



Full wwPDB NMR Structure Validation Report ⓘ

Feb 20, 2018 – 08:13 am GMT

PDB ID : 2L6H
Title : Fat domain of focal adhesion kinase tethered to LD4 motif of paxillin via GGS linker
Authors : Bertolucci, C.M.; Guibao, C.; Zhang, C.; Zheng, J.
Deposited on : 2010-11-19

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 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	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk30686
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30686

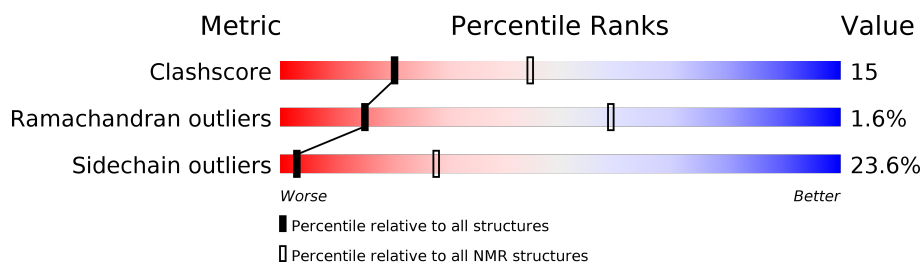
1 Overall quality at a glance

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	180	

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:137, A:170-A:183 (140)	0.46	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 5 clusters and 7 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2435 atoms, of which 1240 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Focal adhesion kinase 1, linker, Paxillin.

Mol	Chain	Residues	Atoms						Trace
1	A	154	Total	C	H	N	O	S	0
			2435	748	1240	204	234	9	

There are 28 discrepancies between the modelled and reference sequences:

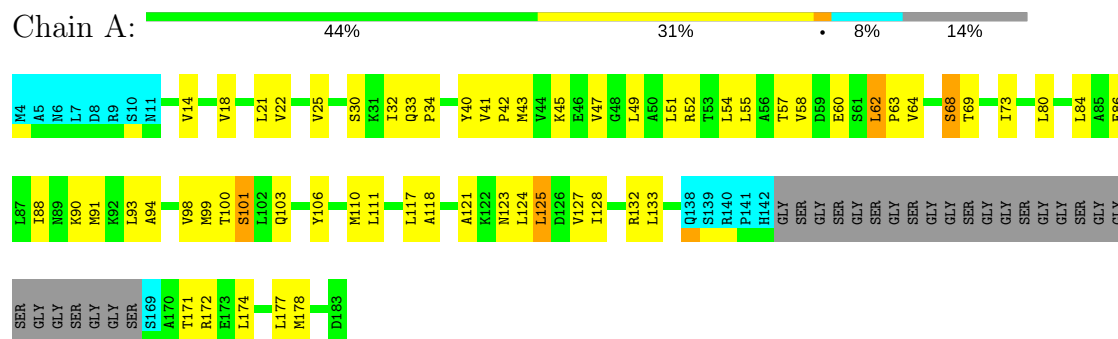
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	INITIATING METHIONINE	UNP Q00944
A	143	GLY	-	LINKER	UNP Q00944
A	144	SER	-	LINKER	UNP Q00944
A	145	GLY	-	LINKER	UNP Q00944
A	146	SER	-	LINKER	UNP Q00944
A	147	GLY	-	LINKER	UNP Q00944
A	148	SER	-	LINKER	UNP Q00944
A	149	GLY	-	LINKER	UNP Q00944
A	150	SER	-	LINKER	UNP Q00944
A	151	GLY	-	LINKER	UNP Q00944
A	152	GLY	-	LINKER	UNP Q00944
A	153	SER	-	LINKER	UNP Q00944
A	154	GLY	-	LINKER	UNP Q00944
A	155	GLY	-	LINKER	UNP Q00944
A	156	SER	-	LINKER	UNP Q00944
A	157	GLY	-	LINKER	UNP Q00944
A	158	GLY	-	LINKER	UNP Q00944
A	159	SER	-	LINKER	UNP Q00944
A	160	GLY	-	LINKER	UNP Q00944
A	161	GLY	-	LINKER	UNP Q00944
A	162	SER	-	LINKER	UNP Q00944
A	163	GLY	-	LINKER	UNP Q00944
A	164	GLY	-	LINKER	UNP Q00944
A	165	SER	-	LINKER	UNP Q00944
A	166	GLY	-	LINKER	UNP Q00944
A	167	GLY	-	LINKER	UNP Q00944
A	168	SER	-	LINKER	UNP Q00944
A	169	SER	-	LINKER	UNP Q00944

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: Focal adhesion kinase 1, linker, Paxillin

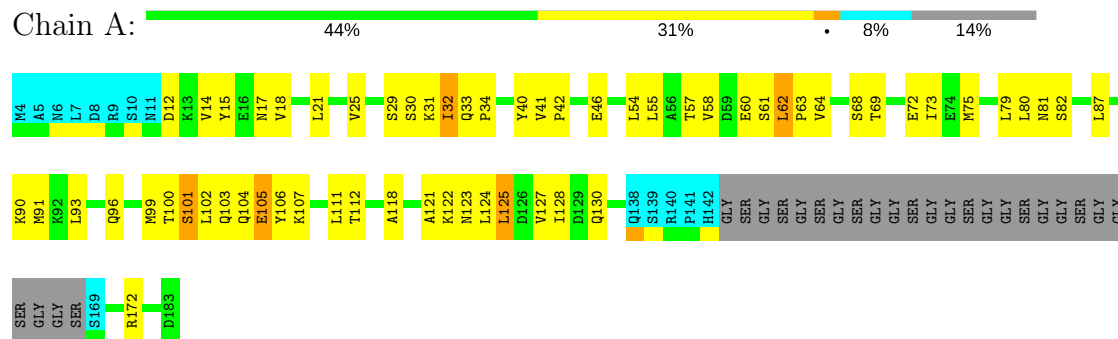


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

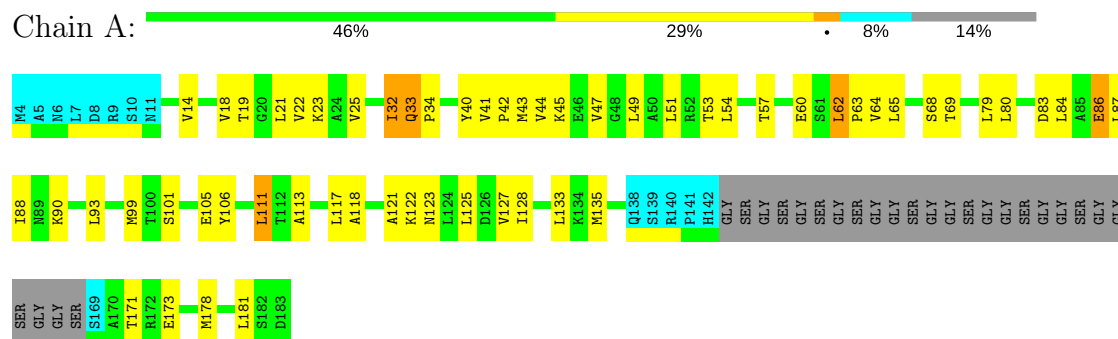
4.2.1 Score per residue for model 1

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



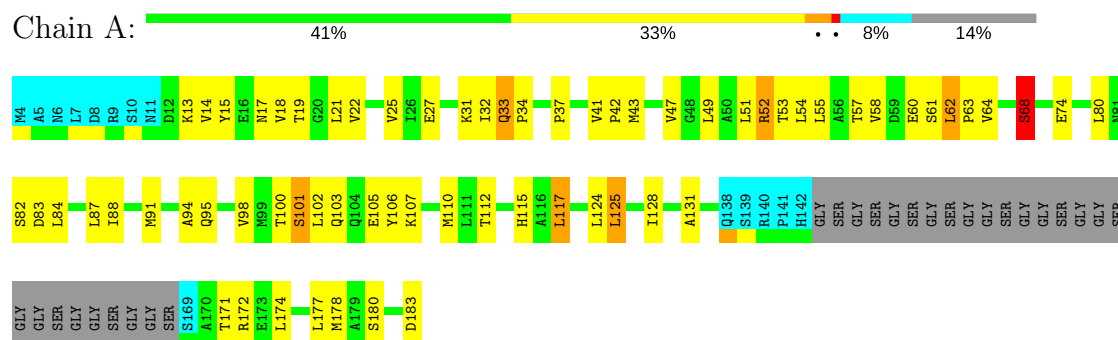
4.2.2 Score per residue for model 2

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



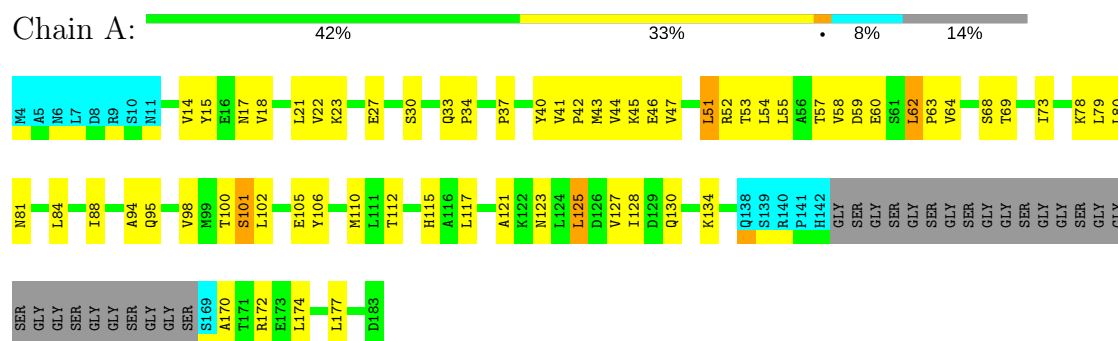
4.2.3 Score per residue for model 3

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



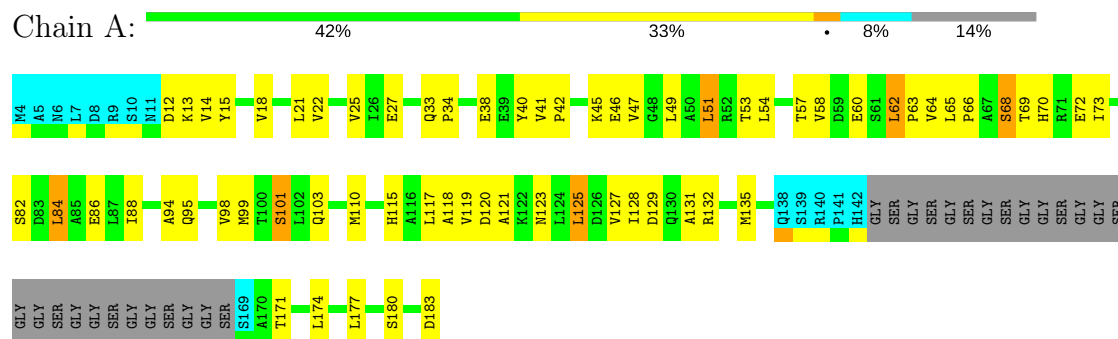
4.2.4 Score per residue for model 4

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



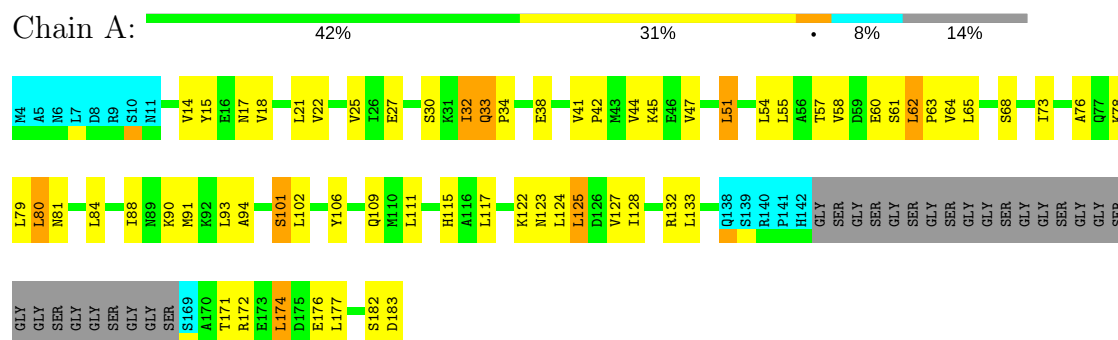
4.2.5 Score per residue for model 5

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



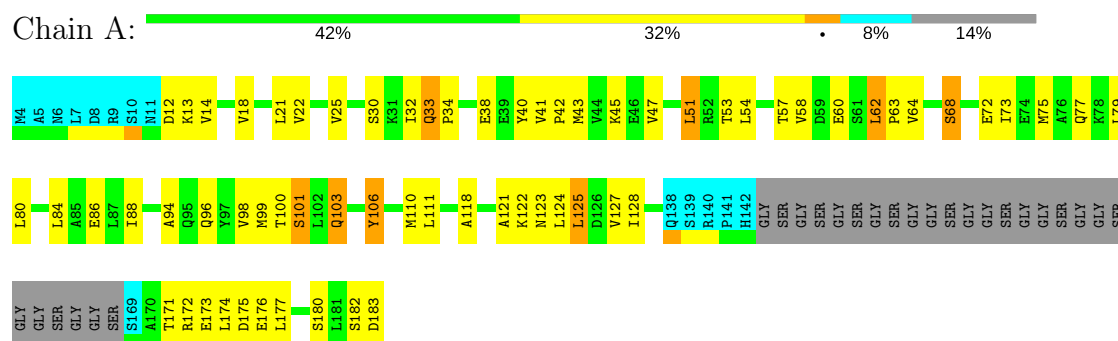
4.2.6 Score per residue for model 6

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



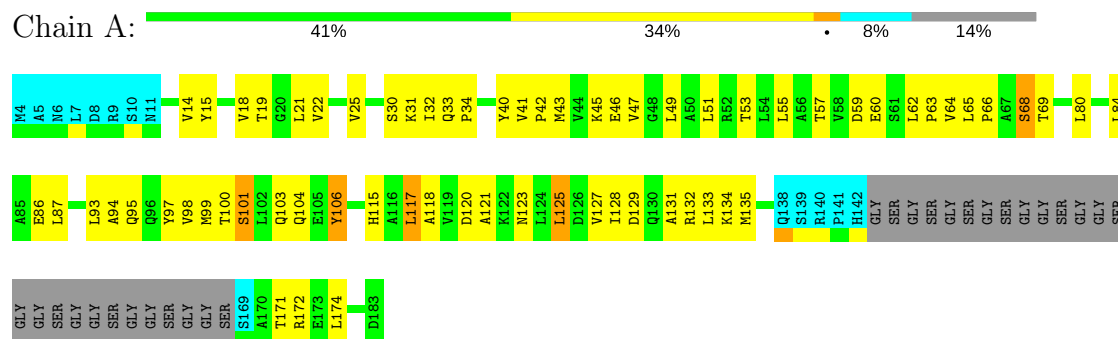
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



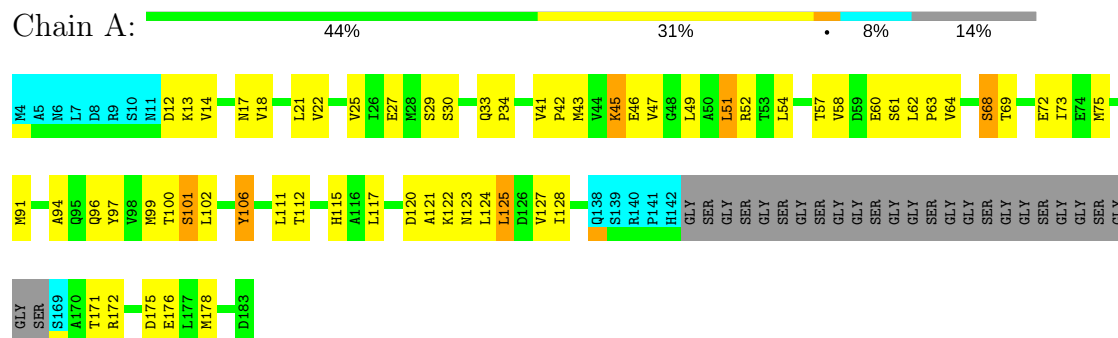
4.2.8 Score per residue for model 8

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



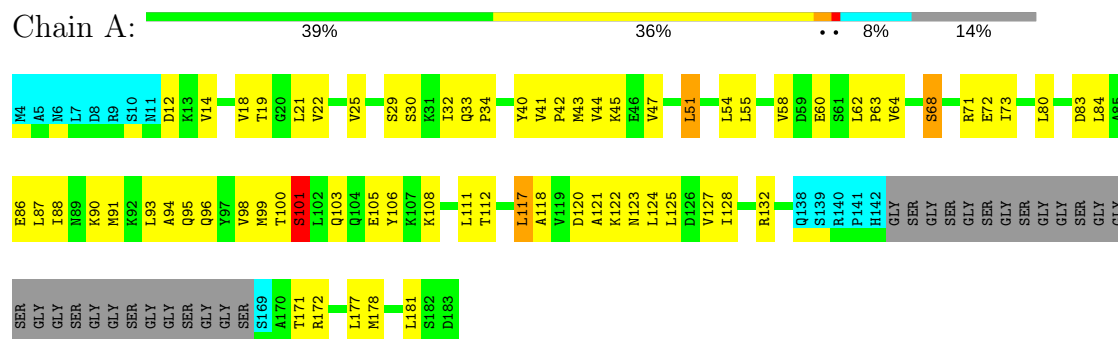
4.2.9 Score per residue for model 9

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



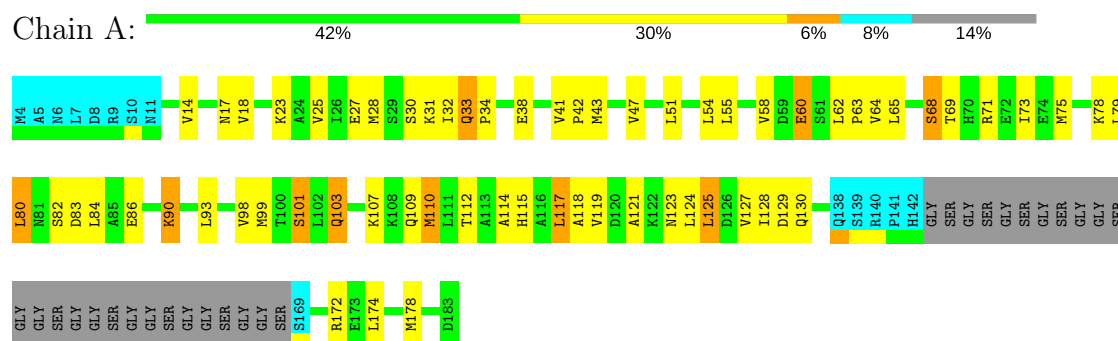
4.2.10 Score per residue for model 10

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



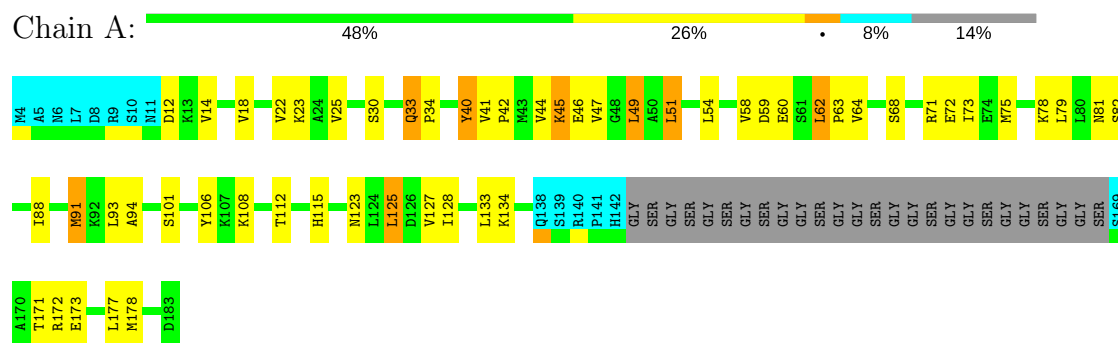
4.2.11 Score per residue for model 11

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



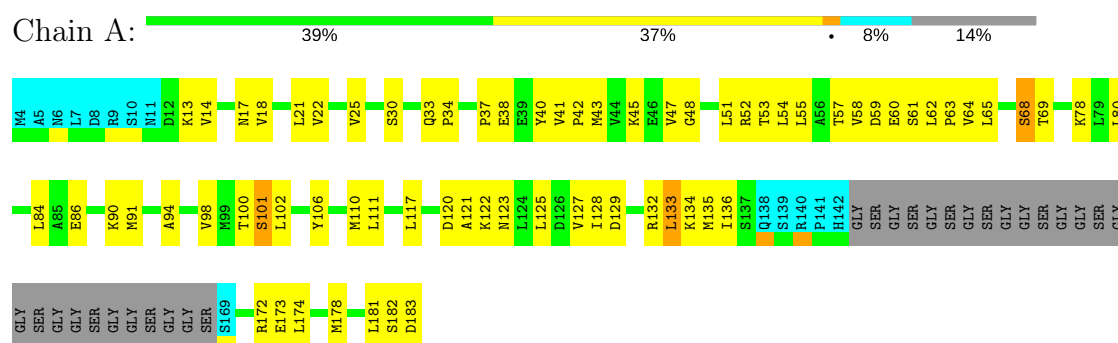
4.2.12 Score per residue for model 12

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



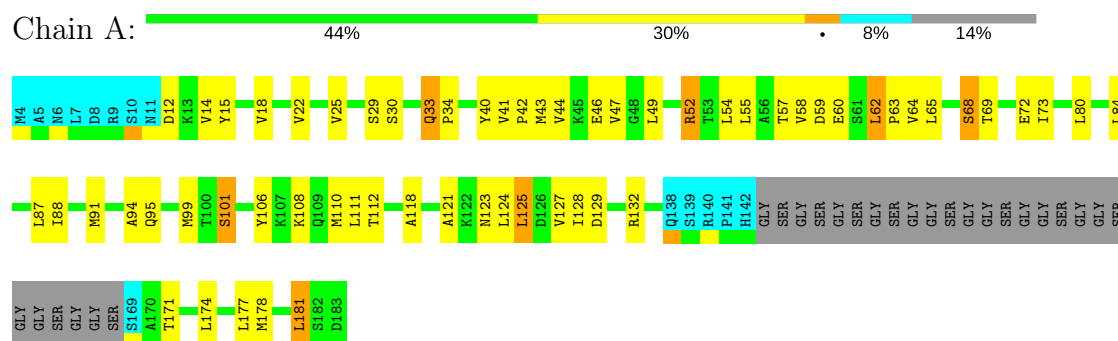
4.2.13 Score per residue for model 13

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



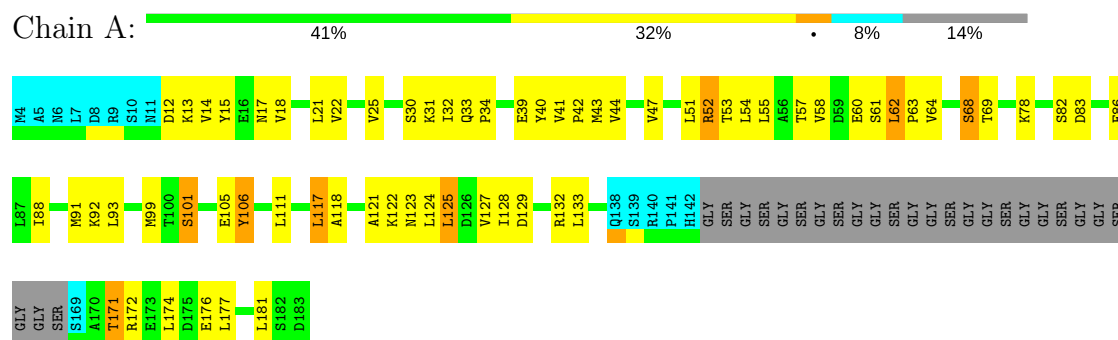
4.2.14 Score per residue for model 14

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



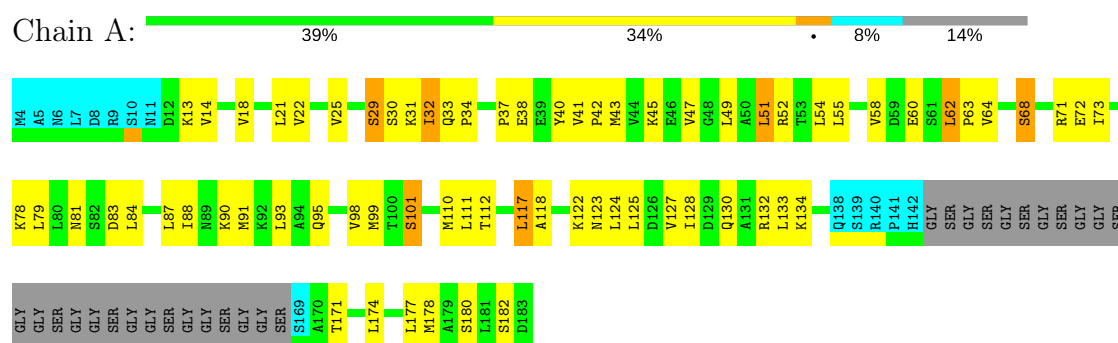
4.2.15 Score per residue for model 15

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



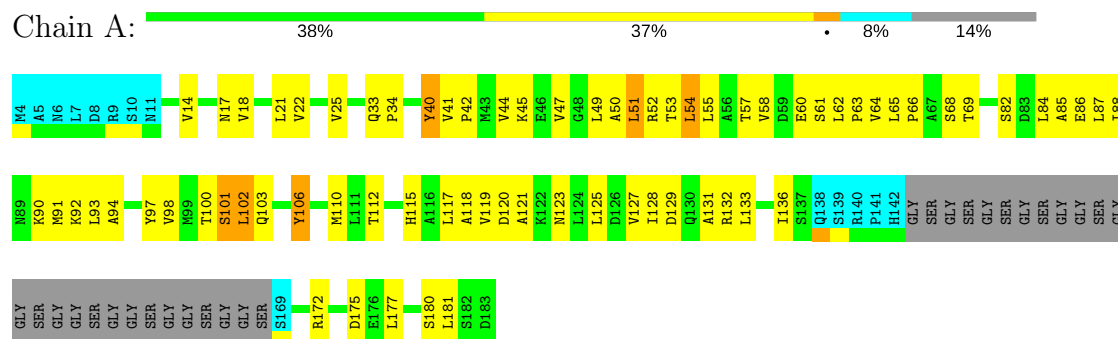
4.2.16 Score per residue for model 16

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



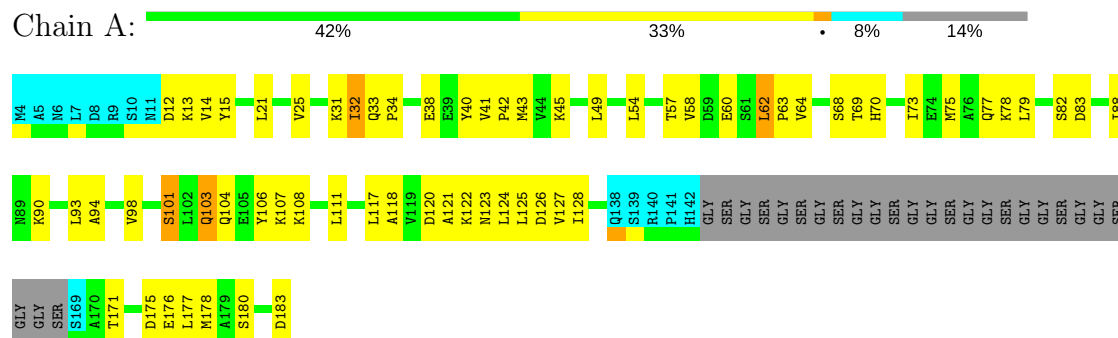
4.2.17 Score per residue for model 17

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



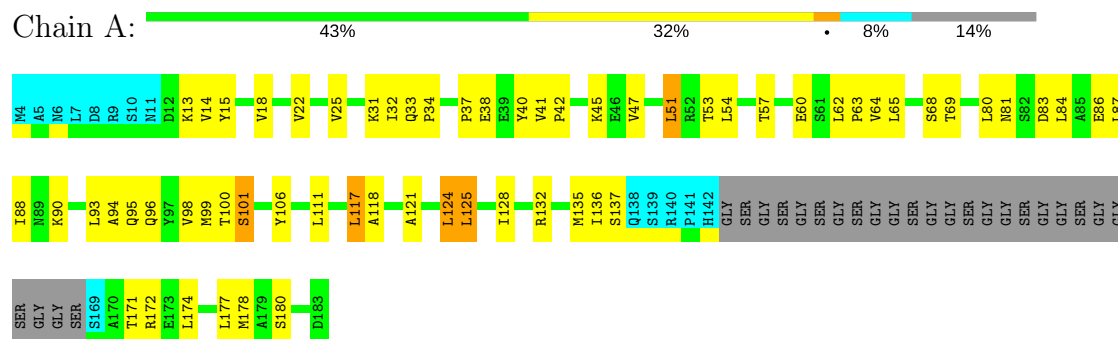
4.2.18 Score per residue for model 18

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



4.2.19 Score per residue for model 19

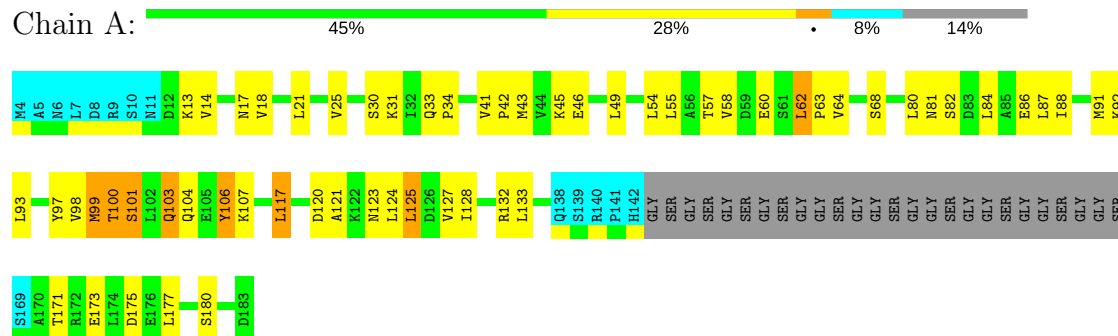
- Molecule 1: Focal adhesion kinase 1, linker, Paxillin



4.2.20 Score per residue for model 20

- Molecule 1: Focal adhesion kinase 1, linker, Paxillin

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING*, *TORSION ANGLE DYNAMICS*.

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	
CYANA	structure solution	
SPARKY	structure solution	
NMRPIPE	structure solution	
MOLMOL	structure solution	

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	1084	1136	1136	33±5
All	All	21680	22720	22720	651

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:THR:HG21	1:A:128:ILE:HG22	0.98	1.31	18	6
1:A:88:ILE:HD12	1:A:177:LEU:HD13	0.98	1.35	17	4
1:A:25:VAL:HG21	1:A:118:ALA:HB2	0.96	1.37	10	10
1:A:88:ILE:HG21	1:A:177:LEU:HD22	0.84	1.50	20	6
1:A:44:VAL:HG11	1:A:181:LEU:HD22	0.84	1.46	17	4
1:A:87:LEU:HD11	1:A:117:LEU:HD12	0.81	1.51	10	4
1:A:14:VAL:HG22	1:A:57:THR:HG22	0.74	1.59	1	1
1:A:47:VAL:HG11	1:A:87:LEU:HD13	0.74	1.60	14	2
1:A:14:VAL:HG12	1:A:57:THR:HG23	0.73	1.61	18	1
1:A:54:LEU:HD13	1:A:80:LEU:HD21	0.72	1.61	19	3
1:A:84:LEU:HD22	1:A:174:LEU:HD23	0.72	1.61	16	1
1:A:88:ILE:HG21	1:A:177:LEU:HD12	0.70	1.62	16	4
1:A:51:LEU:HD21	1:A:117:LEU:HD11	0.70	1.61	10	2
1:A:51:LEU:HD13	1:A:84:LEU:HD13	0.69	1.63	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:ALA:HB2	1:A:106:TYR:HB3	0.67	1.67	14	7
1:A:32:ILE:HG21	1:A:111:LEU:HD11	0.66	1.65	15	5
1:A:51:LEU:HB2	1:A:84:LEU:HD13	0.64	1.70	3	2
1:A:93:LEU:HD22	1:A:97:TYR:CE2	0.64	2.28	8	1
1:A:88:ILE:HG23	1:A:181:LEU:HD11	0.63	1.70	15	1
1:A:21:LEU:O	1:A:25:VAL:HG23	0.63	1.93	6	11
1:A:69:THR:HG21	1:A:128:ILE:CG2	0.63	2.23	17	3
1:A:47:VAL:HG11	1:A:87:LEU:HD11	0.62	1.69	17	1
1:A:88:ILE:HD12	1:A:181:LEU:HD11	0.62	1.72	2	2
1:A:53:THR:O	1:A:57:THR:HG23	0.61	1.95	8	8
1:A:58:VAL:CG2	1:A:73:ILE:HD12	0.61	2.24	14	2
1:A:98:VAL:HG13	1:A:103:GLN:OE1	0.61	1.94	5	2
1:A:14:VAL:HG22	1:A:57:THR:CG2	0.61	2.25	1	1
1:A:47:VAL:O	1:A:51:LEU:HD12	0.61	1.96	17	11
1:A:51:LEU:CD1	1:A:84:LEU:HD13	0.60	2.26	13	2
1:A:52:ARG:CG	1:A:174:LEU:HD22	0.60	2.27	3	2
1:A:54:LEU:O	1:A:58:VAL:HG12	0.60	1.97	18	7
1:A:98:VAL:HG13	1:A:103:GLN:NE2	0.60	2.12	10	1
1:A:54:LEU:HD21	1:A:121:ALA:HB1	0.60	1.72	15	1
1:A:58:VAL:HG22	1:A:124:LEU:HD13	0.60	1.71	6	4
1:A:21:LEU:HD11	1:A:121:ALA:HB3	0.59	1.71	18	3
1:A:94:ALA:O	1:A:98:VAL:HG23	0.59	1.98	8	3
1:A:58:VAL:HG21	1:A:73:ILE:HD12	0.59	1.74	14	1
1:A:90:LYS:HA	1:A:93:LEU:HD12	0.59	1.74	18	9
1:A:15:TYR:CD1	1:A:125:LEU:HD22	0.59	2.33	3	6
1:A:98:VAL:HG23	1:A:103:GLN:OE1	0.58	1.98	7	2
1:A:58:VAL:HG12	1:A:73:ILE:HG23	0.58	1.74	1	2
1:A:25:VAL:HG11	1:A:118:ALA:HB2	0.58	1.74	5	3
1:A:14:VAL:O	1:A:18:VAL:HG23	0.58	1.98	12	7
1:A:88:ILE:CD1	1:A:177:LEU:HD13	0.58	2.28	15	2
1:A:48:GLY:HA2	1:A:51:LEU:HD12	0.58	1.75	13	1
1:A:93:LEU:HD13	1:A:106:TYR:CE1	0.58	2.33	20	1
1:A:51:LEU:O	1:A:80:LEU:HD23	0.58	1.97	4	1
1:A:94:ALA:HB2	1:A:106:TYR:CD2	0.58	2.33	7	3
1:A:54:LEU:O	1:A:58:VAL:HG22	0.58	1.98	16	1
1:A:69:THR:O	1:A:73:ILE:HD13	0.58	1.99	11	1
1:A:14:VAL:HG23	1:A:57:THR:HB	0.58	1.75	13	2
1:A:47:VAL:HG12	1:A:51:LEU:CD1	0.58	2.28	17	5
1:A:123:ASN:O	1:A:127:VAL:HG23	0.57	1.99	17	18
1:A:58:VAL:CG1	1:A:73:ILE:HG23	0.57	2.28	1	5
1:A:18:VAL:HG23	1:A:121:ALA:O	0.57	1.99	20	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:ALA:HB2	1:A:106:TYR:CB	0.57	2.28	14	4
1:A:83:ASP:CG	1:A:117:LEU:HD21	0.56	2.21	15	2
1:A:18:VAL:HG12	1:A:54:LEU:HD21	0.56	1.76	17	2
1:A:44:VAL:HG12	1:A:88:ILE:HD13	0.56	1.76	4	1
1:A:54:LEU:O	1:A:58:VAL:HG23	0.56	2.00	15	7
1:A:84:LEU:HA	1:A:87:LEU:HD12	0.56	1.75	19	2
1:A:32:ILE:HD13	1:A:111:LEU:CD1	0.56	2.30	6	1
1:A:51:LEU:HD13	1:A:84:LEU:HD12	0.56	1.77	7	2
1:A:72:GLU:OE1	1:A:127:VAL:HG11	0.56	2.00	5	3
1:A:65:LEU:HG	1:A:128:ILE:HD12	0.55	1.78	17	7
1:A:25:VAL:HG21	1:A:118:ALA:CB	0.55	2.29	11	8
1:A:47:VAL:CG1	1:A:87:LEU:HD13	0.55	2.30	14	1
1:A:44:VAL:HG11	1:A:181:LEU:CD2	0.55	2.32	2	2
1:A:14:VAL:HG13	1:A:57:THR:HB	0.55	1.78	2	3
1:A:93:LEU:HD22	1:A:106:TYR:CE2	0.55	2.35	1	1
1:A:14:VAL:HG22	1:A:57:THR:HB	0.55	1.79	20	2
1:A:98:VAL:HG23	1:A:103:GLN:NE2	0.55	2.17	17	2
1:A:121:ALA:HA	1:A:124:LEU:HD12	0.55	1.79	18	2
1:A:171:THR:HA	1:A:174:LEU:HD12	0.55	1.77	14	7
1:A:86:GLU:CD	1:A:113:ALA:HB1	0.55	2.22	2	1
1:A:60:GLU:O	1:A:64:VAL:HG23	0.54	2.02	18	20
1:A:115:HIS:O	1:A:119:VAL:HG23	0.54	2.03	5	3
1:A:97:TYR:CD1	1:A:102:LEU:HD11	0.54	2.37	17	1
1:A:54:LEU:HD11	1:A:121:ALA:HB2	0.54	1.80	14	6
1:A:40:TYR:O	1:A:44:VAL:HG23	0.54	2.03	12	1
1:A:44:VAL:HG22	1:A:91:MET:SD	0.54	2.43	15	1
1:A:32:ILE:HD13	1:A:111:LEU:HG	0.54	1.79	2	3
1:A:47:VAL:HG12	1:A:51:LEU:HD23	0.53	1.80	11	3
1:A:25:VAL:HG11	1:A:118:ALA:CB	0.53	2.33	5	3
1:A:69:THR:CG2	1:A:128:ILE:HG22	0.53	2.33	15	8
1:A:54:LEU:HD11	1:A:121:ALA:HB1	0.53	1.78	17	3
1:A:54:LEU:HD11	1:A:121:ALA:CB	0.53	2.33	13	8
1:A:44:VAL:CG1	1:A:88:ILE:HD13	0.53	2.34	4	1
1:A:44:VAL:HG21	1:A:91:MET:SD	0.53	2.43	12	1
1:A:88:ILE:CG2	1:A:177:LEU:HD22	0.53	2.32	15	1
1:A:21:LEU:HD12	1:A:22:VAL:N	0.52	2.19	13	7
1:A:83:ASP:HB3	1:A:117:LEU:HD21	0.52	1.80	15	4
1:A:70:HIS:HA	1:A:73:ILE:HD12	0.52	1.81	5	1
1:A:54:LEU:HD22	1:A:124:LEU:CD1	0.52	2.34	19	8
1:A:83:ASP:CB	1:A:117:LEU:HD21	0.52	2.35	15	4
1:A:58:VAL:HG13	1:A:73:ILE:HD12	0.52	1.80	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:ARG:HG3	1:A:174:LEU:HD22	0.52	1.81	4	1
1:A:72:GLU:CD	1:A:127:VAL:HG11	0.52	2.25	9	1
1:A:73:ILE:HD11	1:A:128:ILE:HD12	0.52	1.81	16	2
1:A:58:VAL:CG2	1:A:124:LEU:HD13	0.52	2.35	9	4
1:A:51:LEU:HD13	1:A:84:LEU:CD1	0.52	2.35	7	5
1:A:44:VAL:HG21	1:A:91:MET:HG2	0.51	1.83	14	1
1:A:51:LEU:HD22	1:A:84:LEU:HA	0.51	1.82	3	1
1:A:58:VAL:CG2	1:A:73:ILE:HG23	0.51	2.36	10	3
1:A:51:LEU:HD12	1:A:80:LEU:HG	0.51	1.81	2	1
1:A:29:SER:CB	1:A:111:LEU:HD21	0.51	2.36	9	2
1:A:51:LEU:HD11	1:A:117:LEU:HD11	0.51	1.82	10	2
1:A:87:LEU:CD1	1:A:117:LEU:HD12	0.51	2.35	8	2
1:A:14:VAL:HG13	1:A:15:TYR:CD1	0.51	2.41	4	1
1:A:97:TYR:CE2	1:A:102:LEU:HD12	0.50	2.41	9	1
1:A:99:MET:CE	1:A:100:THR:HG23	0.50	2.35	20	1
1:A:21:LEU:CD2	1:A:50:ALA:HB1	0.50	2.36	17	1
1:A:102:LEU:HD12	1:A:106:TYR:CD1	0.50	2.40	17	1
1:A:15:TYR:CD1	1:A:125:LEU:HD21	0.50	2.41	4	1
1:A:76:ALA:O	1:A:80:LEU:HD12	0.50	2.07	6	1
1:A:72:GLU:OE1	1:A:127:VAL:HG21	0.50	2.07	9	6
1:A:102:LEU:HD22	1:A:105:GLU:OE2	0.49	2.07	1	2
1:A:52:ARG:HG3	1:A:174:LEU:HD13	0.49	1.83	15	1
1:A:41:VAL:N	1:A:42:PRO:HD2	0.49	2.22	3	20
1:A:72:GLU:OE2	1:A:127:VAL:HG11	0.49	2.07	9	1
1:A:93:LEU:HD13	1:A:106:TYR:OH	0.49	2.06	15	1
1:A:18:VAL:O	1:A:22:VAL:HG23	0.49	2.07	7	9
1:A:41:VAL:O	1:A:44:VAL:HG12	0.49	2.08	6	3
1:A:69:THR:CG2	1:A:128:ILE:HD12	0.49	2.37	14	4
1:A:21:LEU:HD21	1:A:121:ALA:HB1	0.49	1.84	18	2
1:A:83:ASP:CB	1:A:117:LEU:HD23	0.49	2.37	2	1
1:A:84:LEU:HD23	1:A:174:LEU:CD2	0.49	2.38	11	1
1:A:133:LEU:HD13	1:A:136:ILE:HD12	0.49	1.84	17	1
1:A:15:TYR:HA	1:A:125:LEU:HD13	0.49	1.85	6	5
1:A:58:VAL:CG1	1:A:73:ILE:HD12	0.49	2.38	1	1
1:A:68:SER:OG	1:A:131:ALA:HB2	0.49	2.08	3	1
1:A:52:ARG:HA	1:A:55:LEU:HD12	0.48	1.85	3	1
1:A:33:GLN:CB	1:A:34:PRO:CD	0.48	2.91	19	20
1:A:51:LEU:HD11	1:A:117:LEU:CD1	0.48	2.38	10	1
1:A:22:VAL:O	1:A:25:VAL:HG12	0.48	2.09	13	2
1:A:17:ASN:OD1	1:A:53:THR:HG21	0.48	2.08	13	1
1:A:75:MET:O	1:A:79:LEU:HD13	0.48	2.09	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:PRO:HB3	1:A:98:VAL:HG21	0.47	1.85	3	5
1:A:66:PRO:HG2	1:A:131:ALA:HB1	0.47	1.86	17	3
1:A:52:ARG:CG	1:A:174:LEU:HD13	0.47	2.39	15	1
1:A:81:ASN:OD1	1:A:170:ALA:HB1	0.47	2.09	4	1
1:A:37:PRO:HB3	1:A:98:VAL:HG11	0.47	1.85	19	2
1:A:14:VAL:HG12	1:A:57:THR:CG2	0.47	2.35	18	1
1:A:88:ILE:CG2	1:A:177:LEU:HD12	0.47	2.40	5	1
1:A:62:LEU:CB	1:A:63:PRO:CD	0.47	2.93	17	20
1:A:47:VAL:HG12	1:A:51:LEU:CD2	0.47	2.38	11	3
1:A:94:ALA:HB2	1:A:106:TYR:CD1	0.47	2.45	8	1
1:A:54:LEU:HD21	1:A:121:ALA:CB	0.47	2.40	15	1
1:A:53:THR:HG22	1:A:57:THR:CG2	0.47	2.39	17	5
1:A:98:VAL:HG22	1:A:103:GLN:NE2	0.47	2.25	8	2
1:A:14:VAL:HG22	1:A:125:LEU:HD12	0.47	1.87	11	1
1:A:98:VAL:HG23	1:A:103:GLN:CD	0.47	2.30	3	2
1:A:69:THR:HG23	1:A:73:ILE:CD1	0.46	2.39	18	2
1:A:88:ILE:HD12	1:A:177:LEU:HD23	0.46	1.86	19	1
1:A:86:GLU:OE2	1:A:113:ALA:HB1	0.46	2.10	2	1
1:A:51:LEU:O	1:A:80:LEU:HD11	0.46	2.10	11	1
1:A:62:LEU:N	1:A:63:PRO:HD2	0.46	2.25	9	20
1:A:47:VAL:HG12	1:A:51:LEU:HD11	0.46	1.86	5	8
1:A:51:LEU:CD2	1:A:117:LEU:HD11	0.46	2.37	10	1
1:A:133:LEU:HA	1:A:136:ILE:HD12	0.46	1.86	17	2
1:A:54:LEU:HD22	1:A:124:LEU:HD12	0.46	1.87	19	1
1:A:51:LEU:HD22	1:A:84:LEU:HB2	0.46	1.87	10	2
1:A:18:VAL:HG13	1:A:121:ALA:O	0.46	2.11	8	3
1:A:84:LEU:CD2	1:A:174:LEU:HD23	0.45	2.39	16	3
1:A:83:ASP:CG	1:A:117:LEU:HD23	0.45	2.32	18	2
1:A:33:GLN:N	1:A:34:PRO:HD2	0.45	2.27	4	19
1:A:125:LEU:HA	1:A:128:ILE:HG22	0.45	1.89	6	10
1:A:14:VAL:HG23	1:A:15:TYR:CD1	0.45	2.46	18	1
1:A:51:LEU:HD22	1:A:84:LEU:CA	0.44	2.42	3	1
1:A:29:SER:O	1:A:32:ILE:HG22	0.44	2.13	10	3
1:A:93:LEU:HD13	1:A:106:TYR:CE2	0.44	2.48	2	2
1:A:52:ARG:HB2	1:A:174:LEU:HD22	0.44	1.90	14	1
1:A:14:VAL:O	1:A:18:VAL:HG13	0.43	2.12	10	4
1:A:88:ILE:CD1	1:A:181:LEU:HD11	0.43	2.40	2	1
1:A:85:ALA:HA	1:A:177:LEU:HD11	0.43	1.89	17	1
1:A:65:LEU:HD11	1:A:132:ARG:NE	0.43	2.28	6	1
1:A:47:VAL:HG11	1:A:87:LEU:CD1	0.43	2.42	17	1
1:A:125:LEU:HG	1:A:128:ILE:HD11	0.43	1.90	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:THR:HG22	1:A:57:THR:HG23	0.43	1.91	7	2
1:A:32:ILE:HG21	1:A:111:LEU:CD1	0.43	2.42	18	1
1:A:40:TYR:CE2	1:A:94:ALA:HB3	0.43	2.49	4	2
1:A:95:GLN:O	1:A:98:VAL:HG12	0.43	2.14	16	1
1:A:52:ARG:HG2	1:A:174:LEU:HD22	0.43	1.89	3	1
1:A:32:ILE:HD13	1:A:111:LEU:CG	0.43	2.44	6	1
1:A:88:ILE:CG2	1:A:181:LEU:HD21	0.43	2.43	17	1
1:A:88:ILE:HG13	1:A:177:LEU:HD13	0.42	1.90	20	1
1:A:45:LYS:O	1:A:49:LEU:HD23	0.42	2.14	9	1
1:A:110:MET:CE	1:A:114:ALA:HB2	0.42	2.44	11	1
1:A:47:VAL:O	1:A:51:LEU:HD23	0.42	2.15	15	1
1:A:69:THR:HG21	1:A:128:ILE:HD12	0.42	1.92	9	1
1:A:54:LEU:HD12	1:A:124:LEU:CD1	0.42	2.45	16	2
1:A:18:VAL:HA	1:A:21:LEU:HD21	0.42	1.91	13	4
1:A:50:ALA:O	1:A:54:LEU:HD12	0.41	2.15	17	1
1:A:100:THR:HG22	1:A:101:SER:OG	0.41	2.15	10	1
1:A:87:LEU:HD11	1:A:117:LEU:CD1	0.41	2.37	10	1
1:A:58:VAL:CG1	1:A:124:LEU:HD13	0.41	2.46	16	1
1:A:99:MET:HE3	1:A:100:THR:HG23	0.41	1.92	20	1
1:A:45:LYS:O	1:A:49:LEU:HD12	0.40	2.15	12	1
1:A:41:VAL:CB	1:A:42:PRO:CD	0.40	3.00	19	4
1:A:58:VAL:HG22	1:A:73:ILE:HG23	0.40	1.94	10	1
1:A:14:VAL:HG22	1:A:125:LEU:HD13	0.40	1.93	9	1
1:A:52:ARG:CB	1:A:174:LEU:HD22	0.40	2.46	4	1
1:A:136:ILE:HD12	1:A:137:SER:N	0.40	2.32	19	1
1:A:117:LEU:HD13	1:A:117:LEU:C	0.40	2.37	17	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	139/180 (77%)	128±2 (92±1%)	9±2 (7±1%)	2±0 (2±0%)	15	59
All	All	2780/3600 (77%)	2550 (92%)	185 (7%)	45 (2%)	15	59

All 5 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	101	SER	20
1	A	68	SER	20
1	A	105	GLU	3
1	A	124	LEU	1
1	A	77	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	122/145 (84%)	93±4 (76±3%)	29±4 (24±3%)	3	28
All	All	2440/2900 (84%)	1863 (76%)	577 (24%)	3	28

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	125	LEU	18
1	A	101	SER	18
1	A	45	LYS	15
1	A	30	SER	14
1	A	40	TYR	14
1	A	172	ARG	14
1	A	43	MET	14
1	A	99	MET	13
1	A	62	LEU	13
1	A	117	LEU	13
1	A	55	LEU	12
1	A	68	SER	11
1	A	178	MET	11
1	A	86	GLU	11
1	A	112	THR	10
1	A	132	ARG	10
1	A	51	LEU	10
1	A	100	THR	10
1	A	122	LYS	10

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Mol	Chain	Res	Type	Models (Total)
1	A	91	MET	10
1	A	13	LYS	10
1	A	49	LEU	10
1	A	171	THR	9
1	A	12	ASP	9
1	A	31	LYS	9
1	A	82	SER	9
1	A	110	MET	9
1	A	17	ASN	9
1	A	80	LEU	9
1	A	133	LEU	8
1	A	38	GLU	8
1	A	46	GLU	8
1	A	120	ASP	8
1	A	32	ILE	8
1	A	78	LYS	8
1	A	180	SER	8
1	A	52	ARG	7
1	A	33	GLN	7
1	A	129	ASP	7
1	A	95	GLN	7
1	A	61	SER	7
1	A	183	ASP	6
1	A	79	LEU	6
1	A	115	HIS	6
1	A	27	GLU	6
1	A	106	TYR	6
1	A	81	ASN	6
1	A	59	ASP	5
1	A	96	GLN	5
1	A	135	MET	5
1	A	176	GLU	5
1	A	134	LYS	5
1	A	173	GLU	5
1	A	111	LEU	5
1	A	107	LYS	5
1	A	103	GLN	5
1	A	175	ASP	5
1	A	108	LYS	4
1	A	102	LEU	4
1	A	19	THR	4
1	A	104	GLN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	23	LYS	4
1	A	71	ARG	4
1	A	182	SER	4
1	A	130	GLN	4
1	A	75	MET	3
1	A	92	LYS	3
1	A	105	GLU	2
1	A	83	ASP	2
1	A	109	GLN	2
1	A	181	LEU	2
1	A	84	LEU	2
1	A	29	SER	2
1	A	174	LEU	2
1	A	90	LYS	2
1	A	57	THR	1
1	A	93	LEU	1
1	A	126	ASP	1
1	A	60	GLU	1
1	A	74	GLU	1
1	A	77	GLN	1
1	A	54	LEU	1
1	A	39	GLU	1
1	A	70	HIS	1
1	A	97	TYR	1
1	A	28	MET	1
1	A	87	LEU	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

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