Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 01:15 PM EDT

PDB ID	:	2L6L
Title	:	Solution structure of human J-protein co-chaperone, Dph4
Authors	:	Thakur, A.; Chitoor, B.S.; Atreya, H.S.; Silva, P.D.
Deposited on	:	2010-11-23

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

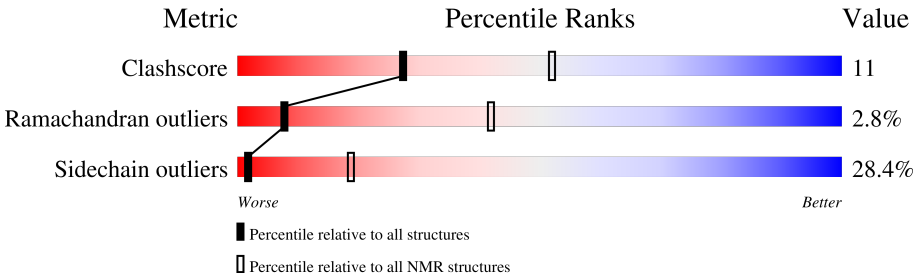
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	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	155	53% 30% • 17%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 14 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 target function*.

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:73 (64)	1.91	14
2	A:78-A:88 (11)	0.11	11
3	A:94-A:147 (54)	0.99	11

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2238 atoms, of which 980 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DnaJ homolog subfamily C member 24.

Mol	Chain	Residues	Atoms						Trace
1	A	155	Total	C	H	N	O	S	0
			2237	786	980	212	248	11	

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	SEE REMARK 999	UNP Q6P3W2
A	150	HIS	-	expression tag	UNP Q6P3W2
A	151	HIS	-	expression tag	UNP Q6P3W2
A	152	HIS	-	expression tag	UNP Q6P3W2
A	153	HIS	-	expression tag	UNP Q6P3W2
A	154	HIS	-	expression tag	UNP Q6P3W2
A	155	HIS	-	expression tag	UNP Q6P3W2

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

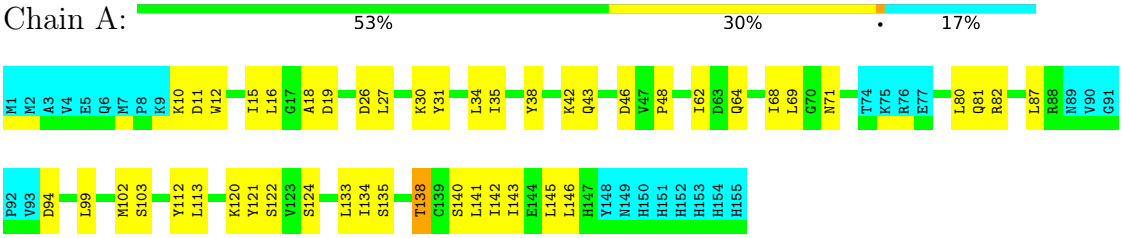
4 Residue-property plots

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: DnaJ homolog subfamily C member 24

Chain A:



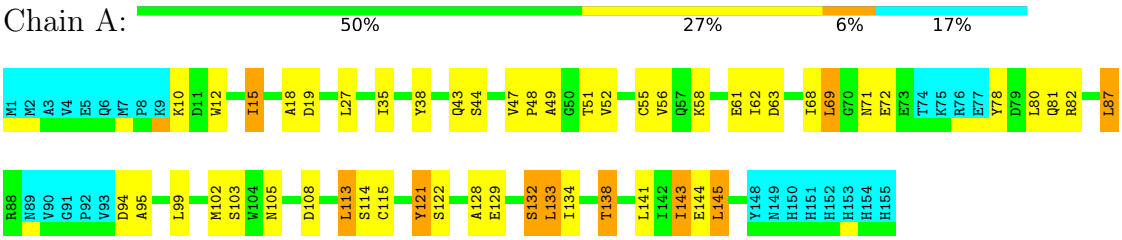
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: DnaJ homolog subfamily C member 24

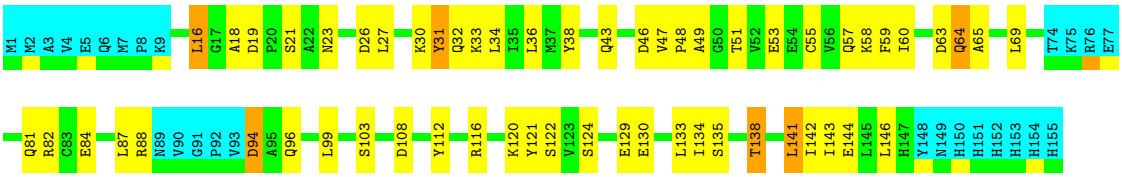
Chain A:



4.2.2 Score per residue for model 2

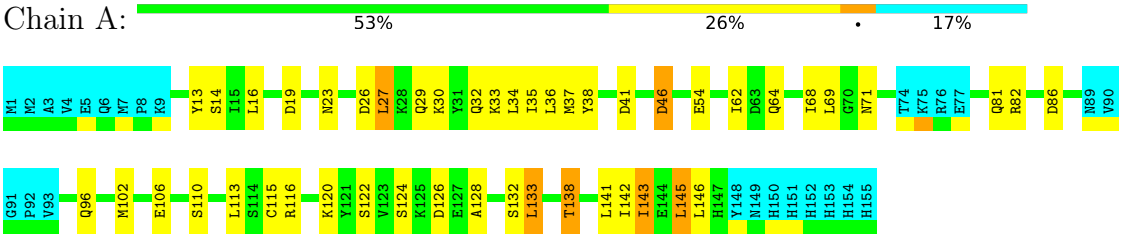
• Molecule 1: DnaJ homolog subfamily C member 24

Chain A:



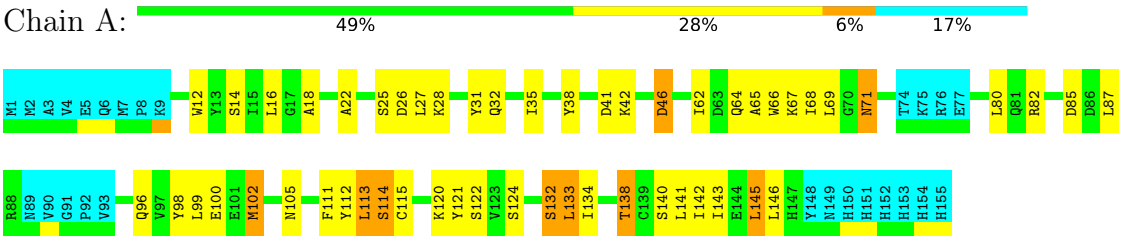
4.2.3 Score per residue for model 3

• Molecule 1: DnaJ homolog subfamily C member 24



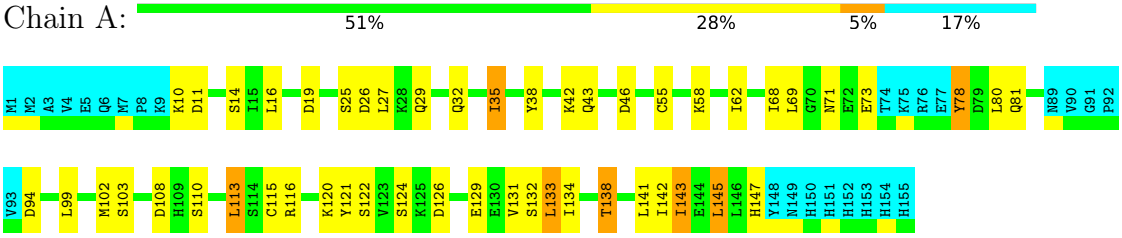
4.2.4 Score per residue for model 4

• Molecule 1: DnaJ homolog subfamily C member 24



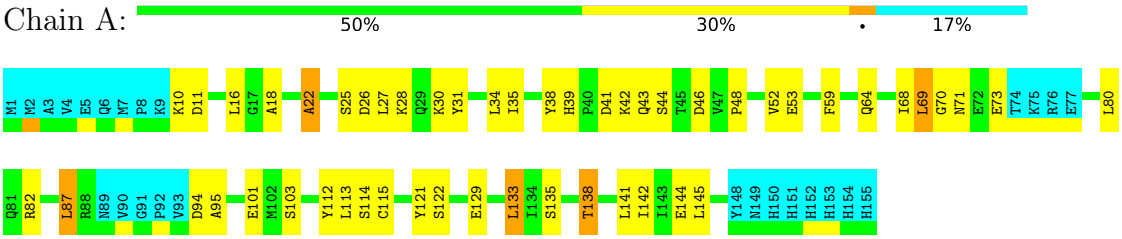
4.2.5 Score per residue for model 5

• Molecule 1: DnaJ homolog subfamily C member 24



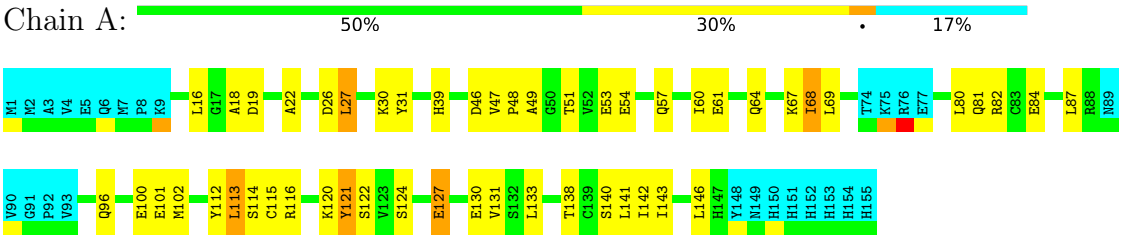
4.2.6 Score per residue for model 6

• Molecule 1: DnaJ homolog subfamily C member 24



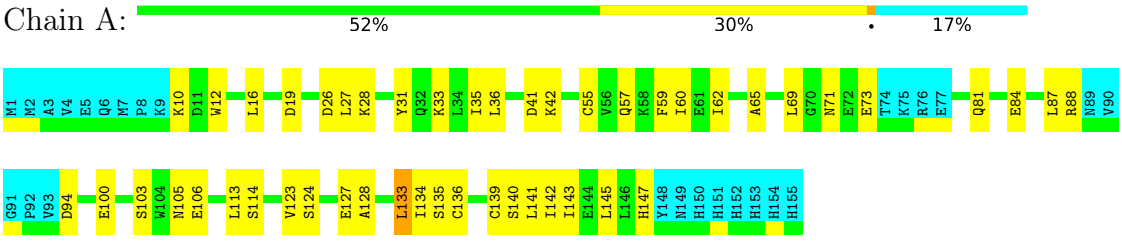
4.2.7 Score per residue for model 7

• Molecule 1: DnaJ homolog subfamily C member 24



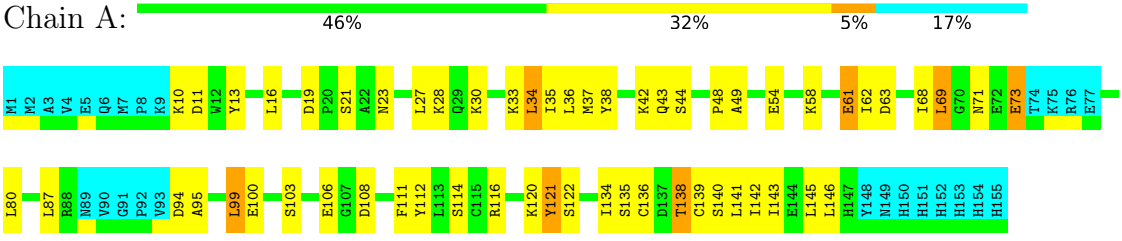
4.2.8 Score per residue for model 8

• Molecule 1: DnaJ homolog subfamily C member 24



4.2.9 Score per residue for model 9

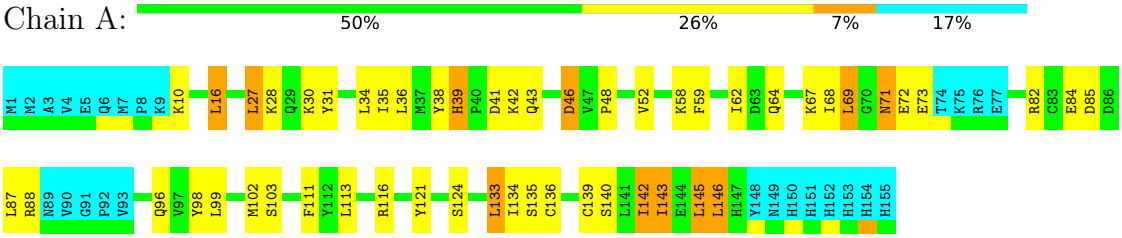
• Molecule 1: DnaJ homolog subfamily C member 24



4.2.10 Score per residue for model 10

• Molecule 1: DnaJ homolog subfamily C member 24

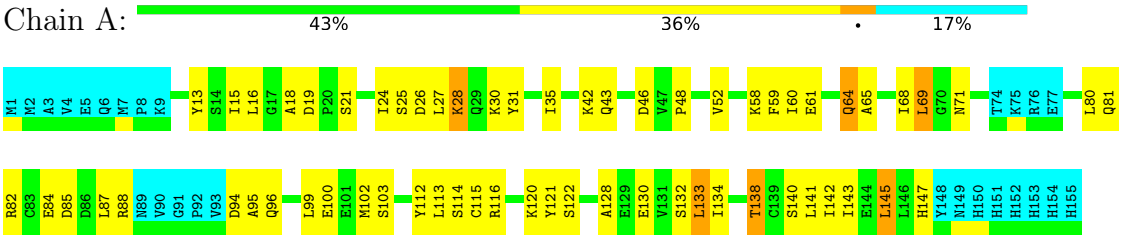
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: DnaJ homolog subfamily C member 24

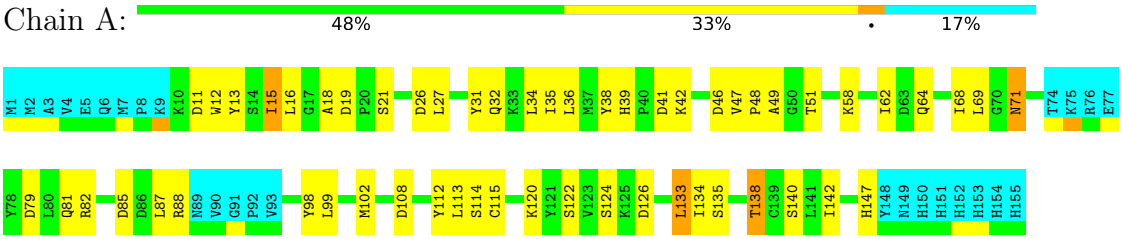
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: DnaJ homolog subfamily C member 24

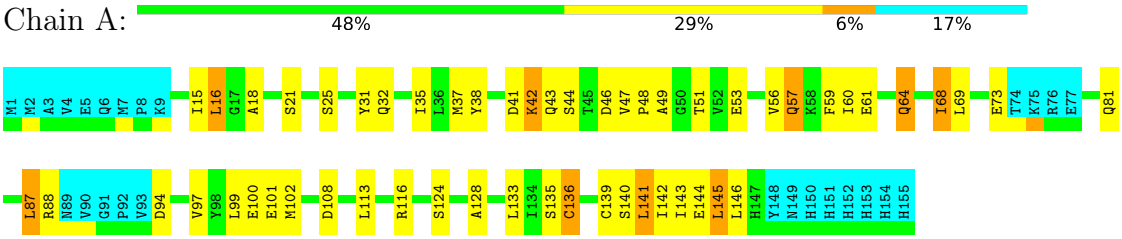
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: DnaJ homolog subfamily C member 24

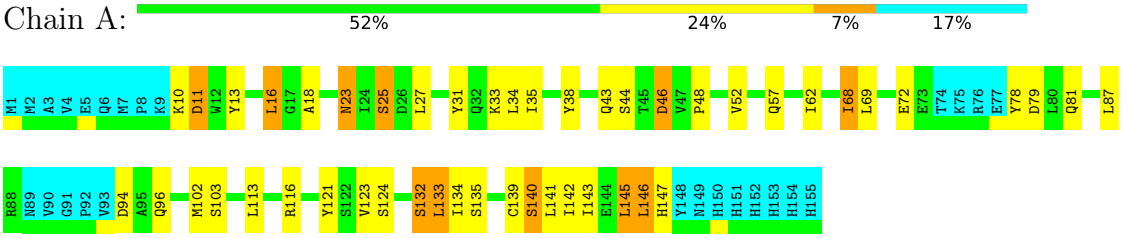
Chain A:



4.2.14 Score per residue for model 14 (medoid)

• Molecule 1: DnaJ homolog subfamily C member 24

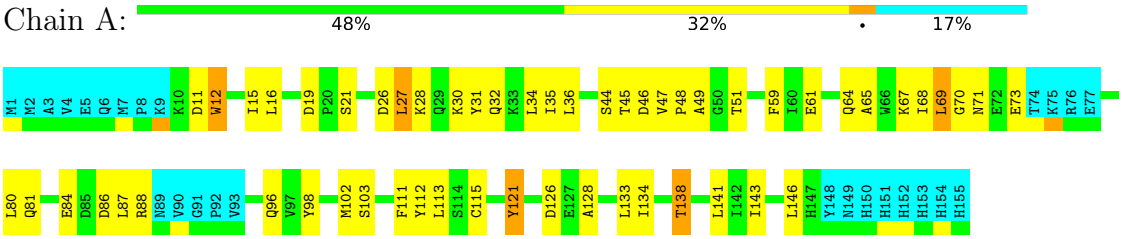
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: DnaJ homolog subfamily C member 24

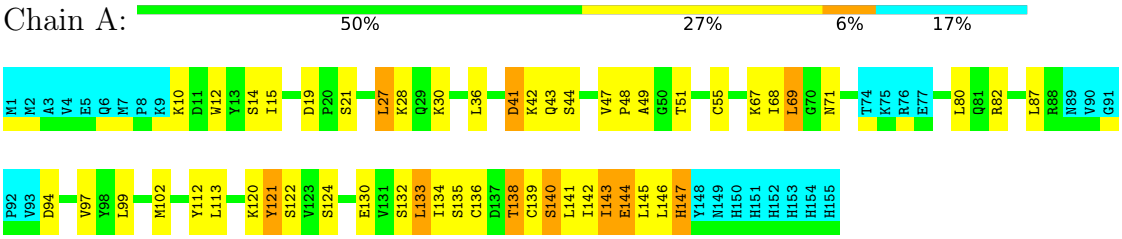
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: DnaJ homolog subfamily C member 24

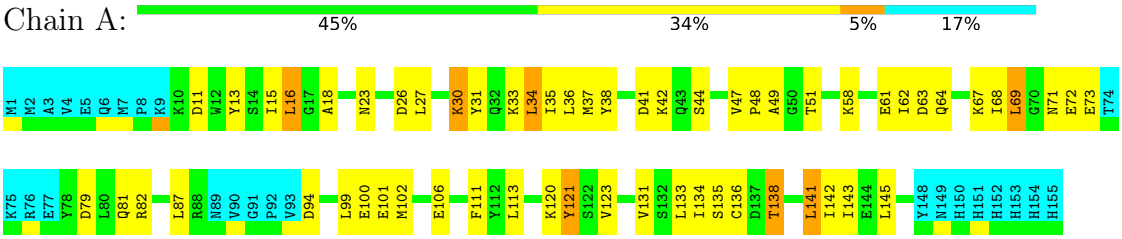
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: DnaJ homolog subfamily C member 24

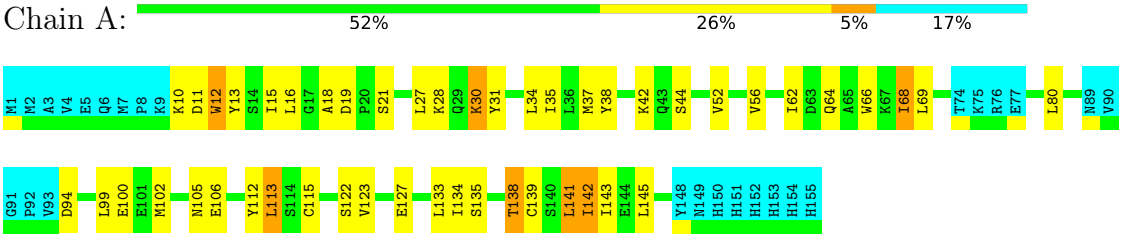
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: DnaJ homolog subfamily C member 24

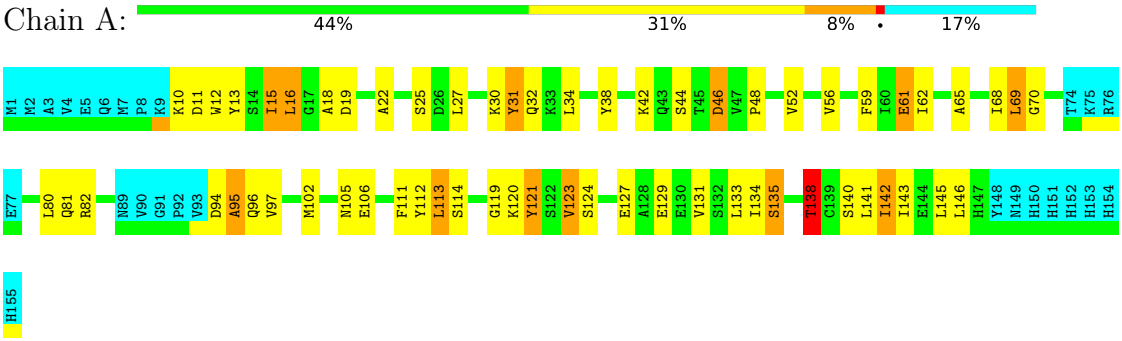
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: DnaJ homolog subfamily C member 24

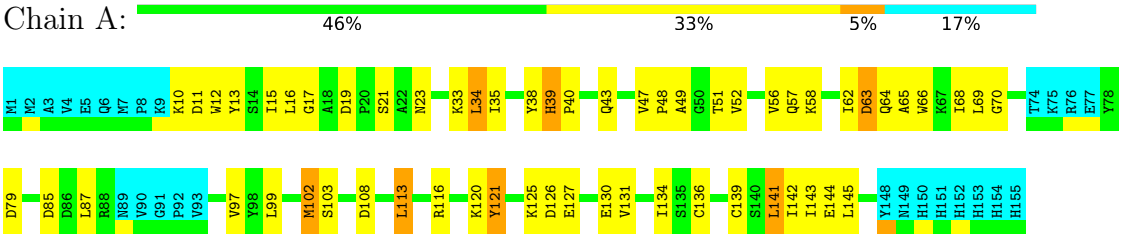
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: DnaJ homolog subfamily C member 24

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, torsion angle dynamics.*

Of the 100 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	structure solution	
CYANA	refinement	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1038	813	986	22±6
All	All	20780	16260	19715	437

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:35:ILE:HG21	1:A:62:ILE:HD12	0.95	1.36	17	1
1:A:35:ILE:HD12	1:A:62:ILE:HG23	0.95	1.34	18	1
1:A:35:ILE:HD12	1:A:62:ILE:HG22	0.93	1.40	3	3
1:A:133:LEU:HD11	1:A:142:ILE:HD13	0.82	1.51	11	2
1:A:18:ALA:HB2	1:A:27:LEU:HD21	0.81	1.52	4	1
1:A:18:ALA:HB2	1:A:27:LEU:HD11	0.81	1.50	14	3
1:A:16:LEU:HD22	1:A:69:LEU:HD21	0.77	1.55	17	2
1:A:131:VAL:HG23	1:A:145:LEU:HD11	0.75	1.58	5	1
1:A:69:LEU:C	1:A:69:LEU:HD22	0.74	2.03	15	1
1:A:133:LEU:HD12	1:A:142:ILE:HG22	0.74	1.59	14	1
1:A:123:VAL:HG11	1:A:145:LEU:HD22	0.73	1.60	14	1
1:A:133:LEU:HD12	1:A:142:ILE:CG2	0.72	2.15	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ALA:HB2	1:A:31:TYR:CE2	0.69	2.22	11	3
1:A:102:MET:HG2	1:A:113:LEU:HD23	0.69	1.65	1	2
1:A:69:LEU:HD13	1:A:70:GLY:N	0.68	2.02	15	1
1:A:39:HIS:CE1	1:A:62:ILE:HG21	0.68	2.23	12	1
1:A:102:MET:HG2	1:A:113:LEU:HD13	0.66	1.67	13	3
1:A:113:LEU:HD13	1:A:121:TYR:CZ	0.66	2.25	19	1
1:A:102:MET:CG	1:A:113:LEU:HD23	0.66	2.21	5	2
1:A:133:LEU:HD11	1:A:142:ILE:HD12	0.66	1.68	8	2
1:A:121:TYR:CB	1:A:134:ILE:HD11	0.66	2.21	9	7
1:A:128:ALA:HB1	1:A:145:LEU:HD11	0.66	1.67	3	2
1:A:31:TYR:O	1:A:35:ILE:HG22	0.66	1.91	8	3
1:A:47:VAL:HG23	1:A:51:THR:OG1	0.65	1.91	16	1
1:A:94:ASP:CG	1:A:141:LEU:HD13	0.65	2.12	19	8
1:A:18:ALA:CB	1:A:27:LEU:HD21	0.65	2.21	4	3
1:A:94:ASP:CB	1:A:141:LEU:HD13	0.64	2.23	17	1
1:A:133:LEU:HD21	1:A:142:ILE:HD13	0.64	1.69	6	2
1:A:94:ASP:OD1	1:A:141:LEU:HD12	0.63	1.92	2	1
1:A:16:LEU:HD12	1:A:69:LEU:HB2	0.63	1.70	12	1
1:A:94:ASP:HB2	1:A:141:LEU:HD13	0.63	1.69	17	1
1:A:18:ALA:CB	1:A:27:LEU:HD11	0.62	2.24	14	3
1:A:102:MET:HG3	1:A:113:LEU:HD23	0.62	1.71	4	2
1:A:35:ILE:HG23	1:A:62:ILE:HB	0.62	1.71	20	1
1:A:145:LEU:O	1:A:146:LEU:HD23	0.62	1.93	16	3
1:A:99:LEU:HD22	1:A:147:HIS:HA	0.62	1.70	12	2
1:A:113:LEU:HD13	1:A:121:TYR:CE2	0.62	2.30	19	1
1:A:27:LEU:HD11	1:A:69:LEU:HD22	0.62	1.70	12	1
1:A:121:TYR:CD1	1:A:134:ILE:HD13	0.61	2.30	19	1
1:A:102:MET:CG	1:A:113:LEU:HD13	0.61	2.24	13	2
1:A:113:LEU:HD11	1:A:123:VAL:HG22	0.61	1.71	18	1
1:A:123:VAL:HG11	1:A:145:LEU:CD2	0.61	2.26	14	1
1:A:35:ILE:CG1	1:A:62:ILE:HG23	0.61	2.25	12	1
1:A:94:ASP:CB	1:A:141:LEU:HD22	0.61	2.24	13	7
1:A:135:SER:OG	1:A:142:ILE:HD12	0.61	1.96	2	1
1:A:133:LEU:HD13	1:A:134:ILE:N	0.61	2.11	17	7
1:A:15:ILE:HG21	1:A:65:ALA:CB	0.61	2.26	20	1
1:A:18:ALA:HB1	1:A:27:LEU:HD21	0.60	1.70	7	2
1:A:57:GLN:HA	1:A:60:ILE:HD12	0.60	1.73	13	3
1:A:35:ILE:HG13	1:A:62:ILE:HG23	0.60	1.74	12	1
1:A:16:LEU:HD23	1:A:69:LEU:HD12	0.60	1.73	6	1
1:A:131:VAL:O	1:A:145:LEU:HD21	0.60	1.97	17	2
1:A:102:MET:HB2	1:A:113:LEU:HD22	0.60	1.74	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:ASP:CA	1:A:141:LEU:HD22	0.59	2.26	9	7
1:A:121:TYR:CG	1:A:134:ILE:HD11	0.59	2.32	15	4
1:A:24:ILE:CD1	1:A:69:LEU:HD21	0.59	2.28	11	1
1:A:16:LEU:HD11	1:A:35:ILE:HG23	0.59	1.75	13	1
1:A:16:LEU:HD11	1:A:31:TYR:CD2	0.59	2.32	10	1
1:A:60:ILE:HG22	1:A:64:GLN:OE1	0.58	1.98	11	2
1:A:69:LEU:HD22	1:A:69:LEU:O	0.58	1.98	15	1
1:A:135:SER:HB3	1:A:142:ILE:HD12	0.58	1.74	17	1
1:A:128:ALA:HB1	1:A:145:LEU:HD21	0.58	1.75	13	1
1:A:97:VAL:HG12	1:A:144:GLU:O	0.58	1.99	20	3
1:A:16:LEU:O	1:A:34:LEU:HD13	0.57	2.00	9	5
1:A:96:GLN:HB2	1:A:146:LEU:HD21	0.57	1.76	14	3
1:A:96:GLN:CG	1:A:146:LEU:HD11	0.57	2.30	15	3
1:A:94:ASP:HB2	1:A:141:LEU:HD22	0.57	1.77	19	4
1:A:35:ILE:HD11	1:A:62:ILE:CB	0.57	2.29	9	1
1:A:35:ILE:HG23	1:A:62:ILE:CG2	0.57	2.29	10	2
1:A:69:LEU:HD13	1:A:69:LEU:O	0.57	1.99	14	4
1:A:22:ALA:HB1	1:A:27:LEU:CD2	0.57	2.30	6	1
1:A:141:LEU:HD12	1:A:142:ILE:N	0.56	2.15	17	5
1:A:35:ILE:HD12	1:A:62:ILE:HB	0.56	1.75	14	2
1:A:15:ILE:HG23	1:A:16:LEU:HD22	0.56	1.77	13	1
1:A:133:LEU:HD13	1:A:143:ILE:O	0.56	2.00	14	1
1:A:27:LEU:HD21	1:A:69:LEU:HG	0.56	1.76	3	1
1:A:16:LEU:HD13	1:A:65:ALA:CB	0.56	2.31	15	2
1:A:102:MET:SD	1:A:113:LEU:HD11	0.55	2.41	16	2
1:A:145:LEU:C	1:A:146:LEU:HD23	0.55	2.21	4	3
1:A:16:LEU:CD2	1:A:69:LEU:HD12	0.55	2.30	6	1
1:A:94:ASP:OD2	1:A:141:LEU:HD13	0.55	2.00	18	1
1:A:102:MET:HA	1:A:113:LEU:HD13	0.55	1.77	10	1
1:A:134:ILE:HG23	1:A:143:ILE:HG13	0.55	1.78	5	5
1:A:16:LEU:HD13	1:A:27:LEU:HD11	0.55	1.77	18	1
1:A:27:LEU:HD23	1:A:69:LEU:CD2	0.55	2.31	19	1
1:A:27:LEU:HD12	1:A:31:TYR:CZ	0.55	2.35	15	1
1:A:13:TYR:CB	1:A:18:ALA:HB3	0.55	2.32	18	1
1:A:18:ALA:HB2	1:A:27:LEU:HD13	0.55	1.77	18	1
1:A:121:TYR:HB3	1:A:134:ILE:HD11	0.55	1.77	20	1
1:A:13:TYR:HB3	1:A:18:ALA:HB3	0.55	1.79	18	1
1:A:141:LEU:O	1:A:142:ILE:HD13	0.55	2.01	17	1
1:A:52:VAL:O	1:A:56:VAL:HG12	0.55	2.01	20	2
1:A:35:ILE:HD11	1:A:62:ILE:HA	0.54	1.79	9	1
1:A:87:LEU:HD23	1:A:133:LEU:HD12	0.54	1.80	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LYS:O	1:A:34:LEU:HD12	0.54	2.03	18	4
1:A:35:ILE:HD11	1:A:62:ILE:CA	0.54	2.33	9	1
1:A:102:MET:SD	1:A:113:LEU:HD21	0.54	2.43	12	1
1:A:113:LEU:HD12	1:A:121:TYR:CD1	0.54	2.38	7	1
1:A:27:LEU:HD12	1:A:31:TYR:CE1	0.54	2.37	15	1
1:A:16:LEU:HD11	1:A:31:TYR:HB2	0.54	1.78	19	1
1:A:96:GLN:HG3	1:A:146:LEU:HD11	0.53	1.80	15	3
1:A:132:SER:O	1:A:145:LEU:HD12	0.53	2.04	14	1
1:A:123:VAL:HG21	1:A:134:ILE:HD13	0.53	1.79	17	1
1:A:16:LEU:HD13	1:A:27:LEU:HD12	0.53	1.81	7	1
1:A:94:ASP:OD1	1:A:141:LEU:HD13	0.53	2.03	9	4
1:A:139:CYS:SG	1:A:141:LEU:HD23	0.53	2.44	18	1
1:A:94:ASP:CG	1:A:141:LEU:HD12	0.53	2.24	2	1
1:A:32:GLN:O	1:A:36:LEU:HD23	0.53	2.03	3	2
1:A:15:ILE:HG23	1:A:35:ILE:HD13	0.53	1.80	11	2
1:A:12:TRP:CB	1:A:69:LEU:HD12	0.53	2.34	16	1
1:A:113:LEU:HD12	1:A:113:LEU:N	0.52	2.19	19	1
1:A:15:ILE:HD11	1:A:61:GLU:HB3	0.52	1.80	17	4
1:A:102:MET:SD	1:A:113:LEU:HD23	0.52	2.44	20	2
1:A:135:SER:HA	1:A:142:ILE:HG22	0.52	1.81	12	3
1:A:15:ILE:HG22	1:A:16:LEU:HD12	0.52	1.81	15	2
1:A:133:LEU:HD21	1:A:142:ILE:CD1	0.52	2.35	11	2
1:A:35:ILE:HD12	1:A:62:ILE:CB	0.52	2.35	14	2
1:A:24:ILE:HD13	1:A:69:LEU:HD11	0.52	1.82	11	1
1:A:113:LEU:HD23	1:A:121:TYR:CD1	0.51	2.40	17	1
1:A:16:LEU:HD12	1:A:69:LEU:HD23	0.51	1.82	5	2
1:A:133:LEU:HD11	1:A:142:ILE:HG21	0.51	1.81	2	4
1:A:121:TYR:CE2	1:A:143:ILE:HD11	0.51	2.41	19	1
1:A:48:PRO:O	1:A:52:VAL:HG23	0.51	2.05	14	5
1:A:127:GLU:O	1:A:131:VAL:HG22	0.51	2.06	7	2
1:A:27:LEU:HD13	1:A:69:LEU:HB3	0.51	1.82	8	3
1:A:102:MET:HG2	1:A:113:LEU:HD22	0.51	1.83	17	1
1:A:56:VAL:HG12	1:A:60:ILE:HD11	0.51	1.80	13	1
1:A:16:LEU:HD21	1:A:31:TYR:CA	0.51	2.35	4	3
1:A:133:LEU:CD1	1:A:142:ILE:HD13	0.51	2.31	11	1
1:A:94:ASP:O	1:A:95:ALA:HB2	0.51	2.06	19	5
1:A:121:TYR:HB2	1:A:134:ILE:HD11	0.50	1.81	9	3
1:A:135:SER:CB	1:A:142:ILE:HD12	0.50	2.36	17	2
1:A:96:GLN:HB2	1:A:146:LEU:HD11	0.50	1.83	7	3
1:A:47:VAL:HG23	1:A:51:THR:HB	0.50	1.83	13	6
1:A:16:LEU:HD21	1:A:31:TYR:HB2	0.50	1.83	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:LEU:HD23	1:A:70:GLY:N	0.50	2.21	6	1
1:A:123:VAL:HG11	1:A:128:ALA:HB2	0.50	1.84	8	1
1:A:35:ILE:HD12	1:A:62:ILE:CG2	0.50	2.22	18	2
1:A:94:ASP:HA	1:A:141:LEU:HD22	0.50	1.83	9	2
1:A:27:LEU:HD13	1:A:69:LEU:CB	0.50	2.37	5	2
1:A:48:PRO:O	1:A:49:ALA:HB3	0.50	2.06	16	10
1:A:133:LEU:HD12	1:A:134:ILE:N	0.50	2.22	18	1
1:A:16:LEU:HD13	1:A:27:LEU:CD1	0.49	2.36	18	1
1:A:12:TRP:CE2	1:A:68:ILE:HD12	0.49	2.43	15	2
1:A:13:TYR:O	1:A:17:GLY:HA2	0.49	2.08	20	1
1:A:69:LEU:HD22	1:A:73:GLU:HG2	0.49	1.84	9	1
1:A:64:GLN:O	1:A:68:ILE:HG22	0.49	2.07	13	1
1:A:16:LEU:HD22	1:A:69:LEU:HD12	0.49	1.83	9	1
1:A:99:LEU:HD12	1:A:147:HIS:CG	0.49	2.43	16	1
1:A:123:VAL:CG1	1:A:134:ILE:HD12	0.49	2.38	19	1
1:A:99:LEU:HD11	1:A:111:PHE:CD1	0.48	2.43	17	1
1:A:15:ILE:CG2	1:A:35:ILE:HD13	0.48	2.39	15	2
1:A:23:ASN:O	1:A:27:LEU:HD23	0.48	2.08	14	2
1:A:27:LEU:CD2	1:A:69:LEU:HD13	0.48	2.37	11	1
1:A:27:LEU:HD23	1:A:28:LYS:N	0.48	2.24	11	1
1:A:99:LEU:HD22	1:A:145:LEU:HD23	0.48	1.86	16	1
1:A:52:VAL:O	1:A:56:VAL:HG23	0.48	2.09	19	2
1:A:68:ILE:O	1:A:68:ILE:HG23	0.47	2.09	17	3
1:A:135:SER:CA	1:A:142:ILE:HG23	0.47	2.39	14	1
1:A:113:LEU:HD23	1:A:143:ILE:CD1	0.47	2.40	3	1
1:A:128:ALA:CB	1:A:145:LEU:HD11	0.47	2.39	3	1
1:A:35:ILE:HG23	1:A:62:ILE:HG22	0.47	1.86	10	1
1:A:113:LEU:HD23	1:A:121:TYR:CE1	0.47	2.44	17	1
1:A:16:LEU:HD21	1:A:31:TYR:HA	0.47	1.87	14	3
1:A:99:LEU:HD12	1:A:111:PHE:CD2	0.47	2.44	9	1
1:A:18:ALA:O	1:A:69:LEU:HD11	0.47	2.08	2	1
1:A:135:SER:N	1:A:142:ILE:HG23	0.47	2.23	14	1
1:A:22:ALA:HB1	1:A:27:LEU:HD21	0.47	1.84	6	1
1:A:35:ILE:HG23	1:A:62:ILE:HG21	0.46	1.87	18	2
1:A:27:LEU:CD1	1:A:69:LEU:HD22	0.46	2.39	12	1
1:A:135:SER:CA	1:A:142:ILE:HG22	0.46	2.40	12	3
1:A:16:LEU:HD12	1:A:65:ALA:HB1	0.46	1.86	8	1
1:A:133:LEU:HD11	1:A:142:ILE:HG13	0.46	1.85	10	1
1:A:16:LEU:HD23	1:A:27:LEU:HD21	0.46	1.88	11	1
1:A:34:LEU:HD23	1:A:35:ILE:N	0.46	2.25	15	1
1:A:99:LEU:HD21	1:A:145:LEU:HG	0.46	1.88	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:TRP:CG	1:A:69:LEU:HD12	0.46	2.46	16	1
1:A:16:LEU:HD11	1:A:35:ILE:HG12	0.46	1.86	20	1
1:A:141:LEU:C	1:A:142:ILE:HD13	0.46	2.31	17	1
1:A:99:LEU:HD12	1:A:111:PHE:CE2	0.46	2.46	4	1
1:A:102:MET:SD	1:A:113:LEU:HD22	0.46	2.50	7	1
1:A:97:VAL:HG11	1:A:113:LEU:CD2	0.46	2.41	20	1
1:A:18:ALA:CB	1:A:69:LEU:HD21	0.46	2.41	6	1
1:A:12:TRP:CD1	1:A:69:LEU:C	0.46	2.89	18	2
1:A:68:ILE:HD11	1:A:78:TYR:CG	0.45	2.45	5	1
1:A:47:VAL:O	1:A:47:VAL:HG13	0.45	2.11	7	1
1:A:16:LEU:HG	1:A:34:LEU:HD13	0.45	1.88	6	1
1:A:18:ALA:HB2	1:A:31:TYR:HE2	0.45	1.71	12	1
1:A:27:LEU:HD13	1:A:31:TYR:CD2	0.45	2.46	12	1
1:A:134:ILE:HG22	1:A:143:ILE:HG13	0.45	1.87	18	1
1:A:39:HIS:CB	1:A:40:PRO:CD	0.45	2.94	20	1
1:A:16:LEU:HD13	1:A:65:ALA:HB1	0.45	1.88	11	2
1:A:27:LEU:HD23	1:A:69:LEU:HD22	0.45	1.87	19	1
1:A:133:LEU:HD22	1:A:143:ILE:O	0.45	2.12	19	1
1:A:119:GLY:N	1:A:138:THR:HG21	0.45	2.27	19	1
1:A:131:VAL:HG23	1:A:145:LEU:CD1	0.45	2.38	5	1
1:A:16:LEU:HD21	1:A:31:TYR:CB	0.45	2.41	4	1
1:A:65:ALA:HB1	1:A:69:LEU:HD23	0.45	1.89	2	1
1:A:128:ALA:HB1	1:A:145:LEU:CD2	0.45	2.41	13	1
1:A:111:PHE:CZ	1:A:128:ALA:HB2	0.45	2.47	15	1
1:A:135:SER:HA	1:A:142:ILE:HG23	0.45	1.89	9	2
1:A:123:VAL:CG1	1:A:128:ALA:HB2	0.44	2.42	8	1
1:A:69:LEU:HD13	1:A:70:GLY:H	0.44	1.72	15	1
1:A:18:ALA:HB2	1:A:27:LEU:CD1	0.44	2.42	6	1
1:A:35:ILE:CD1	1:A:62:ILE:HG23	0.44	2.42	8	1
1:A:12:TRP:HA	1:A:65:ALA:HB2	0.44	1.88	8	1
1:A:16:LEU:HD13	1:A:27:LEU:CG	0.44	2.43	18	1
1:A:22:ALA:HB1	1:A:27:LEU:CD1	0.44	2.43	19	1
1:A:65:ALA:O	1:A:69:LEU:HD13	0.44	2.13	4	1
1:A:123:VAL:HG22	1:A:134:ILE:HD12	0.44	1.89	8	1
1:A:35:ILE:HD11	1:A:62:ILE:CD1	0.44	2.43	12	1
1:A:121:TYR:CE1	1:A:134:ILE:HG21	0.43	2.48	19	1
1:A:69:LEU:C	1:A:69:LEU:HD13	0.43	2.34	7	2
1:A:15:ILE:HG21	1:A:65:ALA:HB2	0.43	1.89	20	1
1:A:68:ILE:HG22	1:A:68:ILE:O	0.43	2.14	4	1
1:A:102:MET:HE3	1:A:145:LEU:HD12	0.43	1.91	4	1
1:A:133:LEU:HD11	1:A:142:ILE:CD1	0.43	2.35	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:LEU:HD23	1:A:145:LEU:O	0.43	2.13	11	1
1:A:133:LEU:HD13	1:A:143:ILE:C	0.43	2.34	14	1
1:A:15:ILE:O	1:A:34:LEU:HD22	0.43	2.13	20	1
1:A:134:ILE:O	1:A:134:ILE:HG23	0.43	2.14	14	1
1:A:16:LEU:HD23	1:A:65:ALA:CB	0.43	2.44	19	1
1:A:16:LEU:CD1	1:A:65:ALA:HB1	0.43	2.44	8	1
1:A:69:LEU:HD12	1:A:71:ASN:ND2	0.43	2.29	10	1
1:A:61:GLU:CD	1:A:62:ILE:HG23	0.42	2.34	9	1
1:A:39:HIS:N	1:A:40:PRO:HD2	0.42	2.28	20	1
1:A:65:ALA:HB1	1:A:69:LEU:CD2	0.42	2.44	2	1
1:A:132:SER:O	1:A:145:LEU:HD22	0.42	2.15	4	1
1:A:141:LEU:HD12	1:A:142:ILE:H	0.42	1.74	7	2
1:A:113:LEU:HD13	1:A:114:SER:H	0.42	1.75	1	1
1:A:15:ILE:HG21	1:A:65:ALA:HB3	0.42	1.90	20	1
1:A:133:LEU:CD2	1:A:142:ILE:HD13	0.42	2.43	6	1
1:A:99:LEU:CD2	1:A:145:LEU:HD23	0.42	2.44	16	1
1:A:16:LEU:HD12	1:A:69:LEU:CD2	0.42	2.45	18	1
1:A:133:LEU:HD11	1:A:142:ILE:CG2	0.42	2.45	5	1
1:A:128:ALA:HB1	1:A:145:LEU:CD1	0.42	2.44	11	1
1:A:47:VAL:HG13	1:A:51:THR:HB	0.42	1.90	7	1
1:A:97:VAL:HG11	1:A:113:LEU:HD22	0.42	1.92	19	1
1:A:113:LEU:HD13	1:A:114:SER:N	0.41	2.30	4	1
1:A:36:LEU:HD13	1:A:36:LEU:C	0.41	2.36	9	1
1:A:27:LEU:HD11	1:A:69:LEU:CD2	0.41	2.44	12	1
1:A:39:HIS:NE2	1:A:62:ILE:HD13	0.41	2.31	10	1
1:A:27:LEU:HD12	1:A:27:LEU:C	0.41	2.36	16	1
1:A:69:LEU:HD13	1:A:69:LEU:C	0.41	2.36	14	1
1:A:65:ALA:O	1:A:66:TRP:C	0.41	2.58	20	1
1:A:27:LEU:HD22	1:A:69:LEU:HD13	0.41	1.92	11	1
1:A:68:ILE:HD11	1:A:72:GLU:HA	0.41	1.91	17	1
1:A:16:LEU:HD23	1:A:27:LEU:HD23	0.41	1.92	10	1
1:A:133:LEU:C	1:A:133:LEU:HD13	0.41	2.36	2	1
1:A:96:GLN:CB	1:A:146:LEU:HD11	0.41	2.45	15	1
1:A:123:VAL:HG21	1:A:145:LEU:CD2	0.41	2.45	18	1
1:A:18:ALA:HB2	1:A:69:LEU:HD11	0.41	1.93	6	1
1:A:16:LEU:HB3	1:A:27:LEU:HD11	0.41	1.93	18	1
1:A:123:VAL:HG21	1:A:145:LEU:HD21	0.40	1.92	18	1
1:A:47:VAL:HG12	1:A:51:THR:N	0.40	2.31	1	1
1:A:113:LEU:HD21	1:A:145:LEU:CD1	0.40	2.46	6	1
1:A:12:TRP:CD1	1:A:68:ILE:HD11	0.40	2.50	12	1
1:A:133:LEU:HD13	1:A:133:LEU:C	0.40	2.36	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:ILE:HD13	1:A:69:LEU:HD21	0.40	1.92	11	1
1:A:135:SER:CB	1:A:142:ILE:HG22	0.40	2.46	16	1
1:A:134:ILE:HG22	1:A:143:ILE:CG1	0.40	2.46	18	1
1:A:62:ILE:HD12	1:A:63:ASP:N	0.40	2.31	20	1
1:A:35:ILE:HG12	1:A:62:ILE:HG22	0.40	1.93	5	1
1:A:27:LEU:HG	1:A:69:LEU:HD22	0.40	1.92	1	1
1:A:95:ALA:O	1:A:143:ILE:HG22	0.40	2.17	1	1
1:A:121:TYR:CD2	1:A:134:ILE:HD11	0.40	2.52	14	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	129/155 (83%)	106±2 (82±2%)	20±3 (15±2%)	4±2 (3±1%)	8	42
All	All	2580/3100 (83%)	2115 (82%)	392 (15%)	73 (3%)	8	42

All 19 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	138	THR	15
1	A	68	ILE	9
1	A	71	ASN	8
1	A	46	ASP	7
1	A	132	SER	4
1	A	140	SER	4
1	A	22	ALA	3
1	A	25	SER	3
1	A	41	ASP	3
1	A	11	ASP	3
1	A	43	GLN	2
1	A	44	SER	2
1	A	42	LYS	2
1	A	12	TRP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	70	GLY	2
1	A	136	CYS	1
1	A	141	LEU	1
1	A	66	TRP	1
1	A	95	ALA	1

6.3.2 Protein sidechains (i)

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	117/141 (83%)	84±4 (72±3%)	33±4 (28±3%)	2 19
All	All	2340/2820 (83%)	1675 (72%)	665 (28%)	2 19

All 99 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	38	TYR	15
1	A	143	ILE	15
1	A	19	ASP	14
1	A	138	THR	14
1	A	81	GLN	13
1	A	133	LEU	13
1	A	64	GLN	13
1	A	82	ARG	12
1	A	87	LEU	12
1	A	122	SER	12
1	A	120	LYS	12
1	A	124	SER	12
1	A	42	LYS	12
1	A	10	LYS	11
1	A	80	LEU	11
1	A	103	SER	11
1	A	121	TYR	11
1	A	26	ASP	11
1	A	46	ASP	11
1	A	112	TYR	11

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Mol	Chain	Res	Type	Models (Total)
1	A	69	LEU	10
1	A	115	CYS	10
1	A	145	LEU	10
1	A	30	LYS	10
1	A	116	ARG	10
1	A	43	GLN	9
1	A	58	LYS	9
1	A	113	LEU	9
1	A	21	SER	9
1	A	28	LYS	9
1	A	140	SER	9
1	A	44	SER	8
1	A	59	PHE	8
1	A	100	GLU	8
1	A	114	SER	8
1	A	11	ASP	8
1	A	73	GLU	8
1	A	99	LEU	7
1	A	108	ASP	7
1	A	33	LYS	7
1	A	34	LEU	7
1	A	88	ARG	7
1	A	13	TYR	7
1	A	41	ASP	7
1	A	136	CYS	7
1	A	139	CYS	7
1	A	71	ASN	6
1	A	16	LEU	6
1	A	32	GLN	6
1	A	36	LEU	6
1	A	84	GLU	6
1	A	141	LEU	6
1	A	27	LEU	6
1	A	106	GLU	6
1	A	67	LYS	6
1	A	15	ILE	5
1	A	55	CYS	5
1	A	63	ASP	5
1	A	105	ASN	5
1	A	129	GLU	5
1	A	23	ASN	5
1	A	130	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	37	MET	5
1	A	126	ASP	5
1	A	85	ASP	5
1	A	25	SER	5
1	A	61	GLU	5
1	A	132	SER	4
1	A	144	GLU	4
1	A	31	TYR	4
1	A	53	GLU	4
1	A	57	GLN	4
1	A	14	SER	4
1	A	98	TYR	4
1	A	147	HIS	4
1	A	39	HIS	4
1	A	101	GLU	4
1	A	127	GLU	4
1	A	79	ASP	4
1	A	72	GLU	3
1	A	78	TYR	3
1	A	54	GLU	3
1	A	96	GLN	3
1	A	102	MET	3
1	A	135	SER	3
1	A	142	ILE	3
1	A	146	LEU	3
1	A	94	ASP	2
1	A	29	GLN	2
1	A	110	SER	2
1	A	12	TRP	2
1	A	111	PHE	2
1	A	68	ILE	2
1	A	66	TRP	1
1	A	35	ILE	1
1	A	45	THR	1
1	A	62	ILE	1
1	A	123	VAL	1
1	A	125	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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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)

No chemical shift data were provided