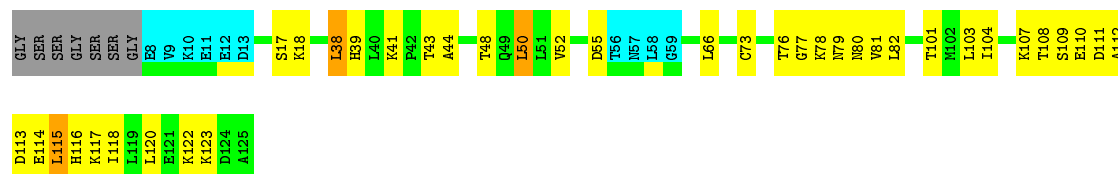




4.2.11 Score per residue for model 11

- Molecule 1: Nucleoporin 50 kDa

Chain A: 56% 28% 8% 6%



4.2.12 Score per residue for model 12

- Molecule 1: Nucleoporin 50 kDa

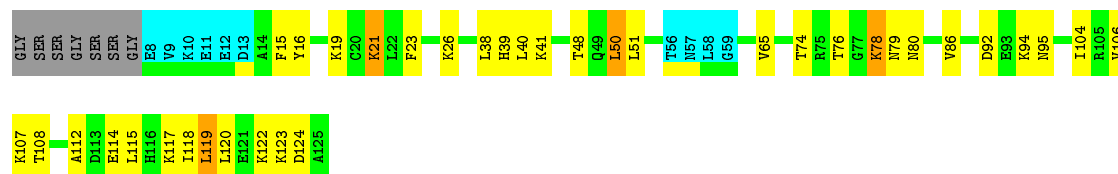
Chain A: 63% 22% 8% 6%



4.2.13 Score per residue for model 13

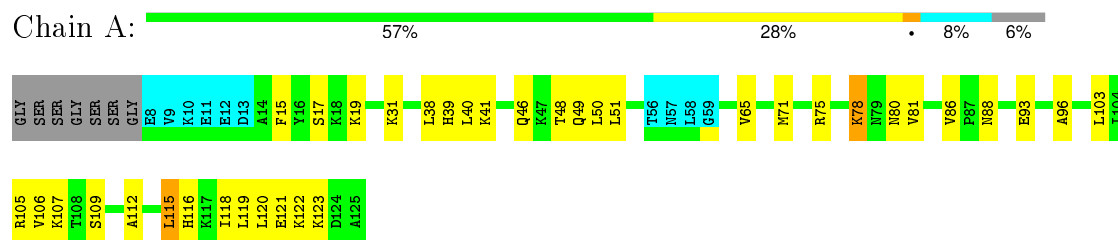
- Molecule 1: Nucleoporin 50 kDa

Chain A: 57% 26% 8% 6%



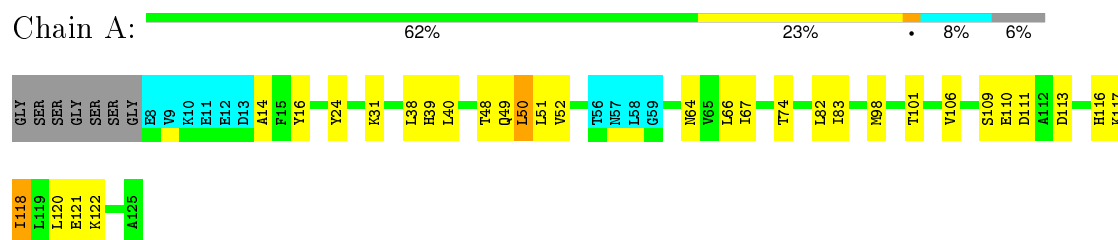
4.2.14 Score per residue for model 14

- Molecule 1: Nucleoporin 50 kDa



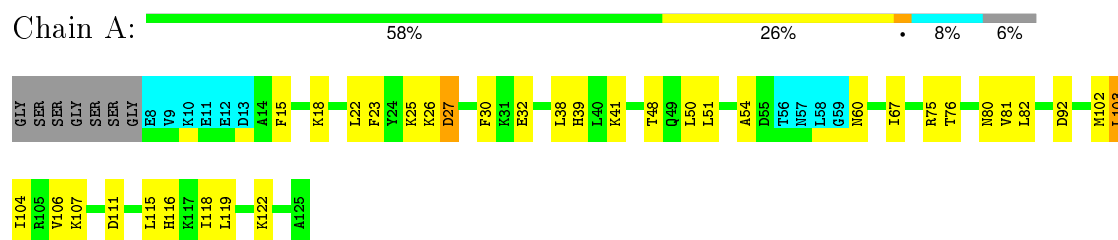
4.2.15 Score per residue for model 15

- Molecule 1: Nucleoporin 50 kDa



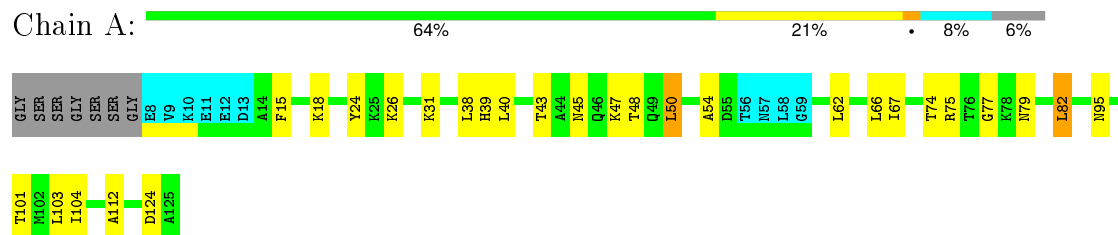
4.2.16 Score per residue for model 16

- Molecule 1: Nucleoporin 50 kDa



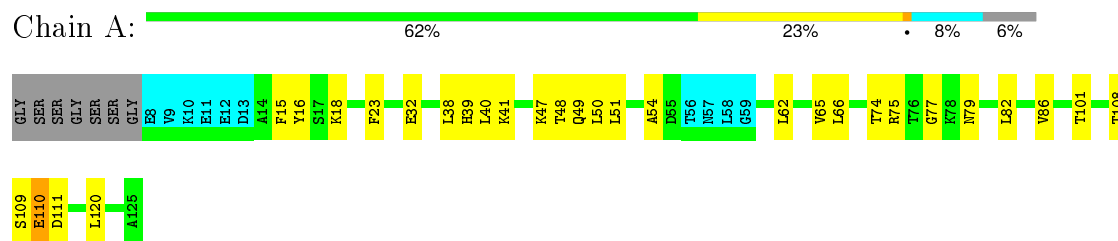
4.2.17 Score per residue for model 17

- Molecule 1: Nucleoporin 50 kDa



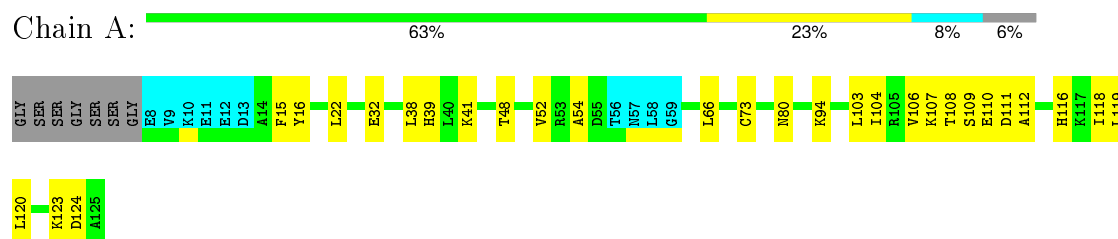
4.2.18 Score per residue for model 18

- Molecule 1: Nucleoporin 50 kDa



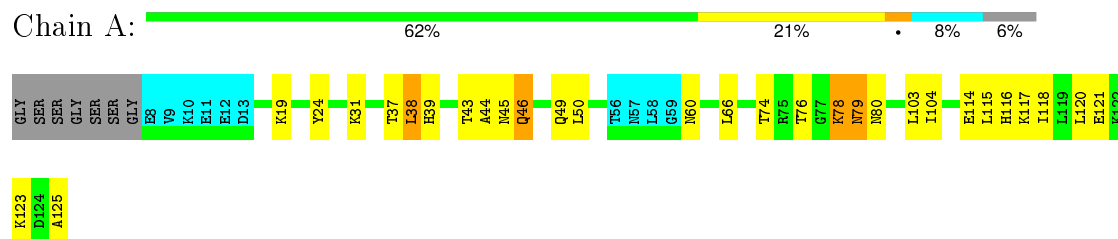
4.2.19 Score per residue for model 19

- Molecule 1: Nucleoporin 50 kDa



4.2.20 Score per residue for model 20

- Molecule 1: Nucleoporin 50 kDa



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy, target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

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

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	854	909	909	22±5
All	All	17080	18180	18180	437

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LEU:HD13	1:A:39:HIS:N	0.82	1.89	15	11
1:A:65:VAL:HG11	1:A:86:VAL:O	0.81	1.75	14	8
1:A:116:HIS:O	1:A:120:LEU:HD23	0.81	1.76	20	3
1:A:119:LEU:C	1:A:119:LEU:HD12	0.80	1.97	13	1
1:A:54:ALA:HB2	1:A:62:LEU:HG	0.79	1.54	18	3
1:A:38:LEU:HD23	1:A:52:VAL:HG22	0.78	1.54	11	3
1:A:48:THR:O	1:A:66:LEU:HD12	0.77	1.79	3	9
1:A:38:LEU:C	1:A:38:LEU:HD13	0.77	2.00	18	9
1:A:92:ASP:O	1:A:96:ALA:HB2	0.76	1.80	5	3
1:A:38:LEU:HD13	1:A:38:LEU:C	0.76	2.00	20	3
1:A:24:TYR:CD2	1:A:91:ILE:HD13	0.73	2.19	9	1
1:A:120:LEU:HD23	1:A:123:LYS:CE	0.71	2.14	14	2
1:A:38:LEU:HD21	1:A:50:LEU:HD21	0.69	1.62	11	2
1:A:116:HIS:CE1	1:A:120:LEU:HD11	0.69	2.22	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:THR:HG22	1:A:47:LYS:C	0.69	2.08	12	1
1:A:106:VAL:HG21	1:A:112:ALA:N	0.66	2.05	12	3
1:A:38:LEU:HD21	1:A:50:LEU:CD2	0.66	2.20	11	3
1:A:80:ASN:HB3	1:A:103:LEU:HD21	0.66	1.67	19	2
1:A:47:LYS:HB3	1:A:66:LEU:HD11	0.66	1.68	10	5
1:A:14:ALA:HB1	1:A:40:LEU:H	0.65	1.51	15	1
1:A:40:LEU:HD23	1:A:49:GLN:O	0.65	1.92	6	4
1:A:50:LEU:C	1:A:50:LEU:HD13	0.64	2.13	5	4
1:A:76:THR:HG23	1:A:80:ASN:HB2	0.62	1.69	11	8
1:A:22:LEU:HD23	1:A:104:ILE:HD11	0.62	1.70	19	1
1:A:76:THR:HG23	1:A:80:ASN:CB	0.61	2.24	11	5
1:A:38:LEU:HD21	1:A:50:LEU:CD1	0.61	2.25	20	2
1:A:38:LEU:HD23	1:A:52:VAL:CG2	0.61	2.25	11	1
1:A:82:LEU:HD11	1:A:101:THR:HG23	0.60	1.72	18	2
1:A:119:LEU:CD1	1:A:119:LEU:C	0.60	2.70	13	1
1:A:46:GLN:CG	1:A:46:GLN:O	0.60	2.49	20	1
1:A:75:ARG:NH1	1:A:112:ALA:HB1	0.59	2.11	8	1
1:A:15:PHE:CE2	1:A:40:LEU:O	0.59	2.55	8	1
1:A:38:LEU:C	1:A:38:LEU:CD1	0.58	2.72	18	6
1:A:67:ILE:HG23	1:A:71:MET:SD	0.58	2.39	9	1
1:A:38:LEU:CD2	1:A:52:VAL:CG2	0.58	2.82	15	1
1:A:120:LEU:HD23	1:A:123:LYS:HE2	0.58	1.76	14	1
1:A:82:LEU:HD13	1:A:103:LEU:HD23	0.58	1.73	16	1
1:A:38:LEU:HD22	1:A:52:VAL:CG2	0.57	2.29	15	1
1:A:38:LEU:HD22	1:A:39:HIS:N	0.57	2.15	16	4
1:A:15:PHE:CD1	1:A:16:TYR:N	0.56	2.72	13	6
1:A:48:THR:HG21	1:A:122:LYS:HD3	0.56	1.77	16	1
1:A:15:PHE:CE1	1:A:40:LEU:O	0.56	2.59	12	3
1:A:82:LEU:HD21	1:A:101:THR:HG23	0.56	1.77	17	1
1:A:103:LEU:HD23	1:A:104:ILE:N	0.56	2.15	20	4
1:A:50:LEU:HD13	1:A:51:LEU:N	0.56	2.16	12	7
1:A:104:ILE:HD13	1:A:115:LEU:HD21	0.56	1.78	12	1
1:A:50:LEU:CD1	1:A:50:LEU:C	0.56	2.74	12	2
1:A:73:CYS:HG	1:A:116:HIS:CD2	0.56	2.18	9	1
1:A:71:MET:N	1:A:123:LYS:HZ3	0.55	1.98	4	1
1:A:15:PHE:CD1	1:A:40:LEU:O	0.55	2.59	14	2
1:A:123:LYS:O	1:A:123:LYS:CG	0.55	2.54	20	2
1:A:38:LEU:CD1	1:A:38:LEU:C	0.55	2.73	20	4
1:A:24:TYR:CZ	1:A:31:LYS:CB	0.55	2.91	15	3
1:A:24:TYR:CD1	1:A:31:LYS:O	0.54	2.60	6	1
1:A:40:LEU:HD22	1:A:48:THR:CG2	0.54	2.32	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LEU:CD2	1:A:50:LEU:HD12	0.54	2.33	2	1
1:A:50:LEU:C	1:A:50:LEU:CD1	0.54	2.75	5	1
1:A:38:LEU:HD22	1:A:52:VAL:HG22	0.53	1.79	15	1
1:A:82:LEU:HD11	1:A:101:THR:CG2	0.53	2.33	18	1
1:A:106:VAL:HG22	1:A:107:LYS:N	0.53	2.18	4	6
1:A:82:LEU:HD22	1:A:101:THR:CG2	0.53	2.33	1	6
1:A:67:ILE:CD1	1:A:122:LYS:NZ	0.53	2.72	15	1
1:A:82:LEU:HD21	1:A:101:THR:CG2	0.53	2.33	15	1
1:A:23:PHE:CZ	1:A:32:GLU:OE1	0.53	2.62	16	1
1:A:48:THR:HB	1:A:67:ILE:HD12	0.52	1.81	16	3
1:A:47:LYS:HD2	1:A:66:LEU:HD21	0.52	1.80	3	1
1:A:103:LEU:HD13	1:A:104:ILE:N	0.52	2.19	16	5
1:A:119:LEU:H	1:A:119:LEU:HD12	0.52	1.64	2	1
1:A:38:LEU:HD22	1:A:51:LEU:O	0.52	2.05	18	2
1:A:21:LYS:HB3	1:A:23:PHE:CE2	0.52	2.40	6	3
1:A:82:LEU:HD23	1:A:102:MET:O	0.52	2.05	1	4
1:A:116:HIS:HE1	1:A:120:LEU:HD11	0.51	1.64	14	1
1:A:73:CYS:SG	1:A:120:LEU:HD21	0.51	2.45	11	1
1:A:48:THR:HG21	1:A:122:LYS:HB3	0.51	1.82	14	1
1:A:15:PHE:CD2	1:A:40:LEU:O	0.51	2.64	8	1
1:A:40:LEU:HD21	1:A:50:LEU:HD23	0.51	1.81	14	1
1:A:116:HIS:CE1	1:A:120:LEU:HD21	0.51	2.41	19	1
1:A:119:LEU:HD12	1:A:119:LEU:H	0.51	1.65	19	1
1:A:21:LYS:HB3	1:A:23:PHE:CE1	0.51	2.41	13	2
1:A:18:LYS:C	1:A:37:THR:HG23	0.50	2.26	1	1
1:A:15:PHE:CZ	1:A:40:LEU:HB3	0.50	2.40	3	4
1:A:84:VAL:HG12	1:A:99:PRO:HB2	0.50	1.83	7	2
1:A:93:GLU:HA	1:A:96:ALA:HB2	0.50	1.84	14	1
1:A:106:VAL:HG11	1:A:112:ALA:N	0.50	2.22	19	2
1:A:103:LEU:HD13	1:A:103:LEU:C	0.50	2.26	8	3
1:A:78:LYS:O	1:A:109:SER:CB	0.50	2.60	14	1
1:A:109:SER:O	1:A:112:ALA:N	0.49	2.45	14	5
1:A:38:LEU:CD2	1:A:52:VAL:HG22	0.49	2.35	11	2
1:A:14:ALA:HB2	1:A:41:LYS:HD2	0.49	1.85	7	1
1:A:118:ILE:HG22	1:A:122:LYS:CD	0.49	2.36	12	1
1:A:24:TYR:CE2	1:A:31:LYS:HB2	0.49	2.42	15	1
1:A:40:LEU:HD21	1:A:50:LEU:HD12	0.49	1.83	2	3
1:A:75:ARG:HG2	1:A:116:HIS:CD2	0.49	2.42	16	2
1:A:118:ILE:O	1:A:121:GLU:N	0.49	2.45	20	5
1:A:22:LEU:HD11	1:A:52:VAL:HG11	0.49	1.84	7	1
1:A:38:LEU:HD22	1:A:39:HIS:H	0.48	1.69	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:LEU:HD12	1:A:120:LEU:N	0.48	2.22	13	1
1:A:26:LYS:O	1:A:27:ASP:CG	0.48	2.51	16	1
1:A:17:SER:HB2	1:A:39:HIS:CE1	0.48	2.44	11	2
1:A:24:TYR:CZ	1:A:31:LYS:HB2	0.48	2.43	15	5
1:A:71:MET:N	1:A:123:LYS:NZ	0.48	2.62	4	1
1:A:75:ARG:CZ	1:A:112:ALA:HB3	0.47	2.39	17	1
1:A:24:TYR:CE1	1:A:31:LYS:HB2	0.47	2.44	1	4
1:A:67:ILE:HD11	1:A:119:LEU:CD2	0.47	2.39	10	1
1:A:108:THR:HG23	1:A:110:GLU:CG	0.47	2.39	19	1
1:A:107:LYS:HG3	1:A:108:THR:HG22	0.47	1.86	11	1
1:A:82:LEU:HD13	1:A:103:LEU:HD12	0.47	1.86	2	1
1:A:82:LEU:HD13	1:A:103:LEU:CD2	0.47	2.38	16	1
1:A:38:LEU:HD11	1:A:50:LEU:HD21	0.47	1.87	14	1
1:A:118:ILE:HG22	1:A:122:LYS:HD3	0.47	1.87	12	1
1:A:65:VAL:HG12	1:A:88:ASN:HB2	0.47	1.87	14	1
1:A:82:LEU:HD22	1:A:103:LEU:HD12	0.47	1.86	6	1
1:A:26:LYS:C	1:A:27:ASP:CG	0.47	2.73	16	1
1:A:21:LYS:HB3	1:A:23:PHE:CZ	0.47	2.45	1	1
1:A:23:PHE:CD1	1:A:32:GLU:HA	0.47	2.45	3	3
1:A:80:ASN:CB	1:A:103:LEU:HD21	0.47	2.38	19	1
1:A:114:GLU:CG	1:A:118:ILE:HD11	0.47	2.39	11	1
1:A:18:LYS:HD3	1:A:106:VAL:HG23	0.47	1.87	16	1
1:A:22:LEU:CD2	1:A:104:ILE:HD11	0.47	2.39	19	1
1:A:121:GLU:O	1:A:125:ALA:HB2	0.47	2.09	20	1
1:A:106:VAL:HG21	1:A:111:ASP:HB3	0.47	1.87	16	2
1:A:49:GLN:HA	1:A:66:LEU:HD23	0.46	1.87	20	1
1:A:75:ARG:NH1	1:A:80:ASN:O	0.46	2.48	12	1
1:A:23:PHE:CE1	1:A:32:GLU:HG3	0.46	2.45	1	3
1:A:24:TYR:CE1	1:A:26:LYS:HD2	0.46	2.46	4	1
1:A:24:TYR:CE1	1:A:26:LYS:HE2	0.46	2.45	17	1
1:A:43:THR:O	1:A:46:GLN:N	0.46	2.48	20	1
1:A:43:THR:HG22	1:A:47:LYS:O	0.46	2.10	2	4
1:A:47:LYS:CD	1:A:66:LEU:HD21	0.46	2.41	3	1
1:A:106:VAL:CG1	1:A:111:ASP:OD2	0.46	2.63	15	1
1:A:48:THR:O	1:A:66:LEU:HD13	0.46	2.11	12	1
1:A:104:ILE:HD12	1:A:104:ILE:N	0.46	2.25	13	1
1:A:112:ALA:O	1:A:114:GLU:N	0.46	2.48	11	1
1:A:16:TYR:CD2	1:A:118:ILE:CD1	0.46	2.98	9	1
1:A:54:ALA:HB3	1:A:60:ASN:HB3	0.46	1.88	16	1
1:A:60:ASN:OD1	1:A:60:ASN:C	0.45	2.52	20	2
1:A:43:THR:CG2	1:A:47:LYS:CB	0.45	2.94	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:ILE:O	1:A:119:LEU:C	0.45	2.53	16	2
1:A:79:ASN:C	1:A:79:ASN:OD1	0.45	2.55	3	2
1:A:64:ASN:C	1:A:64:ASN:OD1	0.45	2.55	9	1
1:A:21:LYS:HG3	1:A:35:ILE:HD12	0.45	1.87	7	1
1:A:109:SER:O	1:A:111:ASP:N	0.45	2.50	18	2
1:A:104:ILE:CD1	1:A:115:LEU:HD21	0.45	2.42	12	1
1:A:15:PHE:CE2	1:A:16:TYR:HB2	0.45	2.46	10	1
1:A:108:THR:CG2	1:A:110:GLU:CG	0.45	2.95	19	1
1:A:106:VAL:HG23	1:A:108:THR:O	0.45	2.12	13	2
1:A:108:THR:CG2	1:A:110:GLU:HG2	0.45	2.41	19	2
1:A:124:ASP:OD1	1:A:125:ALA:N	0.45	2.50	5	1
1:A:16:TYR:CD2	1:A:118:ILE:HD13	0.45	2.46	9	1
1:A:25:LYS:HD3	1:A:30:PHE:CE1	0.45	2.47	16	1
1:A:81:VAL:HG13	1:A:81:VAL:O	0.45	2.12	14	2
1:A:15:PHE:CZ	1:A:122:LYS:HE2	0.45	2.47	5	1
1:A:82:LEU:HD23	1:A:83:ILE:N	0.45	2.27	15	1
1:A:43:THR:O	1:A:44:ALA:C	0.44	2.55	11	1
1:A:32:GLU:OE1	1:A:32:GLU:C	0.44	2.55	6	1
1:A:106:VAL:HG11	1:A:111:ASP:OD2	0.44	2.12	15	1
1:A:106:VAL:HG22	1:A:107:LYS:H	0.44	1.71	14	3
1:A:120:LEU:O	1:A:124:ASP:CG	0.44	2.55	4	1
1:A:15:PHE:CZ	1:A:122:LYS:NZ	0.44	2.83	16	1
1:A:119:LEU:N	1:A:119:LEU:CD2	0.44	2.80	7	1
1:A:24:TYR:CZ	1:A:31:LYS:HB3	0.44	2.48	15	2
1:A:41:LYS:NZ	1:A:51:LEU:HD22	0.44	2.27	13	1
1:A:93:GLU:O	1:A:94:LYS:C	0.44	2.55	12	1
1:A:48:THR:CG2	1:A:67:ILE:HD12	0.44	2.42	17	2
1:A:106:VAL:CG1	1:A:108:THR:O	0.44	2.66	5	1
1:A:81:VAL:HG21	1:A:115:LEU:HD23	0.44	1.89	16	2
1:A:23:PHE:CE2	1:A:32:GLU:OE1	0.44	2.71	16	1
1:A:113:ASP:OD2	1:A:117:LYS:NZ	0.44	2.50	15	1
1:A:40:LEU:HD21	1:A:50:LEU:CD2	0.43	2.43	14	1
1:A:106:VAL:HG13	1:A:108:THR:O	0.43	2.12	9	1
1:A:79:ASN:ND2	1:A:106:VAL:O	0.43	2.50	7	1
1:A:109:SER:O	1:A:110:GLU:C	0.43	2.57	4	2
1:A:115:LEU:CD1	1:A:115:LEU:C	0.43	2.86	14	1
1:A:114:GLU:O	1:A:117:LYS:N	0.43	2.51	13	2
1:A:78:LYS:HG2	1:A:79:ASN:N	0.43	2.29	9	2
1:A:114:GLU:O	1:A:116:HIS:N	0.43	2.52	11	1
1:A:82:LEU:O	1:A:83:ILE:CG2	0.43	2.67	12	1
1:A:21:LYS:HG2	1:A:35:ILE:HD12	0.43	1.89	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:THR:HG21	1:A:82:LEU:CD1	0.43	2.43	7	1
1:A:75:ARG:NH1	1:A:112:ALA:CB	0.43	2.80	8	1
1:A:114:GLU:HG3	1:A:118:ILE:HD11	0.43	1.89	1	1
1:A:114:GLU:O	1:A:118:ILE:HD12	0.43	2.14	13	1
1:A:117:LYS:O	1:A:120:LEU:N	0.43	2.52	2	2
1:A:32:GLU:OE1	1:A:33:LYS:C	0.43	2.57	6	1
1:A:109:SER:C	1:A:111:ASP:N	0.43	2.72	18	1
1:A:103:LEU:CD2	1:A:105:ARG:HG3	0.42	2.43	14	1
1:A:114:GLU:O	1:A:115:LEU:C	0.42	2.56	10	2
1:A:88:ASN:OD1	1:A:88:ASN:C	0.42	2.57	8	1
1:A:43:THR:CG2	1:A:47:LYS:HB2	0.42	2.44	12	1
1:A:21:LYS:HE3	1:A:21:LYS:N	0.42	2.30	7	1
1:A:64:ASN:OD1	1:A:64:ASN:C	0.42	2.56	4	1
1:A:73:CYS:HB2	1:A:116:HIS:CE1	0.42	2.49	19	1
1:A:123:LYS:HG3	1:A:123:LYS:O	0.42	2.15	14	1
1:A:82:LEU:O	1:A:83:ILE:HG23	0.42	2.15	9	1
1:A:120:LEU:O	1:A:120:LEU:HD12	0.42	2.14	18	1
1:A:43:THR:O	1:A:45:ASN:N	0.42	2.53	20	1
1:A:16:TYR:CE2	1:A:118:ILE:CD1	0.42	3.02	9	1
1:A:22:LEU:O	1:A:32:GLU:CD	0.42	2.58	16	1
1:A:16:TYR:CB	1:A:40:LEU:HD12	0.42	2.44	15	1
1:A:120:LEU:O	1:A:124:ASP:CB	0.42	2.67	4	1
1:A:75:ARG:CD	1:A:81:VAL:HG23	0.42	2.44	14	1
1:A:110:GLU:HG3	1:A:111:ASP:N	0.42	2.29	19	2
1:A:38:LEU:HD11	1:A:50:LEU:HD11	0.42	1.90	8	1
1:A:118:ILE:HG23	1:A:122:LYS:HE2	0.42	1.91	12	1
1:A:116:HIS:O	1:A:117:LYS:C	0.42	2.58	2	1
1:A:96:ALA:O	1:A:97:THR:C	0.42	2.57	12	2
1:A:16:TYR:CE2	1:A:115:LEU:HB2	0.41	2.50	13	1
1:A:123:LYS:HG3	1:A:124:ASP:N	0.41	2.30	19	3
1:A:50:LEU:CD2	1:A:51:LEU:N	0.41	2.83	15	1
1:A:46:GLN:O	1:A:46:GLN:CD	0.41	2.59	14	1
1:A:118:ILE:CG2	1:A:122:LYS:CD	0.41	2.98	12	1
1:A:81:VAL:HG21	1:A:116:HIS:HB2	0.41	1.91	12	1
1:A:78:LYS:HD2	1:A:79:ASN:N	0.41	2.30	13	1
1:A:95:ASN:O	1:A:96:ALA:C	0.41	2.58	10	1
1:A:80:ASN:HB3	1:A:103:LEU:HD11	0.41	1.91	3	1
1:A:112:ALA:C	1:A:114:GLU:N	0.41	2.72	11	1
1:A:38:LEU:C	1:A:38:LEU:HD23	0.41	2.35	7	1
1:A:118:ILE:HD12	1:A:118:ILE:H	0.41	1.75	13	1
1:A:71:MET:O	1:A:71:MET:SD	0.41	2.79	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:THR:O	1:A:45:ASN:O	0.41	2.39	3	4
1:A:48:THR:OG1	1:A:122:LYS:CG	0.41	2.69	13	1
1:A:114:GLU:HA	1:A:117:LYS:CG	0.41	2.46	11	1
1:A:115:LEU:O	1:A:116:HIS:C	0.41	2.58	2	1
1:A:123:LYS:O	1:A:124:ASP:C	0.41	2.59	7	1
1:A:103:LEU:C	1:A:103:LEU:HD13	0.41	2.36	11	1
1:A:36:GLY:HA2	1:A:55:ASP:N	0.41	2.31	2	1
1:A:75:ARG:NH1	1:A:76:THR:N	0.41	2.69	12	1
1:A:94:LYS:HG3	1:A:95:ASN:N	0.41	2.31	13	1
1:A:51:LEU:HD13	1:A:64:ASN:ND2	0.41	2.31	15	1
1:A:118:ILE:CG2	1:A:122:LYS:HE2	0.41	2.46	12	1
1:A:32:GLU:CG	1:A:32:GLU:O	0.40	2.69	19	1
1:A:49:GLN:HG2	1:A:50:LEU:N	0.40	2.30	15	1
1:A:78:LYS:HG3	1:A:79:ASN:N	0.40	2.32	11	1
1:A:82:LEU:HD12	1:A:102:MET:O	0.40	2.16	16	1
1:A:103:LEU:CD1	1:A:103:LEU:C	0.40	2.89	8	1
1:A:55:ASP:OD1	1:A:55:ASP:C	0.40	2.59	5	1
1:A:19:LYS:HA	1:A:37:THR:HG23	0.40	1.94	20	1
1:A:110:GLU:OE2	1:A:110:GLU:O	0.40	2.40	7	1
1:A:76:THR:O	1:A:80:ASN:O	0.40	2.39	12	1
1:A:50:LEU:HD13	1:A:50:LEU:C	0.40	2.37	17	1
1:A:119:LEU:CD1	1:A:119:LEU:H	0.40	2.30	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	107/125 (86%)	99±3 (92±3%)	8±3 (7±3%)	1±1 (1±1%)	34	78
All	All	2140/2500 (86%)	1973 (92%)	155 (7%)	12 (1%)	34	78

All 7 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	77	GLY	3
1	A	118	ILE	3
1	A	110	GLU	2
1	A	115	LEU	1
1	A	113	ASP	1
1	A	54	ALA	1
1	A	44	ALA	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	99/112 (88%)	94±2 (95±2%)	5±2 (5±2%)	33	77
All	All	1980/2240 (88%)	1876 (95%)	104 (5%)	33	77

All 42 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	41	LYS	9
1	A	74	THR	9
1	A	19	LYS	8
1	A	18	LYS	6
1	A	50	LEU	5
1	A	92	ASP	4
1	A	79	ASN	4
1	A	123	LYS	4
1	A	78	LYS	4
1	A	94	LYS	4
1	A	21	LYS	3
1	A	98	MET	3
1	A	124	ASP	2
1	A	55	ASP	2
1	A	32	GLU	2
1	A	60	ASN	2
1	A	33	LYS	2
1	A	107	LYS	2
1	A	122	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	82	LEU	2
1	A	119	LEU	2
1	A	26	LYS	2
1	A	38	LEU	2
1	A	31	LYS	1
1	A	109	SER	1
1	A	110	GLU	1
1	A	115	LEU	1
1	A	121	GLU	1
1	A	75	ARG	1
1	A	46	GLN	1
1	A	95	ASN	1
1	A	103	LEU	1
1	A	117	LYS	1
1	A	93	GLU	1
1	A	108	THR	1
1	A	27	ASP	1
1	A	105	ARG	1
1	A	53	ARG	1
1	A	80	ASN	1
1	A	45	ASN	1
1	A	70	ASN	1
1	A	113	ASP	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 carbohydrates in this entry.

6.6 Ligand geometry ⓘ

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