



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 10:38 pm GMT

PDB ID : 2K2R
Title : The NMR structure of alpha-parvin CH2/paxillin LD1 complex
Authors : Wang, X.; Fukuda, K.; Byeon, I.; Velyvis, A.; Wu, C.; Gronenborn, A.; Qin, J.
Deposited on : 2008-04-10

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

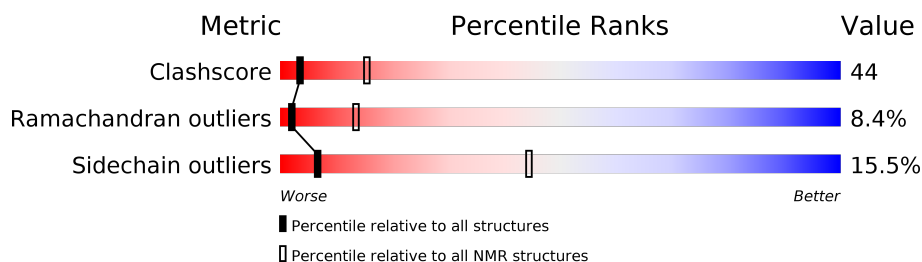
1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	129	<div> <div></div> <div>36%</div> <div>40%</div> <div>9%</div> <div>16%</div> </div>
2	B	10	<div> <div></div> <div>100%</div> </div>

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 10 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:9-A:62, A:74-A:128 (109)	0.29	10

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2275 atoms, of which 1139 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Alpha-parvin.

Mol	Chain	Residues	Atoms						Trace
1	A	129	Total	C	H	N	O	S	0
			2125	689	1065	173	195	3	

- Molecule 2 is a protein called Paxillin.

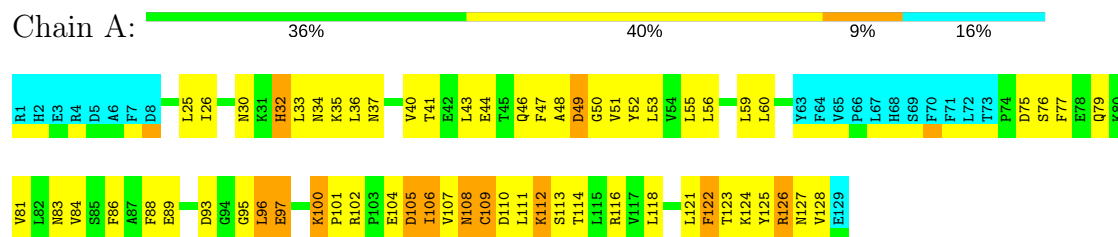
Mol	Chain	Residues	Atoms					Trace
2	B	10	Total	C	H	N	O	0
			150	47	74	10	19	

4 Residue-property plots [i](#)

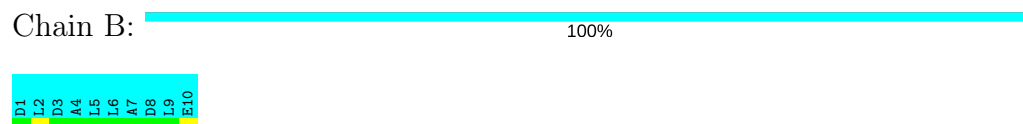
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Alpha-parvin



- Molecule 2: Paxillin

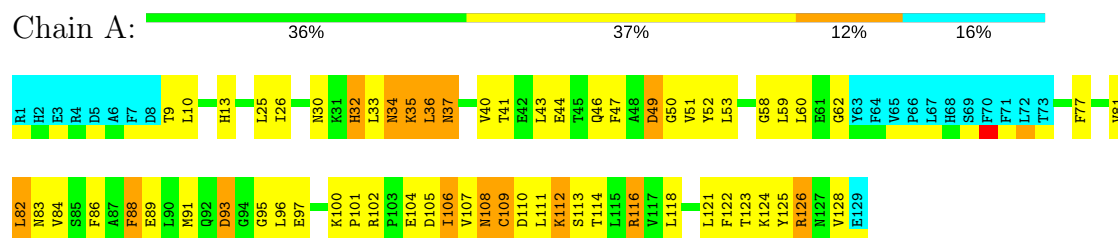


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

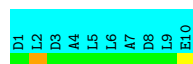
4.2.1 Score per residue for model 1

- Molecule 1: Alpha-parvin



- Molecule 2: Paxillin

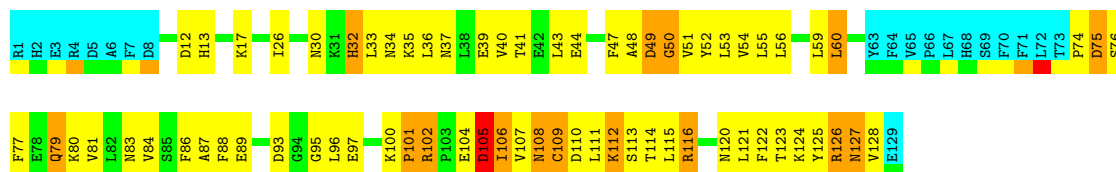
Chain B:  100%



4.2.2 Score per residue for model 2

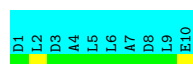
- Molecule 1: Alpha-parvin

Chain A:  30% 42% 12% 16%



- Molecule 2: Paxillin

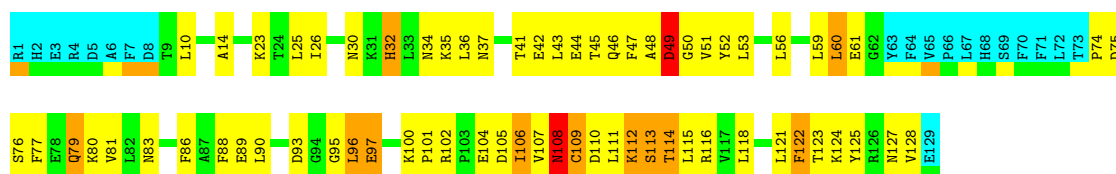
Chain B:  100%



4.2.3 Score per residue for model 3

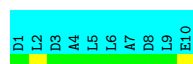
- Molecule 1: Alpha-parvin

Chain A:  32% 43% 9% 16%



- Molecule 2: Paxillin

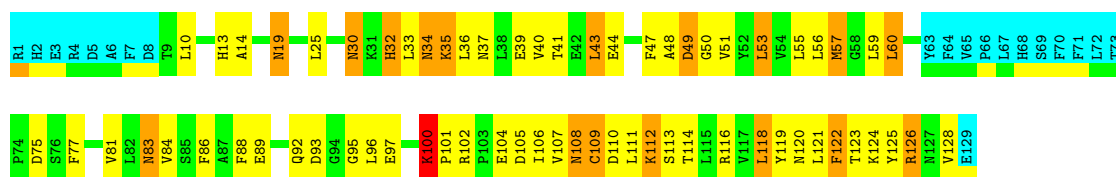
Chain B:  100%



4.2.4 Score per residue for model 4

- Molecule 1: Alpha-parvin

Chain A:  33% 37% 13% 16%



- Molecule 2: Paxillin

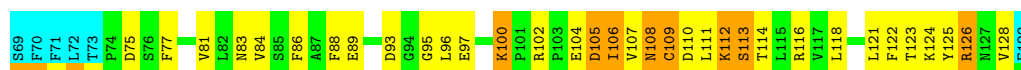
Chain B: 100%



4.2.5 Score per residue for model 5

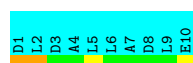
- Molecule 1: Alpha-parvin

Chain A: 32% 42% 11% 16%



- Molecule 2: Paxillin

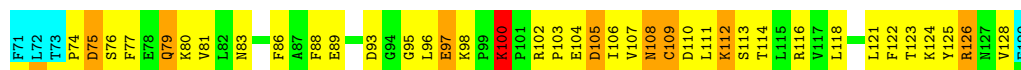
Chain B: 100%



4.2.6 Score per residue for model 6

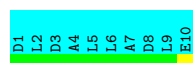
- Molecule 1: Alpha-parvin

Chain A: 31% 43% 9% 16%



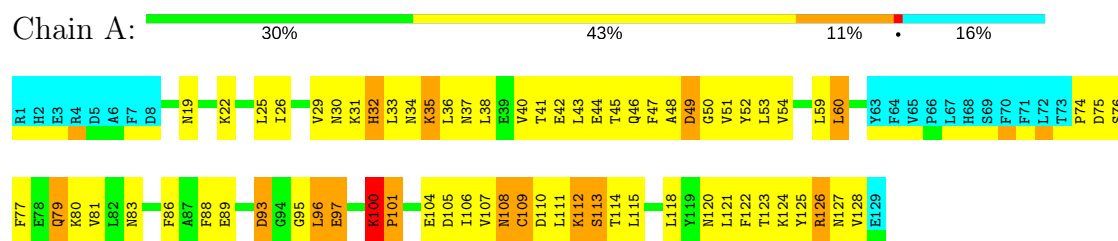
- Molecule 2: Paxillin

Chain B: 100%

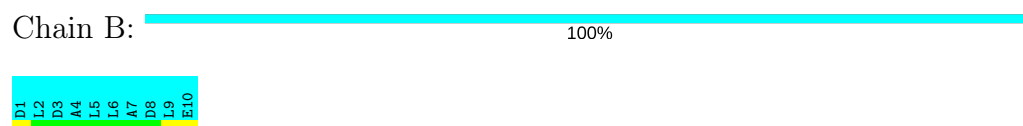


4.2.7 Score per residue for model 7

• Molecule 1: Alpha-parvin

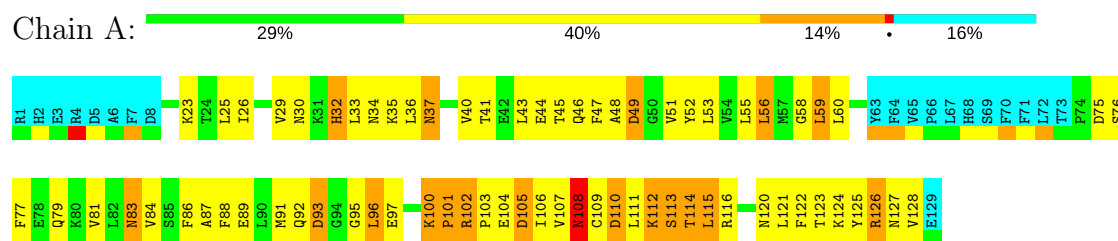


• Molecule 2: Paxillin

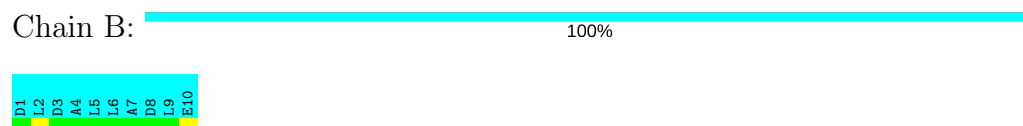


4.2.8 Score per residue for model 8

• Molecule 1: Alpha-parvin

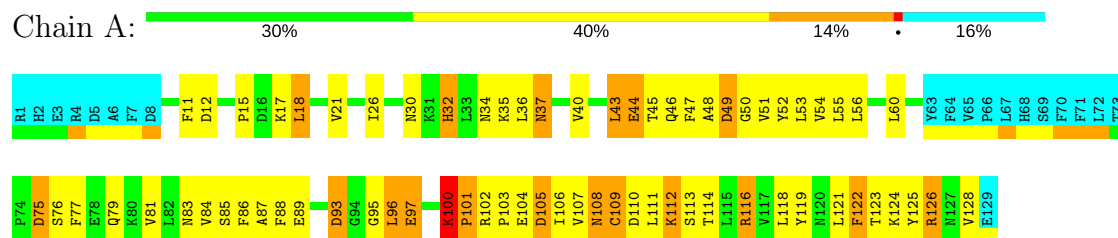


• Molecule 2: Paxillin



4.2.9 Score per residue for model 9

• Molecule 1: Alpha-parvin



- Molecule 2: Paxillin

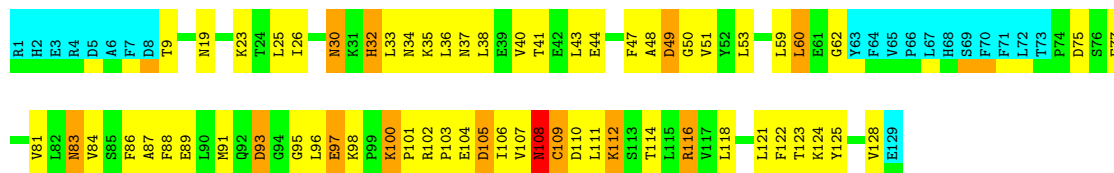
Chain B:  100%



4.2.10 Score per residue for model 10 (medoid)

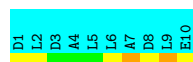
- Molecule 1: Alpha-parvin

Chain A:  36% 39% 9% 16%



- Molecule 2: Paxillin

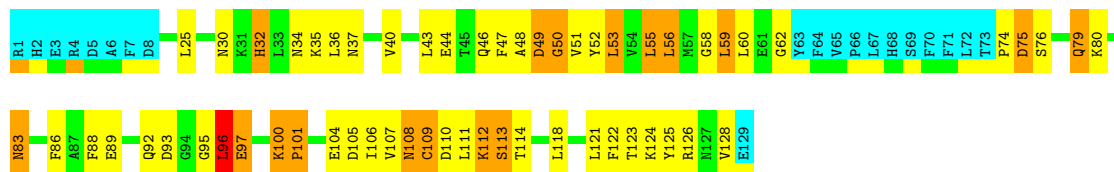
Chain B:  100%



4.2.11 Score per residue for model 11

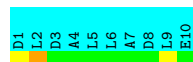
- Molecule 1: Alpha-parvin

Chain A:  39% 32% 13% 16%



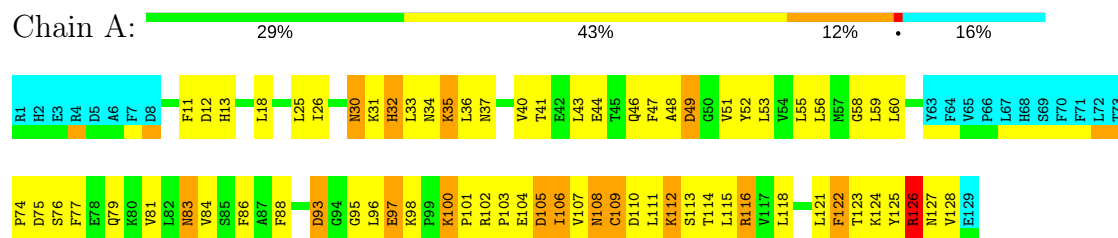
- Molecule 2: Paxillin

Chain B:  100%

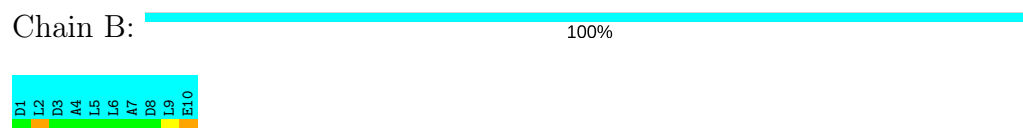


4.2.12 Score per residue for model 12

- Molecule 1: Alpha-parvin

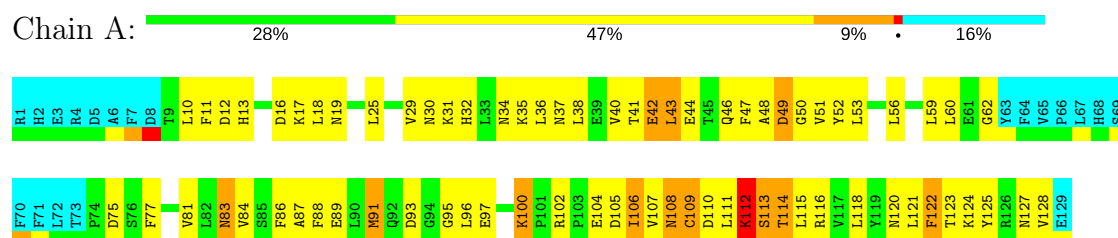


- Molecule 2: Paxillin

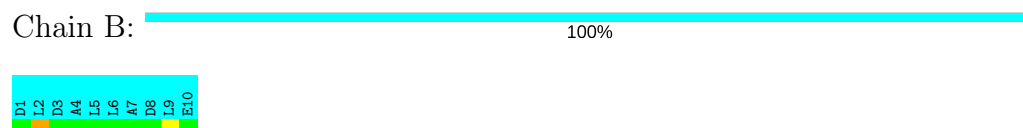


4.2.13 Score per residue for model 13

- Molecule 1: Alpha-parvin

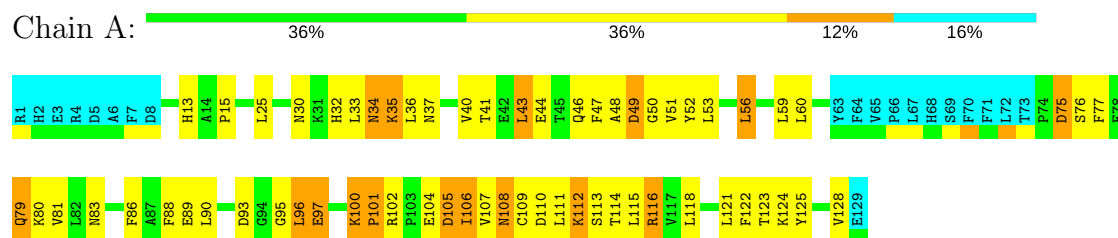


- Molecule 2: Paxillin



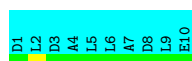
4.2.14 Score per residue for model 14

- Molecule 1: Alpha-parvin



- Molecule 2: Paxillin

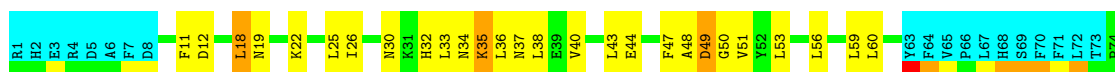




4.2.15 Score per residue for model 15

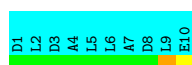
- Molecule 1: Alpha-parvin

Chain A: 37% 36% 10% • 16%



- Molecule 2: Paxillin

Chain B: 100%



4.2.16 Score per residue for model 16

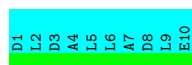
- Molecule 1: Alpha-parvin

Chain A: 33% 40% 11% 16%



- Molecule 2: Paxillin

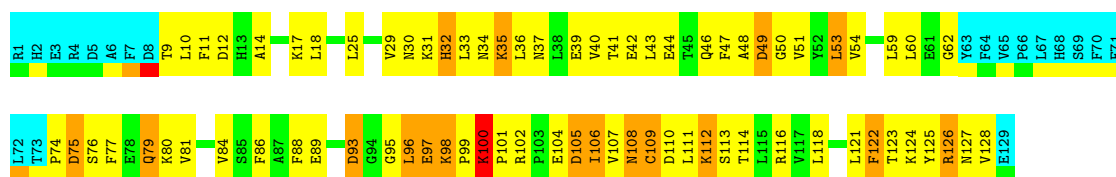
Chain B: 100%



4.2.17 Score per residue for model 17

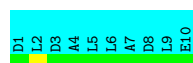
- Molecule 1: Alpha-parvin

Chain A: 26% 44% 13% • 16%



- Molecule 2: Paxillin

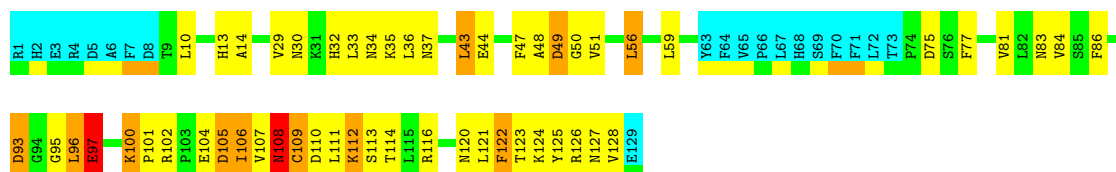
Chain B: 100%



4.2.18 Score per residue for model 18

- Molecule 1: Alpha-parvin

Chain A: 43% 32% 9% 16%



- Molecule 2: Paxillin

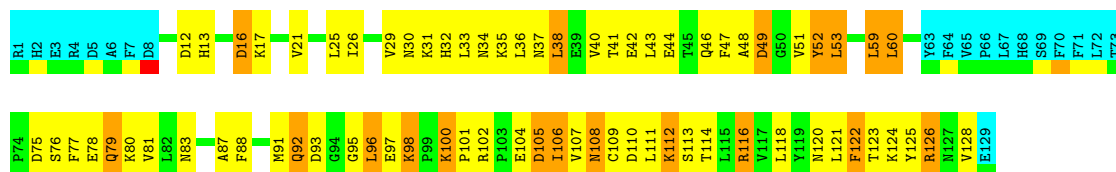
Chain B: 100%



4.2.19 Score per residue for model 19

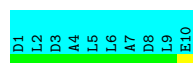
- Molecule 1: Alpha-parvin

Chain A: 29% 41% 15% 16%



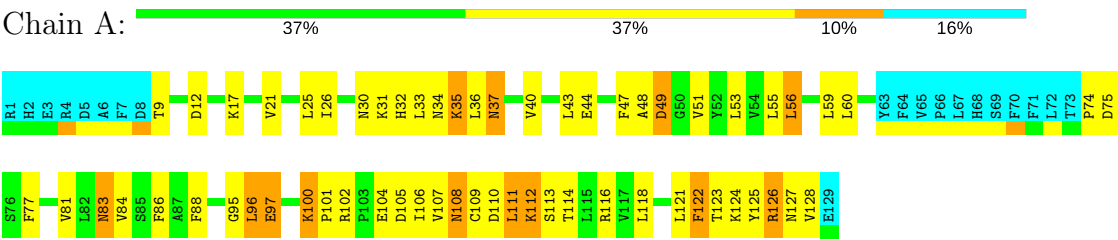
- Molecule 2: Paxillin

Chain B: 100%

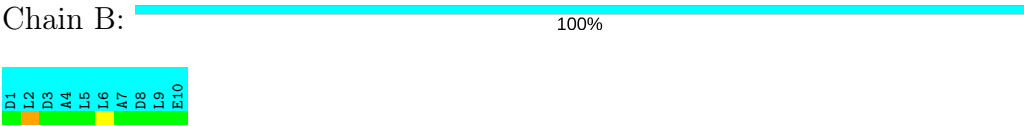


4.2.20 Score per residue for model 20

• Molecule 1: Alpha-parvin



• Molecule 2: Paxillin



5 Refinement protocol and experimental data overview ⓘ

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

Of the 200 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
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

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	879	903	903	78±12
2	B	0	0	0	0±0
All	All	17580	18060	18060	1563

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 44.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:LEU:HD22	1:A:111:LEU:H	0.83	1.34	20	1
1:A:111:LEU:HD22	1:A:111:LEU:N	0.76	1.96	20	4
1:A:11:PHE:CE2	1:A:18:LEU:HD11	0.75	2.16	12	3
1:A:35:LYS:H	1:A:35:LYS:HZ2	0.75	1.22	7	1
1:A:35:LYS:HZ2	1:A:35:LYS:N	0.73	1.81	7	1
1:A:59:LEU:H	1:A:59:LEU:HD22	0.72	1.44	12	2
1:A:47:PHE:CZ	1:A:53:LEU:HD21	0.72	2.19	11	4
1:A:11:PHE:CZ	1:A:18:LEU:HD11	0.72	2.18	12	2
1:A:76:SER:H	1:A:79:GLN:CG	0.72	1.97	7	9
1:A:47:PHE:CD2	1:A:53:LEU:HD11	0.70	2.21	1	1
1:A:96:LEU:N	1:A:124:LYS:NZ	0.70	2.40	5	18
1:A:47:PHE:CE2	1:A:53:LEU:HD21	0.70	2.22	12	6
1:A:75:ASP:N	1:A:79:GLN:NE2	0.69	2.41	19	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:LEU:H	1:A:124:LYS:HZ2	0.69	1.31	3	9
1:A:96:LEU:H	1:A:124:LYS:NZ	0.69	1.85	1	20
1:A:31:LYS:O	1:A:35:LYS:NZ	0.69	2.26	7	1
1:A:43:LEU:C	1:A:43:LEU:HD13	0.67	2.10	12	7
1:A:35:LYS:NZ	1:A:35:LYS:N	0.67	2.42	7	1
1:A:43:LEU:HD13	1:A:43:LEU:C	0.67	2.09	15	8
1:A:96:LEU:H	1:A:124:LYS:HZ3	0.66	1.32	13	3
1:A:60:LEU:HD13	1:A:60:LEU:C	0.65	2.12	15	5
1:A:60:LEU:C	1:A:60:LEU:HD13	0.65	2.10	11	4
1:A:31:LYS:NZ	1:A:35:LYS:NZ	0.64	2.45	12	1
1:A:26:ILE:HG23	1:A:40:VAL:HG13	0.64	1.67	10	11
1:A:79:GLN:NE2	1:A:80:LYS:N	0.64	2.45	3	1
1:A:46:GLN:NE2	1:A:52:TYR:CE2	0.64	2.66	8	3
1:A:47:PHE:CZ	1:A:118:LEU:HD21	0.64	2.28	19	1
1:A:76:SER:H	1:A:79:GLN:HG2	0.63	1.53	11	9
1:A:100:LYS:NZ	1:A:116:ARG:NH1	0.63	2.46	13	1
1:A:46:GLN:NE2	1:A:52:TYR:CD1	0.62	2.67	6	4
1:A:47:PHE:C	1:A:49:ASP:H	0.62	1.98	6	20
1:A:111:LEU:N	1:A:111:LEU:HD22	0.62	2.09	11	2
1:A:100:LYS:H	1:A:101:PRO:CD	0.62	2.08	17	10
1:A:46:GLN:NE2	1:A:52:TYR:CD2	0.62	2.68	13	7
1:A:46:GLN:NE2	1:A:52:TYR:CG	0.61	2.68	11	5
1:A:112:LYS:O	1:A:116:ARG:NH1	0.61	2.33	2	3
1:A:100:LYS:N	1:A:101:PRO:CD	0.61	2.63	2	5
1:A:43:LEU:HD13	1:A:44:GLU:N	0.60	2.11	9	1
1:A:36:LEU:O	1:A:37:ASN:ND2	0.60	2.35	18	12
1:A:56:LEU:C	1:A:56:LEU:HD12	0.60	2.17	5	1
1:A:79:GLN:C	1:A:79:GLN:HE21	0.60	2.00	3	1
1:A:56:LEU:HD12	1:A:56:LEU:C	0.60	2.17	14	4
1:A:76:SER:N	1:A:79:GLN:HE21	0.60	1.94	7	8
1:A:30:ASN:HD22	1:A:40:VAL:HG12	0.60	1.57	4	8
1:A:100:LYS:NZ	1:A:116:ARG:CZ	0.59	2.65	13	1
1:A:25:LEU:HD13	1:A:118:LEU:CB	0.59	2.27	4	12
1:A:33:LEU:O	1:A:37:ASN:N	0.59	2.35	19	3
1:A:49:ASP:OD1	1:A:51:VAL:HG23	0.59	1.96	20	1
1:A:100:LYS:HZ1	1:A:116:ARG:NH1	0.59	1.94	13	1
1:A:88:PHE:O	1:A:88:PHE:CD1	0.59	2.56	1	8
1:A:53:LEU:HD23	1:A:87:ALA:CB	0.59	2.27	2	2
1:A:37:ASN:O	1:A:37:ASN:ND2	0.59	2.36	1	2
1:A:29:VAL:HG21	1:A:43:LEU:HD21	0.59	1.75	5	1
1:A:55:LEU:O	1:A:59:LEU:HD22	0.59	1.97	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:SER:O	1:A:79:GLN:NE2	0.59	2.36	11	8
1:A:10:LEU:O	1:A:14:ALA:N	0.58	2.36	3	3
1:A:111:LEU:N	1:A:111:LEU:CD2	0.58	2.66	4	4
1:A:96:LEU:CA	1:A:124:LYS:NZ	0.58	2.67	15	4
1:A:49:ASP:O	1:A:51:VAL:N	0.58	2.36	7	15
1:A:125:TYR:O	1:A:128:VAL:N	0.58	2.37	7	12
1:A:47:PHE:CE2	1:A:53:LEU:HD11	0.58	2.34	1	1
1:A:37:ASN:ND2	1:A:37:ASN:O	0.57	2.37	8	6
1:A:96:LEU:H	1:A:124:LYS:HZ1	0.57	1.40	1	3
1:A:37:ASN:O	1:A:38:LEU:HD22	0.57	1.99	19	3
1:A:95:GLY:O	1:A:97:GLU:N	0.57	2.37	16	13
1:A:45:THR:HG22	1:A:109:CYS:SG	0.57	2.40	9	1
1:A:59:LEU:N	1:A:59:LEU:CD2	0.57	2.67	19	2
1:A:79:GLN:OE1	1:A:80:LYS:N	0.57	2.38	6	8
1:A:111:LEU:CD2	1:A:111:LEU:N	0.56	2.67	20	2
1:A:121:LEU:O	1:A:123:THR:N	0.56	2.39	12	20
1:A:111:LEU:H	1:A:111:LEU:CD2	0.56	2.11	20	1
1:A:105:ASP:OD1	1:A:105:ASP:N	0.56	2.39	14	8
1:A:46:GLN:NE2	1:A:52:TYR:CE1	0.56	2.74	7	2
1:A:96:LEU:N	1:A:124:LYS:HZ2	0.55	1.99	18	10
1:A:32:HIS:ND1	1:A:56:LEU:CD1	0.55	2.69	3	1
1:A:47:PHE:CZ	1:A:53:LEU:HD11	0.55	2.36	4	2
1:A:116:ARG:NE	1:A:116:ARG:O	0.55	2.40	19	1
1:A:126:ARG:CG	1:A:126:ARG:HH11	0.55	2.15	12	6
1:A:32:HIS:O	1:A:59:LEU:CB	0.55	2.55	6	16
1:A:105:ASP:N	1:A:105:ASP:OD1	0.54	2.39	13	10
1:A:108:ASN:O	1:A:110:ASP:N	0.54	2.40	6	20
1:A:102:ARG:NH1	1:A:105:ASP:OD1	0.54	2.41	18	3
1:A:53:LEU:HD13	1:A:87:ALA:CB	0.54	2.33	8	1
1:A:47:PHE:O	1:A:49:ASP:N	0.54	2.41	20	19
1:A:88:PHE:CD1	1:A:88:PHE:O	0.54	2.61	20	9
1:A:100:LYS:HZ1	1:A:116:ARG:NH2	0.54	2.00	9	1
1:A:126:ARG:NH1	1:A:126:ARG:CG	0.54	2.71	9	8
1:A:126:ARG:HH11	1:A:126:ARG:CG	0.54	2.16	4	6
1:A:51:VAL:O	1:A:53:LEU:N	0.54	2.41	2	6
1:A:77:PHE:CE1	1:A:81:VAL:CG2	0.54	2.91	4	16
1:A:59:LEU:N	1:A:59:LEU:HD22	0.54	2.15	12	2
1:A:51:VAL:C	1:A:53:LEU:N	0.53	2.61	17	16
1:A:57:MET:SD	1:A:57:MET:N	0.53	2.81	4	1
1:A:30:ASN:OD1	1:A:34:ASN:ND2	0.53	2.40	17	1
1:A:111:LEU:N	1:A:111:LEU:HD12	0.53	2.18	1	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ARG:N	1:A:105:ASP:OD2	0.53	2.41	8	10
1:A:13:HIS:ND1	1:A:13:HIS:O	0.53	2.42	14	3
1:A:76:SER:OG	1:A:79:GLN:NE2	0.53	2.41	9	2
1:A:35:LYS:NZ	1:A:35:LYS:CB	0.53	2.71	7	1
1:A:49:ASP:OD1	1:A:51:VAL:N	0.53	2.40	1	13
1:A:111:LEU:HD12	1:A:111:LEU:N	0.53	2.17	10	1
1:A:107:VAL:C	1:A:109:CYS:H	0.53	2.07	9	20
1:A:102:ARG:O	1:A:104:GLU:N	0.53	2.42	12	15
1:A:49:ASP:C	1:A:51:VAL:H	0.53	2.08	17	12
1:A:104:GLU:O	1:A:106:ILE:N	0.53	2.42	17	17
1:A:46:GLN:OE1	1:A:52:TYR:CG	0.53	2.62	1	4
1:A:37:ASN:OD1	1:A:37:ASN:O	0.52	2.27	18	6
1:A:79:GLN:C	1:A:79:GLN:NE2	0.52	2.63	3	1
1:A:42:GLU:N	1:A:42:GLU:OE1	0.52	2.42	17	1
1:A:49:ASP:OD1	1:A:74:PRO:CG	0.52	2.57	20	1
1:A:37:ASN:C	1:A:38:LEU:HD22	0.52	2.25	7	5
1:A:33:LEU:O	1:A:35:LYS:N	0.52	2.43	4	6
1:A:91:MET:O	1:A:95:GLY:N	0.52	2.42	1	1
1:A:30:ASN:ND2	1:A:40:VAL:H	0.52	2.03	13	7
1:A:17:LYS:O	1:A:21:VAL:HG23	0.52	2.05	6	4
1:A:101:PRO:CD	1:A:116:ARG:HH21	0.52	2.18	8	1
1:A:32:HIS:C	1:A:32:HIS:ND1	0.52	2.63	17	4
1:A:43:LEU:HD13	1:A:43:LEU:O	0.52	2.05	14	6
1:A:126:ARG:CG	1:A:126:ARG:NH1	0.52	2.72	5	4
1:A:32:HIS:O	1:A:59:LEU:HD12	0.52	2.04	1	4
1:A:74:PRO:CB	1:A:79:GLN:HE22	0.52	2.18	7	5
1:A:36:LEU:O	1:A:36:LEU:HD23	0.52	2.05	17	1
1:A:75:ASP:N	1:A:79:GLN:OE1	0.52	2.43	3	2
1:A:60:LEU:C	1:A:60:LEU:HD23	0.52	2.25	14	1
1:A:48:ALA:O	1:A:80:LYS:NZ	0.52	2.41	3	1
1:A:87:ALA:O	1:A:91:MET:SD	0.51	2.68	19	2
1:A:19:ASN:OD1	1:A:23:LYS:NZ	0.51	2.43	10	1
1:A:77:PHE:CZ	1:A:81:VAL:CG2	0.51	2.94	7	18
1:A:100:LYS:HZ2	1:A:116:ARG:NH2	0.51	2.03	13	1
1:A:49:ASP:O	1:A:49:ASP:OD1	0.51	2.28	20	1
1:A:19:ASN:OD1	1:A:22:LYS:NZ	0.51	2.43	15	3
1:A:47:PHE:CD2	1:A:53:LEU:HD21	0.51	2.40	14	1
1:A:107:VAL:O	1:A:109:CYS:N	0.51	2.42	9	20
1:A:25:LEU:HD13	1:A:118:LEU:HB3	0.51	1.81	4	10
1:A:31:LYS:HZ2	1:A:35:LYS:NZ	0.51	2.02	12	1
1:A:95:GLY:C	1:A:97:GLU:H	0.51	2.09	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ASN:O	1:A:34:ASN:N	0.51	2.40	5	19
1:A:96:LEU:CA	1:A:124:LYS:HZ2	0.51	2.19	15	2
1:A:49:ASP:OD1	1:A:50:GLY:N	0.50	2.44	11	3
1:A:37:ASN:O	1:A:37:ASN:CG	0.50	2.50	20	3
1:A:47:PHE:C	1:A:49:ASP:N	0.50	2.64	5	20
1:A:26:ILE:CG2	1:A:40:VAL:HG13	0.50	2.37	10	7
1:A:35:LYS:C	1:A:37:ASN:H	0.50	2.09	7	13
1:A:88:PHE:C	1:A:88:PHE:CD1	0.50	2.85	10	8
1:A:96:LEU:N	1:A:124:LYS:HZ1	0.50	2.02	8	5
1:A:46:GLN:OE1	1:A:52:TYR:CB	0.50	2.60	6	4
1:A:53:LEU:HD12	1:A:53:LEU:N	0.50	2.22	3	2
1:A:12:ASP:N	1:A:12:ASP:OD1	0.50	2.42	12	4
1:A:32:HIS:CB	1:A:56:LEU:HD12	0.50	2.36	9	1
1:A:108:ASN:C	1:A:110:ASP:H	0.50	2.10	2	20
1:A:108:ASN:C	1:A:110:ASP:N	0.50	2.65	13	19
1:A:32:HIS:C	1:A:32:HIS:CD2	0.50	2.83	12	1
1:A:13:HIS:CG	1:A:13:HIS:O	0.50	2.63	19	3
1:A:88:PHE:CD1	1:A:88:PHE:C	0.50	2.85	20	10
1:A:36:LEU:O	1:A:37:ASN:OD1	0.50	2.30	1	8
1:A:96:LEU:HD13	1:A:96:LEU:O	0.50	2.07	17	3
1:A:43:LEU:HD12	1:A:118:LEU:HD21	0.50	1.84	4	1
1:A:105:ASP:O	1:A:110:ASP:OD1	0.49	2.30	15	15
1:A:30:ASN:O	1:A:34:ASN:CB	0.49	2.60	5	9
1:A:37:ASN:CG	1:A:37:ASN:O	0.49	2.51	8	2
1:A:109:CYS:SG	1:A:109:CYS:O	0.49	2.70	15	2
1:A:25:LEU:HD11	1:A:115:LEU:HD23	0.49	1.84	12	1
1:A:109:CYS:O	1:A:109:CYS:SG	0.49	2.70	8	4
1:A:10:LEU:HD23	1:A:11:PHE:CE1	0.49	2.42	13	1
1:A:32:HIS:CD2	1:A:32:HIS:C	0.49	2.86	10	1
1:A:92:GLN:O	1:A:92:GLN:NE2	0.49	2.45	11	1
1:A:105:ASP:O	1:A:110:ASP:OD2	0.49	2.31	8	15
1:A:121:LEU:C	1:A:123:THR:N	0.49	2.66	12	20
1:A:75:ASP:H	1:A:79:GLN:HG2	0.49	1.67	19	9
1:A:121:LEU:O	1:A:124:LYS:N	0.49	2.46	4	15
1:A:43:LEU:HD11	1:A:118:LEU:CD1	0.49	2.38	15	2
1:A:49:ASP:O	1:A:51:VAL:HG23	0.49	2.08	3	1
1:A:47:PHE:CD2	1:A:106:ILE:HG21	0.48	2.43	12	6
1:A:31:LYS:NZ	1:A:35:LYS:HZ1	0.48	2.05	12	1
1:A:49:ASP:OD1	1:A:74:PRO:CD	0.48	2.60	20	1
1:A:100:LYS:HZ2	1:A:116:ARG:CZ	0.48	2.20	13	1
1:A:55:LEU:O	1:A:58:GLY:N	0.48	2.43	6	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:PHE:CZ	1:A:53:LEU:HD13	0.48	2.42	16	1
1:A:49:ASP:C	1:A:51:VAL:N	0.48	2.67	17	16
1:A:46:GLN:NE2	1:A:52:TYR:CZ	0.48	2.81	13	2
1:A:60:LEU:HD13	1:A:61:GLU:N	0.48	2.24	5	2
1:A:35:LYS:NZ	1:A:59:LEU:O	0.48	2.44	2	1
1:A:43:LEU:C	1:A:43:LEU:CD1	0.48	2.82	12	7
1:A:97:GLU:O	1:A:98:LYS:C	0.48	2.52	17	5
1:A:98:LYS:CB	1:A:98:LYS:NZ	0.48	2.75	15	1
1:A:32:HIS:O	1:A:59:LEU:CD1	0.48	2.62	2	9
1:A:59:LEU:CD2	1:A:59:LEU:H	0.48	2.20	12	1
1:A:37:ASN:O	1:A:37:ASN:OD1	0.47	2.31	13	6
1:A:74:PRO:C	1:A:79:GLN:NE2	0.47	2.67	2	4
1:A:116:ARG:HH11	1:A:116:ARG:HG2	0.47	1.69	13	1
1:A:60:LEU:HD23	1:A:60:LEU:C	0.47	2.29	20	2
1:A:43:LEU:CD1	1:A:43:LEU:C	0.47	2.83	8	8
1:A:97:GLU:OE2	1:A:120:ASN:ND2	0.47	2.47	18	1
1:A:102:ARG:C	1:A:104:GLU:N	0.47	2.68	12	9
1:A:84:VAL:HG21	1:A:107:VAL:HG23	0.47	1.87	12	12
1:A:102:ARG:H	1:A:105:ASP:CG	0.47	2.13	5	6
1:A:60:LEU:CD1	1:A:60:LEU:C	0.47	2.83	15	4
1:A:59:LEU:HD22	1:A:59:LEU:N	0.47	2.24	19	1
1:A:110:ASP:OD2	1:A:113:SER:N	0.47	2.48	15	1
1:A:86:PHE:CD1	1:A:86:PHE:C	0.46	2.88	3	8
1:A:116:ARG:C	1:A:116:ARG:HE	0.46	2.14	19	1
1:A:43:LEU:O	1:A:43:LEU:HD13	0.46	2.10	20	3
1:A:100:LYS:CE	1:A:116:ARG:HE	0.46	2.24	10	1
1:A:58:GLY:O	1:A:62:GLY:N	0.46	2.44	1	1
1:A:35:LYS:C	1:A:37:ASN:N	0.46	2.69	16	7
1:A:23:LYS:HA	1:A:26:ILE:HD12	0.46	1.87	8	2
1:A:111:LEU:O	1:A:112:LYS:C	0.46	2.54	10	20
1:A:105:ASP:O	1:A:110:ASP:CG	0.46	2.54	13	11
1:A:33:LEU:C	1:A:35:LYS:N	0.46	2.68	4	5
1:A:74:PRO:CB	1:A:79:GLN:NE2	0.46	2.79	7	4
1:A:9:THR:CG2	1:A:10:LEU:N	0.46	2.78	17	1
1:A:56:LEU:HD12	1:A:56:LEU:O	0.46	2.10	14	1
1:A:9:THR:O	1:A:13:HIS:N	0.46	2.49	1	1
1:A:91:MET:HB3	1:A:96:LEU:HD22	0.46	1.88	16	1
1:A:121:LEU:O	1:A:122:PHE:C	0.46	2.54	5	20
1:A:126:ARG:NH1	1:A:127:ASN:ND2	0.46	2.64	2	1
1:A:96:LEU:N	1:A:124:LYS:HZ3	0.46	2.01	13	1
1:A:60:LEU:HD13	1:A:60:LEU:O	0.45	2.11	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:LEU:HD22	1:A:118:LEU:HB3	0.45	1.88	15	3
1:A:125:TYR:O	1:A:128:VAL:O	0.45	2.33	12	11
1:A:34:ASN:O	1:A:37:ASN:N	0.45	2.49	3	3
1:A:50:GLY:O	1:A:53:LEU:CB	0.45	2.64	2	1
1:A:34:ASN:ND2	1:A:34:ASN:C	0.45	2.70	14	1
1:A:75:ASP:H	1:A:79:GLN:CG	0.45	2.24	19	7
1:A:86:PHE:O	1:A:89:GLU:N	0.45	2.50	9	14
1:A:29:VAL:HB	1:A:40:VAL:HG11	0.45	1.89	19	1
1:A:93:ASP:C	1:A:95:GLY:H	0.45	2.15	14	17
1:A:104:GLU:C	1:A:106:ILE:N	0.45	2.70	17	5
1:A:100:LYS:CE	1:A:116:ARG:NE	0.45	2.79	10	1
1:A:125:TYR:O	1:A:127:ASN:N	0.45	2.50	12	1
1:A:29:VAL:HG12	1:A:33:LEU:HD12	0.45	1.88	8	1
1:A:93:ASP:C	1:A:95:GLY:N	0.45	2.70	19	17
1:A:47:PHE:CE1	1:A:118:LEU:HD21	0.45	2.47	6	2
1:A:86:PHE:CE1	1:A:90:LEU:HD11	0.45	2.47	14	1
1:A:106:ILE:N	1:A:106:ILE:HD13	0.45	2.27	13	2
1:A:76:SER:O	1:A:79:GLN:OE1	0.45	2.35	3	1
1:A:107:VAL:C	1:A:109:CYS:N	0.44	2.70	4	19
1:A:101:PRO:CG	1:A:116:ARG:HH21	0.44	2.25	8	1
1:A:35:LYS:H	1:A:35:LYS:NZ	0.44	2.01	7	1
1:A:32:HIS:O	1:A:59:LEU:CG	0.44	2.65	8	1
1:A:32:HIS:ND1	1:A:56:LEU:HD13	0.44	2.28	20	1
1:A:33:LEU:O	1:A:34:ASN:C	0.44	2.56	12	8
1:A:96:LEU:O	1:A:97:GLU:O	0.44	2.36	17	6
1:A:30:ASN:O	1:A:34:ASN:OD1	0.44	2.35	19	2
1:A:56:LEU:C	1:A:56:LEU:CD1	0.44	2.85	14	2
1:A:79:GLN:C	1:A:79:GLN:OE1	0.44	2.55	7	4
1:A:31:LYS:HZ2	1:A:35:LYS:HZ2	0.44	1.55	12	1
1:A:60:LEU:C	1:A:60:LEU:CD1	0.44	2.84	6	3
1:A:116:ARG:HE	1:A:116:ARG:CA	0.44	2.25	19	1
1:A:16:ASP:OD1	1:A:16:ASP:N	0.44	2.50	19	1
1:A:16:ASP:O	1:A:19:ASN:ND2	0.44	2.51	13	1
1:A:95:GLY:O	1:A:96:LEU:CB	0.44	2.64	17	2
1:A:49:ASP:O	1:A:83:ASN:OD1	0.44	2.36	12	8
1:A:108:ASN:OD1	1:A:110:ASP:OD1	0.44	2.36	9	2
1:A:110:ASP:CG	1:A:113:SER:OG	0.44	2.56	15	2
1:A:11:PHE:CE1	1:A:18:LEU:HD13	0.44	2.48	17	1
1:A:12:ASP:OD1	1:A:12:ASP:N	0.44	2.51	15	1
1:A:111:LEU:N	1:A:111:LEU:CD1	0.44	2.80	10	6
1:A:25:LEU:HD11	1:A:115:LEU:CD2	0.43	2.43	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:LYS:CE	1:A:116:ARG:CZ	0.43	2.96	9	1
1:A:91:MET:O	1:A:95:GLY:O	0.43	2.35	1	2
1:A:75:ASP:H	1:A:79:GLN:CD	0.43	2.15	3	5
1:A:116:ARG:CG	1:A:116:ARG:NH1	0.43	2.81	13	1
1:A:40:VAL:HG22	1:A:41:THR:N	0.43	2.27	19	5
1:A:110:ASP:OD1	1:A:110:ASP:C	0.43	2.57	6	5
1:A:108:ASN:OD1	1:A:110:ASP:OD2	0.43	2.37	17	2
1:A:110:ASP:OD2	1:A:113:SER:OG	0.43	2.36	7	3
1:A:74:PRO:CB	1:A:80:LYS:HZ3	0.43	2.27	7	1
1:A:122:PHE:O	1:A:126:ARG:CB	0.43	2.67	8	6
1:A:60:LEU:O	1:A:60:LEU:HD13	0.43	2.14	16	2
1:A:33:LEU:O	1:A:36:LEU:N	0.43	2.51	19	1
1:A:16:ASP:O	1:A:19:ASN:OD1	0.43	2.37	13	1
1:A:110:ASP:C	1:A:110:ASP:OD1	0.43	2.57	12	3
1:A:39:GLU:OE2	1:A:40:VAL:O	0.43	2.36	17	2
1:A:113:SER:O	1:A:114:THR:C	0.43	2.57	8	4
1:A:47:PHE:CD2	1:A:106:ILE:CG2	0.43	3.02	12	1
1:A:51:VAL:C	1:A:53:LEU:H	0.43	2.17	11	3
1:A:111:LEU:CD1	1:A:111:LEU:N	0.43	2.81	1	1
1:A:31:LYS:CB	1:A:31:LYS:NZ	0.43	2.80	20	1
1:A:29:VAL:HG12	1:A:33:LEU:CD1	0.43	2.43	16	2
1:A:14:ALA:HB1	1:A:17:LYS:HB2	0.43	1.91	17	1
1:A:18:LEU:O	1:A:18:LEU:HD23	0.43	2.13	13	1
1:A:79:GLN:OE1	1:A:79:GLN:C	0.43	2.57	16	3
1:A:42:GLU:O	1:A:46:GLN:CG	0.43	2.66	6	4
1:A:113:SER:O	1:A:116:ARG:N	0.43	2.52	5	4
1:A:30:ASN:OD1	1:A:34:ASN:OD1	0.43	2.37	13	1
1:A:46:GLN:CD	1:A:52:TYR:CD2	0.43	2.92	13	1
1:A:30:ASN:O	1:A:34:ASN:CG	0.43	2.58	7	6
1:A:46:GLN:O	1:A:49:ASP:OD2	0.42	2.37	17	1
1:A:46:GLN:CD	1:A:52:TYR:CG	0.42	2.92	13	1
1:A:18:LEU:HD23	1:A:18:LEU:O	0.42	2.15	12	1
1:A:125:TYR:O	1:A:126:ARG:C	0.42	2.58	12	2
1:A:30:ASN:HD21	1:A:39:GLU:CD	0.42	2.17	2	1
1:A:36:LEU:O	1:A:37:ASN:CG	0.42	2.58	13	15
1:A:43:LEU:O	1:A:43:LEU:HD22	0.42	2.14	9	1
1:A:46:GLN:O	1:A:49:ASP:OD1	0.42	2.37	11	1
1:A:115:LEU:O	1:A:116:ARG:C	0.42	2.56	14	3
1:A:121:LEU:N	1:A:121:LEU:HD22	0.42	2.29	3	2
1:A:47:PHE:CG	1:A:106:ILE:HG22	0.42	2.49	5	1
1:A:42:GLU:CB	1:A:45:THR:HG22	0.42	2.44	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:ASN:O	1:A:110:ASP:OD1	0.42	2.37	5	3
1:A:76:SER:O	1:A:80:LYS:NZ	0.42	2.47	2	1
1:A:76:SER:OG	1:A:79:GLN:OE1	0.42	2.36	12	1
1:A:102:ARG:CZ	1:A:105:ASP:OD1	0.42	2.68	18	1
1:A:58:GLY:C	1:A:60:LEU:N	0.42	2.73	6	1
1:A:86:PHE:C	1:A:86:PHE:CD1	0.42	2.91	5	2
1:A:82:LEU:O	1:A:83:ASN:C	0.42	2.58	1	2
1:A:42:GLU:CD	1:A:45:THR:HG1	0.42	2.17	3	1
1:A:76:SER:O	1:A:79:GLN:CD	0.41	2.58	3	7
1:A:32:HIS:ND1	1:A:32:HIS:C	0.41	2.73	2	1
1:A:82:LEU:C	1:A:82:LEU:CD1	0.41	2.88	1	1
1:A:112:LYS:O	1:A:116:ARG:CZ	0.41	2.69	2	1
1:A:19:ASN:C	1:A:19:ASN:HD22	0.41	2.18	4	1
1:A:55:LEU:O	1:A:56:LEU:C	0.41	2.57	8	3
1:A:13:HIS:O	1:A:13:HIS:CG	0.41	2.74	4	1
1:A:52:TYR:CD1	1:A:52:TYR:O	0.41	2.74	19	1
1:A:60:LEU:C	1:A:60:LEU:CD2	0.41	2.89	9	1
1:A:56:LEU:O	1:A:57:MET:C	0.41	2.59	16	1
1:A:116:ARG:NE	1:A:116:ARG:C	0.41	2.74	19	1
1:A:118:LEU:O	1:A:119:TYR:C	0.41	2.59	4	2
1:A:106:ILE:O	1:A:107:VAL:C	0.41	2.58	11	3
1:A:106:ILE:C	1:A:108:ASN:N	0.41	2.73	11	2
1:A:29:VAL:C	1:A:31:LYS:N	0.41	2.74	19	1
1:A:84:VAL:HG21	1:A:107:VAL:CG2	0.41	2.45	12	2
1:A:85:SER:OG	1:A:103:PRO:CB	0.41	2.69	9	1
1:A:47:PHE:CE1	1:A:53:LEU:HD11	0.41	2.51	6	1
1:A:106:ILE:HD13	1:A:106:ILE:N	0.41	2.30	15	1
1:A:56:LEU:CD1	1:A:56:LEU:C	0.41	2.87	20	1
1:A:31:LYS:HZ3	1:A:35:LYS:NZ	0.41	2.13	12	1
1:A:25:LEU:HD11	1:A:115:LEU:HD13	0.41	1.93	8	1
1:A:96:LEU:H	1:A:124:LYS:CE	0.41	2.28	6	1
1:A:74:PRO:HB3	1:A:79:GLN:HE22	0.41	1.76	3	1
1:A:29:VAL:HG13	1:A:32:HIS:CD2	0.41	2.51	17	1
1:A:17:LYS:O	1:A:18:LEU:C	0.40	2.59	13	1
1:A:11:PHE:CD1	1:A:18:LEU:HD13	0.40	2.50	5	1
1:A:79:GLN:O	1:A:83:ASN:OD1	0.40	2.39	2	1
1:A:93:ASP:O	1:A:95:GLY:N	0.40	2.54	19	1
1:A:100:LYS:H	1:A:101:PRO:HD2	0.40	1.77	9	1
1:A:92:GLN:O	1:A:92:GLN:OE1	0.40	2.39	19	1
1:A:77:PHE:O	1:A:80:LYS:N	0.40	2.53	15	1
1:A:60:LEU:CD2	1:A:60:LEU:C	0.40	2.90	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:PHE:CE1	1:A:18:LEU:CD2	0.40	3.04	16	1
1:A:97:GLU:O	1:A:99:PRO:N	0.40	2.54	17	1
1:A:29:VAL:HG21	1:A:43:LEU:CD2	0.40	2.47	13	1
1:A:87:ALA:O	1:A:91:MET:CG	0.40	2.70	13	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	109/129 (84%)	79±2 (73±2%)	21±2 (19±2%)	9±2 (8±2%)	2	13
2	B	0	-	-	-	-	-
All	All	2180/2780 (78%)	1582 (73%)	414 (19%)	184 (8%)	2	13

All 18 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	108	ASN	20
1	A	49	ASP	20
1	A	112	LYS	20
1	A	48	ALA	18
1	A	100	LYS	17
1	A	109	CYS	16
1	A	50	GLY	14
1	A	97	GLU	13
1	A	101	PRO	11
1	A	122	PHE	10
1	A	96	LEU	9
1	A	105	ASP	6
1	A	103	PRO	4
1	A	98	LYS	2
1	A	126	ARG	1
1	A	34	ASN	1
1	A	52	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	74	PRO	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	101/120 (84%)	85±3 (85±3%)	16±3 (15±3%)	7 44
2	B	0	-	-	-
All	All	2020/2560 (79%)	1707 (85%)	313 (15%)	7 44

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	114	THR	20
1	A	44	GLU	20
1	A	113	SER	19
1	A	126	ARG	15
1	A	75	ASP	15
1	A	32	HIS	15
1	A	83	ASN	15
1	A	35	LYS	13
1	A	116	ARG	11
1	A	106	ILE	11
1	A	100	LYS	10
1	A	56	LEU	9
1	A	60	LEU	9
1	A	127	ASN	9
1	A	79	GLN	9
1	A	93	ASP	9
1	A	41	THR	8
1	A	105	ASP	7
1	A	43	LEU	6
1	A	120	ASN	6
1	A	59	LEU	5
1	A	108	ASN	5
1	A	37	ASN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	115	LEU	4
1	A	96	LEU	4
1	A	55	LEU	4
1	A	53	LEU	4
1	A	30	ASN	4
1	A	102	ARG	3
1	A	92	GLN	3
1	A	15	PRO	3
1	A	34	ASN	2
1	A	28	PHE	2
1	A	18	LEU	2
1	A	118	LEU	2
1	A	110	ASP	2
1	A	36	LEU	2
1	A	45	THR	1
1	A	104	GLU	1
1	A	90	LEU	1
1	A	33	LEU	1
1	A	49	ASP	1
1	A	31	LYS	1
1	A	57	MET	1
1	A	111	LEU	1
1	A	38	LEU	1
1	A	78	GLU	1
1	A	82	LEU	1
1	A	97	GLU	1
1	A	52	TYR	1
1	A	29	VAL	1
1	A	88	PHE	1
1	A	112	LYS	1
1	A	13	HIS	1
1	A	10	LEU	1
1	A	16	ASP	1
1	A	19	ASN	1
1	A	42	GLU	1
1	A	91	MET	1

6.3.3 RNA ⓘ

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 carbohydrates 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