Full wwPDB NMR Structure Validation Report (i)

Mar 3, 2022 – 11:03 AM EST

PDB ID	:	2HR9
Title	:	Solution structure of human translationally controlled tumor protein
Authors	:	Feng, Y.; Liu, D.; Yao, H.; Wang, J.
Deposited on	:	2006-07-20

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

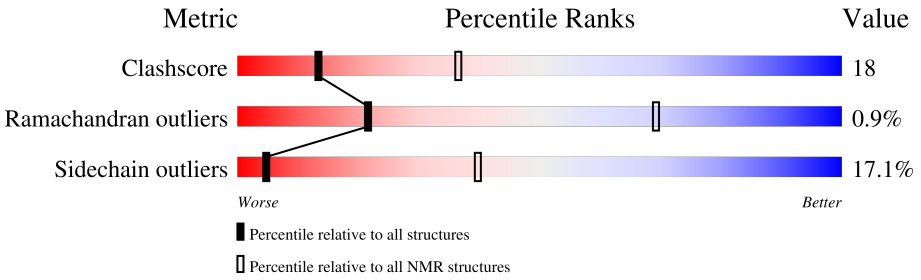
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	180	51% 22% • 21% •

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 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:2-A:36, A:69-A:170 (137)	0.21	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 3 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2752 atoms, of which 1365 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Translationally-controlled tumor protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	174	2752	877	1365	225	273	12	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	173	LEU	-	expression tag	UNP P13693
A	174	GLU	-	expression tag	UNP P13693
A	175	HIS	-	expression tag	UNP P13693
A	176	HIS	-	expression tag	UNP P13693
A	177	HIS	-	expression tag	UNP P13693
A	178	HIS	-	expression tag	UNP P13693
A	179	HIS	-	expression tag	UNP P13693
A	180	HIS	-	expression tag	UNP P13693

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: Translationally-controlled tumor protein

Chain A: 51% 22% • 21% •

M1 I2 I3 Y4 I8 E12 M13 F14 S15 Y18 L27 C28 L29 S37 R38 T39 E40 G41 N42 I43 D44 D45 S46 L47 I48 G49 G50 N51 A52 S53 A54 E55 G56 P57 E58 G59 E60 G61 T62 E63 S64 T65 V66 I67 T68 I72 V73 M74 N75 H76 H77 L78 F83

T84 Y88 Y91 I92 Y95 N96 K97 S98 I99 L103 E104 R107 P108 E109 R110 V111 K112 P113 I122 K123 H124 I125 F129 Y132 Q133 F134 F135 I136 A147 L148 L149 D150 Y151 R152 Y159 M160 K164 L167 E168 M169 E170 K171 C172 L173 E174 HIS HIS HIS

HIS HIS HIS

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: Translationally-controlled tumor protein

Chain A: 46% 26% • • 21% •

M1 I2 I3 Y4 R5 D6 L7 I8 S9 E12 M13 F14 S15 Y18 A24 D25 G26 L27 C28 L29 E30 V31 S37 R38 T39 E40 G41 N42 I43 D44 D45 S46 L47 I48 G49 G50 N51 A52 S53 A54 E55 G56 P57 E58 G59 E60 G61 T62 E63 S64 T65 V66 I67 T68 I72

V73 M74 N75 H76 H77 L78 Q79 F83 T84 K85 Y88 K89 K90 Y91 I92 Y95 L103 E104 E105 Q106 R107 P108 E109 R110 V111 K112 P113 Q121 I122 K123 H124 I125 F129 Y132 I136 V146 A147 L148 L149 D150 Y151 R152 E153 Y159 M160 I161 F162 F163 M169

E170 K171 C172 L173 E174 HIS HIS HIS HIS HIS HIS

4.2.2 Score per residue for model 2

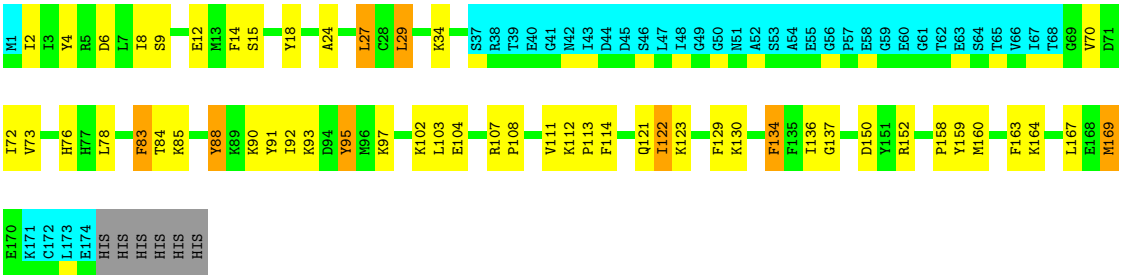
- Molecule 1: Translationally-controlled tumor protein

Chain A: 43% 29% • 21% •

4.2.3 Score per residue for model 3

- Molecule 1: Translationally-controlled tumor protein

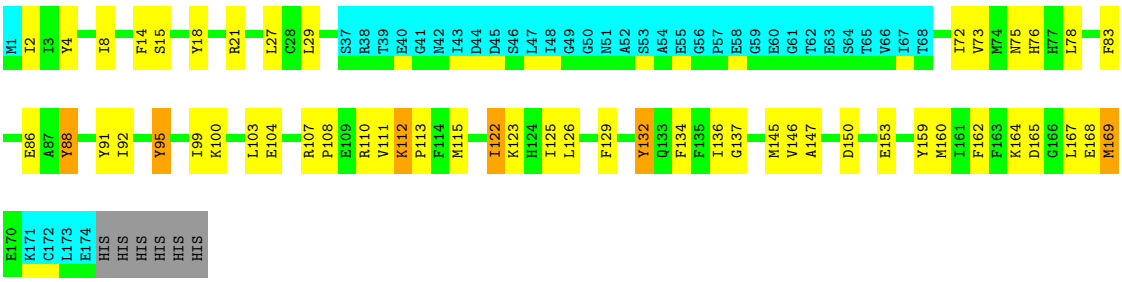
Chain A: 46% 26% • 21% •



4.2.4 Score per residue for model 4

- Molecule 1: Translationally-controlled tumor protein

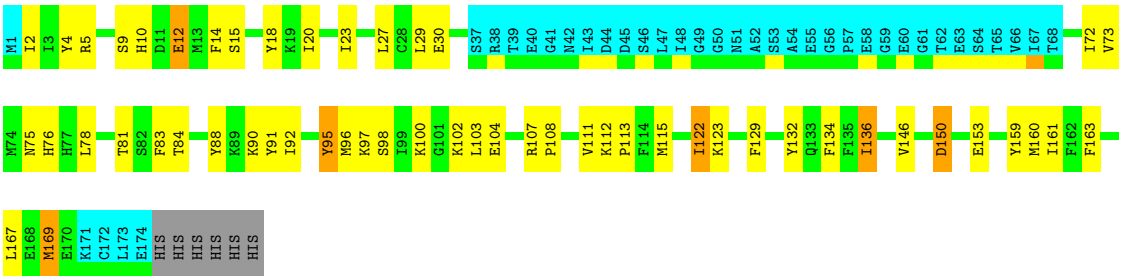
Chain A: 47% 26% • 21% •



4.2.5 Score per residue for model 5

- Molecule 1: Translationally-controlled tumor protein

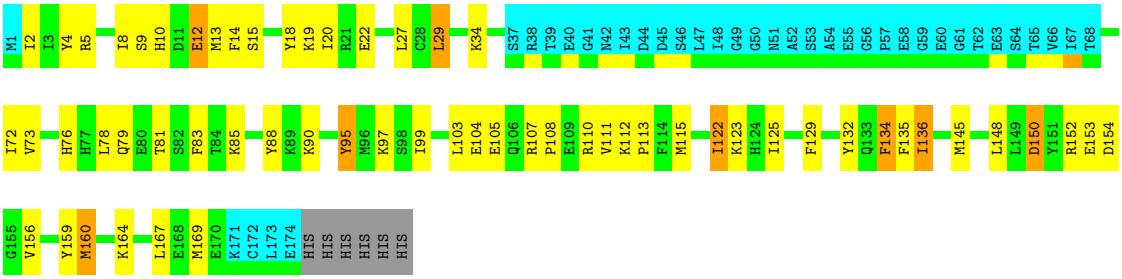
Chain A: 46% 27% • 21% •



4.2.6 Score per residue for model 6

- Molecule 1: Translationally-controlled tumor protein

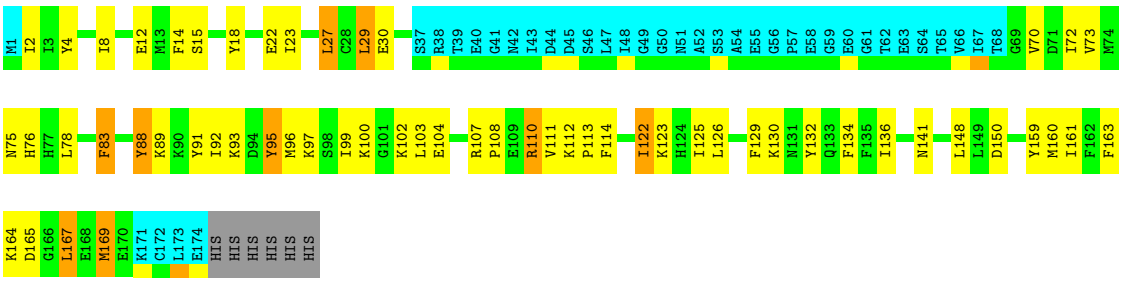
Chain A: 43% 29% • 21% •



4.2.7 Score per residue for model 7

- Molecule 1: Translationally-controlled tumor protein

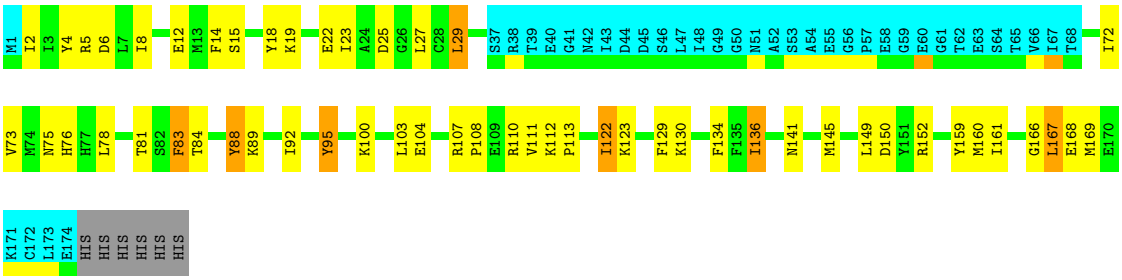
Chain A: 43% 28% 5% 21% •



4.2.8 Score per residue for model 8

- Molecule 1: Translationally-controlled tumor protein

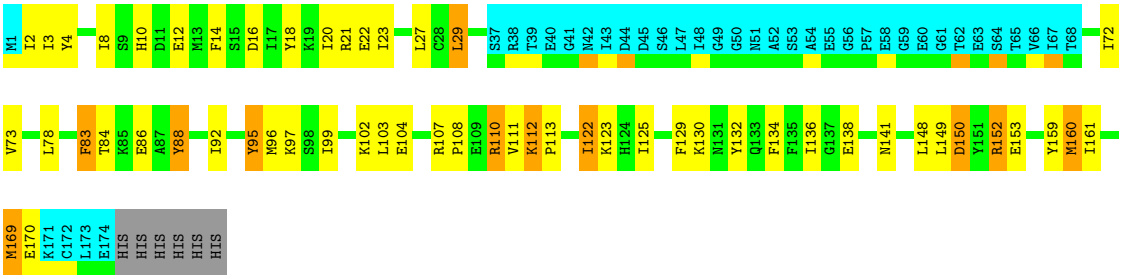
Chain A: 46% 26% • 21% •



4.2.9 Score per residue for model 9

- Molecule 1: Translationally-controlled tumor protein

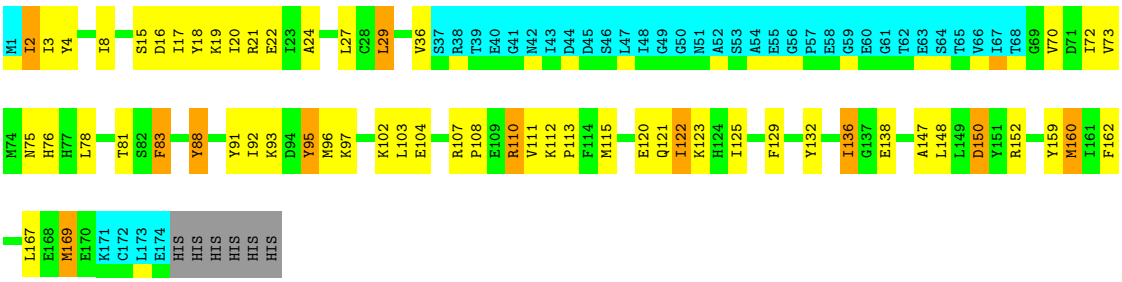
Chain A: 45% 25% 6% 21% •



4.2.10 Score per residue for model 10

- Molecule 1: Translationally-controlled tumor protein

Chain A: 43% 27% 6% 21% •



4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Translationally-controlled tumor protein

Chain A: 48% 22% 7% 21% •

M1 I2 I3 Y4 I8 S9 H10 D11 E12 M13 F14 S15 Y18 E22 L27 C28 L29 E30 V31 K34 S37 R38 T39 E40 G41 N42 I43 D44 D45 S46 L47 I48 G49 G50 N51 A52 S53 A54 E55 G56 P57 E58 G59 E60 G61 T62 E63 S64 T65 V66 I67 T68 G69 V70
D71 I72 V73 M74 N75 H76 H77 L78 Q79 E80 F83 Y88 I92 K93 D94 Y95 M96 K97 S98 I99 L103 E104 R107 P108 E109 R110 V111 K112 P113 F114 M115 I122 K123 H124 I125 F129 F134 F135 I136 A147 L148 L149 D150 Y159 M160 I161 F162 F163 K164
L167 E168 M169 E170 K171 C172 L173 E174 HIS HIS HIS HIS HIS HIS

4.2.12 Score per residue for model 12

- Molecule 1: Translationally-controlled tumor protein

Chain A: 41% 30% 6% 21% •

M1 I2 I3 Y4 R5 D6 L7 I8 S9 H10 D11 E12 M13 F14 Y18 L27 C28 L29 V36 S37 R38 T39 E40 G41 N42 I43 D44 D45 S46 L47 I48 G49 G50 N51 A52 S53 A54 E55 G56 P57 E58 G59 E60 G61 T62 E63 S64 T65 V66 I67 T68 G69 V70 D71 I72 V73 M74
N75 H76 H77 L78 F83 T84 K85 Y88 K89 K90 Y91 I92 Y95 M96 K97 S98 I99 K100 L103 E104 R107 P108 V111 K112 P113 E120 Q121 I122 K123 H124 I125 F129 K130 N131 Y132 Q133 F134 F135 I136 M145 V146 A147 L148 L149 D150 Y151 R152 Y159 M160 I161
F162 F163 K164 D165 G166 L167 E168 M169 E170 K171 C172 L173 E174 HIS HIS HIS HIS HIS HIS

4.2.13 Score per residue for model 13

- Molecule 1: Translationally-controlled tumor protein

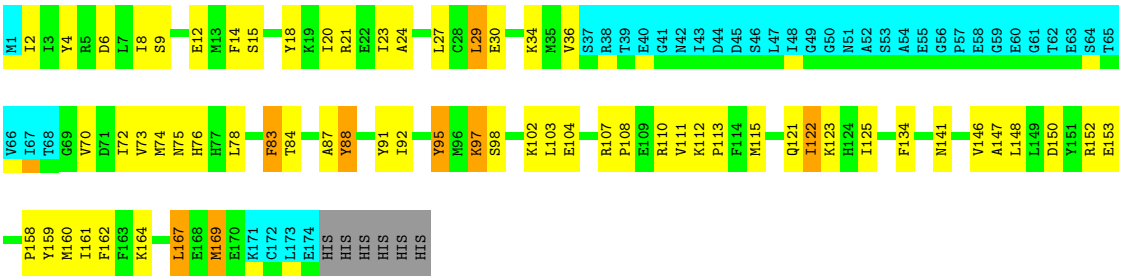
Chain A: 41% 29% 6% 21% •

M1 I2 I3 Y4 R5 D6 L7 I8 S9 E12 M13 F14 S15 Y18 K19 I20 L27 C28 L29 S37 R38 T39 E40 G41 N42 I43 D44 D45 S46 L47 I48 G49 G50 N51 A52 S53 A54 E55 G56 P57 E58 G59 E60 G61 T62 E63 S64 T65 V66 I67 T68 G69 V70 D71 I72 V73
M74 N75 H76 H77 L78 T81 S82 F83 T84 A87 Y88 K89 K90 Y91 I92 Y95 M96 K97 S98 I99 K102 L103 E104 R107 P108 E109 R110 V111 K112 P113 F114 M115 I122 K123 F129 Y132 Q133 F134 F135 I136 M145 V146 A147 D150 Y151 R152 P158 Y159 M160
I161 F162 F163 K164 D165 G166 L167 E168 M169 E170 K171 C172 L173 E174 HIS HIS HIS HIS HIS HIS

4.2.14 Score per residue for model 14

- Molecule 1: Translationally-controlled tumor protein

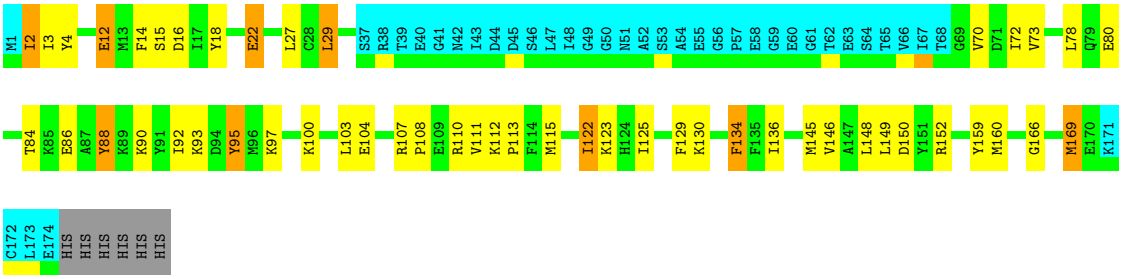
Chain A: 41% 31% • 21% •



4.2.15 Score per residue for model 15

- Molecule 1: Translationally-controlled tumor protein

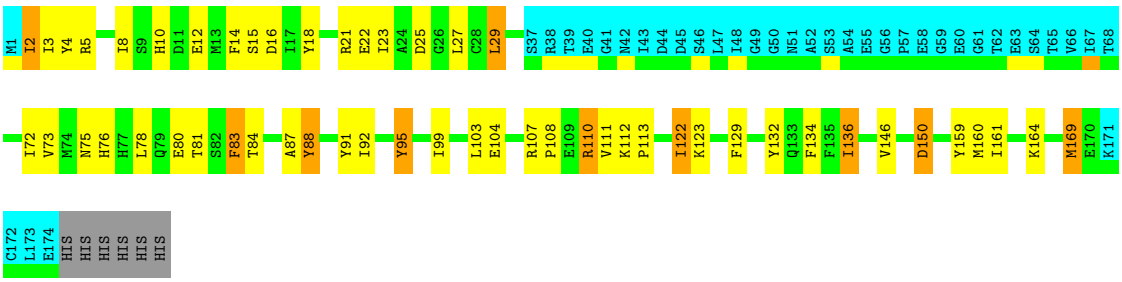
Chain A: 48% 23% 5% 21% •



4.2.16 Score per residue for model 16

- Molecule 1: Translationally-controlled tumor protein

Chain A: 47% 24% 6% 21% •



4.2.17 Score per residue for model 17

- Molecule 1: Translationally-controlled tumor protein

Chain A: 44% 29% • 21% •

4.2.18 Score per residue for model 18

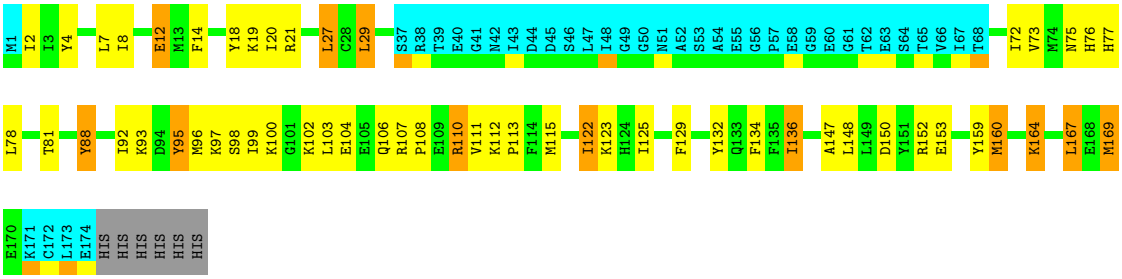
- Molecule 1: Translationally-controlled tumor protein

Chain A: 49% 24% • 21% •

4.2.19 Score per residue for model 19

- Molecule 1: Translationally-controlled tumor protein

Chain A: 45% 24% 7% 21% •



4.2.20 Score per residue for model 20

- Molecule 1: Translationally-controlled tumor protein

Chain A: 45% 24% 7% 21% •

M1 I2 I3 Y4 R5 D6 L7 I8 E12 M13 F14 Y18 E22 I23 L27 C28 L29 E30 V31 S37 R38 T39 E40 G41 N42 I43 D44 D45 S46 L47 T48 G49 G50 N51 A52 S53 A54 E55 G56 P57 E58 G59 E60 G61 T62 E63 S64 T65 V66 I67 T68 I72 V73 M74

N75 H76 H77 L78 T81 S82 F83 Y88 I92 K93 D94 Y95 M96 K97 S98 I99 L103 E104 R107 P108 E109 R110 V111 K112 P113 I122 K123 H124 I125 F129 Y132 Q133 F134 F135 I136 V146 A147 L148 L149 D150 Y159 M160 I161 F162 F163 K164 L167 E168 M169

E170 K171 C172 L173 E174 HIS HIS HIS HIS HIS HIS

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 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
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (i)

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	1127	1120	1116	41±4
All	All	22540	22400	22320	814

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:TYR:CZ	1:A:72:ILE:HG22	0.85	2.07	15	20
1:A:88:TYR:CD2	1:A:122:ILE:HD11	0.84	2.08	3	20
1:A:108:PRO:O	1:A:111:VAL:HG22	0.83	1.73	6	20
1:A:18:TYR:CE2	1:A:72:ILE:HG22	0.82	2.09	14	19
1:A:8:ILE:HD11	1:A:99:ILE:CG1	0.79	2.06	7	13
1:A:125:ILE:HG21	1:A:148:LEU:HD13	0.75	1.58	1	13
1:A:88:TYR:O	1:A:92:ILE:HG22	0.75	1.79	3	3
1:A:78:LEU:HD13	1:A:160:MET:CE	0.75	2.12	11	9
1:A:81:THR:HG21	1:A:136:ILE:HD11	0.73	1.61	8	9
1:A:103:LEU:HD21	1:A:110:ARG:CB	0.72	2.14	13	14
1:A:29:LEU:HD11	1:A:164:LYS:CG	0.72	2.15	12	2
1:A:2:ILE:HG23	1:A:4:TYR:CE1	0.72	2.20	10	13
1:A:103:LEU:HD21	1:A:110:ARG:HB2	0.68	1.64	13	9
1:A:23:ILE:HD11	1:A:161:ILE:HG23	0.68	1.64	5	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:ILE:HD11	1:A:99:ILE:HG13	0.66	1.66	7	12
1:A:92:ILE:HD12	1:A:95:TYR:CE2	0.64	2.27	19	12
1:A:147:ALA:HB1	1:A:160:MET:HE2	0.64	1.69	13	1
1:A:18:TYR:O	1:A:20:ILE:HD12	0.64	1.93	18	4
1:A:27:LEU:HD21	1:A:114:PHE:HA	0.63	1.70	3	1
1:A:78:LEU:HD13	1:A:160:MET:HE1	0.63	1.69	18	6
1:A:2:ILE:HD11	1:A:169:MET:HB3	0.63	1.68	19	14
1:A:73:VAL:HG13	1:A:78:LEU:HB2	0.63	1.71	5	20
1:A:104:GLU:HG3	1:A:111:VAL:HG11	0.63	1.70	19	17
1:A:78:LEU:HD13	1:A:160:MET:HE2	0.62	1.70	11	1
1:A:29:LEU:HD11	1:A:164:LYS:HG3	0.61	1.72	14	3
1:A:73:VAL:HA	1:A:78:LEU:HD12	0.61	1.71	11	7
1:A:29:LEU:HD21	1:A:164:LYS:HD2	0.60	1.73	3	1
1:A:22:GLU:HG3	1:A:29:LEU:HD23	0.60	1.73	16	8
1:A:70:VAL:HG22	1:A:158:PRO:HG2	0.60	1.71	13	1
1:A:147:ALA:HB2	1:A:162:PHE:CE1	0.60	2.31	20	6
1:A:104:GLU:CG	1:A:111:VAL:HG11	0.59	2.27	4	19
1:A:29:LEU:HD11	1:A:164:LYS:HB3	0.59	1.74	19	1
1:A:18:TYR:CE1	1:A:72:ILE:HG22	0.58	2.34	3	5
1:A:78:LEU:HD13	1:A:160:MET:SD	0.58	2.38	16	4
1:A:14:PHE:CD2	1:A:31:VAL:HG21	0.57	2.34	17	4
1:A:72:ILE:HD11	1:A:160:MET:HG3	0.57	1.75	7	3
1:A:70:VAL:HG22	1:A:158:PRO:HG3	0.56	1.77	3	2
1:A:24:ALA:HB2	1:A:121:GLN:NE2	0.55	2.17	1	4
1:A:88:TYR:CE2	1:A:122:ILE:HD11	0.55	2.37	10	18
1:A:125:ILE:HG22	1:A:132:TYR:CD2	0.55	2.37	4	2
1:A:8:ILE:HD11	1:A:99:ILE:HG12	0.55	1.79	19	4
1:A:4:TYR:HB3	1:A:167:LEU:HD21	0.55	1.78	10	5
1:A:95:TYR:C	1:A:95:TYR:CD1	0.54	2.81	17	12
1:A:103:LEU:HB3	1:A:111:VAL:HG12	0.54	1.78	6	8
1:A:2:ILE:HG22	1:A:16:ASP:HB2	0.53	1.80	10	4
1:A:29:LEU:HD11	1:A:164:LYS:HG2	0.52	1.79	12	2
1:A:29:LEU:HD11	1:A:164:LYS:CD	0.52	2.34	2	1
1:A:88:TYR:CZ	1:A:134:PHE:CE1	0.52	2.98	14	12
1:A:4:TYR:CD2	1:A:14:PHE:CZ	0.52	2.98	11	13
1:A:129:PHE:CE1	1:A:134:PHE:CZ	0.52	2.98	4	14
1:A:147:ALA:HB2	1:A:162:PHE:CE2	0.52	2.40	12	3
1:A:4:TYR:CD2	1:A:14:PHE:CE2	0.52	2.98	7	14
1:A:125:ILE:HG22	1:A:132:TYR:CE2	0.51	2.40	4	1
1:A:154:ASP:OD1	1:A:156:VAL:HG23	0.51	2.06	6	2
1:A:129:PHE:CE1	1:A:134:PHE:CE2	0.51	2.98	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:ALA:HB1	1:A:160:MET:HE3	0.51	1.83	1	1
1:A:95:TYR:CZ	1:A:163:PHE:CE2	0.51	2.98	1	1
1:A:83:PHE:CE2	1:A:91:TYR:CE2	0.50	3.00	3	7
1:A:20:ILE:HD12	1:A:20:ILE:N	0.50	2.21	14	6
1:A:93:LYS:O	1:A:97:LYS:CG	0.50	2.60	20	9
1:A:4:TYR:CG	1:A:14:PHE:CE2	0.50	2.99	12	9
1:A:6:ASP:OD1	1:A:8:ILE:HD12	0.49	2.07	3	7
1:A:147:ALA:HB1	1:A:160:MET:SD	0.49	2.47	11	4
1:A:92:ILE:CD1	1:A:95:TYR:CE2	0.49	2.95	3	12
1:A:8:ILE:HD12	1:A:8:ILE:N	0.49	2.23	16	4
1:A:81:THR:CG2	1:A:136:ILE:HD11	0.49	2.35	8	5
1:A:108:PRO:HA	1:A:111:VAL:HG13	0.49	1.84	20	10
1:A:129:PHE:CZ	1:A:134:PHE:CE2	0.49	3.00	4	1
1:A:103:LEU:HD21	1:A:110:ARG:HB3	0.49	1.84	19	3
1:A:122:ILE:CG2	1:A:123:LYS:N	0.48	2.75	8	20
1:A:147:ALA:HB1	1:A:160:MET:CE	0.48	2.39	1	1
1:A:91:TYR:CE2	1:A:146:VAL:HG21	0.47	2.43	4	7
1:A:95:TYR:CD1	1:A:95:TYR:C	0.47	2.86	20	8
1:A:9:SER:O	1:A:10:HIS:CG	0.47	2.68	6	1
1:A:150:ASP:HB2	1:A:159:TYR:CZ	0.47	2.45	7	7
1:A:70:VAL:HG22	1:A:158:PRO:CG	0.47	2.40	13	2
1:A:132:TYR:CD1	1:A:132:TYR:N	0.47	2.81	17	6
1:A:83:PHE:CE2	1:A:87:ALA:HB1	0.47	2.45	14	3
1:A:150:ASP:CB	1:A:159:TYR:CE1	0.46	2.99	4	6
1:A:150:ASP:HB2	1:A:159:TYR:CE1	0.46	2.46	7	4
1:A:135:PHE:CG	1:A:160:MET:CE	0.46	2.99	6	1
1:A:70:VAL:HG12	1:A:72:ILE:HG12	0.46	1.88	7	6
1:A:3:ILE:O	1:A:169:MET:HA	0.46	2.11	15	5
1:A:103:LEU:O	1:A:107:ARG:N	0.46	2.49	5	20
1:A:88:TYR:CZ	1:A:134:PHE:CD1	0.46	3.04	20	1
1:A:27:LEU:HD13	1:A:27:LEU:O	0.46	2.10	12	2
1:A:29:LEU:HD21	1:A:164:LYS:HG3	0.46	1.87	11	1
1:A:17:ILE:HD11	1:A:18:TYR:CZ	0.45	2.47	10	1
1:A:83:PHE:CB	1:A:134:PHE:CE2	0.45	3.00	16	5
1:A:112:LYS:HB2	1:A:113:PRO:HD3	0.45	1.89	4	19
1:A:149:LEU:HD12	1:A:160:MET:HG2	0.45	1.89	9	3
1:A:88:TYR:CE1	1:A:134:PHE:CE1	0.45	3.05	17	4
1:A:29:LEU:HD11	1:A:164:LYS:HB2	0.45	1.87	16	2
1:A:2:ILE:HG23	1:A:4:TYR:HE1	0.45	1.72	17	4
1:A:73:VAL:HG22	1:A:78:LEU:HD12	0.44	1.88	1	1
1:A:150:ASP:HB3	1:A:159:TYR:CE1	0.44	2.47	16	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:ASP:O	1:A:159:TYR:CD1	0.44	2.70	11	18
1:A:83:PHE:CZ	1:A:91:TYR:CG	0.44	3.05	2	1
1:A:14:PHE:CE2	1:A:31:VAL:CG2	0.44	3.00	17	1
1:A:88:TYR:CD2	1:A:126:LEU:HD21	0.44	2.47	4	2
1:A:150:ASP:CB	1:A:159:TYR:CZ	0.44	3.00	5	4
1:A:7:LEU:HD11	1:A:106:GLN:HE22	0.44	1.73	19	1
1:A:7:LEU:HD23	1:A:99:ILE:HG23	0.44	1.89	12	1
1:A:114:PHE:CD1	1:A:165:ASP:HB2	0.44	2.48	13	2
1:A:135:PHE:O	1:A:147:ALA:HB3	0.44	2.12	12	1
1:A:135:PHE:CG	1:A:160:MET:HE2	0.44	2.48	12	1
1:A:3:ILE:HG21	1:A:12:GLU:HB3	0.43	1.91	1	1
1:A:75:ASN:OD1	1:A:76:HIS:CD2	0.43	2.70	20	14
1:A:95:TYR:OH	1:A:163:PHE:CE2	0.43	2.72	13	3
1:A:88:TYR:CE1	1:A:134:PHE:CD1	0.43	3.06	6	1
1:A:132:TYR:CD1	1:A:150:ASP:CG	0.43	2.92	7	3
1:A:132:TYR:CD2	1:A:150:ASP:OD1	0.43	2.72	6	6
1:A:2:ILE:CG2	1:A:4:TYR:CE1	0.43	2.99	10	1
1:A:129:PHE:CD1	1:A:134:PHE:CZ	0.43	3.07	15	1
1:A:89:LYS:O	1:A:92:ILE:CG2	0.43	2.67	17	1
1:A:147:ALA:CB	1:A:162:PHE:CE1	0.42	3.02	20	1
1:A:110:ARG:C	1:A:113:PRO:HD2	0.42	2.34	16	7
1:A:36:VAL:HG23	1:A:36:VAL:O	0.42	2.13	12	1
1:A:83:PHE:HB2	1:A:134:PHE:CE2	0.42	2.50	20	6
1:A:89:LYS:NZ	1:A:126:LEU:HD13	0.42	2.28	7	1
1:A:129:PHE:CD1	1:A:129:PHE:O	0.42	2.73	4	7
1:A:145:MET:HE3	1:A:166:GLY:O	0.42	2.14	12	3
1:A:72:ILE:O	1:A:76:HIS:CG	0.42	2.73	6	3
1:A:97:LYS:HG3	1:A:98:SER:N	0.42	2.30	14	2
1:A:95:TYR:OH	1:A:163:PHE:CD2	0.42	2.73	7	1
1:A:132:TYR:CE1	1:A:150:ASP:OD2	0.42	2.73	1	1
1:A:141:ASN:OD1	1:A:141:ASN:N	0.42	2.53	14	1
1:A:30:GLU:OE1	1:A:159:TYR:CD2	0.42	2.73	14	4
1:A:132:TYR:CZ	1:A:150:ASP:OD2	0.42	2.73	9	3
1:A:78:LEU:HD13	1:A:160:MET:HE3	0.41	1.87	11	1
1:A:3:ILE:HG22	1:A:4:TYR:N	0.41	2.30	20	1
1:A:167:LEU:HD23	1:A:169:MET:CE	0.41	2.45	14	1
1:A:14:PHE:CE2	1:A:31:VAL:HG21	0.41	2.50	17	1
1:A:13:MET:O	1:A:76:HIS:CD2	0.41	2.74	6	2
1:A:71:ASP:O	1:A:75:ASN:ND2	0.41	2.53	2	2
1:A:13:MET:O	1:A:76:HIS:CG	0.41	2.74	13	1
1:A:112:LYS:N	1:A:113:PRO:CD	0.41	2.84	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:TYR:HE2	1:A:146:VAL:HG21	0.41	1.76	4	2
1:A:92:ILE:HD13	1:A:95:TYR:CE2	0.41	2.51	3	1
1:A:92:ILE:HA	1:A:95:TYR:CD2	0.41	2.50	14	1
1:A:132:TYR:CG	1:A:150:ASP:OD2	0.41	2.74	16	1
1:A:132:TYR:CD1	1:A:150:ASP:OD1	0.41	2.74	4	1
1:A:36:VAL:HG23	1:A:74:MET:CE	0.41	2.46	14	1
1:A:75:ASN:OD1	1:A:76:HIS:CG	0.41	2.74	14	1
1:A:132:TYR:CG	1:A:150:ASP:OD1	0.41	2.74	10	3
1:A:8:ILE:HD12	1:A:8:ILE:H	0.41	1.76	18	2
1:A:89:LYS:O	1:A:92:ILE:HG22	0.41	2.16	8	2
1:A:160:MET:HE3	1:A:162:PHE:CZ	0.41	2.51	1	1
1:A:27:LEU:HD21	1:A:113:PRO:O	0.41	2.15	19	1
1:A:77:HIS:CD2	1:A:77:HIS:N	0.40	2.87	19	1
1:A:75:ASN:OD1	1:A:76:HIS:CE1	0.40	2.74	2	1
1:A:141:ASN:N	1:A:141:ASN:OD1	0.40	2.55	8	1
1:A:134:PHE:HB3	1:A:146:VAL:CG1	0.40	2.46	20	1
1:A:95:TYR:OH	1:A:163:PHE:CZ	0.40	2.73	3	1
1:A:71:ASP:N	1:A:71:ASP:OD1	0.40	2.55	13	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	137/180 (76%)	128±1 (94±1%)	7±1 (5±1%)	1±1 (1±0%)	21	69
All	All	2740/3600 (76%)	2567 (94%)	148 (5%)	25 (1%)	21	69

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	12	GLU	17
1	A	152	ARG	6
1	A	137	GLY	2

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	122/157 (78%)	101±3 (83±3%)	21±3 (17±3%)	5 40
All	All	2440/3140 (78%)	2023 (83%)	417 (17%)	5 40

All 58 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	27	LEU	20
1	A	95	TYR	20
1	A	122	ILE	20
1	A	136	ILE	19
1	A	29	LEU	18
1	A	88	TYR	17
1	A	169	MET	17
1	A	15	SER	16
1	A	83	PHE	15
1	A	167	LEU	15
1	A	160	MET	14
1	A	84	THR	11
1	A	12	GLU	10
1	A	115	MET	10
1	A	110	ARG	9
1	A	152	ARG	9
1	A	102	LYS	9
1	A	9	SER	8
1	A	153	GLU	8
1	A	96	MET	8
1	A	100	LYS	8
1	A	90	LYS	7
1	A	150	ASP	7
1	A	5	ARG	7
1	A	97	LYS	7
1	A	164	LYS	7
1	A	21	ARG	7
1	A	85	LYS	6
1	A	19	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	168	GLU	6
1	A	130	LYS	6
1	A	10	HIS	5
1	A	2	ILE	5
1	A	25	ASP	4
1	A	112	LYS	4
1	A	129	PHE	4
1	A	34	LYS	4
1	A	134	PHE	4
1	A	86	GLU	4
1	A	105	GLU	3
1	A	98	SER	3
1	A	145	MET	3
1	A	80	GLU	3
1	A	79	GLN	2
1	A	132	TYR	2
1	A	165	ASP	2
1	A	141	ASN	2
1	A	138	GLU	2
1	A	120	GLU	2
1	A	22	GLU	2
1	A	107	ARG	2
1	A	146	VAL	2
1	A	149	LEU	1
1	A	170	GLU	1
1	A	75	ASN	1
1	A	123	LYS	1
1	A	93	LYS	1
1	A	133	GLN	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 monosaccharides 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 (i)

No chemical shift data were provided