Full wwPDB NMR Structure Validation Report (i)

May 31, 2020 – 11:54 am BST

PDB ID	:	6OB1
Title	:	Structure of WHB in complex with Ubiquitin Variant
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Deposited on	:	2019-03-19

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 (1)) were used in the production of this report:

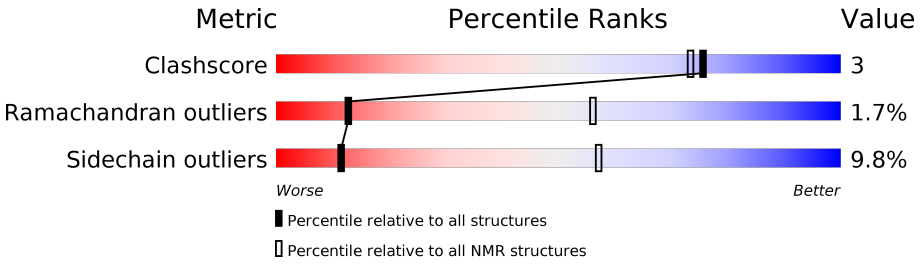
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 67%.

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	75	88% 12%
2	B	75	84% 13% .
3	C	90	72% 11% 17%

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:0-A:6, B:110-B:172 (70)	0.44	14
2	A:7-A:74, B:100-B:109, C:744-C:818 (153)	0.59	7

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3871 atoms, of which 1951 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						Trace
1	A	75	Total	C	H	N	O	S	0
			1222	381	621	100	119	1	

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						Trace
2	B	75	Total	C	H	N	O	S	0
			1215	379	614	100	121	1	

- Molecule 3 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms						Trace
3	C	90	Total	C	H	N	O	S	0
			1434	453	716	118	142	5	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	733	GLY	-	expression tag	UNP Q9UJX6
C	734	SER	-	expression tag	UNP Q9UJX6

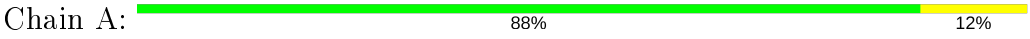
4 Residue-property plots

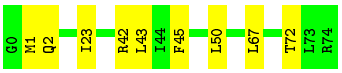
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Ubiquitin

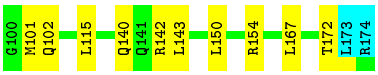
Chain A:





- Molecule 2: Ubiquitin

Chain B:



- Molecule 3: Anaphase-promoting complex subunit 2

Chain C:

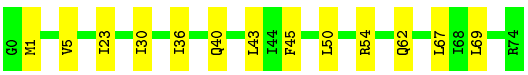
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

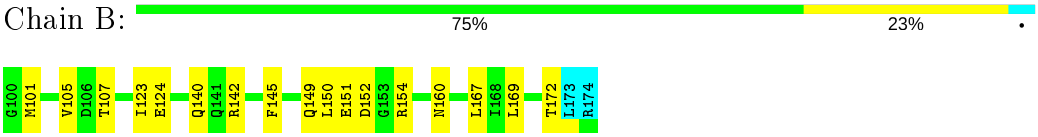
- Molecule 1: Ubiquitin

Chain A:



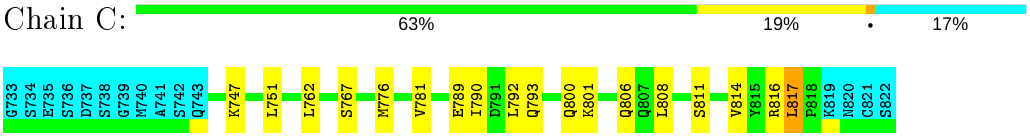
• Molecule 2: Ubiquitin

Chain B:



• Molecule 3: Anaphase-promoting complex subunit 2

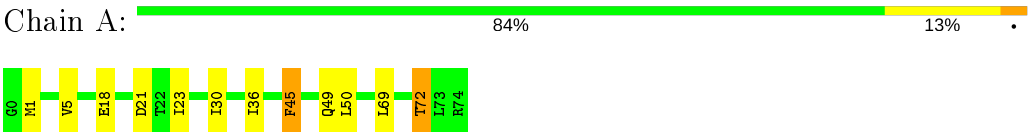
Chain C:



4.2.2 Score per residue for model 2

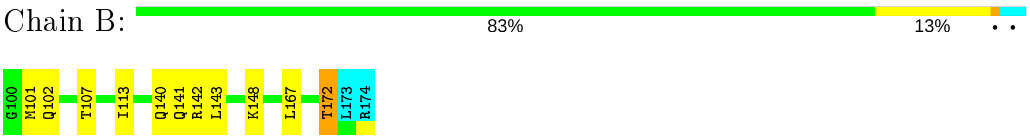
• Molecule 1: Ubiquitin

Chain A:



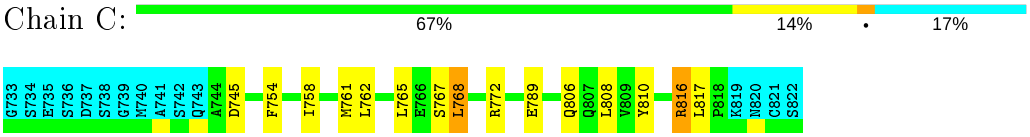
• Molecule 2: Ubiquitin

Chain B:



• Molecule 3: Anaphase-promoting complex subunit 2

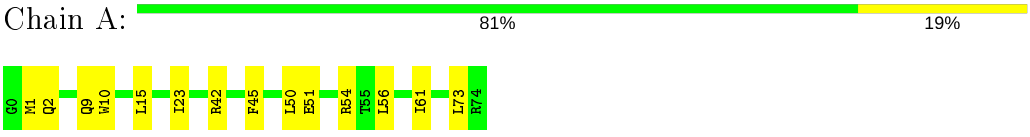
Chain C:



4.2.3 Score per residue for model 3

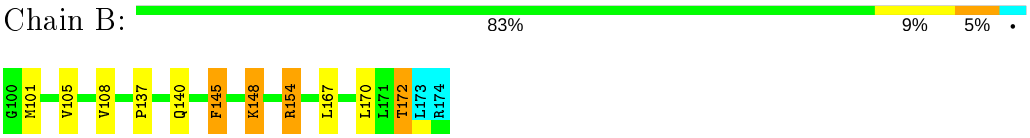
• Molecule 1: Ubiquitin

Chain A:



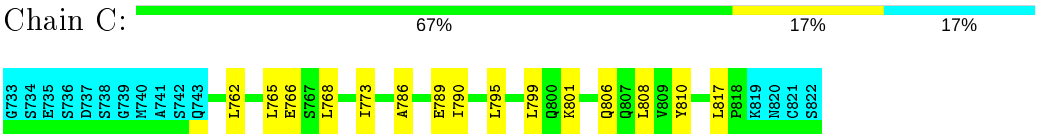
• Molecule 2: Ubiquitin

Chain B:



• Molecule 3: Anaphase-promoting complex subunit 2

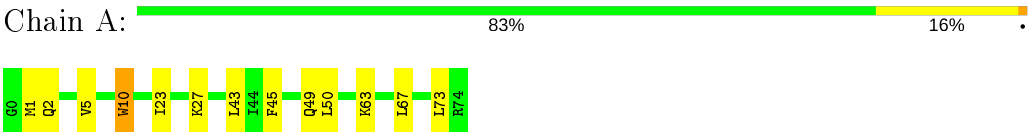
Chain C:



4.2.4 Score per residue for model 4

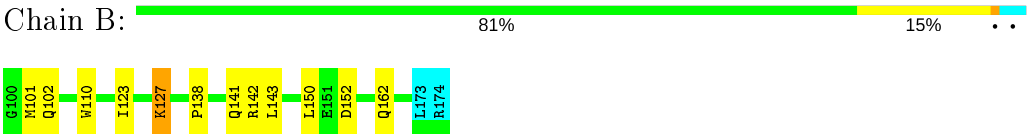
• Molecule 1: Ubiquitin

Chain A:



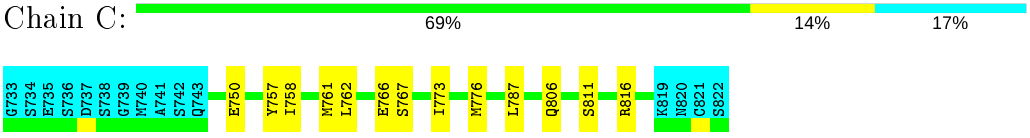
• Molecule 2: Ubiquitin

Chain B:



• Molecule 3: Anaphase-promoting complex subunit 2

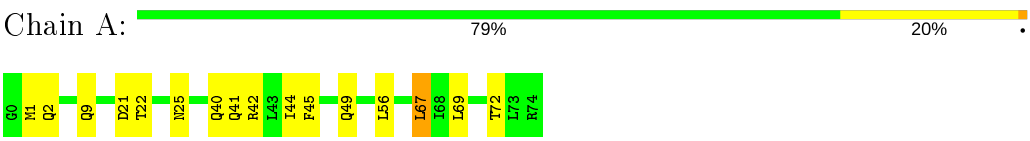
Chain C:



4.2.5 Score per residue for model 5

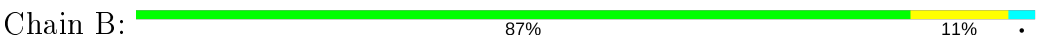
• Molecule 1: Ubiquitin

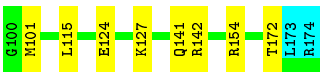
Chain A:



• Molecule 2: Ubiquitin

Chain B:





• Molecule 3: Anaphase-promoting complex subunit 2

Chain C:

4.2.6 Score per residue for model 6

• Molecule 1: Ubiquitin

Chain A:

• Molecule 2: Ubiquitin

Chain B:

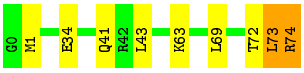
• Molecule 3: Anaphase-promoting complex subunit 2

Chain C:

4.2.7 Score per residue for model 7 (medoid)

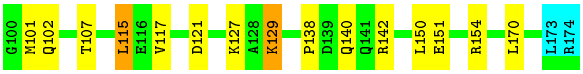
• Molecule 1: Ubiquitin

Chain A:



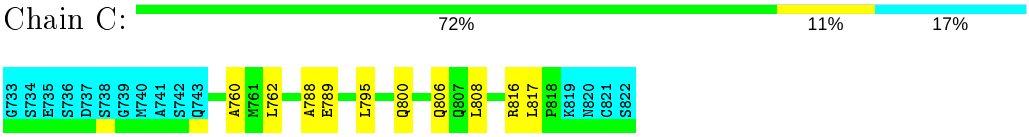
• Molecule 2: Ubiquitin

Chain B:



• Molecule 3: Anaphase-promoting complex subunit 2

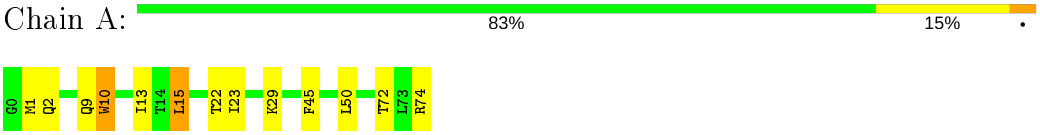
Chain C:



4.2.8 Score per residue for model 8

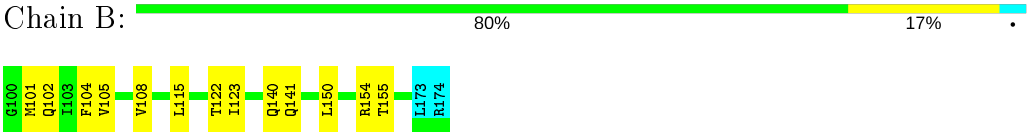
• Molecule 1: Ubiquitin

Chain A:



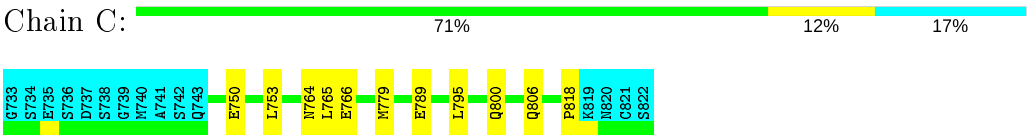
• Molecule 2: Ubiquitin

Chain B:



• Molecule 3: Anaphase-promoting complex subunit 2

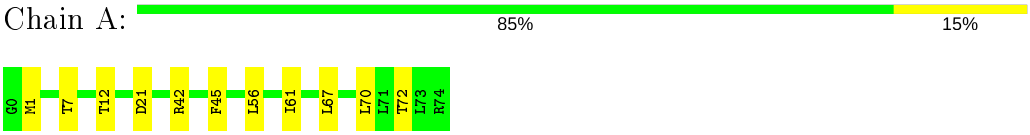
Chain C:



4.2.9 Score per residue for model 9

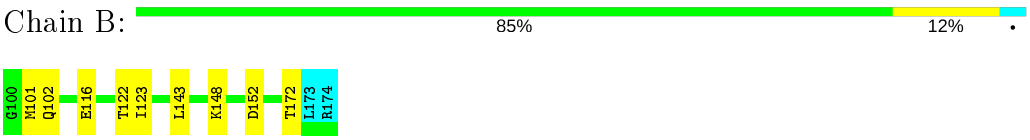
• Molecule 1: Ubiquitin

Chain A:



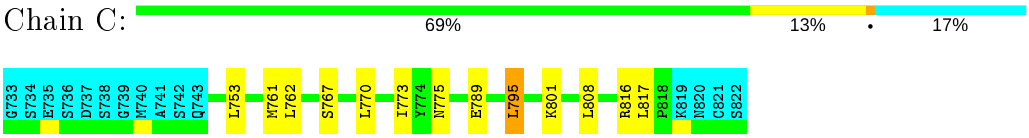
• Molecule 2: Ubiquitin

Chain B:



• Molecule 3: Anaphase-promoting complex subunit 2

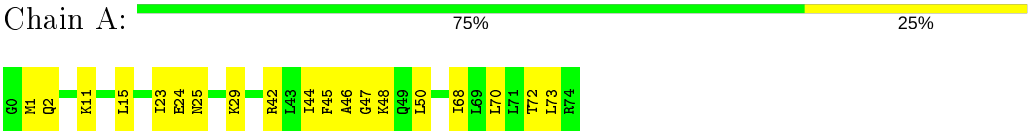
Chain C:



4.2.10 Score per residue for model 10

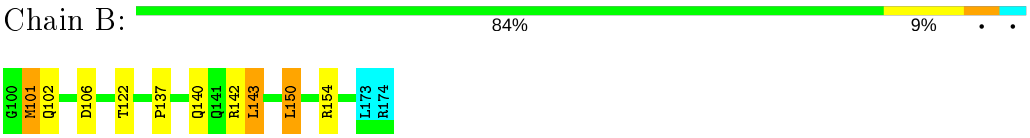
- Molecule 1: Ubiquitin

Chain A:



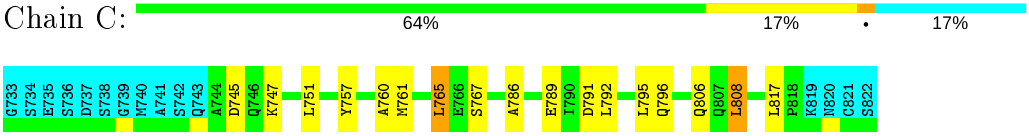
- Molecule 2: Ubiquitin

Chain B:



- Molecule 3: Anaphase-promoting complex subunit 2

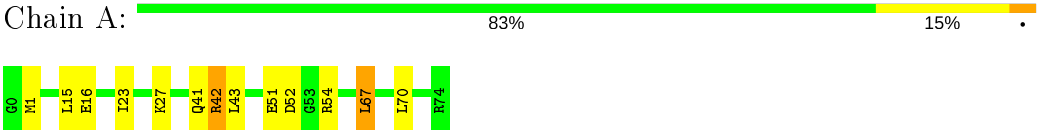
Chain C:



4.2.11 Score per residue for model 11

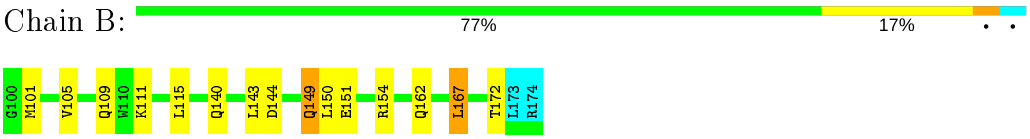
- Molecule 1: Ubiquitin

Chain A:



- Molecule 2: Ubiquitin

Chain B:



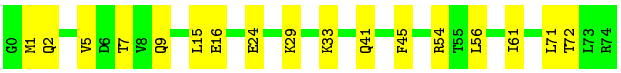
- Molecule 3: Anaphase-promoting complex subunit 2

Chain C:

4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin

Chain A:



- Molecule 2: Ubiquitin

Chain B:

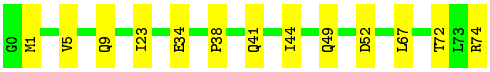
- Molecule 3: Anaphase-promoting complex subunit 2

Chain C:

4.2.13 Score per residue for model 13

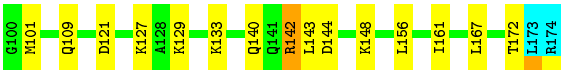
- Molecule 1: Ubiquitin

Chain A:



- Molecule 2: Ubiquitin

Chain B:



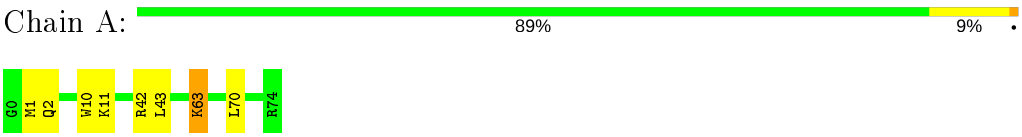
- Molecule 3: Anaphase-promoting complex subunit 2

Chain C:

4.2.14 Score per residue for model 14

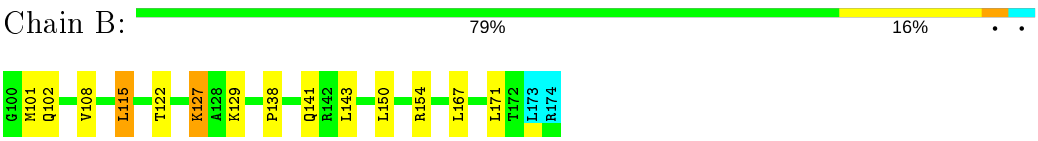
- Molecule 1: Ubiquitin

Chain A:



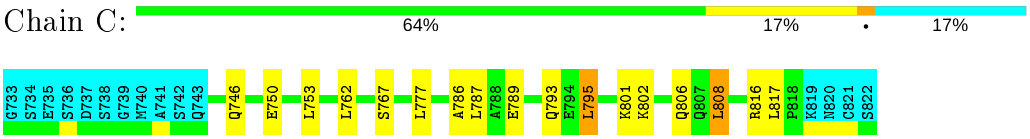
- Molecule 2: Ubiquitin

Chain B:



- Molecule 3: Anaphase-promoting complex subunit 2

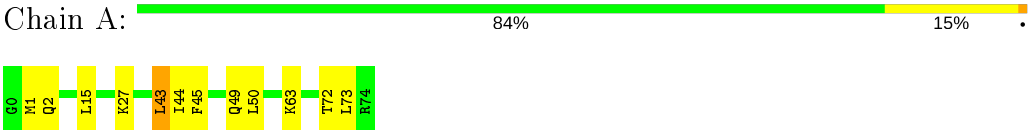
Chain C:



4.2.15 Score per residue for model 15

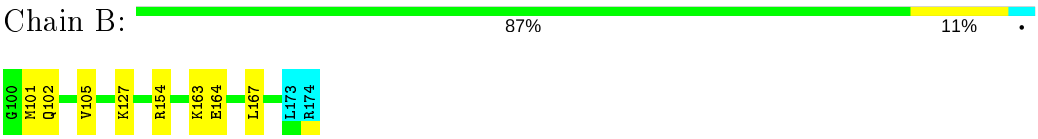
- Molecule 1: Ubiquitin

Chain A:



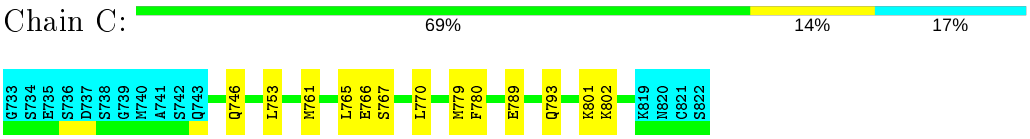
- Molecule 2: Ubiquitin

Chain B:



- Molecule 3: Anaphase-promoting complex subunit 2

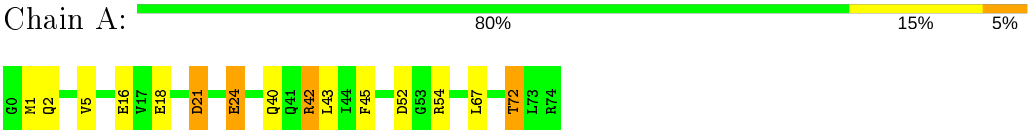
Chain C:



4.2.16 Score per residue for model 16

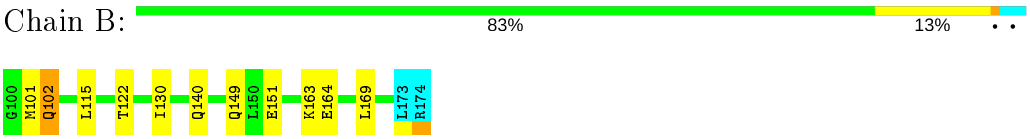
- Molecule 1: Ubiquitin

Chain A:



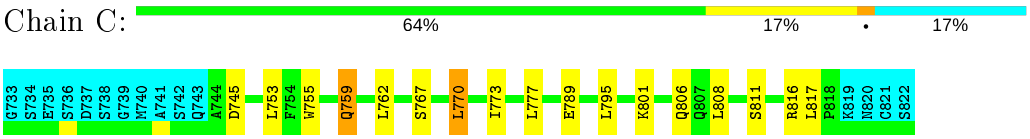
- Molecule 2: Ubiquitin

Chain B:



- Molecule 3: Anaphase-promoting complex subunit 2

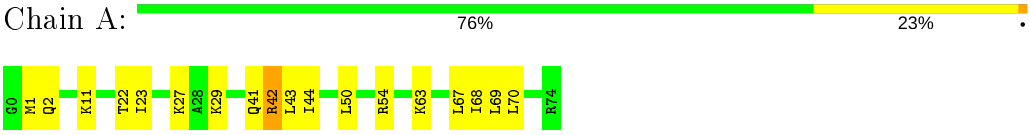
Chain C:



4.2.17 Score per residue for model 17

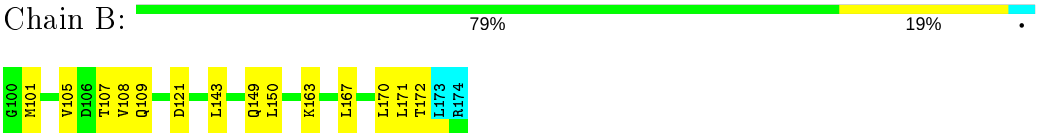
- Molecule 1: Ubiquitin

Chain A:



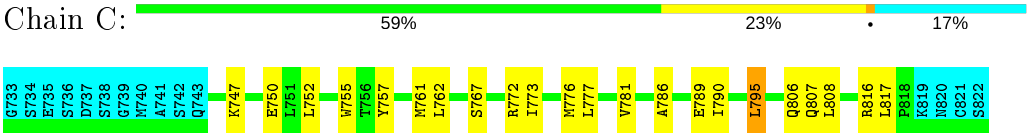
- Molecule 2: Ubiquitin

Chain B:



- Molecule 3: Anaphase-promoting complex subunit 2

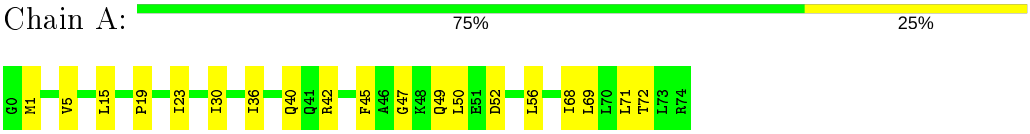
Chain C:



4.2.18 Score per residue for model 18

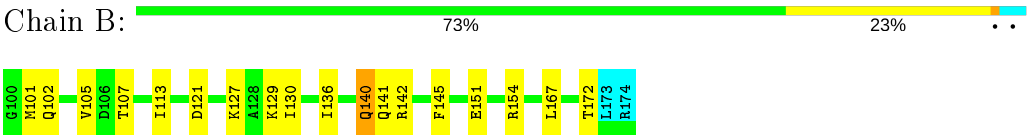
- Molecule 1: Ubiquitin

Chain A:



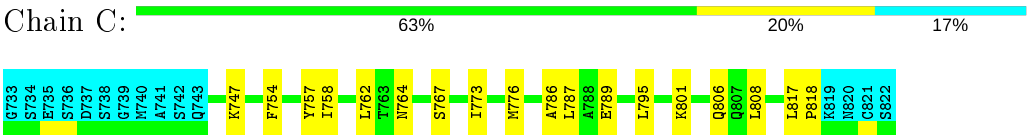
- Molecule 2: Ubiquitin

Chain B:



- Molecule 3: Anaphase-promoting complex subunit 2

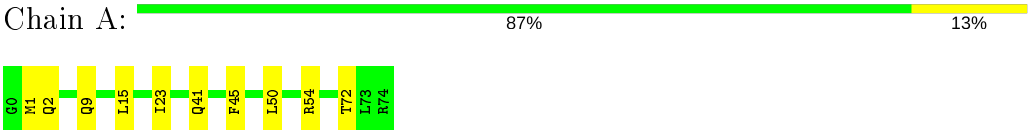
Chain C:



4.2.19 Score per residue for model 19

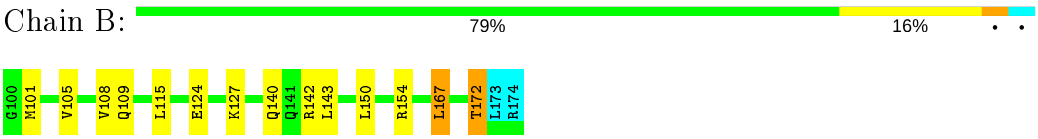
- Molecule 1: Ubiquitin

Chain A:



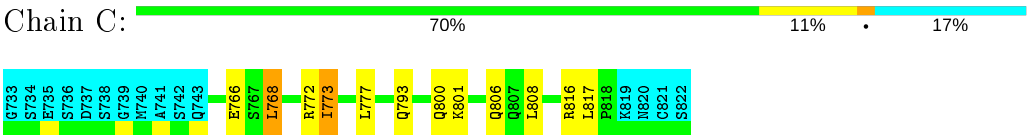
- Molecule 2: Ubiquitin

Chain B:



- Molecule 3: Anaphase-promoting complex subunit 2

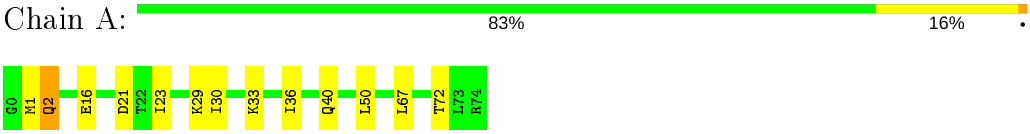
Chain C:



4.2.20 Score per residue for model 20

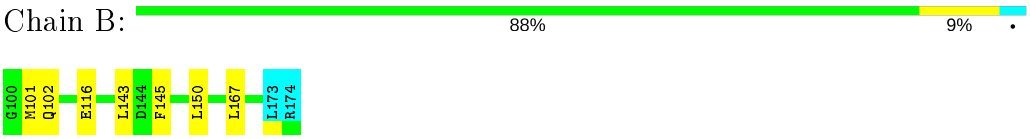
- Molecule 1: Ubiquitin

Chain A:



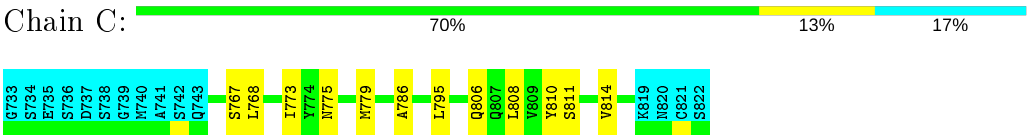
- Molecule 2: Ubiquitin

Chain B:



- Molecule 3: Anaphase-promoting complex subunit 2

Chain C:



5 Refinement protocol and experimental data overview

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

Of the 400 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
CYANA	structure calculation	
CYANA	refinement	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	2295
Number of shifts mapped to atoms	2295
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	67%

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

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	601	621	621	6±2
2	B	581	590	587	4±2
3	C	617	627	627	4±2
All	All	35980	36760	36700	222

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ILE:HG21	1:A:50:LEU:HB3	0.68	1.65	1	11
3:C:761:MET:SD	3:C:765:LEU:HD22	0.65	2.31	2	1
3:C:761:MET:SD	3:C:762:LEU:HD22	0.64	2.32	9	2
3:C:762:LEU:HB3	3:C:817:LEU:HB2	0.63	1.69	18	6
3:C:781:VAL:HG11	3:C:790:ILE:HG12	0.61	1.71	17	1
3:C:758:ILE:HD11	3:C:777:LEU:HD11	0.60	1.72	6	2
1:A:16:GLU:HG2	2:B:102:GLN:HG3	0.59	1.74	20	3
3:C:761:MET:HE1	3:C:765:LEU:HD11	0.58	1.75	10	1
1:A:69:LEU:HD12	2:B:107:THR:HG22	0.57	1.75	7	2
2:B:140:GLN:HA	2:B:172:THR:HB	0.57	1.74	2	3
2:B:142:ARG:HB2	2:B:172:THR:HA	0.56	1.78	19	1
2:B:115:LEU:HD13	2:B:129:LYS:HD3	0.56	1.77	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:GLU:HB2	1:A:21:ASP:HB2	0.56	1.78	2	3
3:C:777:LEU:HB3	3:C:795:LEU:HD21	0.54	1.78	17	1
1:A:11:LYS:HE3	2:B:171:LEU:HD23	0.53	1.79	17	1
1:A:69:LEU:HD22	2:B:107:THR:HG22	0.53	1.81	1	2
3:C:762:LEU:HD22	3:C:816:ARG:HA	0.52	1.81	14	5
1:A:49:GLN:NE2	3:C:753:LEU:HD21	0.52	2.19	15	1
1:A:68:ILE:HD12	3:C:776:MET:SD	0.52	2.44	17	2
2:B:144:ASP:HA	2:B:149:GLN:HA	0.52	1.82	11	1
1:A:56:LEU:HD13	1:A:61:ILE:HD12	0.51	1.80	9	1
1:A:42:ARG:HB2	1:A:70:LEU:HB2	0.51	1.80	9	5
3:C:747:LYS:HA	3:C:787:LEU:HD21	0.51	1.83	18	1
1:A:5:VAL:HB	2:B:113:ILE:HB	0.51	1.82	18	2
1:A:15:LEU:HD21	2:B:105:VAL:HG13	0.51	1.82	19	2
3:C:762:LEU:HD13	3:C:808:LEU:HD21	0.50	1.82	3	1
1:A:44:ILE:HG12	1:A:49:GLN:HG3	0.50	1.82	13	2
1:A:10:TRP:HE3	2:B:108:VAL:HB	0.50	1.67	14	2
1:A:44:ILE:HG21	3:C:757:TYR:CE1	0.50	2.42	17	1
3:C:766:GLU:HG2	3:C:773:ILE:HG23	0.50	1.82	19	1
1:A:41:GLN:HB3	1:A:69:LEU:HB3	0.50	1.83	5	1
2:B:143:LEU:HD21	2:B:150:LEU:H	0.50	1.67	10	1
2:B:143:LEU:HB3	2:B:167:LEU:HD11	0.50	1.84	13	1
3:C:768:LEU:HB2	3:C:772:ARG:HD2	0.49	1.85	2	1
1:A:51:GLU:HB3	1:A:54:ARG:HB2	0.49	1.84	3	1
1:A:9:GLN:HB3	2:B:109:GLN:HG3	0.49	1.82	12	1
2:B:137:PRO:HB2	2:B:140:GLN:HG2	0.49	1.84	10	1
1:A:15:LEU:HD11	2:B:105:VAL:HG13	0.49	1.85	8	1
1:A:11:LYS:NZ	2:B:171:LEU:HB2	0.49	2.23	14	1
1:A:2:GLN:HG3	2:B:116:GLU:HG2	0.49	1.84	20	1
3:C:761:MET:HB2	3:C:765:LEU:HD12	0.49	1.85	15	1
1:A:9:GLN:HB2	2:B:109:GLN:HB2	0.48	1.84	13	2
1:A:68:ILE:HA	2:B:106:ASP:HB2	0.48	1.85	10	1
1:A:10:TRP:HH2	3:C:776:MET:SD	0.48	2.32	4	1
1:A:24:GLU:HB3	1:A:52:ASP:HB3	0.48	1.83	16	1
3:C:811:SER:HB3	3:C:814:VAL:HG13	0.48	1.84	12	2
1:A:45:PHE:HB2	1:A:50:LEU:HD21	0.48	1.86	1	4
2:B:151:GLU:HB2	2:B:154:ARG:HG2	0.48	1.85	1	2
2:B:150:LEU:HD21	2:B:167:LEU:HD23	0.48	1.84	11	1
2:B:123:ILE:HB	2:B:152:ASP:HA	0.47	1.85	4	4
1:A:15:LEU:HD21	2:B:105:VAL:HG23	0.47	1.86	3	1
1:A:15:LEU:HD23	1:A:29:LYS:HD2	0.47	1.86	8	1
1:A:43:LEU:HB3	1:A:67:LEU:HD11	0.47	1.86	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:773:ILE:HD11	3:C:799:LEU:HD11	0.47	1.86	3	1
1:A:44:ILE:HG12	1:A:49:GLN:HG2	0.47	1.85	5	1
1:A:42:ARG:HG2	1:A:70:LEU:HB2	0.47	1.87	17	1
1:A:7:THR:HG22	2:B:169:LEU:HD22	0.47	1.85	12	1
2:B:145:PHE:HB2	2:B:150:LEU:HD21	0.47	1.87	20	2
1:A:30:ILE:HB	1:A:36:ILE:HD12	0.47	1.87	18	4
1:A:47:GLY:HA2	3:C:757:TYR:OH	0.46	2.10	18	2
2:B:115:LEU:HD13	2:B:129:LYS:HD2	0.46	1.88	14	1
2:B:123:ILE:HG21	2:B:150:LEU:HB3	0.46	1.88	8	2
1:A:29:LYS:O	1:A:33:LYS:HG2	0.46	2.11	20	2
1:A:67:LEU:HD23	2:B:105:VAL:HG12	0.46	1.88	17	2
1:A:5:VAL:HG13	2:B:143:LEU:HD21	0.46	1.86	4	2
1:A:38:PRO:HA	1:A:41:GLN:HB3	0.46	1.88	13	1
1:A:41:GLN:NE2	1:A:43:LEU:HD21	0.45	2.26	17	1
1:A:34:GLU:HB3	2:B:109:GLN:NE2	0.45	2.26	13	1
2:B:151:GLU:HB2	2:B:154:ARG:HB2	0.45	1.87	18	1
2:B:129:LYS:O	2:B:133:LYS:HG2	0.45	2.12	13	1
3:C:779:MET:SD	3:C:780:PHE:CD1	0.45	3.10	15	1
3:C:766:GLU:HG2	3:C:816:ARG:HB2	0.45	1.86	6	2
1:A:5:VAL:HB	2:B:169:LEU:HD11	0.45	1.86	1	1
1:A:45:PHE:CD1	1:A:67:LEU:HG	0.45	2.46	5	2
2:B:122:THR:HA	2:B:155:THR:HA	0.45	1.88	8	1
1:A:23:ILE:HB	1:A:52:ASP:HA	0.45	1.88	11	3
2:B:137:PRO:HB2	2:B:140:GLN:HB2	0.45	1.89	3	1
1:A:71:LEU:HB3	3:C:764:ASN:ND2	0.45	2.26	18	1
1:A:9:GLN:HB2	2:B:109:GLN:HB3	0.45	1.87	19	1
2:B:127:LYS:HD3	2:B:138:PRO:HB3	0.45	1.89	14	2
2:B:142:ARG:HB2	2:B:170:LEU:HB2	0.45	1.88	7	1
3:C:792:LEU:O	3:C:796:GLN:HB3	0.45	2.12	10	1
3:C:755:TRP:O	3:C:759:GLN:HG3	0.45	2.12	16	1
1:A:34:GLU:HG2	2:B:107:THR:HG21	0.44	1.89	7	1
1:A:10:TRP:HE1	2:B:108:VAL:HG22	0.44	1.71	8	1
2:B:151:GLU:HB3	2:B:154:ARG:HB2	0.44	1.89	11	1
3:C:746:GLN:O	3:C:750:GLU:HB2	0.44	2.13	12	1
2:B:150:LEU:HD11	2:B:167:LEU:HD23	0.44	1.89	19	2
1:A:25:ASN:O	1:A:29:LYS:HG2	0.44	2.13	10	1
2:B:167:LEU:HD12	2:B:167:LEU:N	0.43	2.27	11	1
3:C:762:LEU:HB3	3:C:817:LEU:HG	0.43	1.89	16	1
1:A:56:LEU:O	1:A:61:ILE:HG12	0.43	2.13	12	2
3:C:802:LYS:HB3	3:C:808:LEU:HB2	0.43	1.89	6	3
2:B:127:LYS:HB2	2:B:138:PRO:HB3	0.43	1.88	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:VAL:HG11	2:B:130:ILE:HG21	0.43	1.88	16	1
3:C:762:LEU:HD12	3:C:816:ARG:HA	0.43	1.91	1	1
3:C:790:ILE:HD12	3:C:795:LEU:HD23	0.43	1.88	3	1
1:A:63:LYS:H	1:A:63:LYS:HD2	0.43	1.73	14	1
2:B:101:MET:SD	2:B:101:MET:N	0.43	2.91	6	1
3:C:772:ARG:HB3	3:C:772:ARG:HH11	0.43	1.74	17	1
2:B:107:THR:HB	2:B:109:GLN:HE22	0.43	1.74	17	1
2:B:101:MET:N	2:B:101:MET:SD	0.43	2.92	10	1
1:A:67:LEU:HD23	2:B:105:VAL:HG22	0.43	1.89	11	1
3:C:777:LEU:HD23	3:C:795:LEU:HD21	0.43	1.89	14	1
2:B:130:ILE:HB	2:B:136:ILE:HD12	0.43	1.91	18	1
1:A:44:ILE:HG21	3:C:757:TYR:HE1	0.43	1.73	10	1
1:A:15:LEU:HD23	2:B:105:VAL:HG21	0.43	1.91	18	1
3:C:770:LEU:HD11	3:C:795:LEU:HD12	0.42	1.90	9	1
1:A:5:VAL:HG23	2:B:113:ILE:HB	0.42	1.91	12	1
1:A:43:LEU:HB3	1:A:67:LEU:HD21	0.42	1.90	16	1
1:A:69:LEU:HD12	2:B:107:THR:HB	0.42	1.91	2	1
3:C:747:LYS:O	3:C:751:LEU:HG	0.42	2.14	10	2
1:A:13:ILE:O	2:B:104:PHE:HA	0.42	2.13	8	1
3:C:808:LEU:HG	3:C:817:LEU:HD23	0.42	1.91	10	1
3:C:778:ARG:HA	3:C:781:VAL:HG12	0.42	1.91	11	1
1:A:22:THR:H	1:A:25:ASN:ND2	0.42	2.12	5	1
3:C:800:GLN:O	3:C:804:ARG:HG2	0.42	2.15	5	1
1:A:45:PHE:O	1:A:47:GLY:N	0.42	2.52	10	1
2:B:124:GLU:HA	2:B:127:LYS:HB3	0.42	1.92	19	1
1:A:21:ASP:O	1:A:56:LEU:HD23	0.42	2.15	5	1
2:B:145:PHE:O	2:B:148:LYS:HG2	0.41	2.14	3	1
1:A:73:LEU:HD23	3:C:760:ALA:HB2	0.41	1.91	7	1
1:A:5:VAL:HG22	2:B:167:LEU:HD23	0.41	1.91	13	1
1:A:19:PRO:HA	1:A:56:LEU:HB2	0.41	1.92	18	1
2:B:129:LYS:HA	2:B:129:LYS:HE2	0.41	1.91	18	1
3:C:762:LEU:HD21	3:C:768:LEU:HG	0.41	1.92	13	1
1:A:42:ARG:NH1	1:A:72:THR:HA	0.41	2.30	16	1
3:C:761:MET:HG3	3:C:762:LEU:HD12	0.41	1.93	17	1
1:A:74:ARG:HA	1:A:74:ARG:HE	0.41	1.76	8	1
2:B:156:LEU:HD12	2:B:161:ILE:HG13	0.41	1.92	13	1
3:C:764:ASN:HB2	3:C:765:LEU:HD12	0.41	1.92	8	1
3:C:754:PHE:O	3:C:758:ILE:HG13	0.41	2.15	18	2
3:C:811:SER:HB2	3:C:814:VAL:HG23	0.41	1.92	20	1
3:C:770:LEU:HD13	3:C:773:ILE:HD11	0.41	1.92	16	1
1:A:9:GLN:O	2:B:108:VAL:HA	0.41	2.16	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:154:ARG:NE	2:B:154:ARG:HA	0.41	2.31	3	1
3:C:755:TRP:HB2	3:C:798:TYR:OH	0.41	2.16	12	1
2:B:144:ASP:HA	2:B:148:LYS:O	0.41	2.15	13	1
3:C:762:LEU:O	3:C:766:GLU:HG3	0.41	2.16	13	1
1:A:16:GLU:HG2	2:B:102:GLN:HB3	0.41	1.91	16	1
2:B:140:GLN:NE2	2:B:141:GLN:HG3	0.41	2.31	18	1
3:C:809:VAL:HB	3:C:816:ARG:HG3	0.41	1.93	6	1
3:C:800:GLN:O	3:C:804:ARG:HD3	0.41	2.15	6	1
1:A:41:GLN:HA	1:A:71:LEU:HA	0.41	1.93	12	1
3:C:746:GLN:O	3:C:750:GLU:HG2	0.41	2.16	14	1
3:C:755:TRP:CZ2	3:C:807:GLN:HG2	0.41	2.51	17	1
1:A:73:LEU:HD12	3:C:760:ALA:HB2	0.40	1.93	10	2
3:C:762:LEU:HG	3:C:817:LEU:HD13	0.40	1.92	9	1
3:C:758:ILE:O	3:C:762:LEU:HB2	0.40	2.15	4	1
1:A:5:VAL:HG13	2:B:169:LEU:HD11	0.40	1.91	16	1
1:A:29:LYS:HE2	1:A:29:LYS:HA	0.40	1.93	17	1
1:A:73:LEU:HD13	1:A:74:ARG:HG3	0.40	1.93	7	1
1:A:43:LEU:HD13	1:A:50:LEU:HB2	0.40	1.94	15	1
3:C:762:LEU:HD21	3:C:768:LEU:HD11	0.40	1.94	2	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	73/75 (97%)	69±1 (94±2%)	4±1 (5±2%)	1±1 (1±1%)	21 69
2	B	72/75 (96%)	70±1 (97±1%)	2±1 (2±2%)	1±0 (1±1%)	24 71
3	C	75/90 (83%)	66±2 (88±3%)	6±2 (8±3%)	3±1 (3±1%)	6 37
All	All	4400/4800 (92%)	4092 (93%)	233 (5%)	75 (2%)	13 56

All 13 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	C	767	SER	15

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Mol	Chain	Res	Type	Models (Total)
3	C	789	GLU	14
2	B	172	THR	12
1	A	72	THR	11
3	C	786	ALA	10
3	C	766	GLU	3
3	C	818	PRO	2
3	C	788	ALA	2
3	C	811	SER	2
3	C	768	LEU	1
3	C	790	ILE	1
1	A	46	ALA	1
1	A	73	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	68/68 (100%)	62±2 (91±3%)	6±2 (9±3%)	14	61
2	B	66/68 (97%)	59±1 (90±2%)	7±1 (10±2%)	11	55
3	C	67/79 (85%)	60±2 (89±2%)	7±2 (11±2%)	10	55
All	All	4020/4300 (93%)	3625 (90%)	395 (10%)	11	57

All 93 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)
2	B	101	MET	20
1	A	1	MET	19
3	C	806	GLN	17
3	C	808	LEU	14
3	C	795	LEU	13
1	A	2	GLN	13
3	C	801	LYS	12
2	B	167	LEU	10
2	B	102	GLN	10
2	B	140	GLN	9
2	B	115	LEU	8

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Mol	Chain	Res	Type	Models (Total)
2	B	142	ARG	8
3	C	773	ILE	8
2	B	143	LEU	8
2	B	154	ARG	8
3	C	816	ARG	7
1	A	45	PHE	7
1	A	42	ARG	6
3	C	800	GLN	6
2	B	127	LYS	6
3	C	768	LEU	6
1	A	43	LEU	6
1	A	67	LEU	6
1	A	54	ARG	6
3	C	753	LEU	6
2	B	141	GLN	5
1	A	63	LYS	5
1	A	15	LEU	5
3	C	793	GLN	5
1	A	40	GLN	5
1	A	27	LYS	4
1	A	72	THR	4
3	C	810	TYR	4
3	C	779	MET	4
3	C	765	LEU	4
1	A	49	GLN	4
2	B	121	ASP	4
2	B	122	THR	4
3	C	750	GLU	4
2	B	149	GLN	4
2	B	163	LYS	3
1	A	41	GLN	3
2	B	148	LYS	3
1	A	21	ASP	3
2	B	150	LEU	3
2	B	145	PHE	3
1	A	73	LEU	3
3	C	770	LEU	3
3	C	775	ASN	3
1	A	24	GLU	3
3	C	817	LEU	3
3	C	745	ASP	2
2	B	124	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	9	GLN	2
1	A	74	ARG	2
3	C	787	LEU	2
2	B	108	VAL	2
3	C	746	GLN	2
1	A	10	TRP	2
2	B	129	LYS	2
3	C	772	ARG	2
3	C	777	LEU	2
2	B	170	LEU	2
2	B	109	GLN	2
1	A	22	THR	2
2	B	162	GLN	2
2	B	164	GLU	2
1	A	7	THR	1
1	A	62	GLN	1
3	C	757	TYR	1
3	C	789	GLU	1
1	A	16	GLU	1
3	C	781	VAL	1
3	C	791	ASP	1
3	C	778	ARG	1
3	C	752	LEU	1
1	A	11	LYS	1
2	B	117	VAL	1
3	C	794	GLU	1
2	B	151	GLU	1
2	B	110	TRP	1
1	A	12	THR	1
1	A	48	LYS	1
3	C	759	GLN	1
2	B	160	ASN	1
3	C	766	GLU	1
2	B	116	GLU	1
3	C	776	MET	1
2	B	111	LYS	1
3	C	747	LYS	1
1	A	51	GLU	1
3	C	802	LYS	1
3	C	792	LEU	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 carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

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

The completeness of assignment taking into account all chemical shift lists is 67% for the well-defined parts and 67% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *WHB_UbVm_deposit_031219.str*

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	2295
Number of shifts mapped to atoms	2295
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	203	-0.21 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	159	0.18 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	142	-0.04 ± 0.11	None needed (< 0.5 ppm)
^{15}N	198	0.66 ± 0.22	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 67%, i.e. 1908 atoms were assigned a chemical shift out of a possible 2836. 27 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	854/1099 (78%)	346/438 (79%)	326/446 (73%)	182/215 (85%)
Sidechain	956/1591 (60%)	592/923 (64%)	346/599 (58%)	18/69 (26%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	98/146 (67%)	62/76 (82%)	33/67 (49%)	3/3 (100%)
Overall	1908/2836 (67%)	1000/1437 (70%)	705/1112 (63%)	203/287 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 67%, i.e. 2034 atoms were assigned a chemical shift out of a possible 3017. 27 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	916/1184 (77%)	374/472 (79%)	345/480 (72%)	197/232 (85%)
Sidechain	1020/1687 (60%)	634/981 (65%)	366/631 (58%)	20/75 (27%)
Aromatic	98/146 (67%)	62/76 (82%)	33/67 (49%)	3/3 (100%)
Overall	2034/3017 (67%)	1070/1529 (70%)	744/1178 (63%)	220/310 (71%)

7.1.4 Statistically unusual chemical shifts (i)

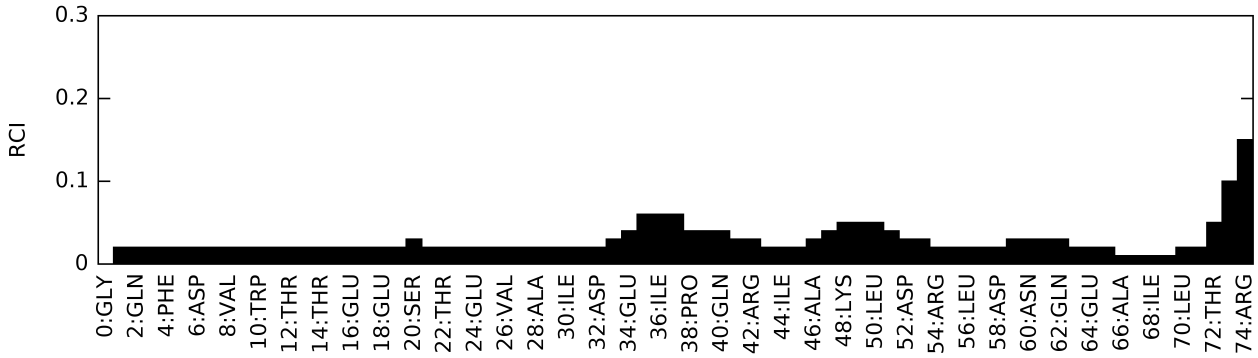
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
3	C	802	LYS	HE2	1.33	3.87 – 1.97	-8.4
3	C	802	LYS	HE3	1.65	3.86 – 1.96	-6.7
3	C	802	LYS	HD2	0.29	2.76 – 0.46	-5.7
3	C	802	LYS	HG2	-0.12	2.67 – 0.07	-5.7

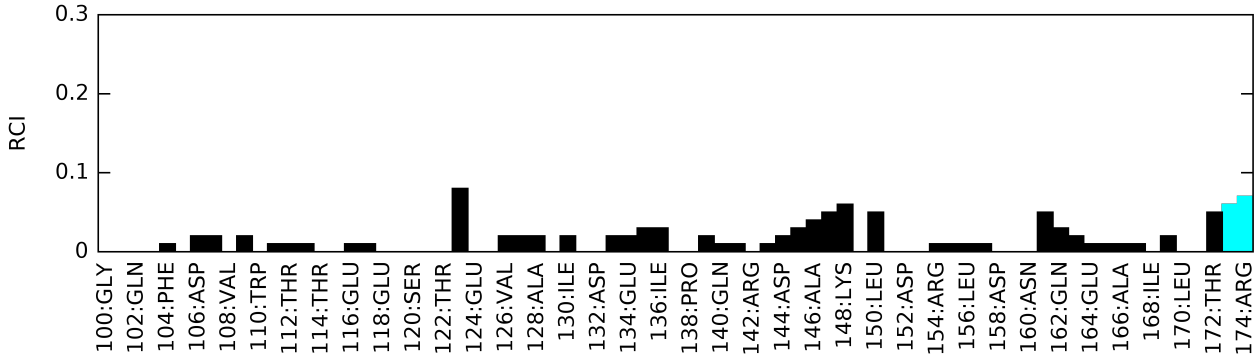
7.1.5 Random Coil Index (RCI) plots (i)

The images below report *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



Random coil index (RCI) for chain C: