Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID	:	7RIK
BMRB ID	:	30936
Title	:	Magic-Angle-Spinning NMR Structure of Kinesin-1 Motor Domain Assembled with Microtubules
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Deposited on	:	2021-07-20

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

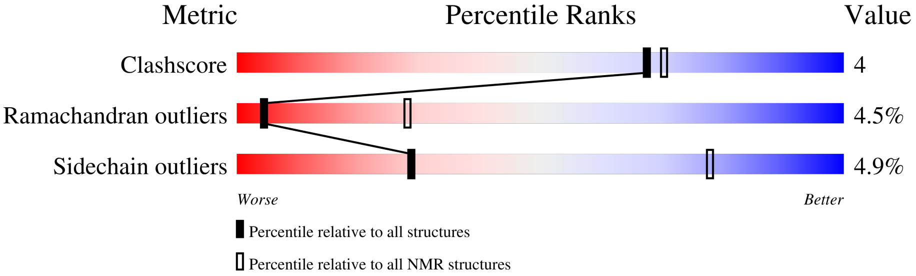
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.31.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 32%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	349	

2 Ensemble composition and analysis ⓘ

This entry contains 22 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:1-A:324 (324)	0.42	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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5488 atoms, of which 2737 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Kinesin-1 heavy chain.

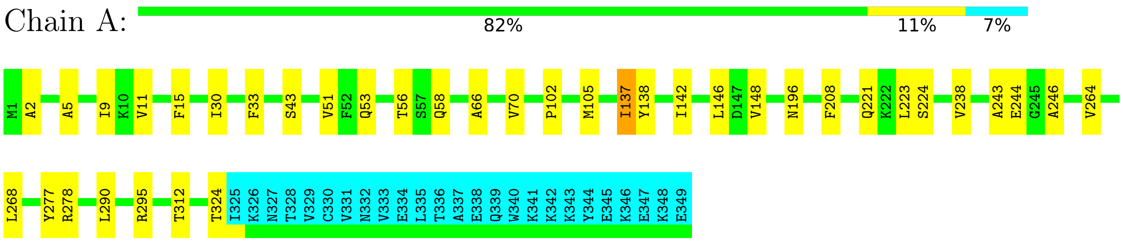
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	349	5488	1715	2737	470	549	17	0

4 Residue-property plots ⓘ

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Kinesin-1 heavy chain

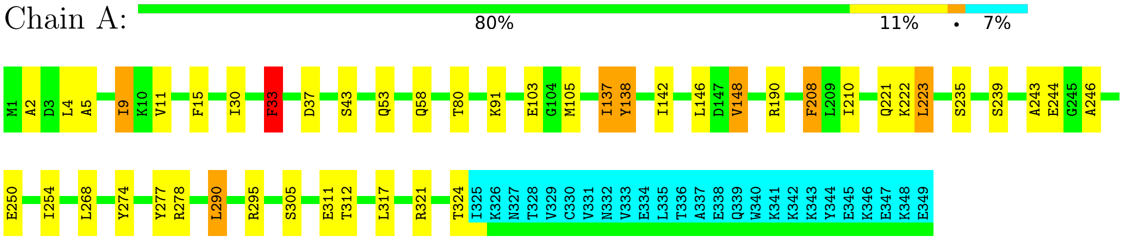


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

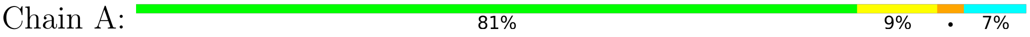
4.2.1 Score per residue for model 1 (medoid)

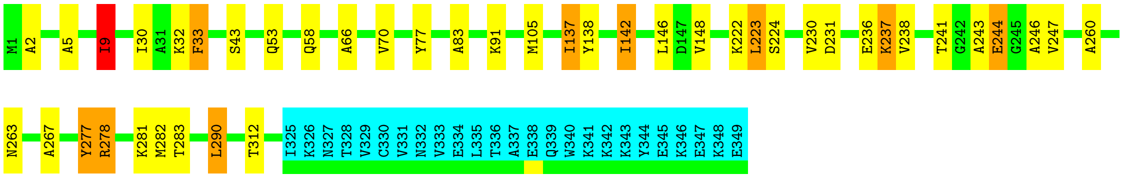
- Molecule 1: Kinesin-1 heavy chain



4.2.2 Score per residue for model 2

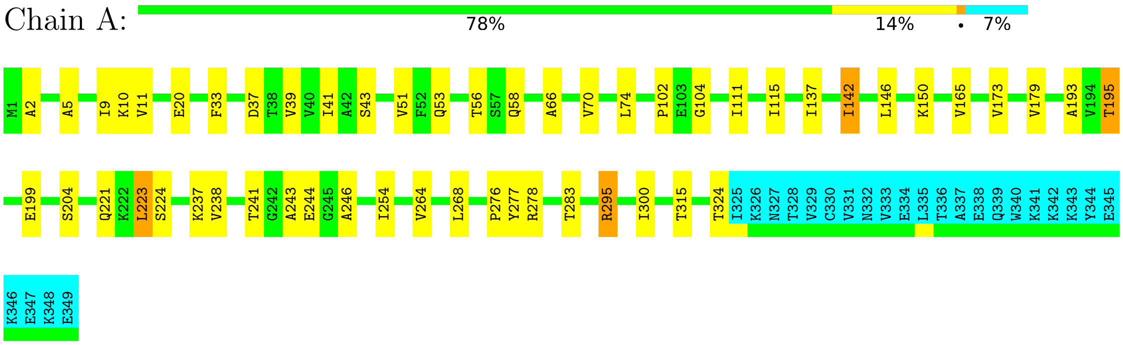
- Molecule 1: Kinesin-1 heavy chain





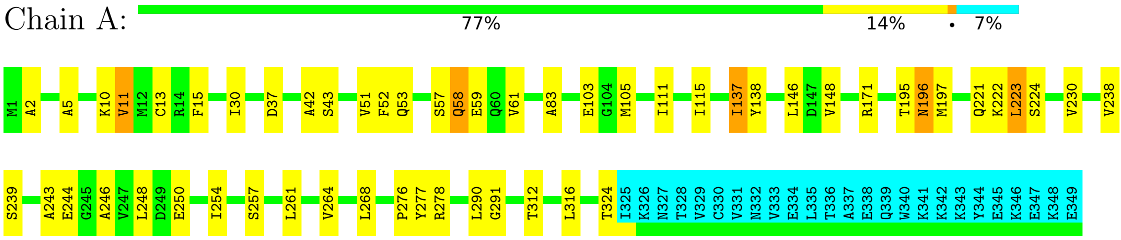
4.2.3 Score per residue for model 3

- Molecule 1: Kinesin-1 heavy chain



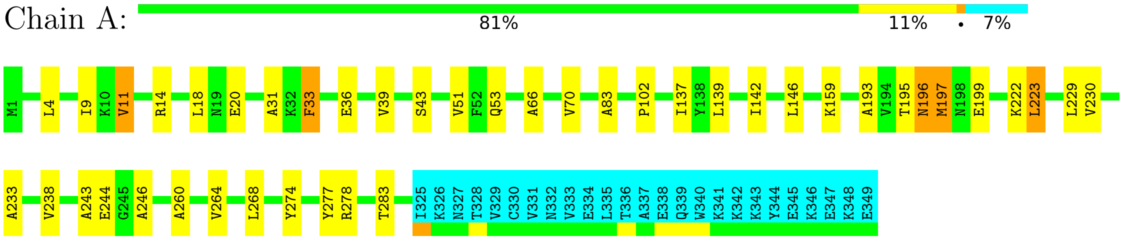
4.2.4 Score per residue for model 4

- Molecule 1: Kinesin-1 heavy chain



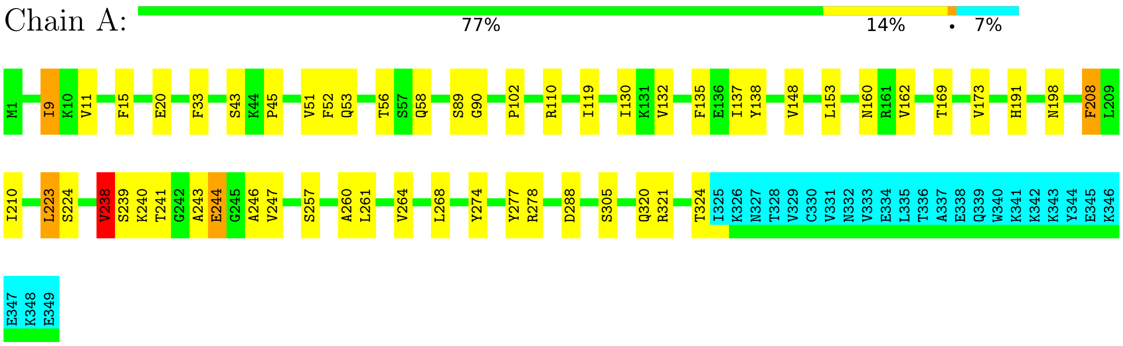
4.2.5 Score per residue for model 5

- Molecule 1: Kinesin-1 heavy chain



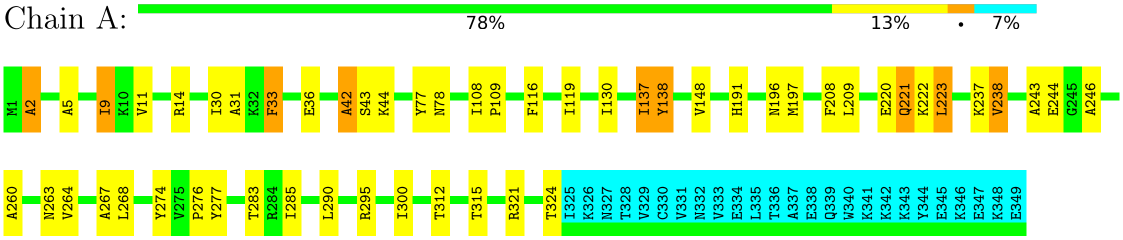
4.2.6 Score per residue for model 6

- Molecule 1: Kinesin-1 heavy chain



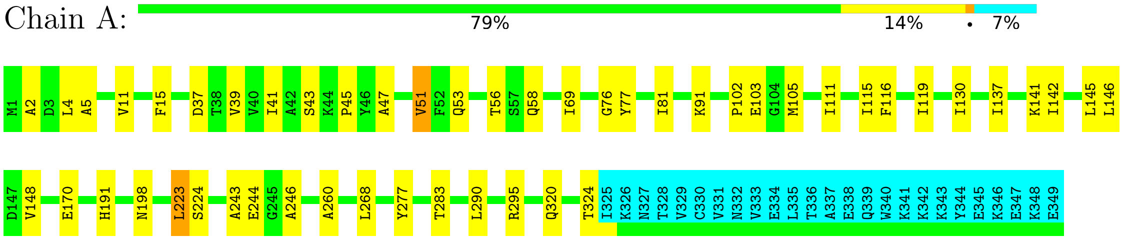
4.2.7 Score per residue for model 7

- Molecule 1: Kinesin-1 heavy chain



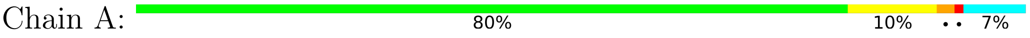
4.2.8 Score per residue for model 8

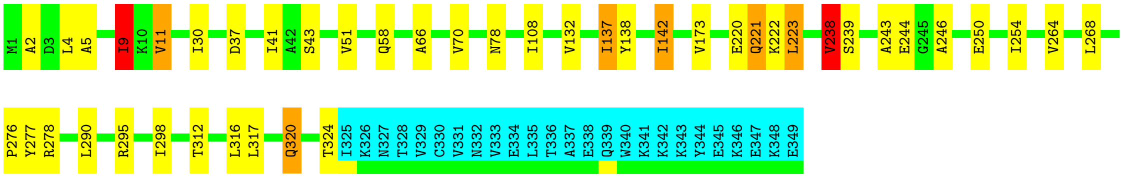
- Molecule 1: Kinesin-1 heavy chain



4.2.9 Score per residue for model 9

- Molecule 1: Kinesin-1 heavy chain

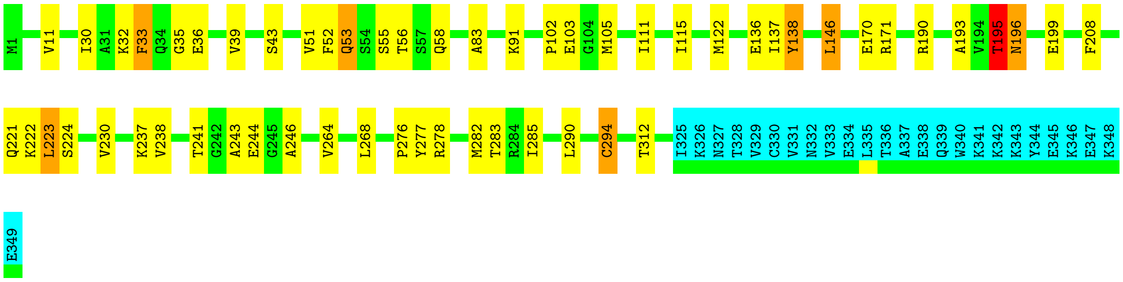




4.2.10 Score per residue for model 10

- Molecule 1: Kinesin-1 heavy chain

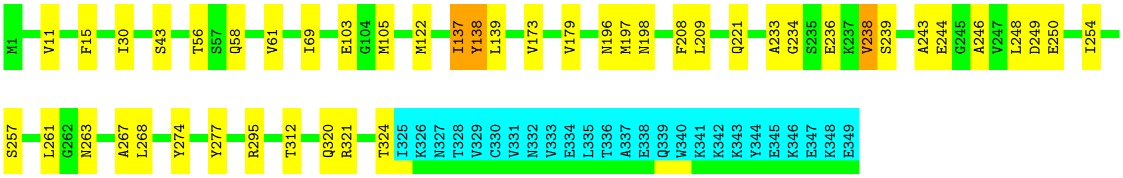
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: Kinesin-1 heavy chain

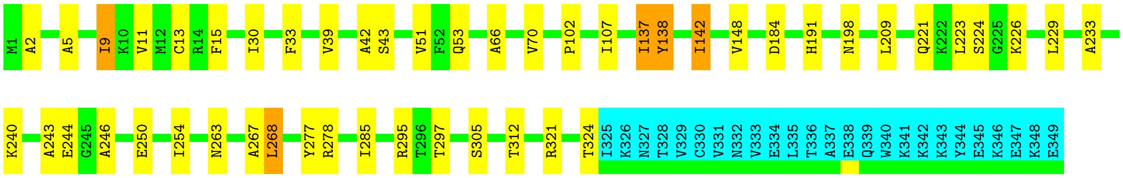
Chain A:



4.2.12 Score per residue for model 12

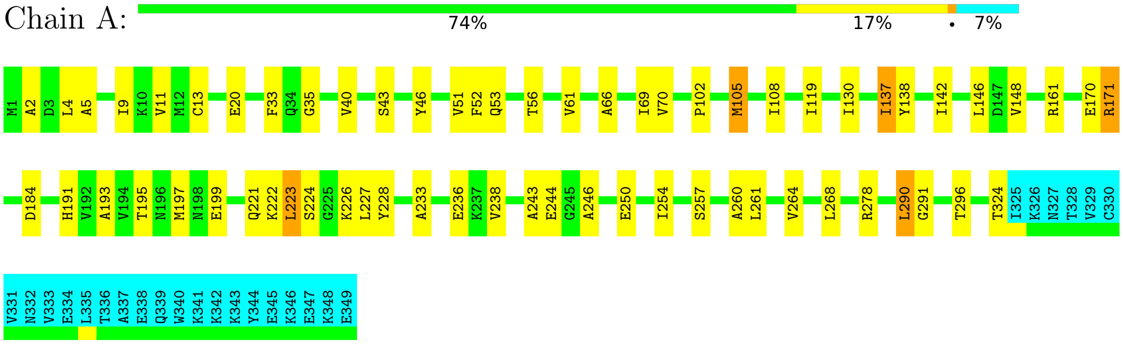
- Molecule 1: Kinesin-1 heavy chain

Chain A:



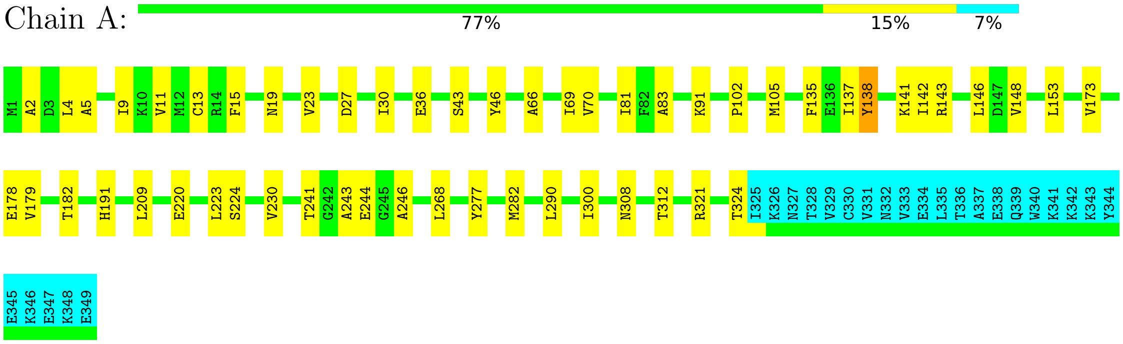
4.2.13 Score per residue for model 13

- Molecule 1: Kinesin-1 heavy chain



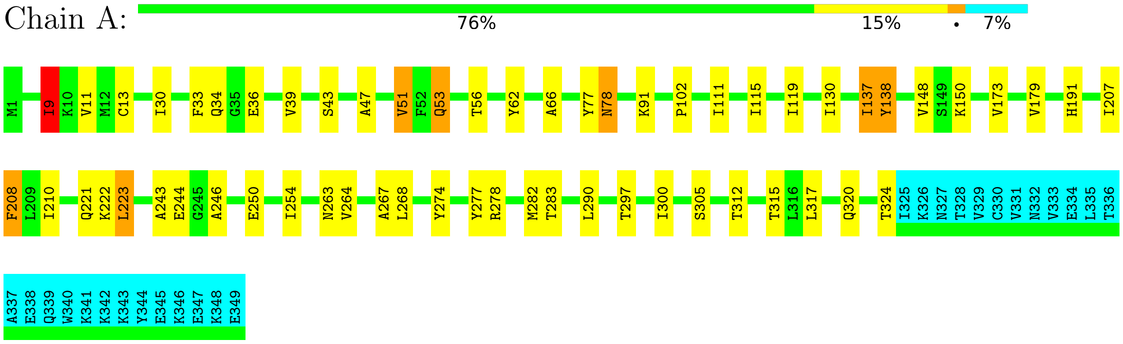
4.2.14 Score per residue for model 14

- Molecule 1: Kinesin-1 heavy chain



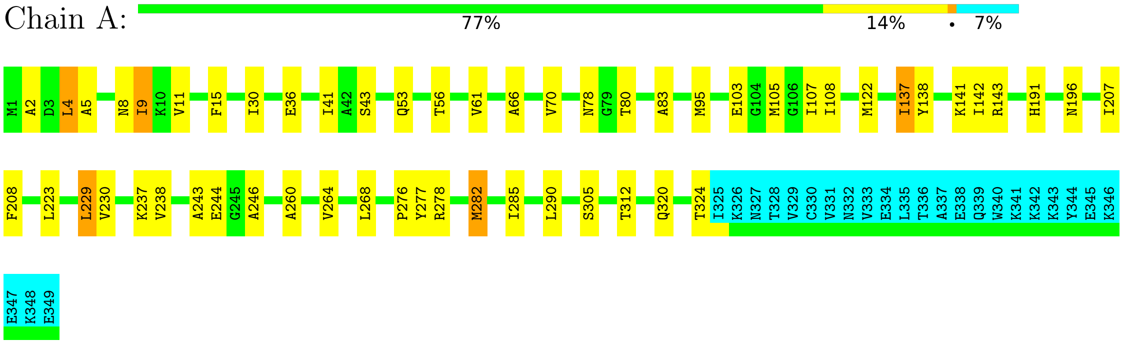
4.2.15 Score per residue for model 15

- Molecule 1: Kinesin-1 heavy chain



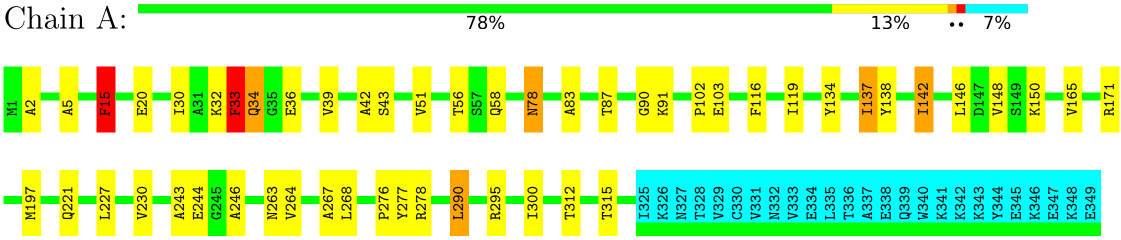
4.2.16 Score per residue for model 16

- Molecule 1: Kinesin-1 heavy chain



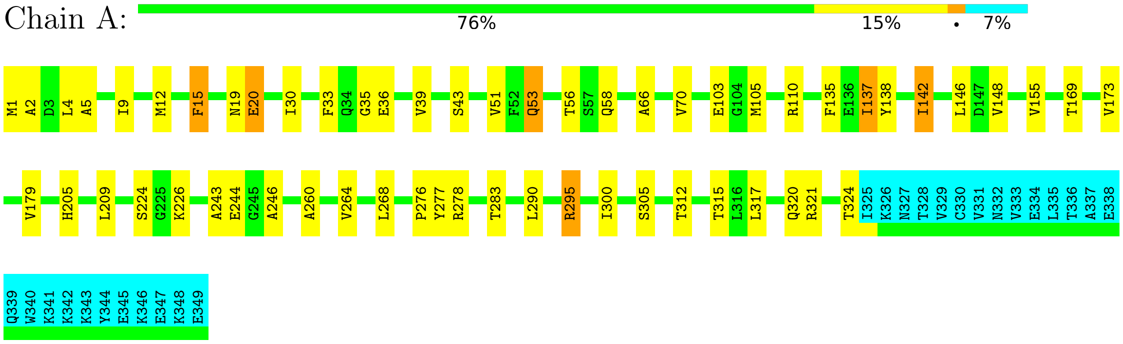
4.2.17 Score per residue for model 17

- Molecule 1: Kinesin-1 heavy chain



4.2.18 Score per residue for model 18

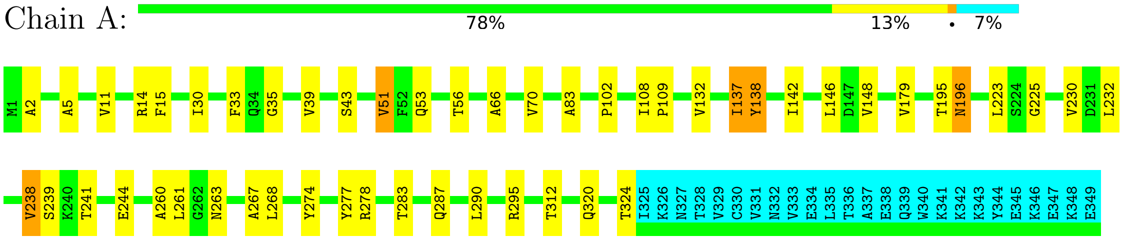
- Molecule 1: Kinesin-1 heavy chain



4.2.19 Score per residue for model 19

- Molecule 1: Kinesin-1 heavy chain

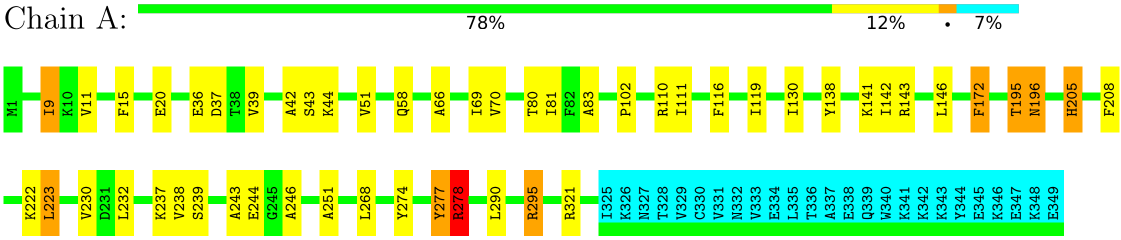
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Kinesin-1 heavy chain

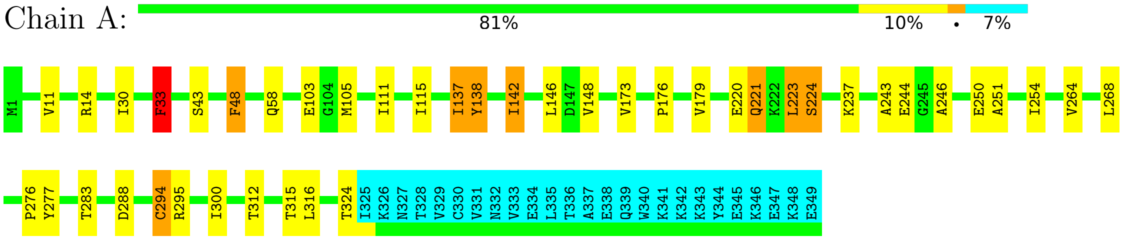
Chain A:



4.2.21 Score per residue for model 21

- Molecule 1: Kinesin-1 heavy chain

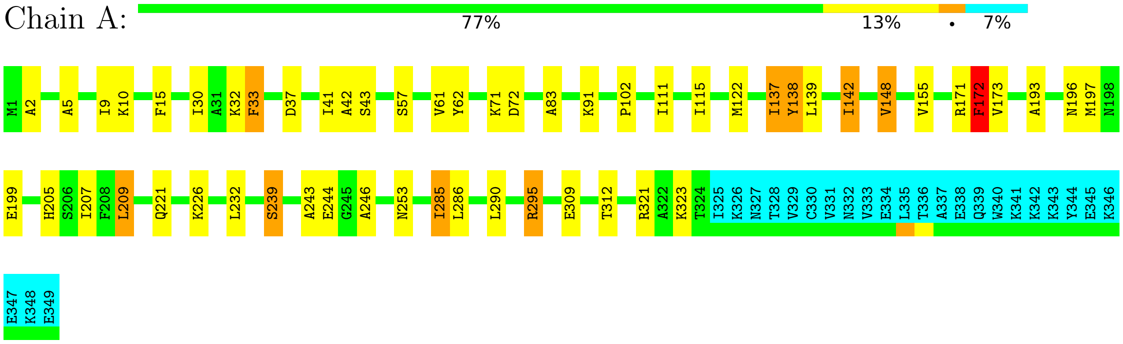
Chain A:



4.2.22 Score per residue for model 22

- Molecule 1: Kinesin-1 heavy chain

Chain A:



5 Refinement protocol and experimental data overview ⓘ

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

Of the 22000 calculated structures, 22 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 calculation	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1376
Number of shifts mapped to atoms	1376
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	32%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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	2538	2517	2510	20±3
All	All	55836	55374	55220	431

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:243:ALA:HB1	1:A:246:ALA:HB3	0.94	1.39	6	21
1:A:119:ILE:HD13	1:A:130:ILE:HD11	0.92	1.40	8	6
1:A:30:ILE:HD11	1:A:312:THR:HG21	0.87	1.43	4	15
1:A:2:ALA:HB3	1:A:5:ALA:HB3	0.80	1.52	17	13
1:A:300:ILE:HG22	1:A:315:THR:HG23	0.75	1.58	17	5
1:A:53:GLN:O	1:A:56:THR:HG23	0.73	1.84	10	6
1:A:160:ASN:O	1:A:162:VAL:HG13	0.72	1.84	6	1
1:A:137:ILE:HD13	1:A:138:TYR:N	0.67	2.04	21	3
1:A:233:ALA:O	1:A:254:ILE:HD13	0.67	1.90	13	3
1:A:45:PRO:HB2	1:A:324:THR:HG22	0.66	1.68	8	1
1:A:1:MET:O	1:A:5:ALA:HB3	0.66	1.91	18	1
1:A:223:LEU:HD13	1:A:224:SER:N	0.65	2.06	3	4
1:A:137:ILE:HD12	1:A:138:TYR:N	0.65	2.07	17	15
1:A:263:ASN:O	1:A:267:ALA:HB3	0.65	1.92	19	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:ILE:HD13	1:A:130:ILE:CD1	0.63	2.23	7	3
1:A:56:THR:HG22	1:A:61:VAL:HG21	0.63	1.69	13	2
1:A:30:ILE:CD1	1:A:312:THR:HG21	0.63	2.23	4	3
1:A:264:VAL:HG21	1:A:283:THR:HG23	0.62	1.70	10	4
1:A:45:PRO:CB	1:A:324:THR:HG22	0.62	2.24	8	1
1:A:260:ALA:O	1:A:264:VAL:HG23	0.61	1.94	7	5
1:A:264:VAL:HG22	1:A:276:PRO:CB	0.61	2.25	3	7
1:A:193:ALA:HB1	1:A:199:GLU:CD	0.61	2.16	5	1
1:A:30:ILE:HD11	1:A:312:THR:OG1	0.61	1.96	15	1
1:A:264:VAL:HG21	1:A:283:THR:HG22	0.61	1.72	3	1
1:A:30:ILE:HD11	1:A:312:THR:CG2	0.60	2.25	4	4
1:A:300:ILE:CG2	1:A:315:THR:HG23	0.60	2.26	7	4
1:A:264:VAL:HG22	1:A:276:PRO:HB3	0.60	1.72	17	3
1:A:290:LEU:HD22	1:A:290:LEU:O	0.58	1.98	2	2
1:A:56:THR:HG23	1:A:58:GLN:H	0.57	1.60	17	2
1:A:9:ILE:O	1:A:9:ILE:HG22	0.56	2.00	1	5
1:A:260:ALA:HB1	1:A:283:THR:HG21	0.55	1.79	2	2
1:A:162:VAL:HG12	1:A:288:ASP:OD2	0.55	2.02	6	1
1:A:47:ALA:HB3	1:A:320:GLN:CD	0.55	2.22	8	2
1:A:39:VAL:HG22	1:A:51:VAL:CG1	0.55	2.32	3	4
1:A:317:LEU:HD12	1:A:324:THR:HG21	0.54	1.79	1	1
1:A:9:ILE:HG23	1:A:9:ILE:O	0.54	2.02	2	3
1:A:260:ALA:HB1	1:A:283:THR:OG1	0.54	2.02	19	3
1:A:264:VAL:HG22	1:A:276:PRO:HB2	0.54	1.80	4	5
1:A:193:ALA:HB1	1:A:199:GLU:HB3	0.54	1.79	22	2
1:A:83:ALA:HB3	1:A:230:VAL:O	0.54	2.03	16	7
1:A:9:ILE:HD11	1:A:295:ARG:NE	0.53	2.17	22	4
1:A:56:THR:HG23	1:A:61:VAL:CG2	0.53	2.33	11	1
1:A:9:ILE:HD11	1:A:295:ARG:HE	0.53	1.64	22	2
1:A:238:VAL:HG13	1:A:239:SER:N	0.53	2.19	9	2
1:A:139:LEU:HD13	1:A:253:ASN:HB2	0.52	1.81	22	1
1:A:31:ALA:HB1	1:A:33:PHE:CZ	0.52	2.39	7	1
1:A:136:GLU:CD	1:A:146:LEU:HD23	0.52	2.24	10	1
1:A:321:ARG:O	1:A:324:THR:HG22	0.52	2.05	6	5
1:A:173:VAL:HG11	1:A:179:VAL:HG13	0.52	1.81	14	5
1:A:260:ALA:HB1	1:A:283:THR:CG2	0.51	2.36	2	2
1:A:193:ALA:HB1	1:A:199:GLU:OE1	0.51	2.05	3	2
1:A:119:ILE:CD1	1:A:130:ILE:HD11	0.51	2.31	20	2
1:A:2:ALA:HB3	1:A:5:ALA:CB	0.51	2.32	13	6
1:A:209:LEU:C	1:A:209:LEU:HD22	0.51	2.26	22	1
1:A:222:LYS:O	1:A:223:LEU:HD22	0.51	2.06	9	10

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:209:LEU:H	1:A:209:LEU:HD23	0.51	1.66	14	1
1:A:56:THR:CG2	1:A:61:VAL:HG21	0.51	2.36	13	1
1:A:250:GLU:HG2	1:A:254:ILE:HD12	0.50	1.83	13	2
1:A:250:GLU:CB	1:A:254:ILE:HD12	0.50	2.36	15	1
1:A:31:ALA:HB1	1:A:33:PHE:CE1	0.49	2.42	5	1
1:A:320:GLN:O	1:A:324:THR:HG22	0.49	2.07	16	3
1:A:52:PHE:HB3	1:A:56:THR:HG22	0.49	1.85	10	2
1:A:237:LYS:HB3	1:A:251:ALA:HB2	0.49	1.83	21	2
1:A:250:GLU:HA	1:A:254:ILE:HD12	0.49	1.85	21	4
1:A:320:GLN:O	1:A:324:THR:HG23	0.49	2.08	8	1
1:A:193:ALA:HB1	1:A:199:GLU:CB	0.49	2.38	22	1
1:A:142:ILE:O	1:A:142:ILE:HG22	0.49	2.08	12	4
1:A:33:PHE:N	1:A:33:PHE:CD1	0.48	2.81	1	1
1:A:69:ILE:CD1	1:A:111:ILE:HD11	0.48	2.37	20	1
1:A:66:ALA:O	1:A:70:VAL:HG23	0.48	2.09	20	11
1:A:320:GLN:HB3	1:A:324:THR:HG23	0.48	1.85	8	1
1:A:15:PHE:CD2	1:A:315:THR:HG21	0.48	2.43	17	1
1:A:39:VAL:HG11	1:A:51:VAL:HG13	0.48	1.86	5	1
1:A:9:ILE:O	1:A:9:ILE:HG23	0.48	2.07	9	1
1:A:9:ILE:O	1:A:9:ILE:CG2	0.47	2.62	1	1
1:A:56:THR:HG23	1:A:61:VAL:HB	0.47	1.86	11	1
1:A:142:ILE:HG22	1:A:142:ILE:O	0.47	2.09	18	4
1:A:148:VAL:HG22	1:A:190:ARG:NH2	0.47	2.24	1	1
1:A:205:HIS:CE1	1:A:230:VAL:HG13	0.47	2.44	20	1
1:A:111:ILE:O	1:A:115:ILE:HG22	0.47	2.09	21	7
1:A:290:LEU:HD23	1:A:296:THR:HG21	0.47	1.86	13	1
1:A:39:VAL:HG22	1:A:51:VAL:HG11	0.47	1.87	20	7
1:A:243:ALA:CB	1:A:246:ALA:HB3	0.47	2.40	17	1
1:A:139:LEU:HD23	1:A:249:ASP:OD1	0.47	2.10	11	1
1:A:107:ILE:HG21	1:A:229:LEU:HD11	0.46	1.86	12	2
1:A:19:ASN:O	1:A:23:VAL:HG23	0.46	2.09	14	1
1:A:83:ALA:O	1:A:232:LEU:HD12	0.46	2.10	22	2
1:A:244:GLU:N	1:A:247:VAL:HG12	0.46	2.25	2	1
1:A:33:PHE:CD1	1:A:33:PHE:N	0.46	2.81	21	2
1:A:135:PHE:CE1	1:A:209:LEU:HD21	0.46	2.46	18	1
1:A:268:LEU:HD23	1:A:268:LEU:O	0.46	2.10	19	1
1:A:116:PHE:HA	1:A:119:ILE:HD12	0.46	1.86	7	4
1:A:69:ILE:HD12	1:A:81:ILE:HD11	0.46	1.87	20	1
1:A:52:PHE:CG	1:A:61:VAL:HG22	0.46	2.46	13	1
1:A:13:CYS:SG	1:A:300:ILE:HD12	0.46	2.51	14	1
1:A:282:MET:O	1:A:285:ILE:HG22	0.46	2.11	16	1

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:30:ILE:HD13	1:A:309:GLU:HG3	0.45	1.88	22	1
1:A:257:SER:O	1:A:261:LEU:HD13	0.45	2.11	13	4
1:A:208:PHE:HZ	1:A:210:ILE:HD12	0.45	1.71	15	1
1:A:83:ALA:HB1	1:A:95:MET:SD	0.45	2.50	16	1
1:A:165:VAL:O	1:A:165:VAL:HG13	0.45	2.11	3	2
1:A:132:VAL:HG11	1:A:179:VAL:CG1	0.45	2.42	19	1
1:A:268:LEU:C	1:A:268:LEU:HD13	0.45	2.32	3	5
1:A:195:THR:O	1:A:196:ASN:CB	0.45	2.65	10	4
1:A:69:ILE:HG21	1:A:81:ILE:HD11	0.45	1.88	8	2
1:A:69:ILE:HD13	1:A:81:ILE:HD11	0.45	1.89	14	1
1:A:69:ILE:HD11	1:A:111:ILE:HD11	0.44	1.87	20	1
1:A:220:GLU:O	1:A:221:GLN:C	0.44	2.56	21	3
1:A:13:CYS:SG	1:A:51:VAL:HG23	0.44	2.53	15	1
1:A:19:ASN:O	1:A:20:GLU:C	0.44	2.56	18	1
1:A:277:TYR:CG	1:A:278:ARG:N	0.44	2.85	2	2
1:A:136:GLU:OE2	1:A:146:LEU:HD23	0.44	2.12	10	1
1:A:61:VAL:HG13	1:A:62:TYR:N	0.44	2.28	22	1
1:A:208:PHE:CZ	1:A:210:ILE:HD11	0.44	2.47	1	2
1:A:32:LYS:C	1:A:33:PHE:CG	0.44	2.91	10	3
1:A:237:LYS:O	1:A:238:VAL:C	0.44	2.57	7	1
1:A:69:ILE:HG21	1:A:81:ILE:CD1	0.44	2.43	8	1
1:A:170:GLU:O	1:A:171:ARG:C	0.44	2.56	13	1
1:A:62:TYR:O	1:A:66:ALA:HB2	0.44	2.12	15	1
1:A:137:ILE:HD13	1:A:137:ILE:C	0.44	2.33	21	1
1:A:32:LYS:O	1:A:33:PHE:HB3	0.44	2.13	22	1
1:A:42:ALA:O	1:A:44:LYS:N	0.43	2.51	7	2
1:A:238:VAL:HG12	1:A:239:SER:N	0.43	2.28	11	1
1:A:39:VAL:HG11	1:A:51:VAL:CG1	0.43	2.43	5	1
1:A:9:ILE:HG21	1:A:297:THR:HG23	0.43	1.89	15	1
1:A:204:SER:HA	1:A:254:ILE:HD11	0.43	1.91	3	1
1:A:196:ASN:O	1:A:197:MET:C	0.43	2.57	5	1
1:A:236:GLU:O	1:A:237:LYS:C	0.43	2.56	2	1
1:A:320:GLN:O	1:A:324:THR:N	0.43	2.51	15	2
1:A:141:LYS:O	1:A:143:ARG:N	0.43	2.51	16	3
1:A:241:THR:HA	1:A:247:VAL:HG11	0.43	1.90	2	1
1:A:290:LEU:C	1:A:290:LEU:HD13	0.43	2.33	4	1
1:A:176:PRO:O	1:A:179:VAL:HG22	0.43	2.14	21	1
1:A:264:VAL:HG21	1:A:283:THR:CG2	0.43	2.40	3	1
1:A:48:PHE:CZ	1:A:316:LEU:HD23	0.43	2.49	21	1
1:A:80:THR:HG21	1:A:290:LEU:HD21	0.43	1.91	20	1
1:A:146:LEU:HD22	1:A:190:ARG:HB2	0.42	1.91	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:ILE:CD1	1:A:81:ILE:HD11	0.42	2.44	14	2
1:A:139:LEU:HD13	1:A:139:LEU:C	0.42	2.35	5	1
1:A:250:GLU:HA	1:A:254:ILE:HD13	0.42	1.91	9	1
1:A:2:ALA:N	1:A:5:ALA:HB3	0.42	2.28	12	1
1:A:87:THR:HG22	1:A:91:LYS:HD2	0.42	1.91	17	1
1:A:290:LEU:HD13	1:A:290:LEU:C	0.42	2.34	10	1
1:A:135:PHE:CD2	1:A:153:LEU:HD11	0.42	2.50	14	2
1:A:53:GLN:O	1:A:56:THR:HG22	0.42	2.14	18	1
1:A:34:GLN:O	1:A:39:VAL:HG12	0.42	2.15	15	1
1:A:80:THR:HG21	1:A:290:LEU:HD23	0.42	1.92	1	1
1:A:290:LEU:HD22	1:A:290:LEU:C	0.42	2.34	13	2
1:A:316:LEU:N	1:A:316:LEU:HD12	0.42	2.30	4	1
1:A:52:PHE:CD1	1:A:61:VAL:HG23	0.42	2.50	4	1
1:A:169:THR:O	1:A:169:THR:HG22	0.42	2.15	6	1
1:A:207:ILE:O	1:A:207:ILE:HG23	0.42	2.15	22	2
1:A:155:VAL:O	1:A:155:VAL:HG13	0.42	2.15	22	1
1:A:80:THR:HG21	1:A:290:LEU:HD12	0.42	1.91	16	1
1:A:235:SER:HG	1:A:311:GLU:CD	0.42	2.18	1	1
1:A:260:ALA:HB2	1:A:278:ARG:HD3	0.42	1.91	6	1
1:A:56:THR:HG23	1:A:61:VAL:CB	0.42	2.45	11	1
1:A:232:LEU:HD22	1:A:261:LEU:HD22	0.42	1.91	19	1
1:A:83:ALA:HB3	1:A:231:ASP:OD1	0.41	2.15	2	1
1:A:57:SER:O	1:A:59:GLU:N	0.41	2.52	4	1
1:A:132:VAL:HG22	1:A:173:VAL:HG21	0.41	1.91	9	1
1:A:8:ASN:O	1:A:9:ILE:HG22	0.41	2.14	16	1
1:A:134:TYR:O	1:A:146:LEU:HD12	0.41	2.15	17	1
1:A:173:VAL:HG11	1:A:179:VAL:HG23	0.41	1.92	18	1
1:A:244:GLU:O	1:A:247:VAL:HG12	0.41	2.16	6	1
1:A:56:THR:HG22	1:A:58:GLN:H	0.41	1.74	11	1
1:A:238:VAL:HG22	1:A:239:SER:N	0.41	2.30	19	1
1:A:240:LYS:O	1:A:241:THR:HG23	0.41	2.15	6	1
1:A:9:ILE:HD12	1:A:297:THR:HG23	0.41	1.91	12	1
1:A:317:LEU:CD1	1:A:324:THR:HG21	0.41	2.44	1	1
1:A:178:GLU:O	1:A:182:THR:HG23	0.41	2.16	14	1
1:A:4:LEU:N	1:A:4:LEU:HD13	0.41	2.31	16	1
1:A:285:ILE:O	1:A:285:ILE:HD13	0.41	2.15	22	1
1:A:108:ILE:HG22	1:A:109:PRO:HD3	0.41	1.92	19	2
1:A:290:LEU:HD23	1:A:296:THR:CG2	0.41	2.46	13	1
1:A:80:THR:HG21	1:A:290:LEU:CD2	0.41	2.46	20	1
1:A:13:CYS:O	1:A:51:VAL:HG23	0.41	2.16	4	1
1:A:132:VAL:HG22	1:A:173:VAL:HG11	0.41	1.93	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:320:GLN:O	1:A:321:ARG:C	0.41	2.59	11	1
1:A:241:THR:HG22	1:A:241:THR:O	0.41	2.15	19	1
1:A:209:LEU:HD23	1:A:226:LYS:HD2	0.41	1.93	22	1
1:A:39:VAL:HG13	1:A:51:VAL:HG13	0.41	1.92	8	1
1:A:11:VAL:HG22	1:A:298:ILE:HD12	0.41	1.92	9	1
1:A:45:PRO:CG	1:A:324:THR:O	0.40	2.70	6	1
1:A:169:THR:HG22	1:A:169:THR:O	0.40	2.16	18	1
1:A:230:VAL:HG12	1:A:232:LEU:CD1	0.40	2.47	20	1
1:A:83:ALA:HB3	1:A:231:ASP:HA	0.40	1.93	2	1
1:A:83:ALA:N	1:A:230:VAL:O	0.40	2.55	2	1
1:A:10:LYS:O	1:A:11:VAL:C	0.40	2.60	4	1
1:A:171:ARG:O	1:A:172:PHE:C	0.40	2.60	22	1
1:A:268:LEU:HD13	1:A:268:LEU:O	0.40	2.17	12	1
1:A:4:LEU:N	1:A:4:LEU:HD22	0.40	2.31	16	1
1:A:139:LEU:HD13	1:A:253:ASN:CB	0.40	2.46	22	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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	323/349 (93%)	280±4 (87±1%)	29±4 (9±1%)	14±3 (4±1%)	4	28
All	All	7106/7678 (93%)	6150 (87%)	639 (9%)	317 (4%)	4	28

All 53 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	43	SER	22
1	A	244	GLU	22
1	A	277	TYR	20
1	A	11	VAL	18
1	A	142	ILE	16
1	A	278	ARG	15
1	A	148	VAL	14

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Mol	Chain	Res	Type	Models (Total)
1	A	221	GLN	13
1	A	238	VAL	13
1	A	102	PRO	13
1	A	9	ILE	12
1	A	58	GLN	9
1	A	103	GLU	9
1	A	36	GLU	9
1	A	33	PHE	8
1	A	196	ASN	8
1	A	37	ASP	7
1	A	105	MET	7
1	A	20	GLU	7
1	A	197	MET	7
1	A	195	THR	5
1	A	42	ALA	5
1	A	237	LYS	4
1	A	171	ARG	4
1	A	35	GLY	4
1	A	239	SER	3
1	A	241	THR	3
1	A	78	ASN	3
1	A	15	PHE	3
1	A	224	SER	2
1	A	291	GLY	2
1	A	90	GLY	2
1	A	2	ALA	2
1	A	77	TYR	2
1	A	170	GLU	2
1	A	294	CYS	2
1	A	236	GLU	2
1	A	13	CYS	2
1	A	172	PHE	2
1	A	104	GLY	1
1	A	14	ARG	1
1	A	233	ALA	1
1	A	76	GLY	1
1	A	234	GLY	1
1	A	240	LYS	1
1	A	27	ASP	1
1	A	317	LEU	1
1	A	34	GLN	1
1	A	290	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	12	MET	1
1	A	225	GLY	1
1	A	57	SER	1
1	A	173	VAL	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	288/312 (92%)	274±3 (95±1%)	14±3 (5±1%)	29	78
All	All	6336/6864 (92%)	6024 (95%)	312 (5%)	29	78

All 79 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	137	ILE	18
1	A	223	LEU	18
1	A	268	LEU	14
1	A	146	LEU	13
1	A	295	ARG	13
1	A	15	PHE	12
1	A	290	LEU	12
1	A	138	TYR	11
1	A	33	PHE	10
1	A	53	GLN	10
1	A	4	LEU	8
1	A	208	PHE	8
1	A	274	TYR	8
1	A	191	HIS	8
1	A	91	LYS	7
1	A	305	SER	6
1	A	224	SER	6
1	A	51	VAL	6
1	A	105	MET	5
1	A	282	MET	5
1	A	41	ILE	5

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Mol	Chain	Res	Type	Models (Total)
1	A	198	ASN	4
1	A	78	ASN	4
1	A	209	LEU	4
1	A	285	ILE	4
1	A	321	ARG	4
1	A	122	MET	4
1	A	9	ILE	3
1	A	150	LYS	3
1	A	110	ARG	3
1	A	14	ARG	3
1	A	324	THR	3
1	A	108	ILE	3
1	A	226	LYS	3
1	A	205	HIS	3
1	A	77	TYR	2
1	A	10	LYS	2
1	A	195	THR	2
1	A	58	GLN	2
1	A	239	SER	2
1	A	248	LEU	2
1	A	229	LEU	2
1	A	238	VAL	2
1	A	317	LEU	2
1	A	320	GLN	2
1	A	294	CYS	2
1	A	69	ILE	2
1	A	184	ASP	2
1	A	46	TYR	2
1	A	227	LEU	2
1	A	148	VAL	2
1	A	172	PHE	2
1	A	281	LYS	1
1	A	56	THR	1
1	A	74	LEU	1
1	A	11	VAL	1
1	A	18	LEU	1
1	A	159	LYS	1
1	A	89	SER	1
1	A	141	LYS	1
1	A	145	LEU	1
1	A	316	LEU	1
1	A	55	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	161	ARG	1
1	A	228	TYR	1
1	A	220	GLU	1
1	A	308	ASN	1
1	A	207	ILE	1
1	A	196	ASN	1
1	A	34	GLN	1
1	A	155	VAL	1
1	A	287	GLN	1
1	A	278	ARG	1
1	A	48	PHE	1
1	A	288	ASP	1
1	A	71	LYS	1
1	A	72	ASP	1
1	A	286	LEU	1
1	A	323	LYS	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 monosaccharides 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 (i)

The completeness of assignment taking into account all chemical shift lists is 32% for the well-defined parts and 31% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1376
Number of shifts mapped to atoms	1376
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	289	-0.20 ± 0.04	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	263	0.40 ± 0.17	None needed (< 0.5 ppm)
$^{13}C'$	262	0.29 ± 0.04	None needed (< 0.5 ppm)
^{15}N	277	0.13 ± 0.15	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 32%, i.e. 1256 atoms were assigned a chemical shift out of a possible 3937. 12 out of 47 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	788/1604 (49%)	0/640 (0%)	525/648 (81%)	263/316 (83%)
Sidechain	427/2066 (21%)	0/1208 (0%)	427/761 (56%)	0/97 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	41/267 (15%)	0/139 (0%)	41/114 (36%)	0/14 (0%)
Overall	1256/3937 (32%)	0/1987 (0%)	993/1523 (65%)	263/427 (62%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 31%, i.e. 1324 atoms were assigned a chemical shift out of a possible 4274. 14 out of 51 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	828/1729 (48%)	0/690 (0%)	551/698 (79%)	277/341 (81%)
Sidechain	453/2258 (20%)	0/1320 (0%)	453/832 (54%)	0/106 (0%)
Aromatic	43/287 (15%)	0/149 (0%)	42/123 (34%)	1/15 (7%)
Overall	1324/4274 (31%)	0/2159 (0%)	1046/1653 (63%)	278/462 (60%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A: