



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:27 AM BST

PDB ID : 2L6G
Title : FAT-LD2 Double labeled construct with free LD4 peptide
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
<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

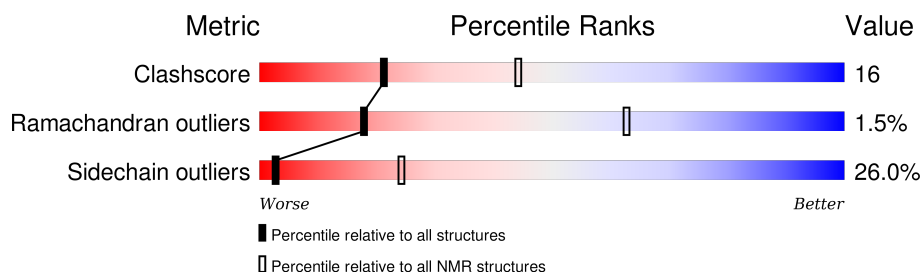
1 Overall quality at a glance

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	176	

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:10-A:137, A:162-A:170 (137)	0.38	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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2559 atoms, of which 1304 are hydrogens and 0 are deuteriums.

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

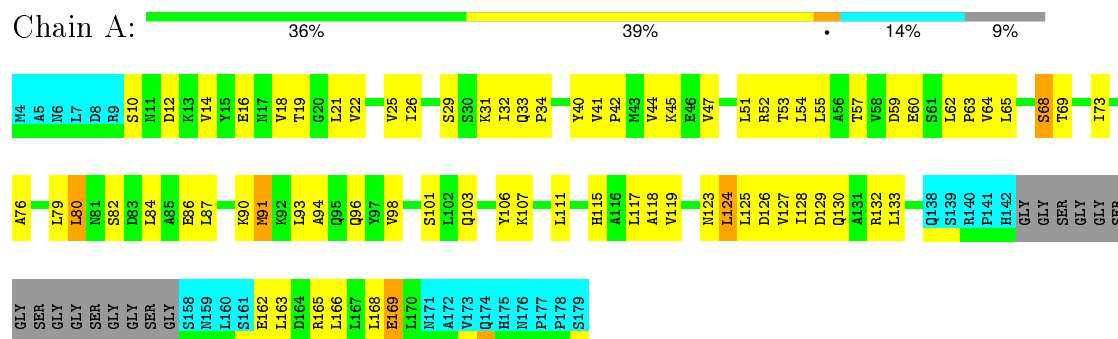
Mol	Chain	Residues	Atoms						Trace
1	A	161	Total	C	H	N	O	S	0
			2559	788	1304	217	242	8	

There are 16 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	GLY	-	LINKER	UNP Q00944
A	145	SER	-	LINKER	UNP Q00944
A	146	GLY	-	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

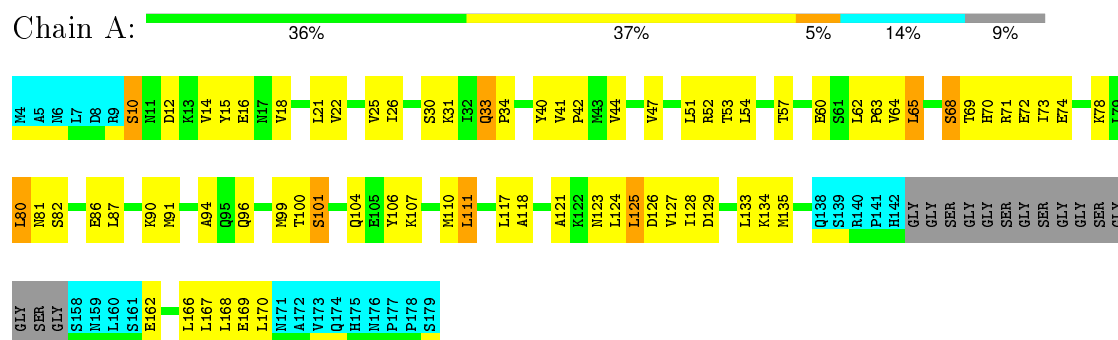
4.2.2 Score per residue for model 2

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



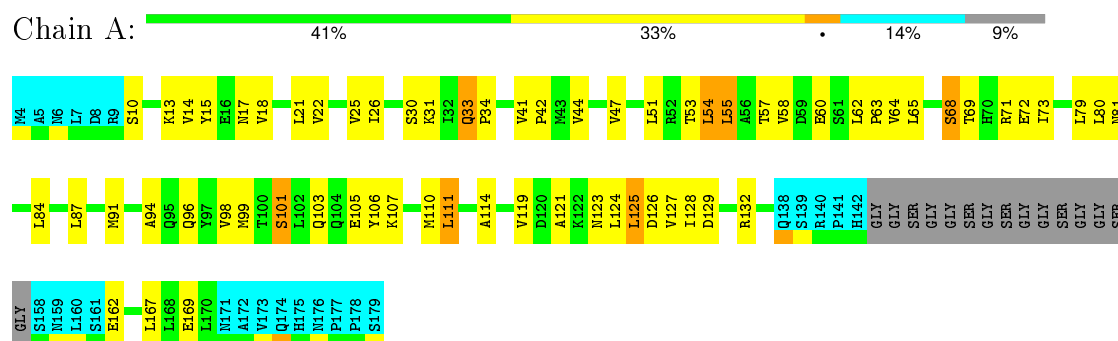
4.2.3 Score per residue for model 3

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



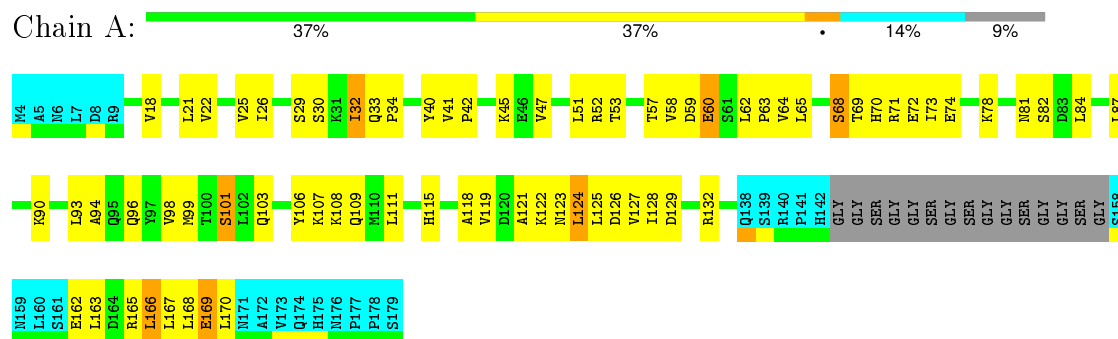
4.2.4 Score per residue for model 4

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



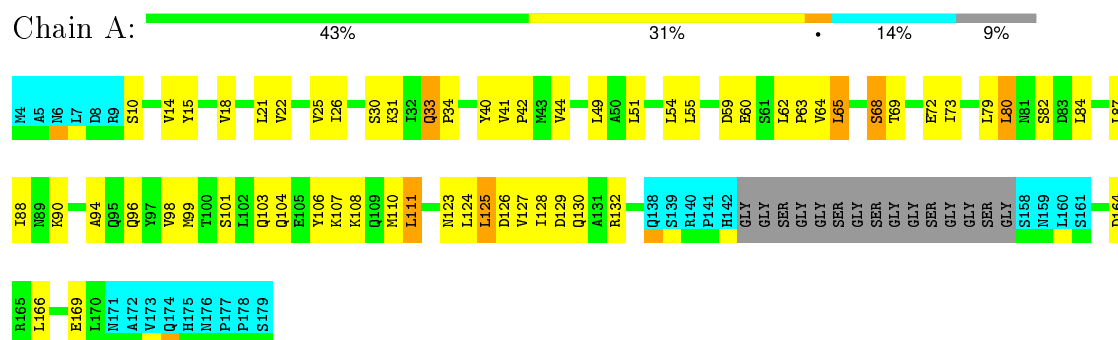
4.2.5 Score per residue for model 5

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



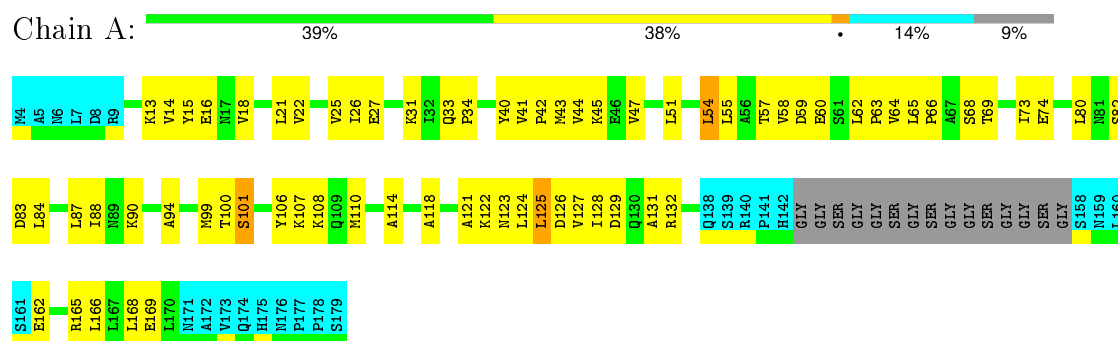
4.2.6 Score per residue for model 6

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



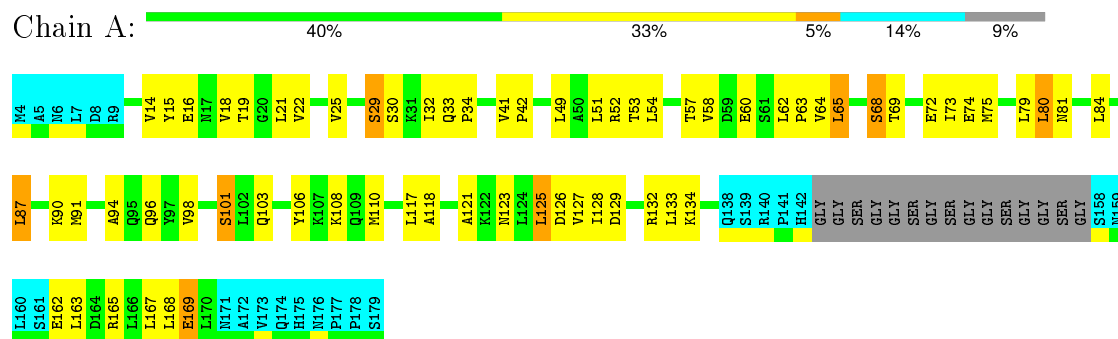
4.2.7 Score per residue for model 7

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



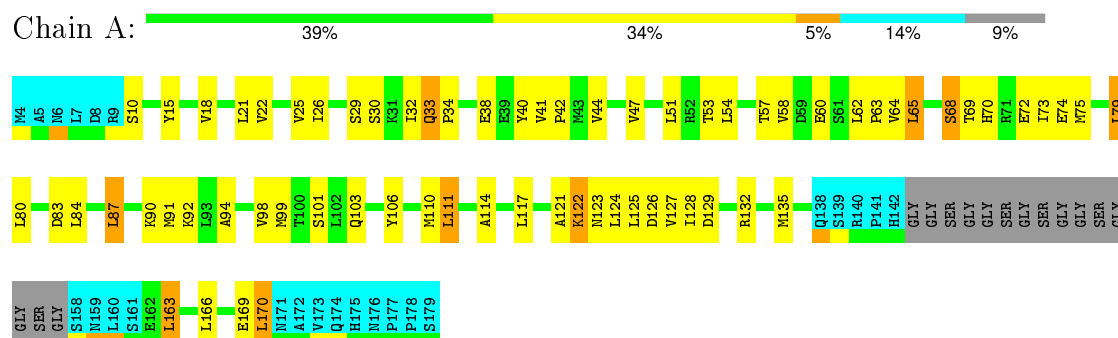
4.2.8 Score per residue for model 8

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



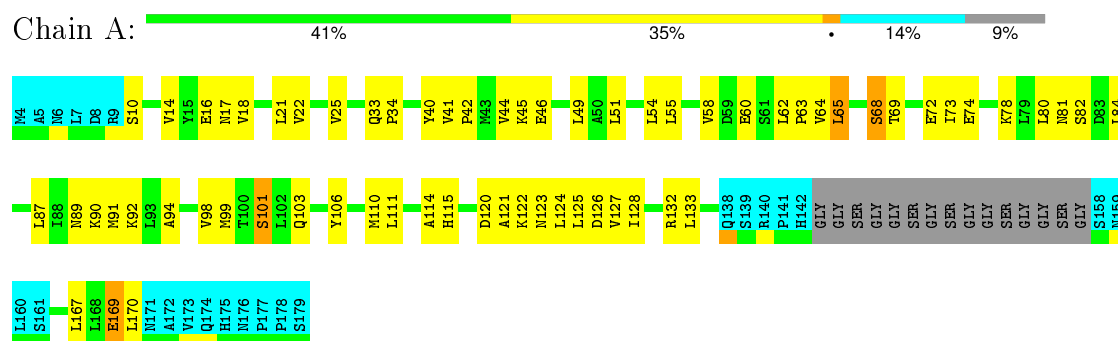
4.2.9 Score per residue for model 9

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



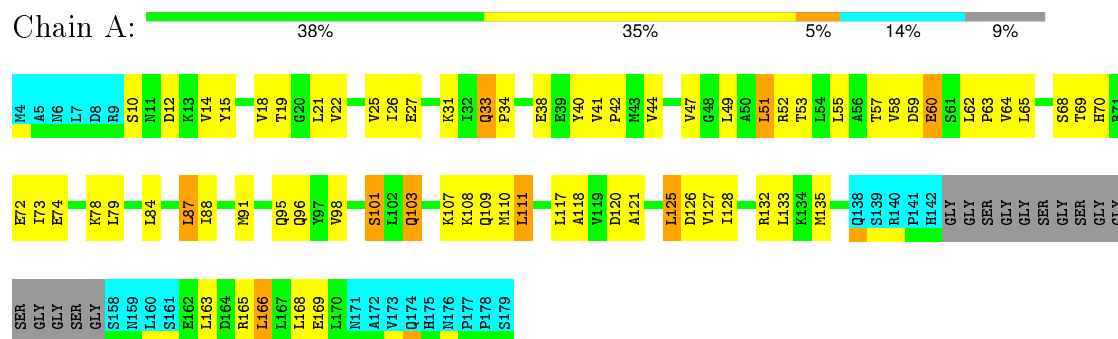
4.2.10 Score per residue for model 10 (medoid)

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



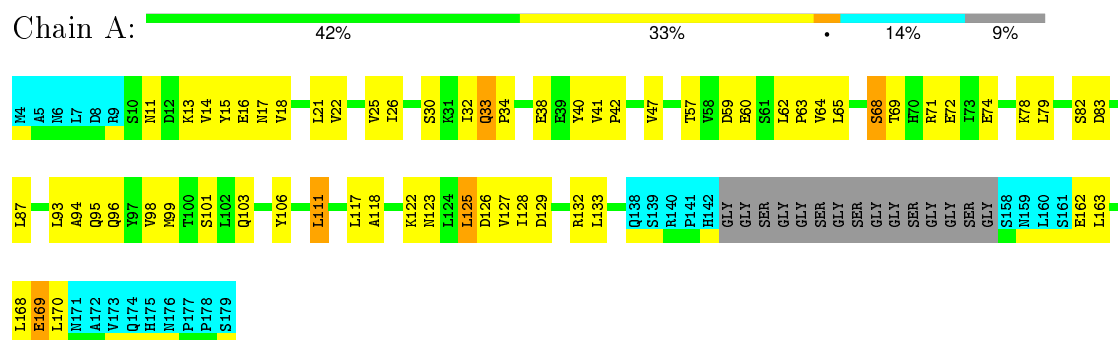
4.2.11 Score per residue for model 11

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



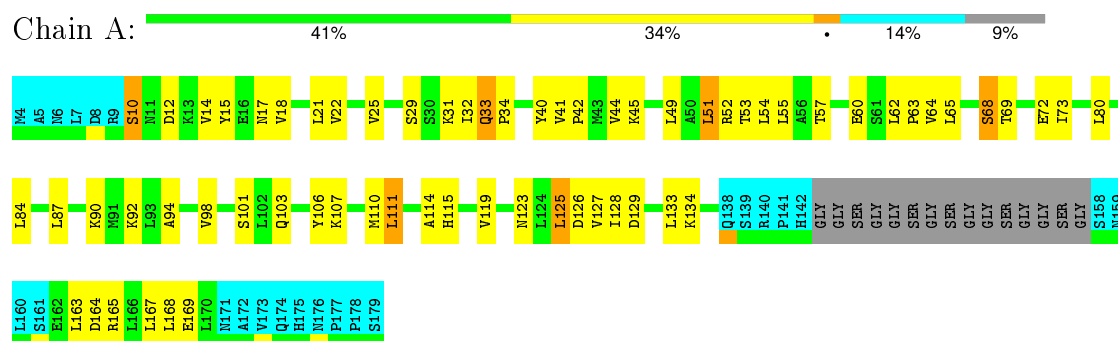
4.2.12 Score per residue for model 12

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



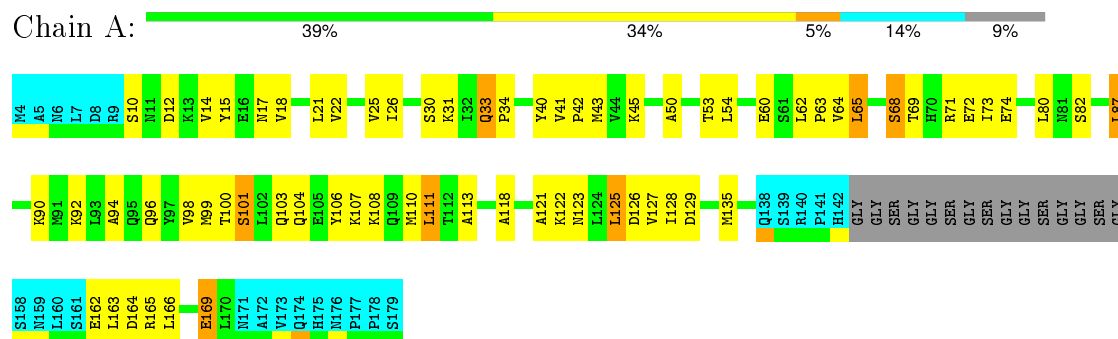
4.2.13 Score per residue for model 13

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



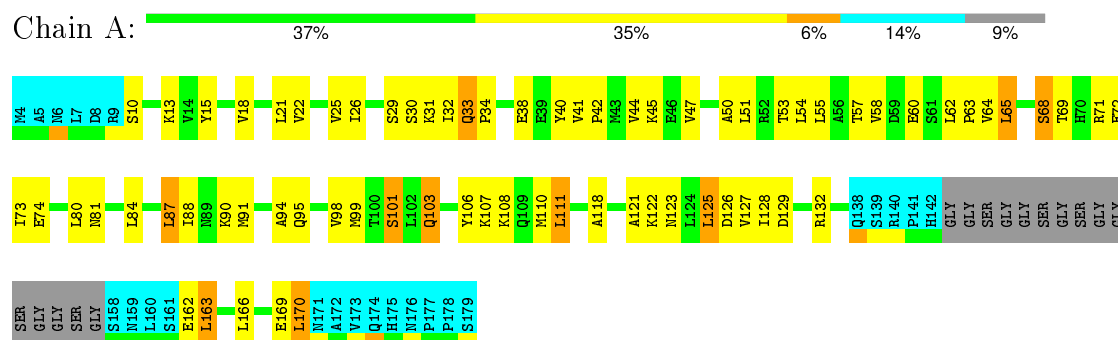
4.2.14 Score per residue for model 14

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



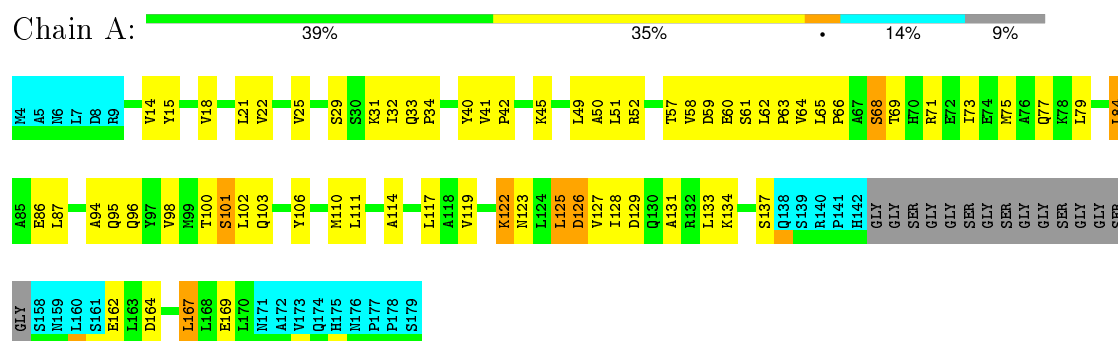
4.2.15 Score per residue for model 15

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



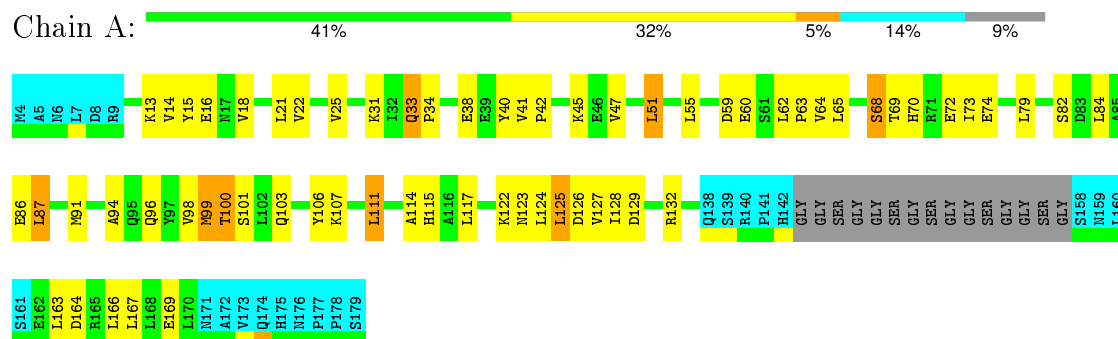
4.2.16 Score per residue for model 16

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



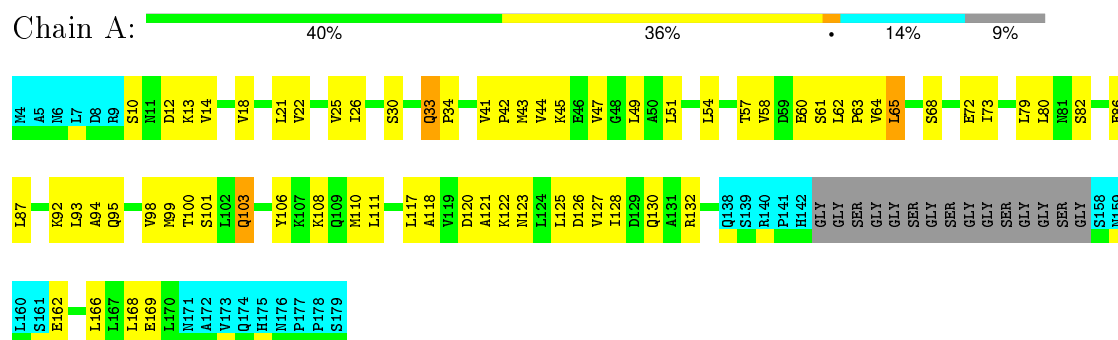
4.2.17 Score per residue for model 17

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



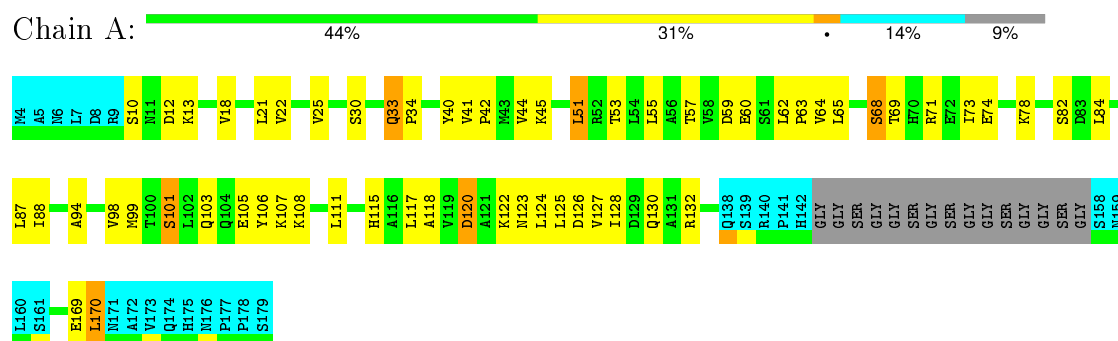
4.2.18 Score per residue for model 18

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



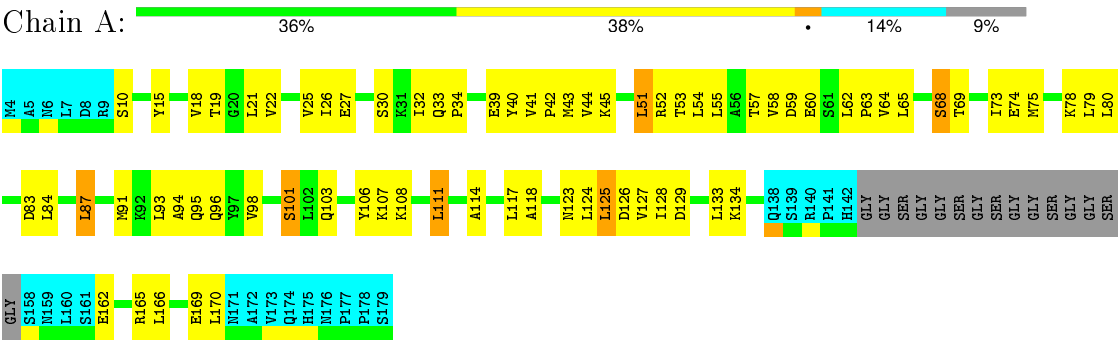
4.2.19 Score per residue for model 19

- 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



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	1069	1129	1129	34±6
All	All	21380	22580	22580	682

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:VAL:HG11	1:A:118:ALA:HB2	0.97	1.35	11	10
1:A:22:VAL:HG21	1:A:163:LEU:HD11	0.96	1.36	9	1
1:A:54:LEU:HD23	1:A:80:LEU:HD21	0.94	1.40	20	4
1:A:54:LEU:HD22	1:A:80:LEU:HD13	0.91	1.39	7	2
1:A:25:VAL:HG21	1:A:118:ALA:HB2	0.90	1.44	12	2
1:A:69:THR:HG21	1:A:128:ILE:HG22	0.89	1.44	17	6
1:A:26:ILE:HG21	1:A:166:LEU:HD12	0.88	1.40	15	4
1:A:58:VAL:HG21	1:A:124:LEU:HD23	0.88	1.43	20	1
1:A:18:VAL:HG11	1:A:125:LEU:HD13	0.79	1.53	14	1
1:A:25:VAL:HG23	1:A:114:ALA:HB1	0.72	1.60	4	1
1:A:47:VAL:HG21	1:A:87:LEU:HD22	0.71	1.63	11	1
1:A:26:ILE:HG21	1:A:166:LEU:HD22	0.70	1.64	18	2
1:A:22:VAL:HG11	1:A:163:LEU:HD23	0.69	1.62	15	3
1:A:111:LEU:HD21	1:A:170:LEU:HD23	0.68	1.65	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LEU:HD11	1:A:117:LEU:HD22	0.68	1.66	1	1
1:A:73:ILE:HD11	1:A:128:ILE:HG21	0.67	1.66	2	3
1:A:19:THR:HG23	1:A:163:LEU:HD11	0.66	1.68	11	1
1:A:79:LEU:HD23	1:A:80:LEU:HD12	0.66	1.66	9	1
1:A:47:VAL:HG11	1:A:87:LEU:HD13	0.65	1.68	15	2
1:A:21:LEU:HD21	1:A:121:ALA:HB1	0.64	1.69	3	8
1:A:21:LEU:O	1:A:25:VAL:HG23	0.63	1.93	2	18
1:A:26:ILE:HD13	1:A:166:LEU:HB3	0.63	1.70	20	2
1:A:25:VAL:HG13	1:A:114:ALA:HB1	0.63	1.68	13	6
1:A:60:GLU:O	1:A:64:VAL:HG23	0.63	1.93	10	20
1:A:25:VAL:CG1	1:A:114:ALA:HB1	0.63	2.23	13	1
1:A:51:LEU:O	1:A:80:LEU:HD21	0.63	1.94	13	2
1:A:69:THR:HG23	1:A:73:ILE:HD11	0.62	1.72	7	9
1:A:14:VAL:O	1:A:18:VAL:HG23	0.61	1.96	17	8
1:A:51:LEU:HD22	1:A:84:LEU:HA	0.61	1.73	2	4
1:A:25:VAL:CG2	1:A:114:ALA:HB1	0.61	2.24	4	1
1:A:98:VAL:HG23	1:A:103:GLN:CG	0.61	2.26	2	14
1:A:53:THR:O	1:A:57:THR:HG23	0.60	1.97	1	11
1:A:25:VAL:CG1	1:A:118:ALA:HB2	0.60	2.27	19	3
1:A:69:THR:HG23	1:A:73:ILE:CD1	0.60	2.27	9	11
1:A:54:LEU:HB3	1:A:80:LEU:HD21	0.60	1.72	14	2
1:A:72:GLU:OE1	1:A:127:VAL:HG11	0.60	1.96	12	13
1:A:15:TYR:CD1	1:A:125:LEU:HD22	0.60	2.31	12	9
1:A:119:VAL:HG22	1:A:167:LEU:CD2	0.60	2.26	1	1
1:A:87:LEU:HD13	1:A:117:LEU:HD11	0.60	1.72	8	1
1:A:98:VAL:HG23	1:A:103:GLN:HG3	0.59	1.73	4	15
1:A:58:VAL:CG2	1:A:124:LEU:HD23	0.59	2.25	20	1
1:A:51:LEU:CB	1:A:84:LEU:HD12	0.59	2.28	19	6
1:A:65:LEU:CD2	1:A:128:ILE:HD12	0.59	2.27	17	1
1:A:22:VAL:O	1:A:26:ILE:HD12	0.58	1.98	12	2
1:A:123:ASN:O	1:A:127:VAL:HG23	0.58	1.99	9	19
1:A:26:ILE:HD13	1:A:166:LEU:CB	0.58	2.28	20	1
1:A:69:THR:CG2	1:A:128:ILE:HG22	0.58	2.24	17	8
1:A:47:VAL:HG11	1:A:87:LEU:CD1	0.58	2.28	17	5
1:A:99:MET:CE	1:A:100:THR:HG23	0.58	2.29	17	1
1:A:58:VAL:CG1	1:A:73:ILE:HD12	0.58	2.28	5	1
1:A:22:VAL:HG21	1:A:163:LEU:HD23	0.58	1.74	17	1
1:A:65:LEU:HB2	1:A:128:ILE:HD11	0.58	1.76	6	8
1:A:94:ALA:HB2	1:A:106:TYR:CG	0.57	2.34	14	12
1:A:26:ILE:HD13	1:A:166:LEU:HD22	0.57	1.77	1	5
1:A:47:VAL:O	1:A:51:LEU:HD12	0.57	1.99	18	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:LEU:HD11	1:A:88:ILE:HD11	0.57	1.75	15	1
1:A:62:LEU:HG	1:A:73:ILE:HG21	0.57	1.76	8	12
1:A:47:VAL:HG11	1:A:87:LEU:HD11	0.57	1.77	2	1
1:A:55:LEU:HD12	1:A:80:LEU:HD23	0.56	1.77	4	1
1:A:72:GLU:CD	1:A:127:VAL:HG11	0.56	2.20	11	7
1:A:54:LEU:O	1:A:58:VAL:HG12	0.56	2.00	18	1
1:A:26:ILE:CG2	1:A:166:LEU:HD12	0.56	2.26	15	1
1:A:58:VAL:CG2	1:A:124:LEU:HD21	0.56	2.31	9	3
1:A:58:VAL:CG1	1:A:73:ILE:HG23	0.56	2.31	1	4
1:A:15:TYR:HA	1:A:125:LEU:HD13	0.55	1.78	1	4
1:A:119:VAL:CG2	1:A:167:LEU:HD21	0.55	2.32	16	1
1:A:18:VAL:HG21	1:A:125:LEU:HD22	0.55	1.77	2	1
1:A:119:VAL:HG22	1:A:167:LEU:HD11	0.55	1.79	16	1
1:A:119:VAL:HG22	1:A:167:LEU:HD13	0.54	1.79	13	1
1:A:19:THR:HA	1:A:163:LEU:HD21	0.54	1.78	11	2
1:A:65:LEU:CB	1:A:128:ILE:HD11	0.54	2.33	10	7
1:A:98:VAL:HG23	1:A:103:GLN:HB3	0.54	1.79	16	1
1:A:47:VAL:HG21	1:A:87:LEU:CD2	0.54	2.31	11	1
1:A:111:LEU:HG	1:A:170:LEU:HD21	0.54	1.78	20	3
1:A:51:LEU:HD22	1:A:84:LEU:CA	0.54	2.33	2	4
1:A:26:ILE:HD13	1:A:166:LEU:HD12	0.53	1.80	11	2
1:A:51:LEU:HB3	1:A:84:LEU:HD12	0.53	1.80	6	4
1:A:58:VAL:HG21	1:A:124:LEU:HD13	0.53	1.79	5	1
1:A:14:VAL:O	1:A:18:VAL:HG13	0.53	2.04	14	4
1:A:47:VAL:HG11	1:A:87:LEU:HD12	0.53	1.79	17	1
1:A:51:LEU:HB2	1:A:84:LEU:HD12	0.53	1.81	19	5
1:A:22:VAL:HG12	1:A:26:ILE:CD1	0.53	2.33	4	6
1:A:115:HIS:CE1	1:A:167:LEU:HD12	0.53	2.39	10	1
1:A:69:THR:HG21	1:A:128:ILE:HG23	0.52	1.80	11	1
1:A:114:ALA:HA	1:A:117:LEU:HD12	0.52	1.80	20	1
1:A:58:VAL:HG13	1:A:73:ILE:HD12	0.52	1.80	5	1
1:A:51:LEU:HB2	1:A:84:LEU:HD13	0.52	1.81	10	1
1:A:14:VAL:HG12	1:A:125:LEU:HD11	0.52	1.81	14	1
1:A:73:ILE:HD13	1:A:124:LEU:HD12	0.52	1.79	19	1
1:A:26:ILE:HG12	1:A:170:LEU:HD12	0.52	1.81	1	1
1:A:98:VAL:HG23	1:A:103:GLN:CB	0.51	2.35	16	1
1:A:72:GLU:OE1	1:A:127:VAL:HG21	0.51	2.05	17	1
1:A:58:VAL:HG22	1:A:73:ILE:HG23	0.51	1.82	11	2
1:A:122:LYS:CG	1:A:163:LEU:HD13	0.51	2.35	9	1
1:A:14:VAL:HG23	1:A:57:THR:HB	0.51	1.83	3	1
1:A:98:VAL:HG23	1:A:103:GLN:CD	0.51	2.26	20	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:VAL:HG22	1:A:91:MET:HG2	0.50	1.81	3	2
1:A:69:THR:HG21	1:A:128:ILE:HB	0.50	1.83	9	4
1:A:111:LEU:CD2	1:A:170:LEU:HD23	0.50	2.36	9	1
1:A:54:LEU:HD23	1:A:80:LEU:CD2	0.50	2.34	10	2
1:A:94:ALA:HB2	1:A:106:TYR:HB3	0.50	1.83	8	6
1:A:26:ILE:CD1	1:A:166:LEU:HD13	0.50	2.36	7	2
1:A:58:VAL:HG12	1:A:73:ILE:HG23	0.50	1.83	8	1
1:A:94:ALA:HB2	1:A:106:TYR:CD1	0.50	2.42	6	5
1:A:26:ILE:HD13	1:A:166:LEU:HD13	0.50	1.83	9	1
1:A:83:ASP:HB3	1:A:117:LEU:HD21	0.49	1.83	9	3
1:A:115:HIS:CD2	1:A:170:LEU:HD13	0.49	2.42	19	1
1:A:41:VAL:N	1:A:42:PRO:HD2	0.49	2.22	7	20
1:A:54:LEU:CD2	1:A:80:LEU:HD13	0.49	2.37	4	1
1:A:115:HIS:O	1:A:119:VAL:HG23	0.49	2.07	2	3
1:A:29:SER:OG	1:A:170:LEU:HD21	0.49	2.07	15	1
1:A:94:ALA:HB2	1:A:106:TYR:CD2	0.49	2.42	13	4
1:A:51:LEU:HD23	1:A:80:LEU:HG	0.49	1.84	7	1
1:A:69:THR:HG21	1:A:128:ILE:CB	0.49	2.38	4	8
1:A:26:ILE:HA	1:A:170:LEU:HD11	0.49	1.85	9	1
1:A:115:HIS:CD2	1:A:170:LEU:HD22	0.48	2.43	1	1
1:A:44:VAL:HG13	1:A:88:ILE:HD12	0.48	1.84	19	2
1:A:54:LEU:HD11	1:A:121:ALA:HB2	0.48	1.85	7	1
1:A:87:LEU:HD12	1:A:117:LEU:CD1	0.48	2.37	12	1
1:A:54:LEU:HD23	1:A:80:LEU:HD13	0.48	1.85	13	1
1:A:14:VAL:HG12	1:A:57:THR:HB	0.48	1.86	18	1
1:A:25:VAL:HG21	1:A:118:ALA:CB	0.48	2.39	2	1
1:A:33:GLN:CB	1:A:34:PRO:CD	0.48	2.92	19	20
1:A:62:LEU:HD22	1:A:70:HIS:CE1	0.47	2.44	11	4
1:A:87:LEU:HD11	1:A:117:LEU:CD1	0.47	2.39	16	1
1:A:51:LEU:CB	1:A:84:LEU:HD23	0.47	2.40	16	2
1:A:66:PRO:HG2	1:A:131:ALA:HB1	0.47	1.85	7	2
1:A:51:LEU:HD11	1:A:87:LEU:HD13	0.47	1.85	11	1
1:A:41:VAL:O	1:A:44:VAL:HG12	0.47	2.10	11	5
1:A:18:VAL:O	1:A:22:VAL:HG23	0.47	2.09	17	19
1:A:14:VAL:HG13	1:A:57:THR:HB	0.47	1.86	16	2
1:A:72:GLU:OE2	1:A:127:VAL:HG11	0.47	2.09	13	2
1:A:69:THR:CG2	1:A:128:ILE:HD12	0.47	2.40	8	7
1:A:122:LYS:HG3	1:A:163:LEU:HD13	0.47	1.85	9	1
1:A:62:LEU:CB	1:A:63:PRO:CD	0.47	2.93	20	20
1:A:44:VAL:HG22	1:A:91:MET:HG3	0.47	1.84	9	2
1:A:87:LEU:HD23	1:A:117:LEU:HD11	0.47	1.86	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:VAL:HG22	1:A:88:ILE:CD1	0.47	2.40	11	1
1:A:44:VAL:HG22	1:A:88:ILE:HD13	0.47	1.87	11	1
1:A:51:LEU:HA	1:A:80:LEU:HD21	0.47	1.86	6	1
1:A:44:VAL:HG13	1:A:88:ILE:CD1	0.46	2.41	7	2
1:A:44:VAL:HG22	1:A:91:MET:CG	0.46	2.40	3	1
1:A:58:VAL:HG22	1:A:124:LEU:HD21	0.46	1.86	9	2
1:A:19:THR:CG2	1:A:163:LEU:HD11	0.46	2.39	11	1
1:A:17:ASN:ND2	1:A:53:THR:HG21	0.46	2.25	4	1
1:A:62:LEU:CD2	1:A:73:ILE:HG21	0.46	2.40	1	1
1:A:69:THR:HG21	1:A:128:ILE:CG2	0.46	2.41	2	2
1:A:14:VAL:HG11	1:A:61:SER:HB2	0.46	1.87	18	1
1:A:54:LEU:CD2	1:A:80:LEU:HD21	0.46	2.27	20	1
1:A:21:LEU:HD11	1:A:121:ALA:CB	0.46	2.41	14	4
1:A:22:VAL:HG12	1:A:26:ILE:HD11	0.46	1.88	4	1
1:A:95:GLN:O	1:A:98:VAL:HG12	0.45	2.10	18	2
1:A:29:SER:O	1:A:32:ILE:HG22	0.45	2.11	8	6
1:A:10:SER:HB2	1:A:64:VAL:HG21	0.45	1.88	1	3
1:A:76:ALA:HB1	1:A:124:LEU:HD11	0.45	1.88	2	1
1:A:19:THR:OG1	1:A:163:LEU:HD21	0.45	2.11	2	1
1:A:14:VAL:HG12	1:A:125:LEU:HD12	0.45	1.88	4	1
1:A:73:ILE:HD13	1:A:124:LEU:CD1	0.45	2.40	19	1
1:A:22:VAL:HG11	1:A:163:LEU:CD2	0.45	2.36	15	1
1:A:17:ASN:OD1	1:A:53:THR:HG21	0.45	2.11	14	1
1:A:14:VAL:HG22	1:A:125:LEU:CD1	0.45	2.42	11	2
1:A:84:LEU:CD1	1:A:88:ILE:HD11	0.44	2.41	15	1
1:A:51:LEU:O	1:A:80:LEU:HD12	0.44	2.12	8	1
1:A:115:HIS:CE1	1:A:167:LEU:HD23	0.44	2.47	17	1
1:A:22:VAL:CG1	1:A:163:LEU:HD23	0.44	2.42	5	1
1:A:54:LEU:HD22	1:A:80:LEU:CD1	0.44	2.42	4	1
1:A:51:LEU:HA	1:A:54:LEU:HD12	0.44	1.90	9	1
1:A:73:ILE:CD1	1:A:124:LEU:HD12	0.44	2.42	19	1
1:A:44:VAL:HG22	1:A:91:MET:CE	0.44	2.43	2	1
1:A:26:ILE:HG21	1:A:166:LEU:CD1	0.44	2.39	5	2
1:A:51:LEU:HD22	1:A:84:LEU:N	0.44	2.28	11	1
1:A:21:LEU:HB2	1:A:50:ALA:HB1	0.43	1.90	15	3
1:A:44:VAL:CG1	1:A:88:ILE:HD12	0.43	2.43	19	4
1:A:54:LEU:HD13	1:A:80:LEU:HD21	0.43	1.90	2	1
1:A:54:LEU:HD21	1:A:121:ALA:HB2	0.43	1.88	10	1
1:A:62:LEU:N	1:A:63:PRO:HD2	0.43	2.28	12	20
1:A:14:VAL:HG12	1:A:125:LEU:CD1	0.43	2.42	4	2
1:A:18:VAL:HG23	1:A:121:ALA:O	0.43	2.13	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:HD21	1:A:121:ALA:CB	0.43	2.43	4	2
1:A:111:LEU:O	1:A:111:LEU:HD13	0.43	2.13	13	1
1:A:21:LEU:HD11	1:A:118:ALA:HA	0.43	1.91	7	1
1:A:44:VAL:HG22	1:A:91:MET:SD	0.43	2.54	2	2
1:A:18:VAL:CG2	1:A:125:LEU:HD22	0.43	2.44	2	1
1:A:119:VAL:HG22	1:A:167:LEU:HD21	0.43	1.90	16	1
1:A:54:LEU:HB3	1:A:80:LEU:HD22	0.43	1.89	7	1
1:A:26:ILE:HD12	1:A:166:LEU:HD13	0.43	1.91	7	1
1:A:26:ILE:CG1	1:A:170:LEU:HD12	0.42	2.44	1	1
1:A:58:VAL:CG2	1:A:124:LEU:HD13	0.42	2.43	5	1
1:A:51:LEU:CD1	1:A:80:LEU:HD23	0.42	2.44	15	1
1:A:33:GLN:N	1:A:34:PRO:HD2	0.42	2.29	13	20
1:A:54:LEU:HD11	1:A:121:ALA:CB	0.42	2.44	7	1
1:A:15:TYR:O	1:A:18:VAL:HG12	0.42	2.15	9	1
1:A:11:ASN:OD1	1:A:64:VAL:HG11	0.42	2.15	12	1
1:A:111:LEU:CD2	1:A:170:LEU:HD21	0.42	2.44	1	1
1:A:29:SER:HB2	1:A:111:LEU:HD11	0.42	1.90	2	1
1:A:79:LEU:HD23	1:A:80:LEU:N	0.41	2.30	8	1
1:A:87:LEU:HD21	1:A:113:ALA:HB1	0.41	1.91	14	1
1:A:21:LEU:HD11	1:A:121:ALA:HB3	0.41	1.91	5	1
1:A:87:LEU:HD12	1:A:117:LEU:HD13	0.41	1.93	20	1
1:A:41:VAL:HG23	1:A:95:GLN:NE2	0.41	2.30	11	1
1:A:119:VAL:HA	1:A:167:LEU:HD21	0.41	1.92	4	1
1:A:51:LEU:HD21	1:A:117:LEU:HD11	0.41	1.92	2	1
1:A:21:LEU:CD2	1:A:54:LEU:HD21	0.41	2.46	15	1
1:A:73:ILE:HD11	1:A:128:ILE:HD12	0.40	1.93	14	1
1:A:22:VAL:HG21	1:A:163:LEU:CD2	0.40	2.47	13	1
1:A:120:ASP:O	1:A:124:LEU:HD23	0.40	2.17	19	1
1:A:54:LEU:O	1:A:58:VAL:HG23	0.40	2.15	7	1
1:A:41:VAL:CB	1:A:42:PRO:CD	0.40	3.00	2	1
1:A:10:SER:HB3	1:A:64:VAL:HG21	0.40	1.94	14	1
1:A:53:THR:HG22	1:A:57:THR:CG2	0.40	2.47	1	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	137/176 (78%)	128±2 (94±1%)	7±2 (5±1%)	2±0 (1±0%)	18	63
All	All	2740/3520 (78%)	2564 (94%)	135 (5%)	41 (1%)	18	63

All 3 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	68	SER	20
1	A	101	SER	20
1	A	89	ASN	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	121/148 (82%)	90±3 (74±3%)	31±3 (26±3%)	3	24
All	All	2420/2960 (82%)	1791 (74%)	629 (26%)	3	24

All 83 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	126	ASP	20
1	A	125	LEU	19
1	A	65	LEU	19
1	A	40	TYR	17
1	A	68	SER	17
1	A	111	LEU	16
1	A	87	LEU	16
1	A	129	ASP	15
1	A	132	ARG	15
1	A	107	LYS	14
1	A	74	GLU	14
1	A	99	MET	14
1	A	110	MET	14
1	A	33	GLN	13
1	A	10	SER	13

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Mol	Chain	Res	Type	Models (Total)
1	A	45	LYS	13
1	A	82	SER	12
1	A	31	LYS	12
1	A	122	LYS	12
1	A	101	SER	12
1	A	162	GLU	12
1	A	30	SER	12
1	A	96	GLN	12
1	A	59	ASP	11
1	A	55	LEU	11
1	A	90	LYS	11
1	A	168	LEU	10
1	A	133	LEU	10
1	A	108	LYS	10
1	A	79	LEU	10
1	A	165	ARG	9
1	A	71	ARG	9
1	A	16	GLU	8
1	A	52	ARG	8
1	A	12	ASP	8
1	A	91	MET	7
1	A	78	LYS	7
1	A	13	LYS	7
1	A	81	ASN	7
1	A	49	LEU	7
1	A	134	LYS	6
1	A	169	GLU	6
1	A	86	GLU	6
1	A	100	THR	6
1	A	124	LEU	6
1	A	92	LYS	5
1	A	38	GLU	5
1	A	170	LEU	5
1	A	93	LEU	5
1	A	51	LEU	5
1	A	164	ASP	5
1	A	80	LEU	4
1	A	135	MET	4
1	A	130	GLN	4
1	A	43	MET	4
1	A	84	LEU	4
1	A	32	ILE	4

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Mol	Chain	Res	Type	Models (Total)
1	A	117	LEU	4
1	A	163	LEU	4
1	A	120	ASP	4
1	A	75	MET	4
1	A	167	LEU	4
1	A	17	ASN	3
1	A	95	GLN	3
1	A	104	GLN	3
1	A	54	LEU	3
1	A	27	GLU	3
1	A	166	LEU	3
1	A	103	GLN	3
1	A	57	THR	3
1	A	46	GLU	2
1	A	60	GLU	2
1	A	109	GLN	2
1	A	105	GLU	2
1	A	61	SER	2
1	A	29	SER	1
1	A	137	SER	1
1	A	102	LEU	1
1	A	77	GLN	1
1	A	83	ASP	1
1	A	70	HIS	1
1	A	39	GLU	1
1	A	15	TYR	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