



Full wwPDB NMR Structure Validation Report ⓘ

May 31, 2020 – 11:04 am BST

PDB ID : 6KJN
Title : The microtubule-binding domains of yeast cytoplasmic dynein in the high affinity state
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Deposited on : 2019-07-22

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 : 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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

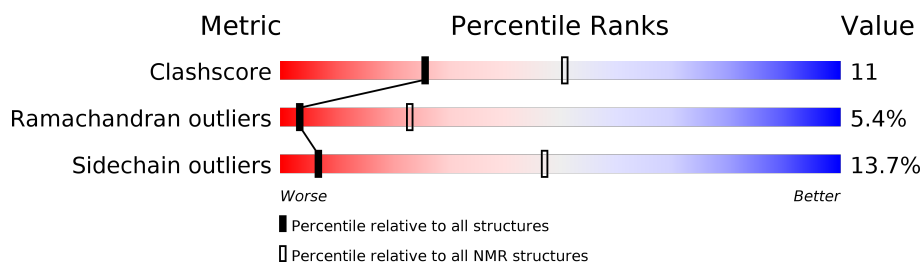
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 71%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	141	

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 6 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:3101-A:3222 (122)	0.83	6

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 6, 8, 10
2	5, 7, 9

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2294 atoms, of which 1139 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms						Trace
1	A	141	Total	C	H	N	O	S	0
			2294	730	1139	202	214	9	

There are 5 discrepancies between the modelled and reference sequences:

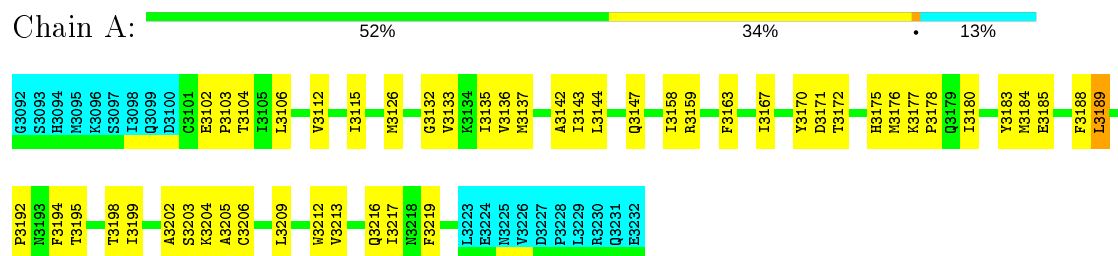
Chain	Residue	Modelled	Actual	Comment	Reference
A	3092	GLY	-	expression tag	UNP P36022
A	3093	SER	-	expression tag	UNP P36022
A	3094	HIS	-	expression tag	UNP P36022
A	3101	CYS	ILE	engineered mutation	UNP P36022
A	3222	CYS	VAL	engineered mutation	UNP P36022

4 Residue-property plots

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: Dynein heavy chain, cytoplasmic

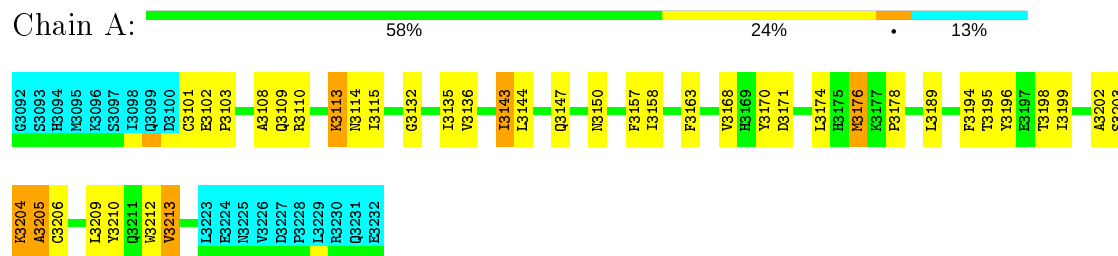


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

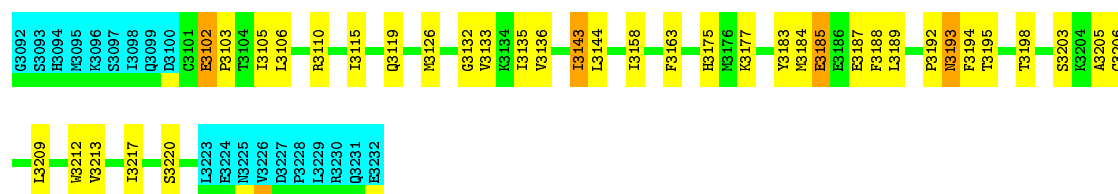
- Molecule 1: Dynein heavy chain, cytoplasmic



4.2.2 Score per residue for model 2

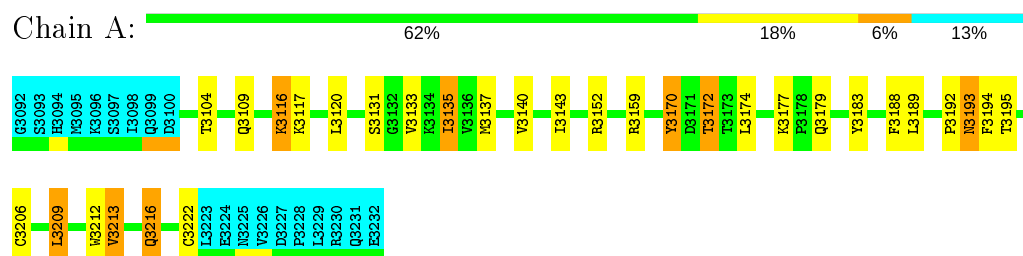
- Molecule 1: Dynein heavy chain, cytoplasmic





4.2.3 Score per residue for model 3

- Molecule 1: Dynein heavy chain, cytoplasmic



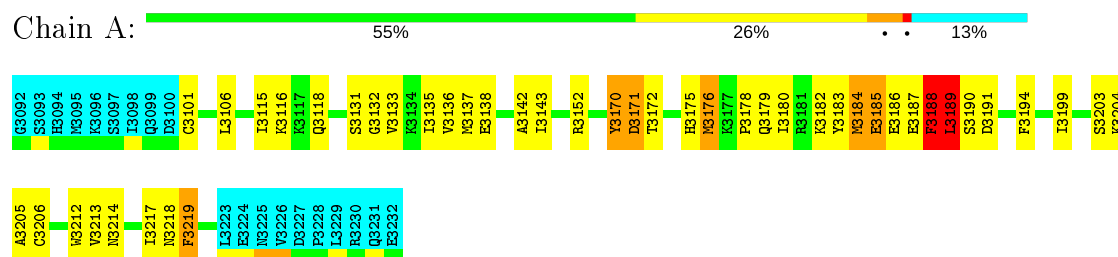
4.2.4 Score per residue for model 4

- Molecule 1: Dynein heavy chain, cytoplasmic



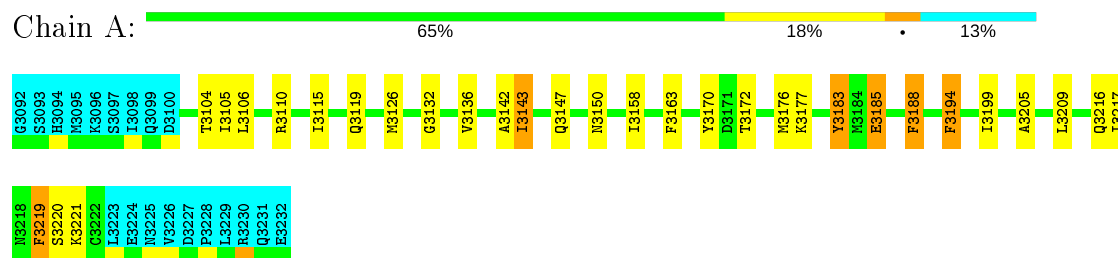
4.2.5 Score per residue for model 5

- Molecule 1: Dynein heavy chain, cytoplasmic



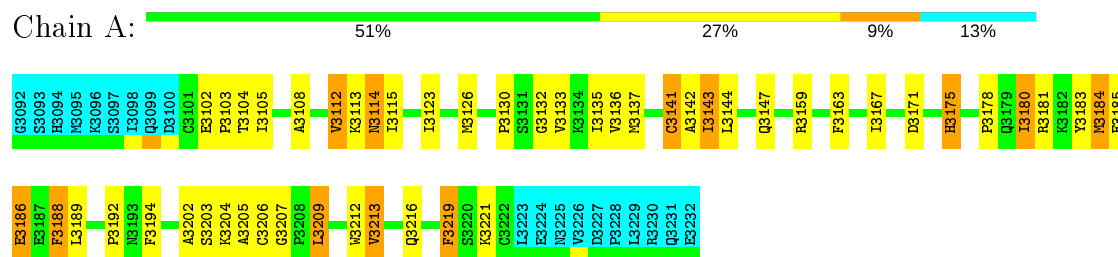
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Dynein heavy chain, cytoplasmic



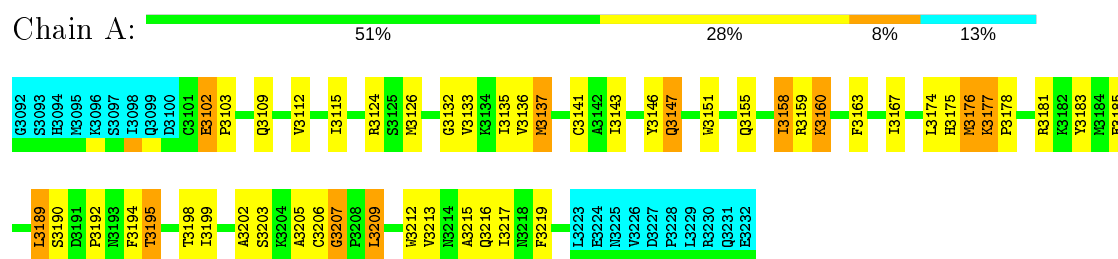
4.2.7 Score per residue for model 7

- Molecule 1: Dynein heavy chain, cytoplasmic



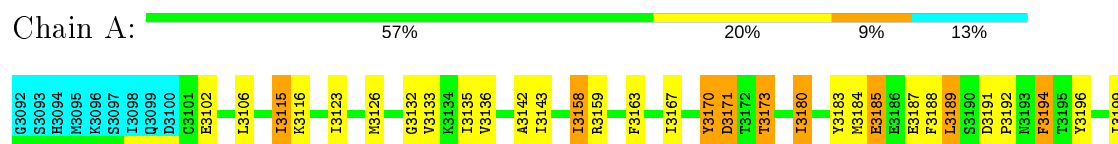
4.2.8 Score per residue for model 8

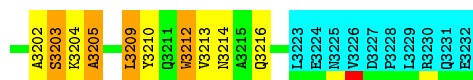
- Molecule 1: Dynein heavy chain, cytoplasmic



4.2.9 Score per residue for model 9

- Molecule 1: Dynein heavy chain, cytoplasmic

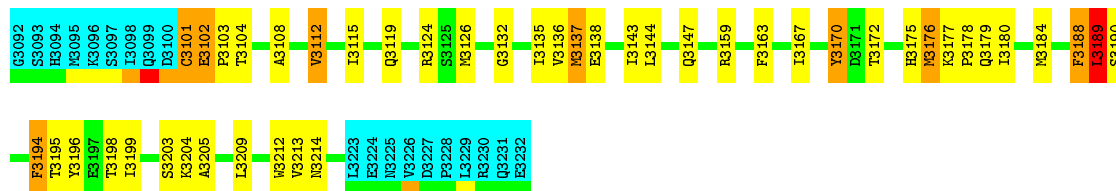




4.2.10 Score per residue for model 10

- Molecule 1: Dynein heavy chain, cytoplasmic

Chain A: 55% 26% 6% 13%



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 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	

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1398
Number of shifts mapped to atoms	1398
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%

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	1003	994	994	22±7
All	All	10030	9940	9940	225

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3115:ILE:HD11	1:A:3164:ILE:HD11	0.92	1.37	4	1
1:A:3212:TRP:CZ3	1:A:3213:VAL:HG13	0.80	2.11	1	1
1:A:3142:ALA:HB1	1:A:3180:ILE:HD12	0.80	1.54	9	2
1:A:3185:GLU:O	1:A:3189:LEU:HD12	0.79	1.78	5	1
1:A:3115:ILE:HG21	1:A:3205:ALA:HA	0.77	1.56	8	2
1:A:3189:LEU:HD13	1:A:3190:SER:N	0.75	1.96	5	1
1:A:3105:ILE:HD11	1:A:3219:PHE:HB2	0.69	1.65	4	2
1:A:3132:GLY:O	1:A:3136:VAL:HG23	0.68	1.89	7	8
1:A:3115:ILE:CD1	1:A:3164:ILE:HD11	0.67	2.19	4	1
1:A:3133:VAL:HG22	1:A:3206:CYS:SG	0.67	2.29	8	5
1:A:3209:LEU:O	1:A:3213:VAL:HG12	0.67	1.90	9	2
1:A:3163:PHE:CZ	1:A:3167:ILE:HD11	0.66	2.25	9	2
1:A:3158:ILE:HG22	1:A:3163:PHE:CE1	0.65	2.26	1	5
1:A:3135:ILE:HD12	1:A:3194:PHE:CD1	0.65	2.26	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3142:ALA:HB1	1:A:3180:ILE:CD1	0.65	2.21	9	2
1:A:3194:PHE:CE2	1:A:3199:ILE:HD11	0.65	2.27	10	4
1:A:3123:ILE:HD12	1:A:3133:VAL:HG11	0.64	1.69	9	1
1:A:3105:ILE:HD11	1:A:3219:PHE:CB	0.64	2.22	6	1
1:A:3194:PHE:CE1	1:A:3199:ILE:HD11	0.63	2.29	5	2
1:A:3167:ILE:HD13	1:A:3209:LEU:HD11	0.63	1.70	7	4
1:A:3163:PHE:CE1	1:A:3167:ILE:HD11	0.62	2.29	4	3
1:A:3189:LEU:HD22	1:A:3189:LEU:O	0.62	1.95	5	1
1:A:3204:LYS:O	1:A:3205:ALA:HB2	0.62	1.94	1	2
1:A:3137:MET:SD	1:A:3137:MET:N	0.61	2.74	10	2
1:A:3192:PRO:O	1:A:3193:ASN:CB	0.60	2.49	2	2
1:A:3130:PRO:HB2	1:A:3202:ALA:HB1	0.60	1.74	4	1
1:A:3189:LEU:HD13	1:A:3189:LEU:C	0.59	2.18	2	1
1:A:3218:ASN:O	1:A:3219:PHE:CB	0.59	2.50	5	2
1:A:3189:LEU:HD22	1:A:3189:LEU:C	0.59	2.18	5	1
1:A:3184:MET:O	1:A:3186:GLU:N	0.58	2.36	5	1
1:A:3101:CYS:O	1:A:3104:THR:N	0.58	2.37	10	1
1:A:3212:TRP:CZ3	1:A:3213:VAL:HG23	0.58	2.33	3	3
1:A:3218:ASN:O	1:A:3219:PHE:HB2	0.58	1.99	4	1
1:A:3115:ILE:HD13	1:A:3205:ALA:HA	0.57	1.76	7	2
1:A:3137:MET:N	1:A:3137:MET:SD	0.57	2.76	7	2
1:A:3130:PRO:CB	1:A:3202:ALA:HB1	0.57	2.29	4	1
1:A:3204:LYS:O	1:A:3205:ALA:CB	0.57	2.52	1	2
1:A:3108:ALA:HB1	1:A:3212:TRP:HA	0.57	1.77	7	2
1:A:3105:ILE:CG2	1:A:3105:ILE:O	0.56	2.53	2	1
1:A:3142:ALA:HB1	1:A:3183:TYR:CE1	0.55	2.37	4	1
1:A:3159:ARG:O	1:A:3160:LYS:HB3	0.55	2.01	8	1
1:A:3185:GLU:O	1:A:3186:GLU:HB2	0.55	2.02	7	1
1:A:3185:GLU:HA	1:A:3189:LEU:HD23	0.55	1.76	9	1
1:A:3142:ALA:HB3	1:A:3180:ILE:HD11	0.55	1.79	7	1
1:A:3105:ILE:HG22	1:A:3105:ILE:O	0.55	2.02	2	1
1:A:3189:LEU:C	1:A:3189:LEU:HD13	0.54	2.23	1	1
1:A:3212:TRP:CE3	1:A:3213:VAL:HG23	0.54	2.37	8	3
1:A:3102:GLU:N	1:A:3103:PRO:CD	0.54	2.71	1	4
1:A:3131:SER:O	1:A:3135:ILE:HG13	0.54	2.03	5	2
1:A:3143:ILE:HD13	1:A:3212:TRP:CH2	0.53	2.38	7	1
1:A:3212:TRP:CE3	1:A:3213:VAL:HG13	0.53	2.39	1	1
1:A:3142:ALA:HB1	1:A:3183:TYR:CE2	0.53	2.39	6	1
1:A:3159:ARG:O	1:A:3160:LYS:CB	0.53	2.57	8	1
1:A:3180:ILE:HG22	1:A:3181:ARG:N	0.52	2.20	7	1
1:A:3135:ILE:HD12	1:A:3194:PHE:HD1	0.52	1.65	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3184:MET:HB2	1:A:3217:ILE:HD11	0.52	1.82	2	1
1:A:3189:LEU:HD23	1:A:3190:SER:N	0.51	2.20	10	3
1:A:3123:ILE:HD11	1:A:3203:SER:OG	0.51	2.05	7	1
1:A:3102:GLU:CB	1:A:3103:PRO:CD	0.51	2.88	10	1
1:A:3185:GLU:O	1:A:3186:GLU:CB	0.51	2.59	7	1
1:A:3143:ILE:HD11	1:A:3216:GLN:HG2	0.51	1.83	7	1
1:A:3170:TYR:CD1	1:A:3170:TYR:N	0.50	2.78	3	1
1:A:3170:TYR:O	1:A:3171:ASP:C	0.49	2.50	5	2
1:A:3109:GLN:OE1	1:A:3168:VAL:HG13	0.49	2.08	1	1
1:A:3195:THR:HG23	1:A:3198:THR:H	0.49	1.66	3	4
1:A:3140:VAL:CG2	1:A:3209:LEU:HD12	0.49	2.38	3	1
1:A:3184:MET:O	1:A:3188:PHE:CB	0.48	2.61	10	1
1:A:3210:TYR:CD2	1:A:3210:TYR:C	0.48	2.86	1	1
1:A:3184:MET:O	1:A:3188:PHE:N	0.48	2.46	7	1
1:A:3105:ILE:HD11	1:A:3219:PHE:CG	0.48	2.42	7	1
1:A:3185:GLU:O	1:A:3189:LEU:HB3	0.48	2.09	8	1
1:A:3101:CYS:O	1:A:3103:PRO:N	0.48	2.47	10	1
1:A:3213:VAL:HG13	1:A:3214:ASN:N	0.48	2.24	10	1
1:A:3102:GLU:CB	1:A:3103:PRO:HD3	0.48	2.39	4	1
1:A:3191:ASP:O	1:A:3191:ASP:OD1	0.48	2.31	5	1
1:A:3170:TYR:CE2	1:A:3172:THR:HG22	0.48	2.43	10	1
1:A:3133:VAL:O	1:A:3136:VAL:HG12	0.48	2.08	4	1
1:A:3170:TYR:O	1:A:3170:TYR:CD1	0.48	2.67	3	1
1:A:3189:LEU:HD23	1:A:3189:LEU:H	0.48	1.69	7	1
1:A:3188:PHE:O	1:A:3191:ASP:CG	0.47	2.52	5	1
1:A:3116:LYS:HA	1:A:3120:LEU:HD23	0.47	1.86	3	1
1:A:3101:CYS:O	1:A:3102:GLU:C	0.47	2.52	10	1
1:A:3130:PRO:HG2	1:A:3202:ALA:HB1	0.47	1.87	7	1
1:A:3113:LYS:O	1:A:3114:ASN:C	0.47	2.52	7	1
1:A:3176:MET:O	1:A:3177:LYS:C	0.47	2.52	10	1
1:A:3213:VAL:HG13	1:A:3214:ASN:H	0.47	1.70	9	1
1:A:3143:ILE:HG22	1:A:3144:LEU:N	0.47	2.25	1	1
1:A:3115:ILE:CG2	1:A:3205:ALA:HB1	0.47	2.40	10	3
1:A:3133:VAL:HG23	1:A:3202:ALA:HB1	0.46	1.87	8	2
1:A:3115:ILE:HG22	1:A:3205:ALA:HA	0.46	1.85	2	4
1:A:3123:ILE:HD13	1:A:3126:MET:SD	0.46	2.50	9	1
1:A:3194:PHE:CD2	1:A:3199:ILE:HD11	0.46	2.46	9	1
1:A:3115:ILE:HG21	1:A:3205:ALA:CA	0.46	2.37	8	2
1:A:3188:PHE:CE1	1:A:3194:PHE:CZ	0.45	3.03	10	1
1:A:3143:ILE:HD11	1:A:3216:GLN:CB	0.45	2.41	6	1
1:A:3194:PHE:CD1	1:A:3199:ILE:HD11	0.45	2.46	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3143:ILE:HD13	1:A:3213:VAL:HG23	0.45	1.89	9	1
1:A:3143:ILE:HG21	1:A:3212:TRP:CH2	0.45	2.46	1	1
1:A:3105:ILE:HD11	1:A:3219:PHE:CD1	0.45	2.47	7	1
1:A:3183:TYR:O	1:A:3184:MET:O	0.45	2.34	5	1
1:A:3112:VAL:CG2	1:A:3209:LEU:HD22	0.45	2.42	7	1
1:A:3108:ALA:O	1:A:3112:VAL:HG13	0.45	2.12	10	1
1:A:3115:ILE:HD12	1:A:3119:GLN:OE1	0.45	2.11	10	1
1:A:3196:TYR:HA	1:A:3210:TYR:CD2	0.45	2.46	1	1
1:A:3199:ILE:O	1:A:3202:ALA:HB3	0.45	2.12	1	1
1:A:3183:TYR:O	1:A:3185:GLU:N	0.44	2.50	9	1
1:A:3206:CYS:O	1:A:3209:LEU:N	0.44	2.50	7	1
1:A:3112:VAL:HG12	1:A:3164:ILE:HD12	0.44	1.89	4	1
1:A:3143:ILE:CG2	1:A:3144:LEU:N	0.44	2.81	1	4
1:A:3115:ILE:HG22	1:A:3205:ALA:CB	0.44	2.43	9	1
1:A:3170:TYR:O	1:A:3172:THR:N	0.44	2.50	5	1
1:A:3183:TYR:O	1:A:3184:MET:C	0.44	2.56	7	2
1:A:3195:THR:HG23	1:A:3198:THR:OG1	0.44	2.13	8	1
1:A:3194:PHE:CE2	1:A:3210:TYR:CD1	0.44	3.06	9	1
1:A:3209:LEU:HD13	1:A:3212:TRP:CE3	0.43	2.48	9	1
1:A:3180:ILE:O	1:A:3183:TYR:N	0.43	2.51	9	2
1:A:3143:ILE:HD11	1:A:3216:GLN:CG	0.43	2.44	7	1
1:A:3135:ILE:HD12	1:A:3194:PHE:CG	0.43	2.48	9	1
1:A:3144:LEU:HD11	1:A:3166:ASN:OD1	0.43	2.14	4	1
1:A:3113:LYS:HE2	1:A:3168:VAL:HG11	0.42	1.92	1	1
1:A:3170:TYR:HD1	1:A:3170:TYR:N	0.42	2.11	3	1
1:A:3189:LEU:HD23	1:A:3189:LEU:N	0.42	2.29	7	1
1:A:3178:PRO:C	1:A:3180:ILE:H	0.42	2.17	10	1
1:A:3143:ILE:HG21	1:A:3212:TRP:HH2	0.42	1.74	1	1
1:A:3170:TYR:O	1:A:3170:TYR:CG	0.42	2.71	4	2
1:A:3199:ILE:O	1:A:3206:CYS:SG	0.42	2.76	4	1
1:A:3176:MET:O	1:A:3177:LYS:CB	0.42	2.68	8	1
1:A:3219:PHE:CD1	1:A:3219:PHE:N	0.42	2.86	8	1
1:A:3146:TYR:O	1:A:3147:GLN:C	0.42	2.58	8	1
1:A:3189:LEU:HD23	1:A:3190:SER:H	0.42	1.75	8	1
1:A:3158:ILE:HG22	1:A:3163:PHE:CD1	0.41	2.50	6	2
1:A:3215:ALA:O	1:A:3218:ASN:O	0.41	2.38	4	1
1:A:3206:CYS:O	1:A:3207:GLY:C	0.41	2.59	8	2
1:A:3215:ALA:O	1:A:3219:PHE:HB2	0.41	2.15	8	1
1:A:3115:ILE:HG22	1:A:3205:ALA:CA	0.41	2.46	9	1
1:A:3204:LYS:O	1:A:3204:LYS:CG	0.41	2.69	1	1
1:A:3188:PHE:O	1:A:3190:SER:N	0.41	2.53	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3155:GLN:HA	1:A:3158:ILE:HG13	0.41	1.92	8	1
1:A:3214:ASN:O	1:A:3217:ILE:HB	0.41	2.15	5	1
1:A:3170:TYR:CE1	1:A:3172:THR:HG22	0.41	2.51	6	1
1:A:3219:PHE:C	1:A:3221:LYS:H	0.41	2.18	6	2
1:A:3141:CYS:SG	1:A:3142:ALA:N	0.41	2.92	7	1
1:A:3189:LEU:CD1	1:A:3189:LEU:C	0.41	2.89	2	1
1:A:3109:GLN:O	1:A:3112:VAL:HG22	0.41	2.16	8	1
1:A:3114:ASN:O	1:A:3115:ILE:C	0.41	2.59	1	1
1:A:3190:SER:O	1:A:3192:PRO:HD3	0.41	2.15	8	1
1:A:3143:ILE:HD11	1:A:3216:GLN:CD	0.41	2.36	7	1
1:A:3188:PHE:O	1:A:3188:PHE:CD2	0.40	2.73	10	1
1:A:3184:MET:O	1:A:3185:GLU:C	0.40	2.58	5	1
1:A:3189:LEU:CD2	1:A:3189:LEU:C	0.40	2.86	5	1
1:A:3172:THR:HG22	1:A:3216:GLN:OE1	0.40	2.17	3	1
1:A:3196:TYR:CD2	1:A:3196:TYR:O	0.40	2.74	9	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	122/141 (87%)	104±5 (85±4%)	12±4 (10±3%)	7±2 (5±1%)	3	23
All	All	1220/1410 (87%)	1037 (85%)	117 (10%)	66 (5%)	3	23

All 31 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	3147	GLN	6
1	A	3178	PRO	5
1	A	3185	GLU	5
1	A	3188	PHE	5
1	A	3184	MET	3
1	A	3176	MET	3
1	A	3171	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	3175	HIS	3
1	A	3220	SER	2
1	A	3219	PHE	2
1	A	3180	ILE	2
1	A	3192	PRO	2
1	A	3102	GLU	2
1	A	3174	LEU	2
1	A	3177	LYS	2
1	A	3189	LEU	2
1	A	3193	ASN	2
1	A	3205	ALA	2
1	A	3116	LYS	1
1	A	3186	GLU	1
1	A	3160	LYS	1
1	A	3204	LYS	1
1	A	3207	GLY	1
1	A	3173	THR	1
1	A	3101	CYS	1
1	A	3170	TYR	1
1	A	3179	GLN	1
1	A	3114	ASN	1
1	A	3203	SER	1
1	A	3117	LYS	1
1	A	3187	GLU	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	112/130 (86%)	97±3 (86±2%)	15±3 (14±2%)	7	47
All	All	1120/1300 (86%)	967 (86%)	153 (14%)	7	47

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	3143	ILE	8

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Mol	Chain	Res	Type	Models (Total)
1	A	3203	SER	8
1	A	3209	LEU	7
1	A	3189	LEU	6
1	A	3183	TYR	5
1	A	3126	MET	5
1	A	3170	TYR	5
1	A	3106	LEU	5
1	A	3204	LYS	4
1	A	3176	MET	4
1	A	3104	THR	4
1	A	3194	PHE	4
1	A	3137	MET	4
1	A	3159	ARG	4
1	A	3213	VAL	4
1	A	3188	PHE	4
1	A	3216	GLN	4
1	A	3124	ARG	3
1	A	3217	ILE	3
1	A	3110	ARG	3
1	A	3185	GLU	3
1	A	3175	HIS	3
1	A	3116	LYS	2
1	A	3219	PHE	2
1	A	3109	GLN	2
1	A	3150	ASN	2
1	A	3152	ARG	2
1	A	3177	LYS	2
1	A	3212	TRP	2
1	A	3158	ILE	2
1	A	3112	VAL	2
1	A	3102	GLU	2
1	A	3141	CYS	2
1	A	3179	GLN	2
1	A	3138	GLU	2
1	A	3187	GLU	2
1	A	3195	THR	2
1	A	3119	GLN	2
1	A	3221	LYS	1
1	A	3191	ASP	1
1	A	3157	PHE	1
1	A	3115	ILE	1
1	A	3173	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	3151	TRP	1
1	A	3182	LYS	1
1	A	3171	ASP	1
1	A	3174	LEU	1
1	A	3118	GLN	1
1	A	3101	CYS	1
1	A	3199	ILE	1
1	A	3206	CYS	1
1	A	3181	ARG	1
1	A	3135	ILE	1
1	A	3201	ARG	1
1	A	3113	LYS	1
1	A	3196	TYR	1
1	A	3148	PHE	1
1	A	3222	CYS	1
1	A	3172	THR	1

6.3.3 RNA [i](#)

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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 71% for the well-defined parts and 71% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	1398
Number of shifts mapped to atoms	1398
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	130	2.60 ± 0.16	Should be applied
$^{13}\text{C}_\beta$	125	2.82 ± 0.08	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	121	1.15 ± 0.18	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 71%, i.e. 1134 atoms were assigned a chemical shift out of a possible 1588. 13 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	440/598 (74%)	220/238 (92%)	112/244 (46%)	108/116 (93%)
Sidechain	605/851 (71%)	373/503 (74%)	232/304 (76%)	0/44 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	89/139 (64%)	47/74 (64%)	40/60 (67%)	2/5 (40%)
Overall	1134/1588 (71%)	640/815 (79%)	384/608 (63%)	110/165 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 71%, i.e. 1306 atoms were assigned a chemical shift out of a possible 1827. 16 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	502/691 (73%)	251/275 (91%)	130/282 (46%)	121/134 (90%)
Sidechain	715/990 (72%)	442/585 (76%)	273/354 (77%)	0/51 (0%)
Aromatic	89/146 (61%)	47/78 (60%)	40/62 (65%)	2/6 (33%)
Overall	1306/1827 (71%)	740/938 (79%)	443/698 (63%)	123/191 (64%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	3129	PRO	HG2	-0.07	3.48 – 0.38	-6.5
1	A	3216	GLN	HG2	0.66	3.67 – 0.97	-6.2
1	A	3151	TRP	CZ3	111.93	129.20 – 113.60	-6.1
1	A	3167	ILE	HG23	-0.78	2.13 – -0.57	-5.8
1	A	3167	ILE	HG22	-0.78	2.13 – -0.57	-5.8
1	A	3167	ILE	HG21	-0.78	2.13 – -0.57	-5.8
1	A	3212	TRP	CZ3	113.53	129.20 – 113.60	-5.0

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:

