



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 01:58 am BST

PDB ID : 2YUJ
Title : Solution structure of human ubiquitin fusion degradation protein 1 homolog UFD1
Authors : Saito, K.; Tomizawa, T.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-04-06

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

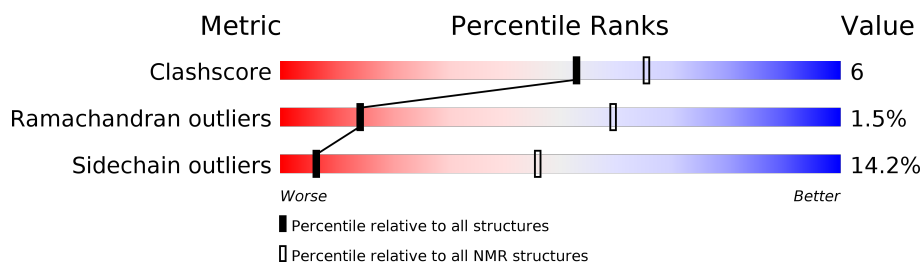
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	190	 74% 13% 13%

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:16-A:26, A:37-A:190 (165)	0.35	2

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 5 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2958 atoms, of which 1471 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin fusion degradation 1-like.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	190	2958	937	1471	249	288	13	0

There are 7 discrepancies between the modelled and reference sequences:

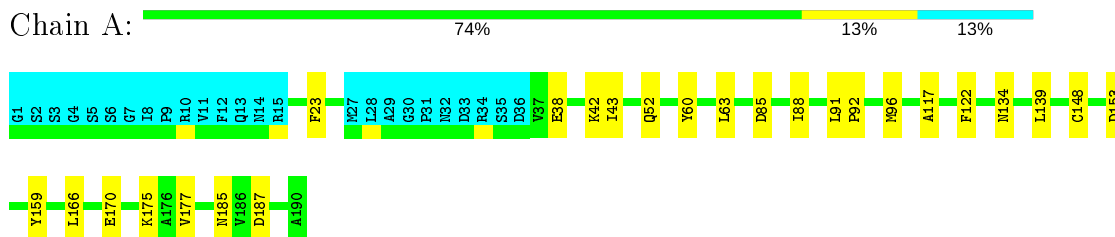
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q541A5
A	2	SER	-	expression tag	UNP Q541A5
A	3	SER	-	expression tag	UNP Q541A5
A	4	GLY	-	expression tag	UNP Q541A5
A	5	SER	-	expression tag	UNP Q541A5
A	6	SER	-	expression tag	UNP Q541A5
A	7	GLY	-	expression tag	UNP Q541A5

4 Residue-property plots [i](#)

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: Ubiquitin fusion degradation 1-like

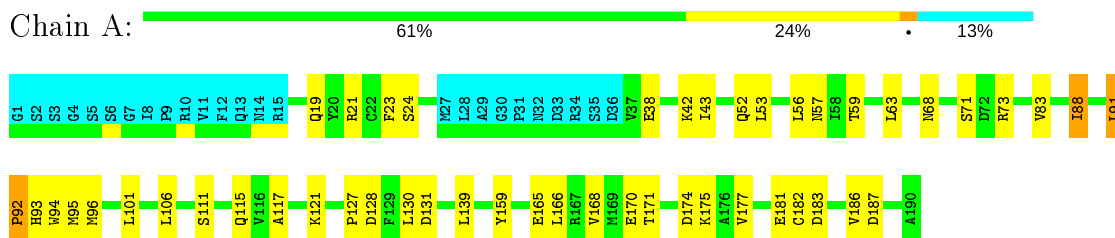


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

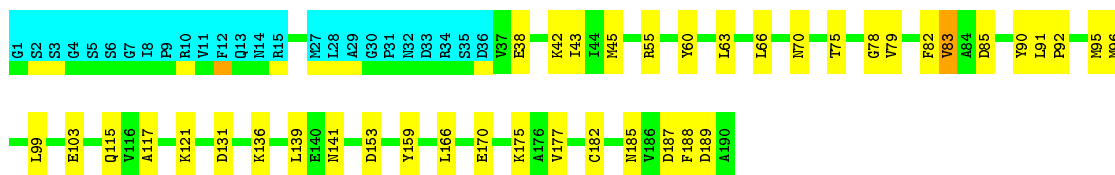
- Molecule 1: Ubiquitin fusion degradation 1-like



4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Ubiquitin fusion degradation 1-like

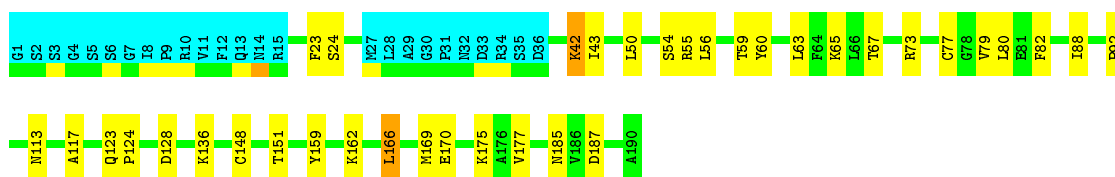




4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin fusion degradation 1-like

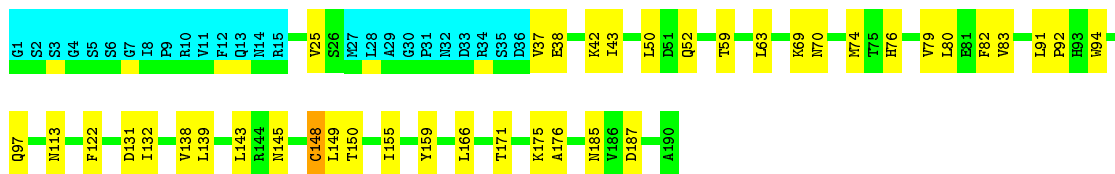
Chain A: 67% 18% 13%



4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin fusion degradation 1-like

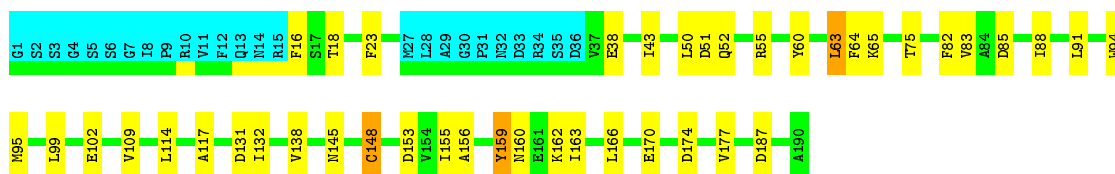
Chain A: 66% 21% 13%



4.2.5 Score per residue for model 5

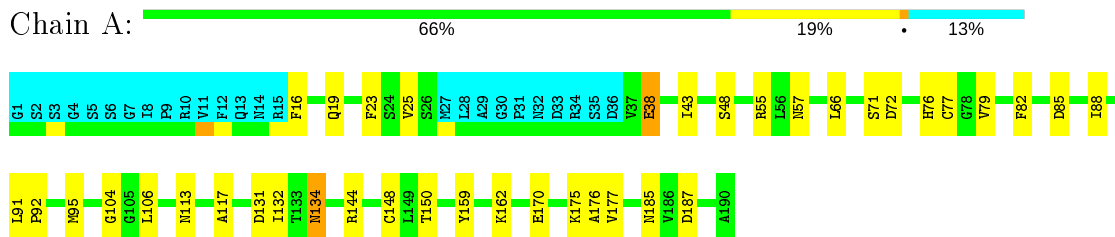
- Molecule 1: Ubiquitin fusion degradation 1-like

Chain A: 64% 21% 13%



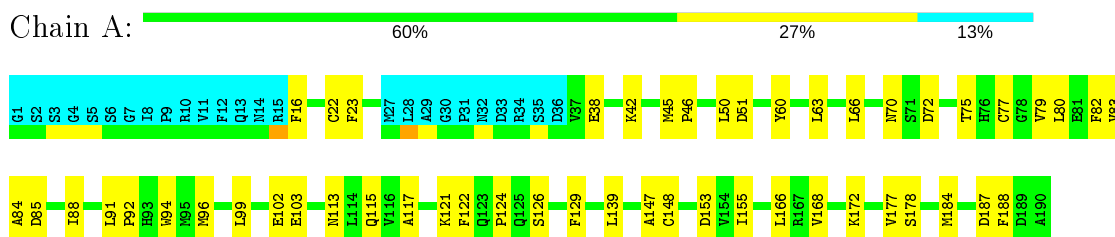
4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin fusion degradation 1-like



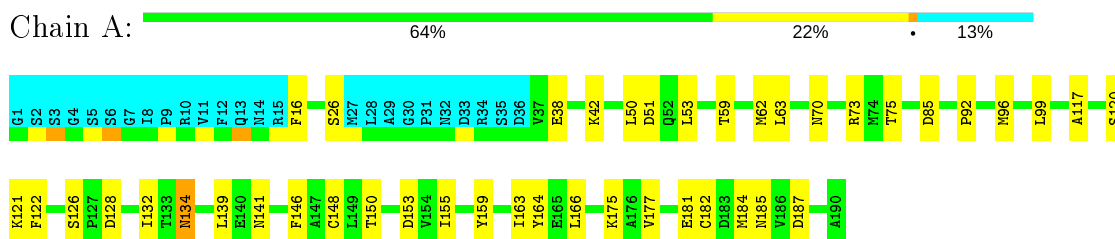
4.2.7 Score per residue for model 7

- Molecule 1: Ubiquitin fusion degradation 1-like



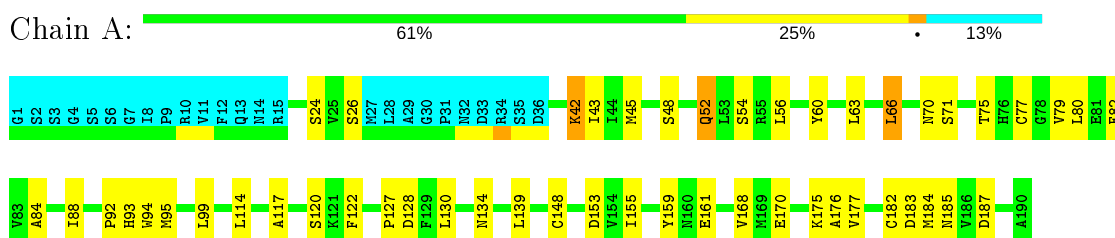
4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin fusion degradation 1-like



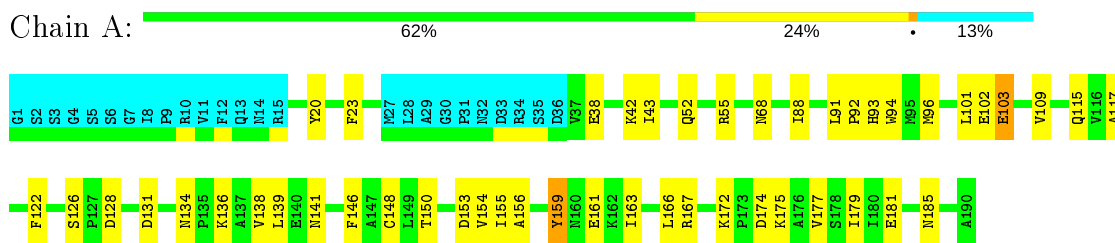
4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin fusion degradation 1-like



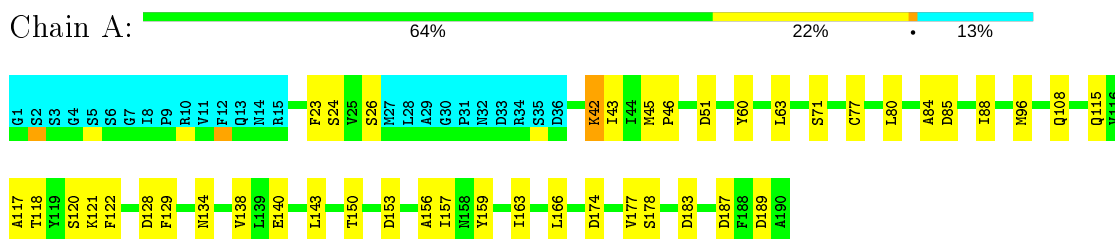
4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin fusion degradation 1-like



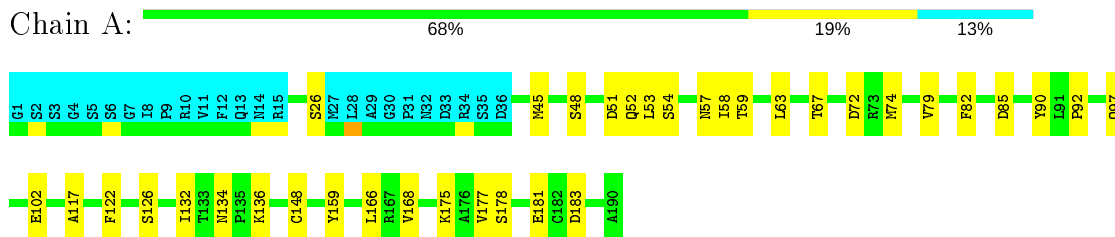
4.2.11 Score per residue for model 11

- Molecule 1: Ubiquitin fusion degradation 1-like



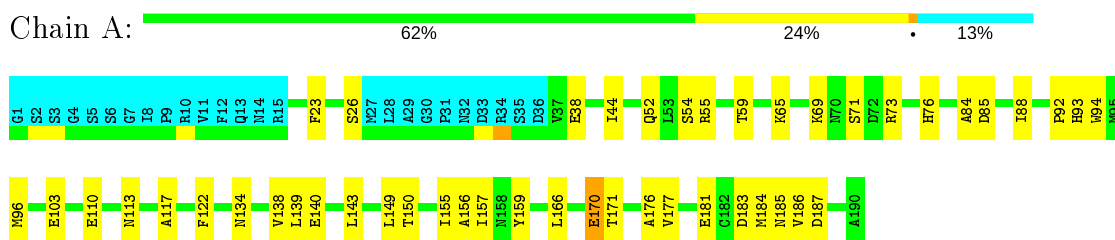
4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin fusion degradation 1-like



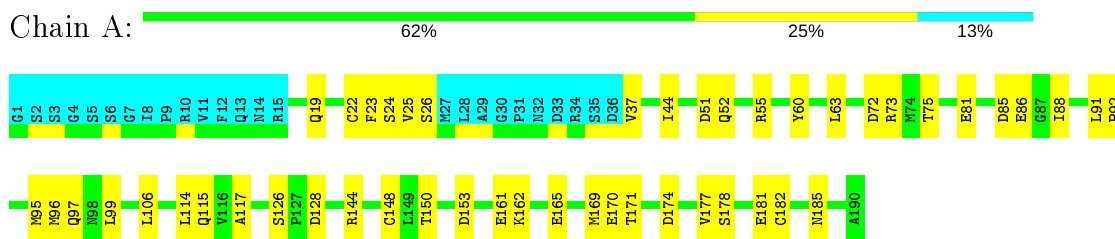
4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin fusion degradation 1-like



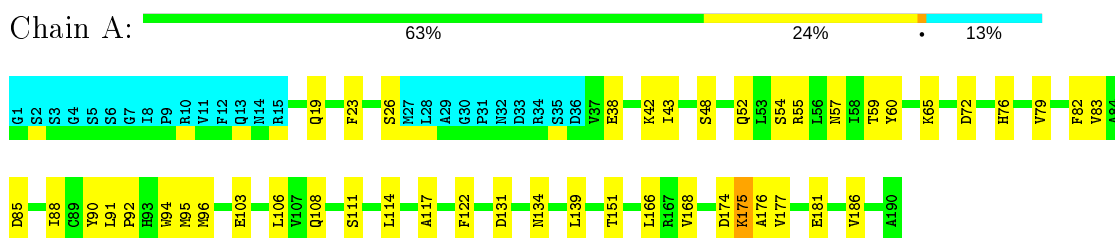
4.2.14 Score per residue for model 14

- Molecule 1: Ubiquitin fusion degradation 1-like



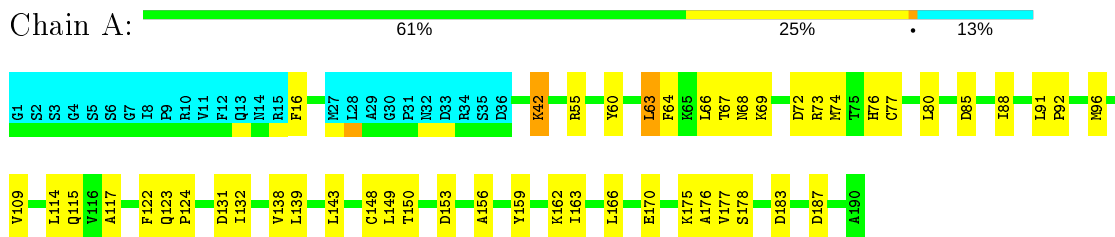
4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin fusion degradation 1-like



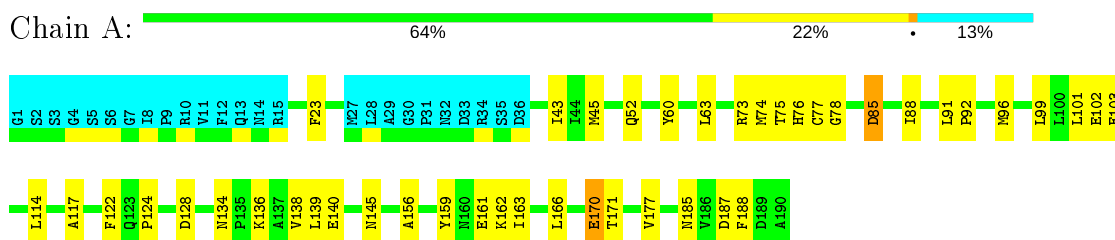
4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin fusion degradation 1-like



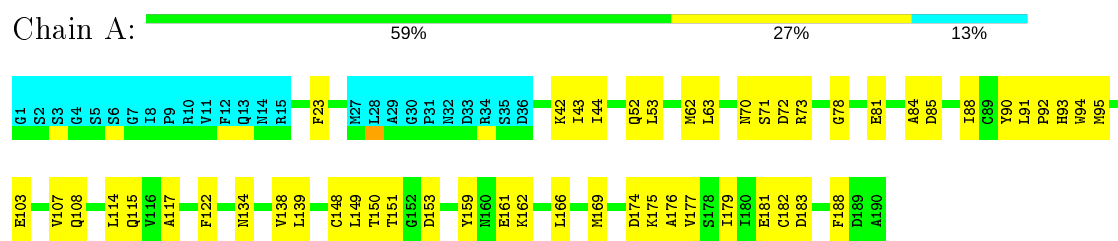
4.2.17 Score per residue for model 17

- Molecule 1: Ubiquitin fusion degradation 1-like



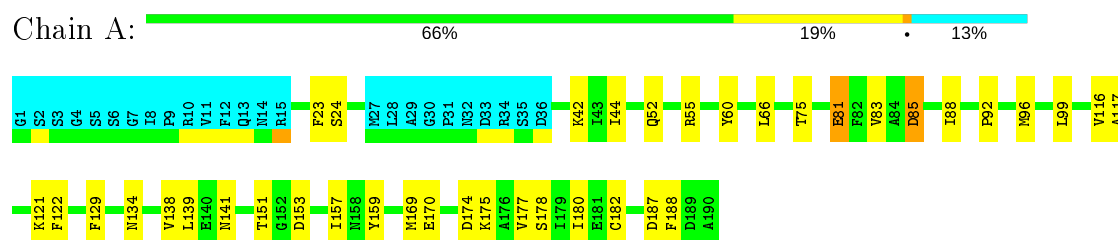
4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin fusion degradation 1-like



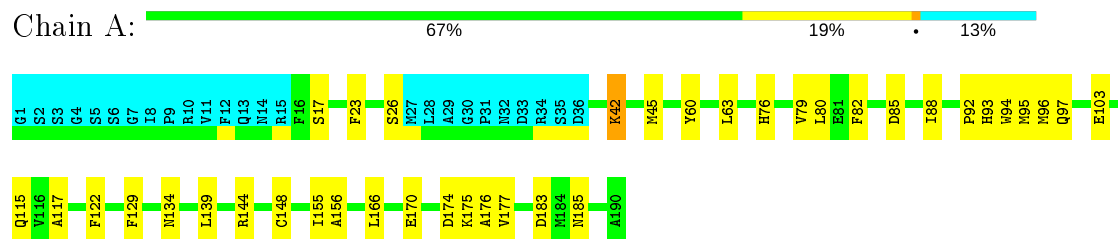
4.2.19 Score per residue for model 19

- Molecule 1: Ubiquitin fusion degradation 1-like



4.2.20 Score per residue for model 20

- Molecule 1: Ubiquitin fusion degradation 1-like



5 Refinement protocol and experimental data overview

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. No validations of the models with respect to experimental NMR restraints is performed at this time.

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	1306	1297	1297	15±4
All	All	26120	25940	25940	293

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:ALA:HB2	1:A:177:VAL:HG21	0.79	1.52	9	19
1:A:79:VAL:HG21	1:A:82:PHE:CZ	0.78	2.12	3	7
1:A:74:MET:O	1:A:150:THR:HG21	0.73	1.83	16	1
1:A:43:ILE:HG21	1:A:91:LEU:HD23	0.70	1.62	1	7
1:A:122:PHE:CG	1:A:139:LEU:HD21	0.69	2.22	17	3
1:A:94:TRP:CZ3	1:A:155:ILE:HG22	0.68	2.24	7	6
1:A:139:LEU:HD22	1:A:188:PHE:CZ	0.66	2.25	2	4
1:A:132:ILE:HG21	1:A:138:VAL:HG21	0.66	1.66	16	1
1:A:122:PHE:CD2	1:A:139:LEU:HD21	0.66	2.25	9	3
1:A:23:PHE:CD2	1:A:88:ILE:HG23	0.64	2.27	3	14
1:A:63:LEU:HD13	1:A:148:CYS:SG	0.64	2.32	4	3
1:A:75:THR:HG21	1:A:99:LEU:HD11	0.63	1.71	19	4
1:A:50:LEU:HD13	1:A:82:PHE:CD2	0.62	2.28	3	2
1:A:50:LEU:HD13	1:A:82:PHE:CE2	0.62	2.30	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:ASN:O	1:A:138:VAL:HG23	0.61	1.95	18	4
1:A:117:ALA:HB2	1:A:177:VAL:CG2	0.61	2.25	10	11
1:A:85:ASP:CB	1:A:88:ILE:HD12	0.61	2.26	19	3
1:A:43:ILE:HG22	1:A:92:PRO:HD3	0.61	1.72	1	2
1:A:139:LEU:HD12	1:A:166:LEU:HD13	0.60	1.70	1	1
1:A:151:THR:HG22	1:A:175:LYS:CB	0.60	2.26	15	1
1:A:122:PHE:CD1	1:A:139:LEU:HD21	0.60	2.32	19	5
1:A:43:ILE:CG2	1:A:91:LEU:HD23	0.60	2.27	1	4
1:A:138:VAL:HG11	1:A:159:TYR:CZ	0.59	2.33	19	1
1:A:63:LEU:HD13	1:A:114:LEU:HD12	0.58	1.75	14	2
1:A:151:THR:HG23	1:A:169:MET:O	0.58	1.99	18	2
1:A:156:ALA:HB1	1:A:163:ILE:CG2	0.57	2.29	10	5
1:A:114:LEU:HD13	1:A:176:ALA:O	0.57	1.99	9	1
1:A:132:ILE:HD13	1:A:138:VAL:HG21	0.57	1.77	4	2
1:A:124:PRO:HA	1:A:166:LEU:HD23	0.56	1.77	17	1
1:A:139:LEU:HD22	1:A:188:PHE:CE1	0.56	2.35	7	1
1:A:19:GLN:HB3	1:A:106:LEU:HD22	0.56	1.78	15	4
1:A:63:LEU:HD23	1:A:78:GLY:HA2	0.56	1.78	17	1
1:A:146:PHE:HB3	1:A:179:ILE:HD11	0.55	1.79	10	1
1:A:151:THR:HG22	1:A:175:LYS:HB2	0.55	1.79	15	1
1:A:63:LEU:HD23	1:A:78:GLY:CA	0.55	2.32	2	2
1:A:85:ASP:HB2	1:A:88:ILE:HD12	0.54	1.79	16	2
1:A:64:PHE:CD1	1:A:109:VAL:HG12	0.54	2.38	16	2
1:A:75:THR:HG22	1:A:99:LEU:HD21	0.54	1.80	14	4
1:A:122:PHE:CE2	1:A:139:LEU:HD21	0.54	2.36	9	1
1:A:122:PHE:CE2	1:A:168:VAL:HG22	0.54	2.37	7	3
1:A:116:VAL:HG21	1:A:182:CYS:SG	0.53	2.43	19	1
1:A:43:ILE:HD13	1:A:77:CYS:SG	0.53	2.44	3	4
1:A:172:LYS:O	1:A:177:VAL:HG11	0.53	2.04	7	2
1:A:66:LEU:HB2	1:A:75:THR:HG23	0.52	1.82	19	2
1:A:76:HIS:CE1	1:A:176:ALA:HB2	0.52	2.39	4	5
1:A:52:GLN:HG2	1:A:56:LEU:HD11	0.52	1.80	9	1
1:A:124:PRO:HG3	1:A:166:LEU:HD21	0.52	1.80	3	1
1:A:143:LEU:HD22	1:A:149:LEU:HD11	0.51	1.82	16	1
1:A:42:LYS:HB3	1:A:80:LEU:HD22	0.51	1.81	16	2
1:A:84:ALA:HB1	1:A:88:ILE:O	0.51	2.05	9	2
1:A:53:LEU:HA	1:A:56:LEU:HD12	0.51	1.82	1	1
1:A:63:LEU:HD21	1:A:147:ALA:HB1	0.51	1.81	7	1
1:A:132:ILE:HG21	1:A:138:VAL:CG2	0.51	2.35	16	1
1:A:63:LEU:HD22	1:A:148:CYS:HB2	0.51	1.81	3	3
1:A:53:LEU:HD13	1:A:62:MET:SD	0.51	2.45	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LEU:HD11	1:A:178:SER:OG	0.51	2.05	14	3
1:A:140:GLU:HA	1:A:143:LEU:HD12	0.51	1.83	11	1
1:A:85:ASP:HB3	1:A:88:ILE:HD12	0.51	1.81	15	4
1:A:46:PRO:N	1:A:84:ALA:HB3	0.50	2.20	11	2
1:A:75:THR:CG2	1:A:99:LEU:HD21	0.50	2.36	9	1
1:A:146:PHE:CE2	1:A:155:ILE:HD13	0.50	2.41	8	1
1:A:50:LEU:HA	1:A:53:LEU:HD12	0.50	1.84	8	1
1:A:94:TRP:HB3	1:A:156:ALA:HB3	0.50	1.84	13	2
1:A:122:PHE:CZ	1:A:143:LEU:HD21	0.50	2.42	11	1
1:A:155:ILE:HD12	1:A:157:ILE:HG23	0.50	1.82	13	1
1:A:129:PHE:CE2	1:A:166:LEU:HD11	0.50	2.42	11	2
1:A:117:ALA:HB2	1:A:177:VAL:CB	0.49	2.37	13	4
1:A:75:THR:CG2	1:A:99:LEU:HD11	0.49	2.38	7	1
1:A:151:THR:HG23	1:A:151:THR:O	0.49	2.07	15	1
1:A:68:ASN:OD1	1:A:101:LEU:HD21	0.48	2.08	1	2
1:A:117:ALA:HB3	1:A:184:MET:SD	0.48	2.49	9	1
1:A:25:VAL:HG11	1:A:37:VAL:HG21	0.47	1.85	14	1
1:A:94:TRP:CH2	1:A:95:MET:HE2	0.47	2.45	9	1
1:A:154:VAL:HG22	1:A:167:ARG:HG3	0.47	1.87	10	1
1:A:44:ILE:HG22	1:A:84:ALA:HB2	0.47	1.84	18	1
1:A:122:PHE:CZ	1:A:143:LEU:HD11	0.47	2.44	4	1
1:A:44:ILE:HG23	1:A:81:GLU:HB3	0.47	1.86	19	1
1:A:139:LEU:CD1	1:A:166:LEU:HD13	0.47	2.39	1	1
1:A:76:HIS:CD2	1:A:114:LEU:HD11	0.47	2.45	15	2
1:A:114:LEU:HD22	1:A:176:ALA:O	0.46	2.10	18	2
1:A:91:LEU:HD22	1:A:95:MET:SD	0.46	2.50	6	1
1:A:20:TYR:HB2	1:A:109:VAL:HG21	0.46	1.87	10	1
1:A:157:ILE:HG12	1:A:166:LEU:HD12	0.46	1.88	11	1
1:A:124:PRO:CA	1:A:166:LEU:HD23	0.46	2.39	17	1
1:A:178:SER:OG	1:A:180:ILE:HD11	0.46	2.10	19	1
1:A:146:PHE:CZ	1:A:155:ILE:HD13	0.46	2.45	10	1
1:A:138:VAL:HG11	1:A:159:TYR:CE1	0.46	2.46	19	1
1:A:42:LYS:HG2	1:A:80:LEU:HD13	0.46	1.87	3	3
1:A:163:ILE:N	1:A:163:ILE:HD12	0.46	2.26	8	1
1:A:170:GLU:O	1:A:171:THR:HG23	0.46	2.11	17	2
1:A:114:LEU:HD13	1:A:148:CYS:SG	0.45	2.52	5	1
1:A:45:MET:C	1:A:84:ALA:HB3	0.45	2.32	11	1
1:A:43:ILE:HG21	1:A:91:LEU:CD2	0.45	2.42	18	1
1:A:159:TYR:CD1	1:A:159:TYR:N	0.45	2.85	19	1
1:A:159:TYR:CD1	1:A:160:ASN:N	0.45	2.85	5	1
1:A:66:LEU:HD11	1:A:77:CYS:SG	0.45	2.52	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:LEU:HD23	1:A:186:VAL:HG11	0.45	1.88	15	1
1:A:25:VAL:HG11	1:A:37:VAL:HG11	0.45	1.88	4	1
1:A:138:VAL:HG13	1:A:159:TYR:OH	0.45	2.11	10	1
1:A:94:TRP:CD2	1:A:95:MET:N	0.45	2.85	5	2
1:A:73:ARG:HB3	1:A:99:LEU:HD23	0.45	1.89	8	2
1:A:63:LEU:HD22	1:A:148:CYS:SG	0.44	2.52	16	1
1:A:132:ILE:HG22	1:A:134:ASN:H	0.44	1.72	12	3
1:A:99:LEU:HD13	1:A:101:LEU:HD11	0.44	1.89	17	1
1:A:127:PRO:HA	1:A:130:LEU:HD12	0.44	1.88	1	2
1:A:138:VAL:CG1	1:A:159:TYR:CE2	0.44	3.01	5	1
1:A:79:VAL:HG21	1:A:82:PHE:CE2	0.44	2.47	2	1
1:A:23:PHE:CZ	1:A:104:GLY:CA	0.44	3.01	6	1
1:A:143:LEU:CD2	1:A:149:LEU:HD11	0.44	2.43	4	1
1:A:140:GLU:OE2	1:A:186:VAL:HG21	0.43	2.13	13	1
1:A:22:CYS:HB2	1:A:91:LEU:HD13	0.43	1.89	14	1
1:A:42:LYS:HG2	1:A:80:LEU:HD22	0.43	1.91	11	2
1:A:63:LEU:CD2	1:A:147:ALA:HB1	0.43	2.43	7	1
1:A:129:PHE:CE1	1:A:166:LEU:HD11	0.43	2.49	7	1
1:A:66:LEU:HD12	1:A:77:CYS:SG	0.43	2.54	16	3
1:A:76:HIS:CE1	1:A:176:ALA:CB	0.42	3.02	16	1
1:A:129:PHE:CE1	1:A:157:ILE:HD11	0.42	2.49	19	1
1:A:79:VAL:HG21	1:A:82:PHE:CE1	0.42	2.49	15	1
1:A:79:VAL:HG22	1:A:80:LEU:N	0.42	2.29	4	1
1:A:66:LEU:HD23	1:A:109:VAL:HG22	0.42	1.91	16	1
1:A:159:TYR:CE1	1:A:164:TYR:CD1	0.42	3.08	8	1
1:A:44:ILE:HG23	1:A:81:GLU:HB2	0.42	1.91	14	1
1:A:107:VAL:HG12	1:A:108:GLN:N	0.42	2.29	18	1
1:A:149:LEU:HD12	1:A:179:ILE:HG21	0.42	1.91	18	1
1:A:22:CYS:HB2	1:A:91:LEU:HD12	0.42	1.91	7	1
1:A:44:ILE:O	1:A:84:ALA:HB2	0.42	2.14	13	1
1:A:79:VAL:CG2	1:A:82:PHE:CZ	0.42	3.03	9	1
1:A:42:LYS:HG3	1:A:80:LEU:HD22	0.41	1.92	7	1
1:A:121:LYS:O	1:A:168:VAL:HG13	0.41	2.15	1	1
1:A:129:PHE:CD1	1:A:166:LEU:HD11	0.41	2.50	7	1
1:A:94:TRP:CE3	1:A:95:MET:N	0.41	2.88	15	1
1:A:94:TRP:CH2	1:A:95:MET:CE	0.41	3.04	9	3
1:A:63:LEU:HD22	1:A:78:GLY:CA	0.41	2.46	18	1
1:A:63:LEU:HD23	1:A:78:GLY:HA3	0.41	1.91	2	1
1:A:82:PHE:O	1:A:83:VAL:HG13	0.41	2.16	2	1
1:A:64:PHE:CD1	1:A:109:VAL:CG1	0.41	3.04	16	1
1:A:159:TYR:N	1:A:159:TYR:CD1	0.41	2.89	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:VAL:HG21	1:A:38:GLU:OE1	0.41	2.15	6	1
1:A:122:PHE:CE1	1:A:168:VAL:HG22	0.41	2.50	9	1
1:A:53:LEU:HD23	1:A:58:ILE:HD12	0.41	1.93	12	1
1:A:38:GLU:O	1:A:94:TRP:CD1	0.41	2.74	4	1
1:A:139:LEU:CD2	1:A:186:VAL:HG11	0.40	2.46	1	1
1:A:143:LEU:HD13	1:A:184:MET:CE	0.40	2.46	13	1
1:A:75:THR:HG23	1:A:75:THR:O	0.40	2.16	7	1
1:A:42:LYS:HE3	1:A:80:LEU:HD13	0.40	1.93	7	1
1:A:16:PHE:CE2	1:A:18:THR:HG22	0.40	2.51	5	1
1:A:156:ALA:HB1	1:A:163:ILE:HG22	0.40	1.91	10	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	164/190 (86%)	146±2 (89±1%)	15±3 (9±2%)	2±1 (1±0%)	14	59
All	All	3280/3800 (86%)	2928 (89%)	303 (9%)	49 (1%)	14	59

All 10 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	92	PRO	17
1	A	159	TYR	13
1	A	83	VAL	7
1	A	103	GLU	5
1	A	124	PRO	2
1	A	70	ASN	1
1	A	181	GLU	1
1	A	88	ILE	1
1	A	16	PHE	1
1	A	66	LEU	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	149/169 (88%)	128±3 (86±2%)	21±3 (14±2%)	6	46
All	All	2980/3380 (88%)	2558 (86%)	422 (14%)	6	46

All 76 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	187	ASP	14
1	A	175	LYS	14
1	A	42	LYS	13
1	A	96	MET	13
1	A	60	TYR	12
1	A	52	GLN	12
1	A	170	GLU	12
1	A	153	ASP	11
1	A	85	ASP	11
1	A	166	LEU	11
1	A	185	ASN	11
1	A	55	ARG	10
1	A	115	GLN	9
1	A	174	ASP	9
1	A	38	GLU	9
1	A	183	ASP	8
1	A	150	THR	8
1	A	128	ASP	8
1	A	148	CYS	8
1	A	131	ASP	8
1	A	26	SER	8
1	A	162	LYS	7
1	A	72	ASP	7
1	A	59	THR	7
1	A	181	GLU	7
1	A	134	ASN	7
1	A	71	SER	6
1	A	182	CYS	6
1	A	24	SER	6

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Mol	Chain	Res	Type	Models (Total)
1	A	93	HIS	6
1	A	73	ARG	6
1	A	51	ASP	6
1	A	45	MET	6
1	A	63	LEU	5
1	A	161	GLU	5
1	A	70	ASN	5
1	A	102	GLU	5
1	A	113	ASN	5
1	A	126	SER	5
1	A	54	SER	5
1	A	136	LYS	5
1	A	121	LYS	5
1	A	48	SER	4
1	A	57	ASN	4
1	A	65	LYS	4
1	A	97	GLN	4
1	A	103	GLU	4
1	A	141	ASN	4
1	A	74	MET	3
1	A	120	SER	3
1	A	91	LEU	3
1	A	95	MET	3
1	A	67	THR	3
1	A	16	PHE	3
1	A	145	ASN	3
1	A	69	LYS	3
1	A	171	THR	3
1	A	144	ARG	3
1	A	123	GLN	2
1	A	169	MET	2
1	A	108	GLN	2
1	A	111	SER	2
1	A	189	ASP	2
1	A	184	MET	2
1	A	81	GLU	2
1	A	178	SER	2
1	A	165	GLU	2
1	A	86	GLU	1
1	A	17	SER	1
1	A	149	LEU	1
1	A	140	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	21	ARG	1
1	A	151	THR	1
1	A	68	ASN	1
1	A	110	GLU	1
1	A	118	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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided