



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 01:16 PM UTC

PDB ID : 8B7J / pdb_00008b7j
BMRB ID : 34759
Title : Human HSP90 alpha ATP Binding Domain, ATP-lid closed conformation, R46A
Authors : Rioual, E.; Henot, F.; Favier, A.; Macek, P.; Crublet, E.; Josso, P.; Brustcher, B.; Frech, M.; Gans, P.; Loison, C.; Boisbouvier, J.
Deposited on : 2022-09-30

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

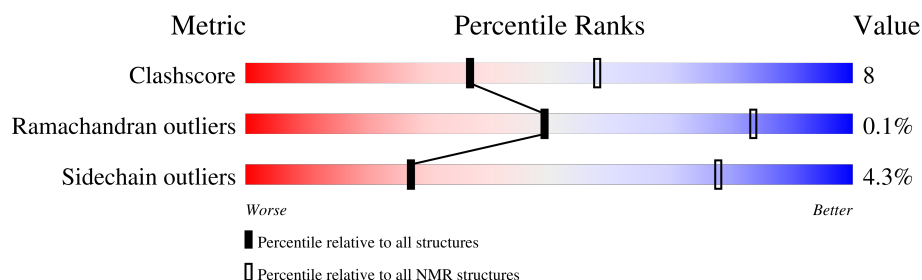
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 42%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	266	

2 Ensemble composition and analysis

This entry contains 20 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:16-A:100, A:137-A:223 (172)	0.38	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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3349 atoms, of which 1671 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HSP90AA1 protein.

Mol	Chain	Residues	Atoms						Trace
1	A	213	Total	C	H	N	O	S	0
			3349	1064	1671	274	334	6	

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	MET	-	initiating methionine	UNP Q2VPJ6
A	-28	GLY	-	expression tag	UNP Q2VPJ6
A	-27	SER	-	expression tag	UNP Q2VPJ6
A	-26	SER	-	expression tag	UNP Q2VPJ6
A	-25	HIS	-	expression tag	UNP Q2VPJ6
A	-24	HIS	-	expression tag	UNP Q2VPJ6
A	-23	HIS	-	expression tag	UNP Q2VPJ6
A	-22	HIS	-	expression tag	UNP Q2VPJ6
A	-21	HIS	-	expression tag	UNP Q2VPJ6
A	-20	HIS	-	expression tag	UNP Q2VPJ6
A	-19	SER	-	expression tag	UNP Q2VPJ6
A	-18	SER	-	expression tag	UNP Q2VPJ6
A	-17	GLY	-	expression tag	UNP Q2VPJ6
A	-16	LEU	-	expression tag	UNP Q2VPJ6
A	-15	VAL	-	expression tag	UNP Q2VPJ6
A	-14	PRO	-	expression tag	UNP Q2VPJ6
A	-13	ARG	-	expression tag	UNP Q2VPJ6
A	-12	GLY	-	expression tag	UNP Q2VPJ6
A	-11	SER	-	expression tag	UNP Q2VPJ6
A	-10	HIS	-	expression tag	UNP Q2VPJ6
A	-9	ASN	-	expression tag	UNP Q2VPJ6
A	-8	GLN	-	expression tag	UNP Q2VPJ6
A	-7	THR	-	expression tag	UNP Q2VPJ6
A	-6	SER	-	expression tag	UNP Q2VPJ6
A	-5	LEU	-	expression tag	UNP Q2VPJ6
A	-4	TYR	-	expression tag	UNP Q2VPJ6
A	-3	LYS	-	expression tag	UNP Q2VPJ6
A	-2	LYS	-	expression tag	UNP Q2VPJ6
A	-1	ALA	-	expression tag	UNP Q2VPJ6
A	0	GLY	-	expression tag	UNP Q2VPJ6
A	1	PHE	-	expression tag	UNP Q2VPJ6

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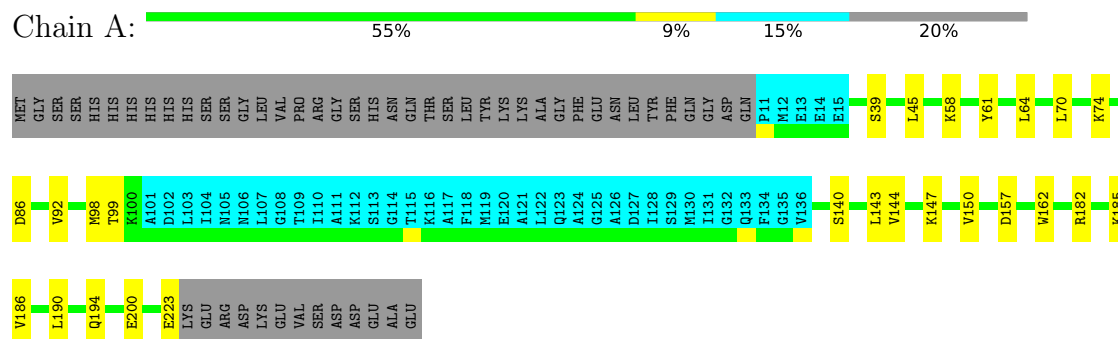
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	-	expression tag	UNP Q2VPJ6
A	3	ASN	-	expression tag	UNP Q2VPJ6
A	4	LEU	-	expression tag	UNP Q2VPJ6
A	5	TYR	-	expression tag	UNP Q2VPJ6
A	6	PHE	-	expression tag	UNP Q2VPJ6
A	7	GLN	-	expression tag	UNP Q2VPJ6
A	8	GLY	-	expression tag	UNP Q2VPJ6
A	63	THR	SER	conflict	UNP Q2VPJ6

4 Residue-property plots [i](#)

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: HSP90AA1 protein

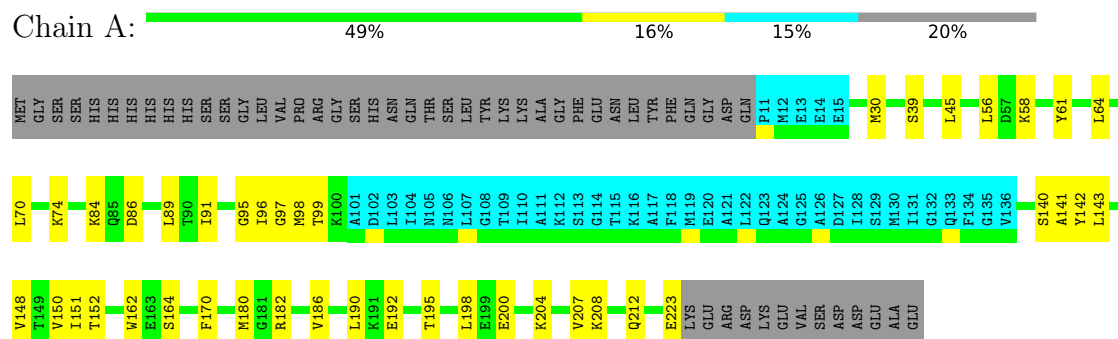


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

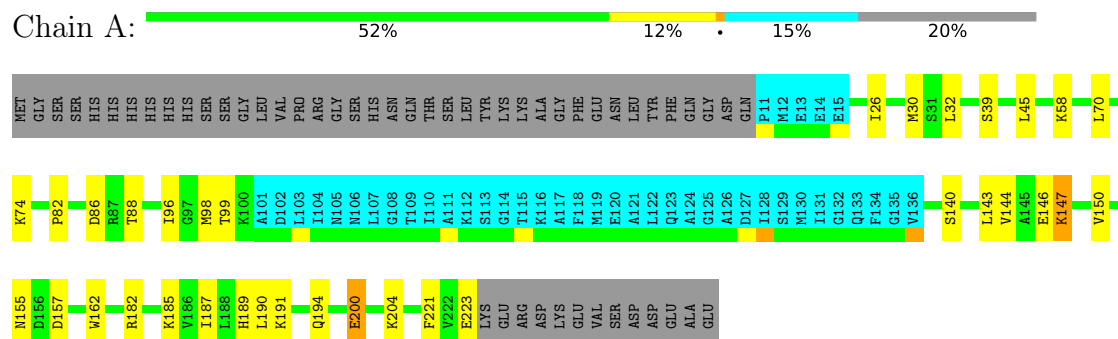
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: HSP90AA1 protein



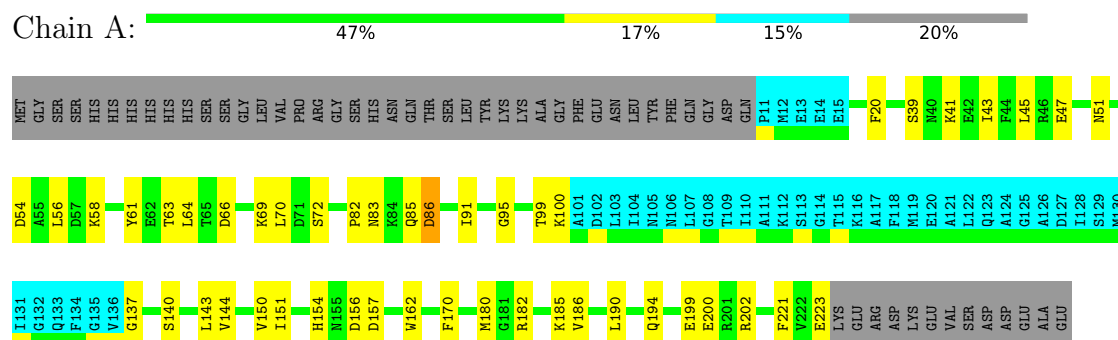
4.2.2 Score per residue for model 2

- Molecule 1: HSP90AA1 protein



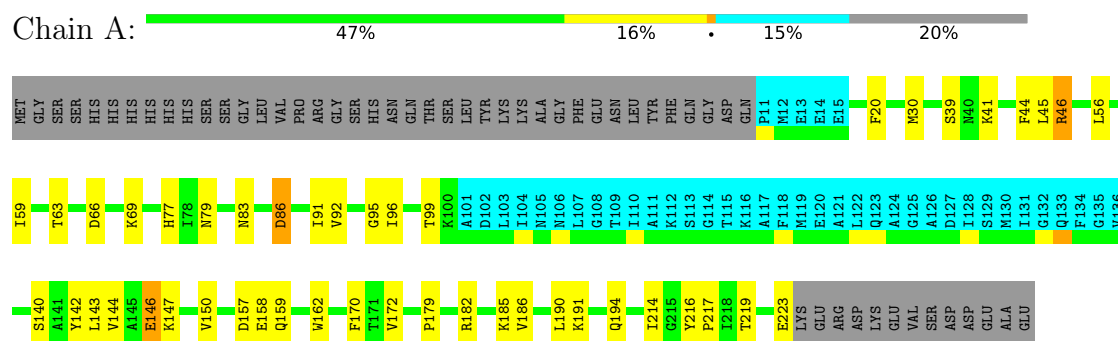
4.2.3 Score per residue for model 3

- Molecule 1: HSP90AA1 protein



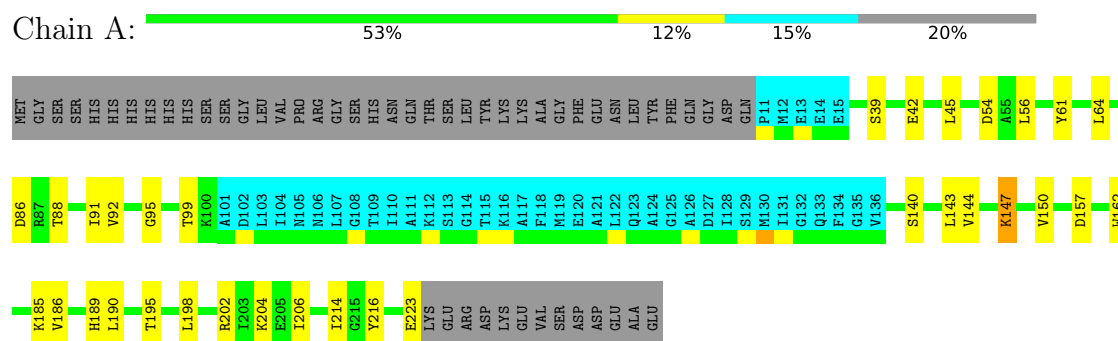
4.2.4 Score per residue for model 4

- Molecule 1: HSP90AA1 protein



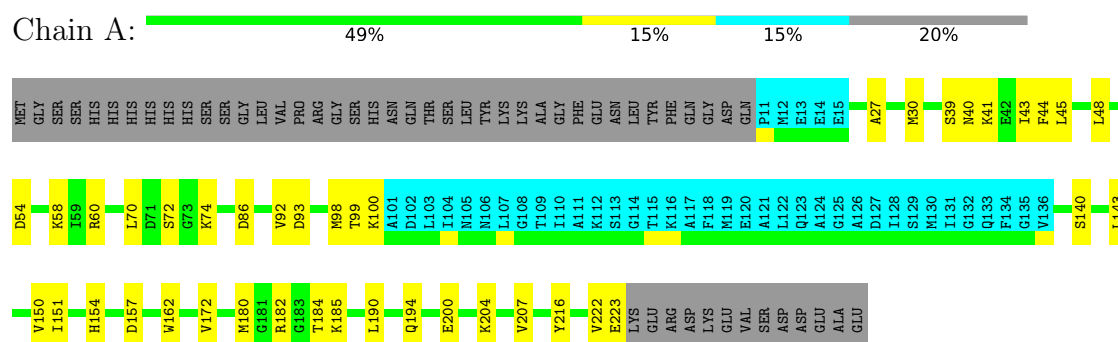
4.2.5 Score per residue for model 5

- Molecule 1: HSP90AA1 protein



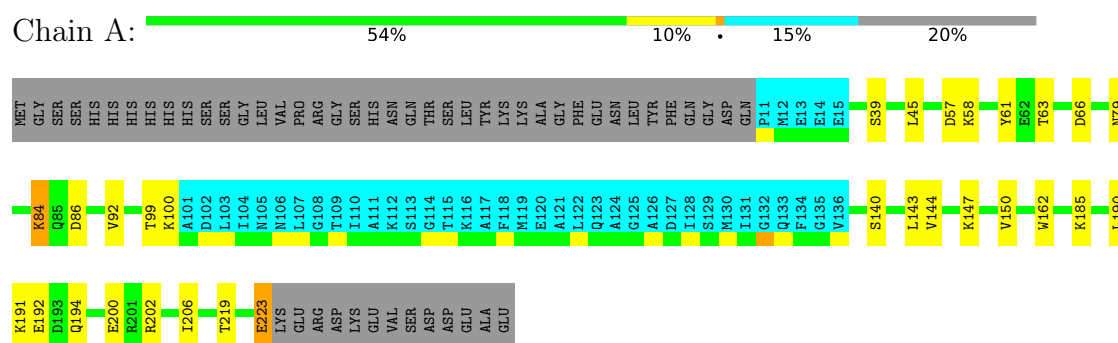
4.2.6 Score per residue for model 6

- Molecule 1: HSP90AA1 protein



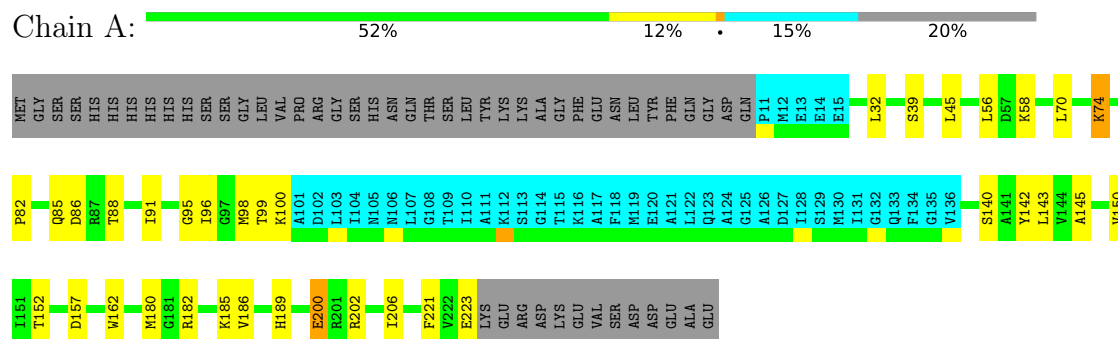
4.2.7 Score per residue for model 7

- Molecule 1: HSP90AA1 protein



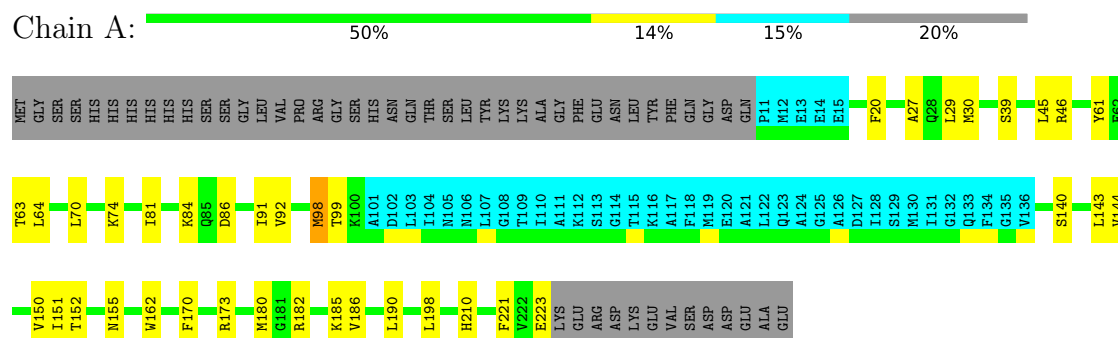
4.2.8 Score per residue for model 8

- Molecule 1: HSP90AA1 protein



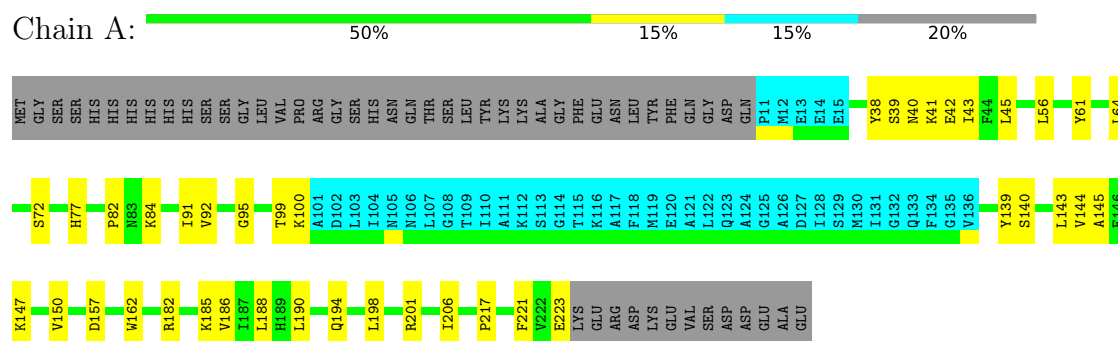
4.2.9 Score per residue for model 9

- Molecule 1: HSP90AA1 protein



4.2.10 Score per residue for model 10

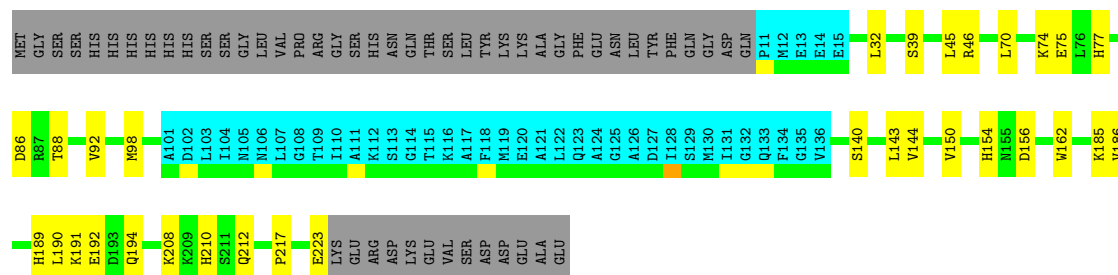
- Molecule 1: HSP90AA1 protein



4.2.11 Score per residue for model 11

- Molecule 1: HSP90AA1 protein

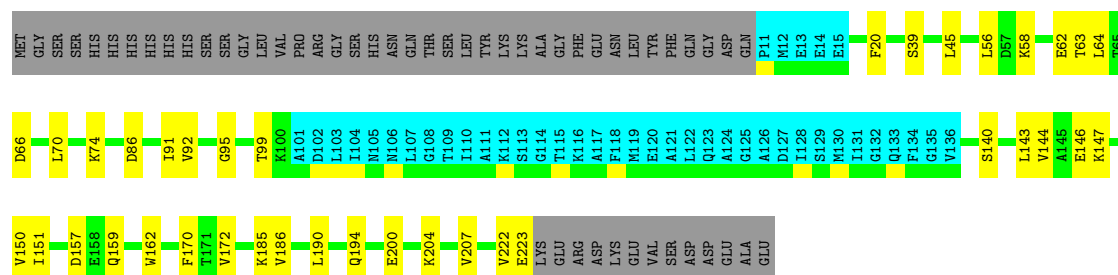
Chain A: 53% 12% 15% 20%



4.2.12 Score per residue for model 12

- Molecule 1: HSP90AA1 protein

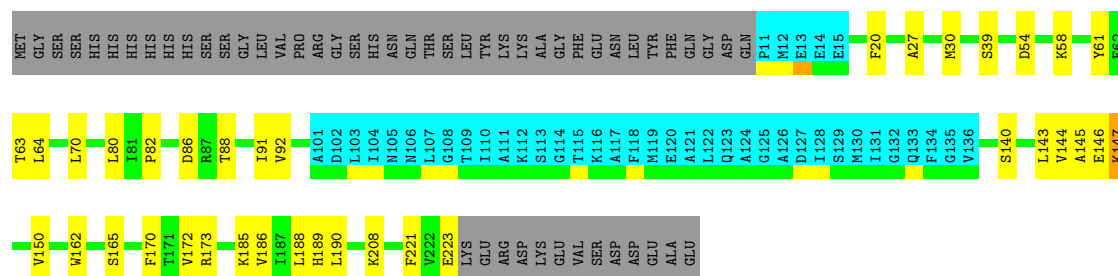
Chain A:



4.2.13 Score per residue for model 13

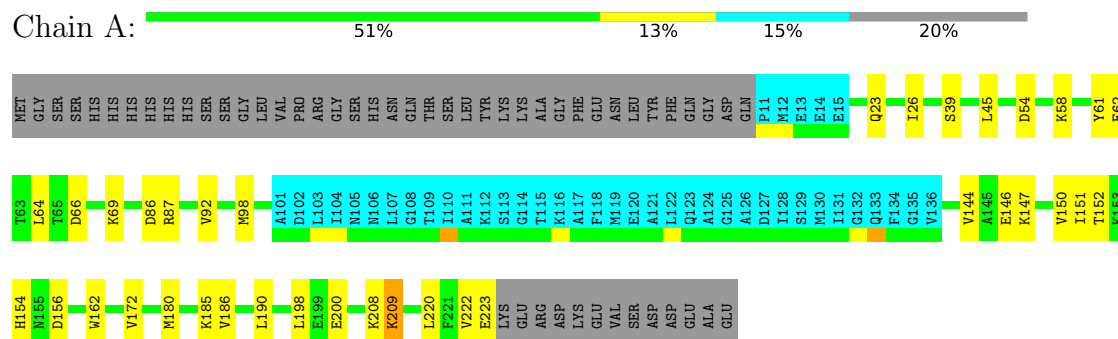
- Molecule 1: HSP90AA1 protein

Chain A: 51% 13% 15% 20%



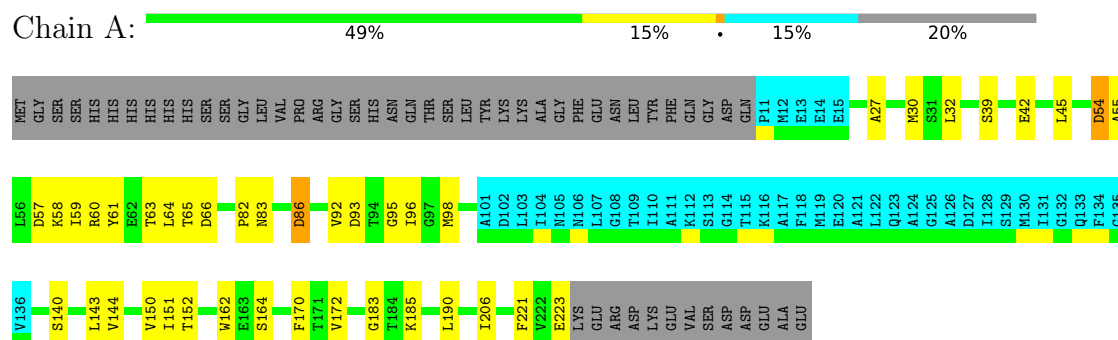
4.2.14 Score per residue for model 14

- Molecule 1: HSP90AA1 protein



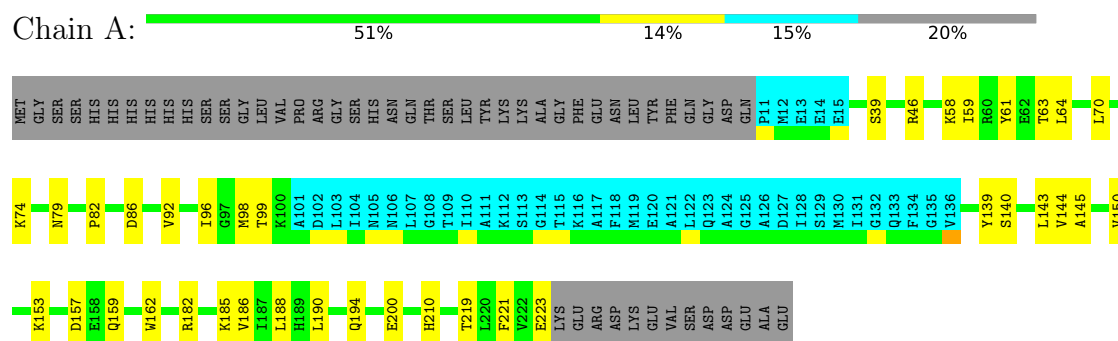
4.2.15 Score per residue for model 15

- Molecule 1: HSP90AA1 protein



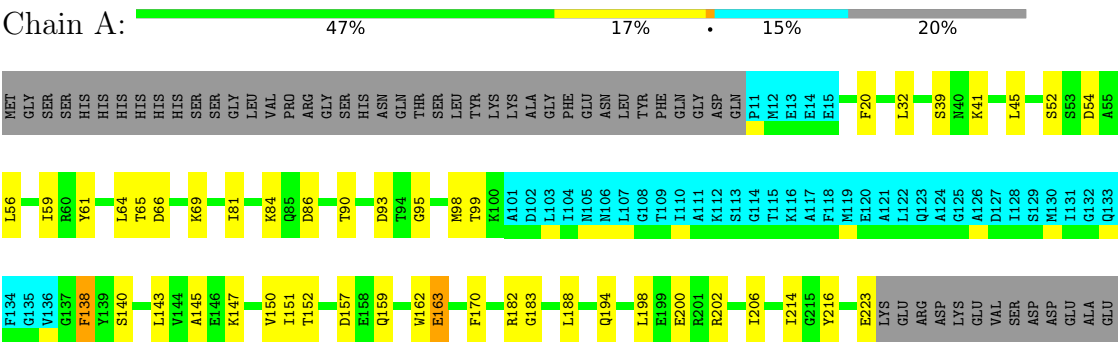
4.2.16 Score per residue for model 16

- Molecule 1: HSP90AA1 protein



4.2.20 Score per residue for model 20

● Molecule 1: HSP90AA1 protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 1000 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
CNS	refinement	
CYANA	structure calculation	3.98.13

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	1217
Number of shifts mapped to atoms	1193
Number of unparsed shifts	0
Number of shifts with mapping errors	24
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	42%

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	1382	1378	1378	21±5
All	All	27640	27560	27560	421

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:LYS:HE3	1:A:96:ILE:HG21	0.82	1.52	18	1
1:A:96:ILE:HA	1:A:182:ARG:HH21	0.80	1.35	17	3
1:A:140:SER:HA	1:A:143:LEU:HD23	0.73	1.58	10	10
1:A:98:MET:HB2	1:A:152:THR:HG21	0.71	1.59	14	6
1:A:27:ALA:HA	1:A:30:MET:HE2	0.69	1.64	6	5
1:A:151:ILE:HG22	1:A:159:GLN:HE21	0.69	1.48	19	3
1:A:140:SER:HA	1:A:143:LEU:HD13	0.68	1.64	8	8
1:A:70:LEU:HB3	1:A:74:LYS:HG2	0.67	1.66	11	7
1:A:99:THR:HG22	1:A:157:ASP:HB2	0.67	1.64	12	8
1:A:84:LYS:HA	1:A:198:LEU:HD23	0.67	1.66	1	1
1:A:61:TYR:HA	1:A:64:LEU:HD23	0.65	1.67	10	2
1:A:150:VAL:HG12	1:A:186:VAL:HG12	0.64	1.70	19	13
1:A:77:HIS:HB3	1:A:217:PRO:HG2	0.64	1.68	10	4
1:A:70:LEU:HD22	1:A:74:LYS:HA	0.63	1.71	8	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:THR:HG22	1:A:189:HIS:HA	0.62	1.70	19	7
1:A:96:ILE:HA	1:A:182:ARG:NH2	0.62	2.08	17	1
1:A:72:SER:HB2	1:A:182:ARG:HB2	0.62	1.72	19	5
1:A:154:HIS:HD2	1:A:156:ASP:H	0.62	1.37	14	3
1:A:204:LYS:HE2	1:A:204:LYS:HA	0.62	1.72	5	1
1:A:84:LYS:HA	1:A:198:LEU:HD13	0.62	1.70	17	6
1:A:92:VAL:HG12	1:A:185:LYS:HG3	0.61	1.71	4	14
1:A:40:ASN:HD22	1:A:43:ILE:HG23	0.60	1.55	6	1
1:A:41:LYS:HD3	1:A:194:GLN:HE22	0.60	1.57	18	3
1:A:38:TYR:HB2	1:A:41:LYS:HG2	0.59	1.73	17	1
1:A:66:ASP:HB3	1:A:69:LYS:HE2	0.58	1.74	4	2
1:A:144:VAL:HG22	1:A:190:LEU:HD12	0.58	1.76	15	1
1:A:61:TYR:O	1:A:64:LEU:HG	0.57	1.99	3	10
1:A:200:GLU:HB3	1:A:222:VAL:HG21	0.57	1.75	12	4
1:A:163:GLU:HB3	1:A:173:ARG:HH22	0.57	1.60	18	1
1:A:42:GLU:HB2	1:A:206:ILE:HD12	0.56	1.75	10	3
1:A:54:ASP:O	1:A:58:LYS:HG3	0.56	2.01	14	4
1:A:209:LYS:HE3	1:A:209:LYS:HA	0.56	1.78	14	1
1:A:80:LEU:HG	1:A:91:ILE:HD12	0.55	1.77	13	1
1:A:28:GLN:HA	1:A:28:GLN:OE1	0.55	2.02	19	1
1:A:144:VAL:HG22	1:A:190:LEU:HD22	0.54	1.79	2	13
1:A:58:LYS:HD2	1:A:96:ILE:HG21	0.54	1.79	17	4
1:A:23:GLN:HB3	1:A:26:ILE:HD13	0.54	1.79	14	1
1:A:96:ILE:HG13	1:A:182:ARG:HH21	0.53	1.63	16	1
1:A:150:VAL:HG22	1:A:162:TRP:HB3	0.53	1.81	13	7
1:A:180:MET:SD	1:A:185:LYS:HB2	0.53	2.43	18	3
1:A:59:ILE:HB	1:A:96:ILE:HB	0.52	1.80	15	2
1:A:144:VAL:HG23	1:A:194:GLN:HB3	0.52	1.82	3	5
1:A:99:THR:HG23	1:A:157:ASP:HB2	0.52	1.81	4	3
1:A:58:LYS:HB3	1:A:96:ILE:HD12	0.52	1.82	17	5
1:A:91:ILE:HB	1:A:186:VAL:CG2	0.52	2.35	1	9
1:A:82:PRO:HD2	1:A:221:PHE:O	0.52	2.05	16	9
1:A:150:VAL:CG2	1:A:162:TRP:HB3	0.51	2.34	1	19
1:A:195:THR:HA	1:A:198:LEU:HD13	0.51	1.82	1	1
1:A:185:LYS:HE2	1:A:187:ILE:HD11	0.51	1.83	18	2
1:A:84:LYS:HD3	1:A:223:GLU:OE1	0.51	2.05	7	1
1:A:140:SER:HA	1:A:143:LEU:CD2	0.51	2.34	2	8
1:A:98:MET:HG2	1:A:152:THR:HG21	0.51	1.82	9	1
1:A:59:ILE:HD12	1:A:182:ARG:HE	0.51	1.66	20	1
1:A:63:THR:HG21	1:A:70:LEU:HG	0.50	1.83	9	3
1:A:195:THR:HA	1:A:198:LEU:HD23	0.50	1.84	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ILE:O	1:A:63:THR:HG23	0.50	2.07	4	2
1:A:63:THR:CG2	1:A:70:LEU:HG	0.50	2.37	9	4
1:A:140:SER:CA	1:A:143:LEU:HD23	0.49	2.35	10	6
1:A:38:TYR:HB2	1:A:41:LYS:HE2	0.49	1.83	10	1
1:A:59:ILE:HB	1:A:96:ILE:CA	0.49	2.38	18	1
1:A:150:VAL:HG22	1:A:162:TRP:CE3	0.49	2.43	10	7
1:A:151:ILE:HG22	1:A:180:MET:HE1	0.49	1.84	6	4
1:A:200:GLU:H	1:A:200:GLU:CD	0.49	2.16	14	2
1:A:100:LYS:HG2	1:A:157:ASP:OD1	0.49	2.08	6	1
1:A:61:TYR:CD1	1:A:64:LEU:HD21	0.49	2.43	15	1
1:A:208:LYS:O	1:A:212:GLN:HB3	0.48	2.08	11	2
1:A:140:SER:CA	1:A:143:LEU:HD13	0.48	2.38	8	2
1:A:24:ALA:O	1:A:28:GLN:HG2	0.48	2.09	18	1
1:A:204:LYS:HA	1:A:207:VAL:HG22	0.48	1.84	6	3
1:A:70:LEU:HB3	1:A:74:LYS:HD2	0.48	1.84	2	1
1:A:79:ASN:ND2	1:A:219:THR:HB	0.48	2.23	16	2
1:A:75:GLU:HB3	1:A:77:HIS:CD2	0.48	2.44	11	1
1:A:147:LYS:HE2	1:A:163:GLU:OE2	0.48	2.08	20	1
1:A:190:LEU:HD12	1:A:190:LEU:H	0.47	1.69	1	4
1:A:60:ARG:HD2	1:A:216:TYR:OH	0.47	2.09	6	1
1:A:56:LEU:HD23	1:A:95:GLY:HA2	0.47	1.87	5	9
1:A:89:LEU:HB2	1:A:190:LEU:HD11	0.47	1.87	1	1
1:A:180:MET:SD	1:A:185:LYS:HE3	0.47	2.49	3	2
1:A:145:ALA:HB2	1:A:188:LEU:HB3	0.47	1.86	20	4
1:A:48:LEU:HD11	1:A:188:LEU:HD21	0.47	1.86	19	2
1:A:99:THR:HB	1:A:157:ASP:OD2	0.47	2.10	20	1
1:A:146:GLU:HB3	1:A:191:LYS:HG2	0.46	1.87	4	1
1:A:56:LEU:HA	1:A:59:ILE:HG22	0.46	1.88	17	2
1:A:42:GLU:HB2	1:A:206:ILE:CD1	0.46	2.40	10	1
1:A:202:ARG:O	1:A:206:ILE:HG12	0.46	2.10	20	6
1:A:100:LYS:HD3	1:A:100:LYS:C	0.46	2.36	8	2
1:A:63:THR:HA	1:A:66:ASP:O	0.46	2.11	7	3
1:A:93:ASP:O	1:A:183:GLY:HA3	0.46	2.10	15	2
1:A:26:ILE:O	1:A:30:MET:HG2	0.45	2.11	2	1
1:A:150:VAL:HG22	1:A:162:TRP:HE3	0.45	1.71	12	5
1:A:40:ASN:OD1	1:A:43:ILE:HG23	0.45	2.12	10	1
1:A:147:LYS:HE2	1:A:163:GLU:CD	0.45	2.36	20	1
1:A:159:GLN:OE1	1:A:179:PRO:HA	0.45	2.11	4	1
1:A:151:ILE:HD12	1:A:151:ILE:N	0.45	2.27	15	4
1:A:44:PHE:CE2	1:A:144:VAL:HG11	0.45	2.47	17	1
1:A:20:PHE:HB2	1:A:170:PHE:CZ	0.44	2.47	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:LYS:HB2	1:A:159:GLN:HG3	0.44	1.89	16	1
1:A:84:LYS:HG2	1:A:198:LEU:HB3	0.44	1.89	20	1
1:A:146:GLU:OE1	1:A:147:LYS:HB3	0.44	2.13	2	1
1:A:190:LEU:HD22	1:A:190:LEU:H	0.44	1.73	15	1
1:A:200:GLU:CD	1:A:200:GLU:N	0.44	2.76	14	1
1:A:87:ARG:HA	1:A:198:LEU:HD11	0.44	1.90	14	1
1:A:30:MET:HE1	1:A:142:TYR:CE2	0.43	2.48	4	1
1:A:151:ILE:HD13	1:A:185:LYS:HD2	0.43	1.89	3	1
1:A:214:ILE:HG22	1:A:216:TYR:H	0.43	1.73	20	4
1:A:85:GLN:HA	1:A:85:GLN:OE1	0.43	2.13	8	2
1:A:52:SER:HB3	1:A:93:ASP:HB3	0.43	1.90	20	2
1:A:41:LYS:HD2	1:A:143:LEU:HB3	0.43	1.91	3	1
1:A:46:ARG:HD2	1:A:46:ARG:O	0.43	2.14	4	1
1:A:147:LYS:NZ	1:A:147:LYS:HB2	0.43	2.29	5	1
1:A:30:MET:HE1	1:A:142:TYR:CE1	0.43	2.48	1	1
1:A:155:ASN:OD1	1:A:182:ARG:HD3	0.43	2.14	9	2
1:A:66:ASP:OD1	1:A:69:LYS:HG3	0.43	2.13	14	2
1:A:46:ARG:HB2	1:A:210:HIS:HB3	0.43	1.91	16	3
1:A:84:LYS:HE2	1:A:198:LEU:O	0.43	2.14	18	2
1:A:191:LYS:HB2	1:A:194:GLN:HG2	0.43	1.91	7	3
1:A:46:ARG:HD2	1:A:46:ARG:C	0.42	2.39	4	1
1:A:70:LEU:O	1:A:74:LYS:HE2	0.42	2.14	8	1
1:A:158:GLU:HA	1:A:158:GLU:OE1	0.42	2.14	4	1
1:A:164:SER:HB3	1:A:170:PHE:CB	0.42	2.44	15	2
1:A:142:TYR:HA	1:A:145:ALA:O	0.42	2.15	8	1
1:A:144:VAL:HA	1:A:194:GLN:NE2	0.42	2.29	11	1
1:A:55:ALA:HB1	1:A:95:GLY:HA3	0.42	1.90	15	1
1:A:43:ILE:O	1:A:47:GLU:HG2	0.42	2.14	3	1
1:A:79:ASN:OD1	1:A:219:THR:HB	0.42	2.13	4	1
1:A:62:GLU:OE1	1:A:69:LYS:HE3	0.42	2.15	14	1
1:A:141:ALA:HB1	1:A:148:VAL:HG11	0.42	1.92	1	1
1:A:95:GLY:O	1:A:182:ARG:HD2	0.42	2.14	4	1
1:A:83:ASN:OD1	1:A:86:ASP:HB2	0.42	2.15	4	1
1:A:59:ILE:HB	1:A:96:ILE:HA	0.42	1.92	18	1
1:A:41:LYS:HD2	1:A:194:GLN:HE22	0.42	1.73	20	1
1:A:83:ASN:CG	1:A:86:ASP:HB2	0.42	2.40	15	2
1:A:220:LEU:HG	1:A:222:VAL:HG23	0.42	1.92	14	1
1:A:96:ILE:HG23	1:A:97:GLY:O	0.41	2.15	1	1
1:A:199:GLU:HB2	1:A:202:ARG:HB2	0.41	1.91	3	1
1:A:93:ASP:OD1	1:A:184:THR:HB	0.41	2.15	6	1
1:A:201:ARG:C	1:A:201:ARG:HD3	0.41	2.40	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ARG:C	1:A:46:ARG:HD3	0.41	2.39	16	1
1:A:79:ASN:HB2	1:A:92:VAL:CG2	0.41	2.45	16	1
1:A:147:LYS:HD3	1:A:165:SER:OG	0.41	2.15	13	1
1:A:41:LYS:O	1:A:44:PHE:HD1	0.41	1.98	4	1
1:A:91:ILE:HB	1:A:186:VAL:HG22	0.41	1.92	1	1
1:A:204:LYS:HA	1:A:204:LYS:CE	0.41	2.45	5	1
1:A:60:ARG:HH21	1:A:61:TYR:HE2	0.41	1.59	15	1
1:A:54:ASP:O	1:A:57:ASP:HB2	0.41	2.15	17	1
1:A:200:GLU:O	1:A:204:LYS:HG3	0.40	2.16	2	1
1:A:81:ILE:HB	1:A:90:THR:HB	0.40	1.93	20	1
1:A:44:PHE:O	1:A:48:LEU:HG	0.40	2.17	6	1
1:A:191:LYS:HB2	1:A:194:GLN:CG	0.40	2.45	7	1
1:A:98:MET:C	1:A:154:HIS:HB2	0.40	2.42	6	1
1:A:81:ILE:HG13	1:A:221:PHE:HD1	0.40	1.77	9	1
1:A:64:LEU:HD12	1:A:65:THR:N	0.40	2.32	15	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	171/266 (64%)	168±1 (98±1%)	3±1 (2±1%)	0±0 (0±0%)	49	83
All	All	3420/5320 (64%)	3356 (98%)	62 (2%)	2 (0%)	49	83

All 2 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	137	GLY	1
1	A	138	PHE	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	154/230 (67%)	147±2 (96±1%)	7±2 (4±1%)	27	78
All	All	3080/4600 (67%)	2949 (96%)	131 (4%)	27	78

All 26 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	39	SER	20
1	A	223	GLU	20
1	A	86	ASP	19
1	A	45	LEU	18
1	A	200	GLU	9
1	A	147	LYS	9
1	A	32	LEU	5
1	A	146	GLU	4
1	A	192	GLU	3
1	A	100	LYS	3
1	A	173	ARG	3
1	A	57	ASP	2
1	A	84	LYS	2
1	A	208	LYS	2
1	A	46	ARG	1
1	A	74	LYS	1
1	A	98	MET	1
1	A	62	GLU	1
1	A	64	LEU	1
1	A	209	LYS	1
1	A	54	ASP	1
1	A	59	ILE	1
1	A	60	ARG	1
1	A	65	THR	1
1	A	159	GLN	1
1	A	163	GLU	1

6.3.3 RNA ⓘ

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 oligosaccharides 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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 42% for the well-defined parts and 41% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	1217
Number of shifts mapped to atoms	1193
Number of unparsed shifts	0
Number of shifts with mapping errors	24
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 24 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	224	LYS	H	8.46	0.05	1
1	A	224	LYS	C	176.69	0.05	1
1	A	224	LYS	CA	56.19	0.05	1
1	A	224	LYS	CB	33.41	0.05	1
1	A	224	LYS	N	123.45	0.05	1
1	A	229	GLU	C	176.71	0.05	1
1	A	229	GLU	CA	56.86	0.05	1
1	A	229	GLU	CB	30.36	0.05	1
1	A	230	VAL	HG21	0.95	0.05	1
1	A	230	VAL	HG22	0.95	0.05	1
1	A	230	VAL	HG23	0.95	0.05	1
1	A	230	VAL	C	176.07	0.05	1
1	A	230	VAL	CA	62.44	0.05	1
1	A	230	VAL	CB	33.31	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	230	VAL	CG2	20.65	0.05	1
1	A	231	SER	CA	58.11	0.05	1
1	A	231	SER	CB	64.15	0.05	1
1	A	232	ASP	C	176.37	0.05	1
1	A	232	ASP	CA	54.83	0.05	1
1	A	232	ASP	CB	41.31	0.05	1
1	A	235	ALA	HB1	1.42	0.05	1
1	A	235	ALA	HB2	1.42	0.05	1
1	A	235	ALA	HB3	1.42	0.05	1
1	A	235	ALA	CB	19.65	0.05	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	193	-0.41 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	180	0.08 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	179	-0.30 ± 0.10	None needed (< 0.5 ppm)
^{15}N	166	0.75 ± 0.36	Should be applied

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 42%, i.e. 1013 atoms were assigned a chemical shift out of a possible 2384. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	610/862 (71%)	147/350 (42%)	316/344 (92%)	147/168 (88%)
Sidechain	403/1339 (30%)	198/868 (23%)	205/425 (48%)	0/46 (0%)
Aromatic	0/183 (0%)	0/90 (0%)	0/88 (0%)	0/5 (0%)
Overall	1013/2384 (42%)	345/1308 (26%)	521/857 (61%)	147/219 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 41%, i.e. 1193 atoms were assigned a chemical shift out of a possible 2896. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	693/1070 (65%)	165/436 (38%)	363/426 (85%)	165/208 (79%)

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	Total	¹ H	¹³ C	¹⁵ N
Sidechain	500/1623 (31%)	255/1055 (24%)	245/516 (47%)	0/52 (0%)
Aromatic	0/203 (0%)	0/100 (0%)	0/98 (0%)	0/5 (0%)
Overall	1193/2896 (41%)	420/1591 (26%)	608/1040 (58%)	165/265 (62%)

7.1.4 Statistically unusual chemical shifts [i](#)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	107	LEU	HD21	-0.85	-0.65 – 2.13	-5.7
1	A	107	LEU	HD22	-0.85	-0.65 – 2.13	-5.7
1	A	107	LEU	HD23	-0.85	-0.65 – 2.13	-5.7

7.1.5 Random Coil Index (RCI) plots [i](#)

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

