Full wwPDB NMR Structure Validation Report (i)

May 2, 2016 – 10:42 PM EDT

PDB ID	:	2MWY
Title	:	Mdmx-p53
Authors	:	Grace, C.R.
Deposited on	:	2014-12-03

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

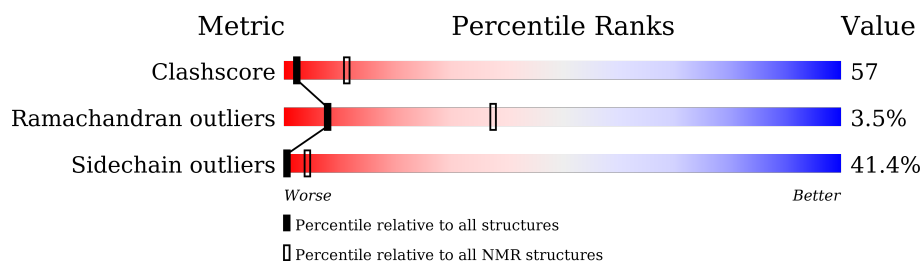|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 34%.

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	Percentile Ranks	Value
Clashscore		57
Ramachandran outliers		3.5%
Sidechain outliers		41.4%

Worse   *Better*

■ Percentile relative to all structures
▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	89	18% 60% 13% • 7%
2	B	15	33% 20% 47%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 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:3-A:85, B:119-B:126 (91)	0.34	4

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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1686 atoms, of which 849 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein Mdm4.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	89	1440	456	730	121	127	6	0

- Molecule 2 is a protein called Cellular tumor antigen p53.

| Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	15	246	82	119	19	26	0

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: Protein Mdm4
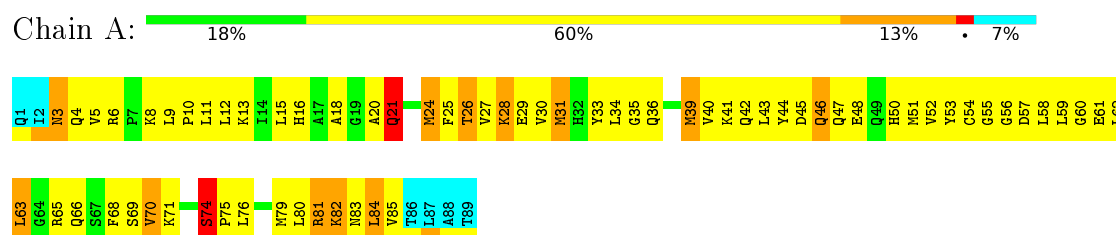
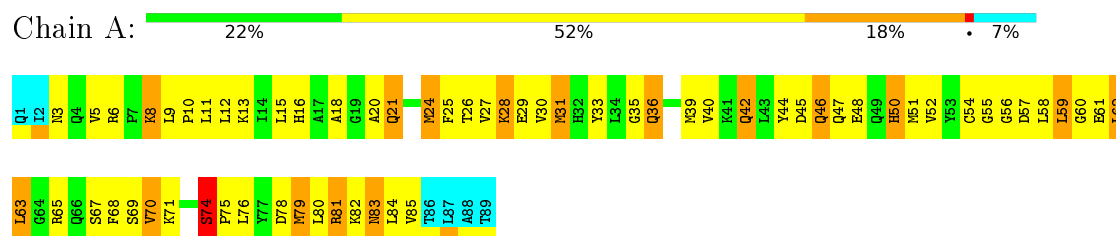- Molecule 2: Cellular tumor antigen p53
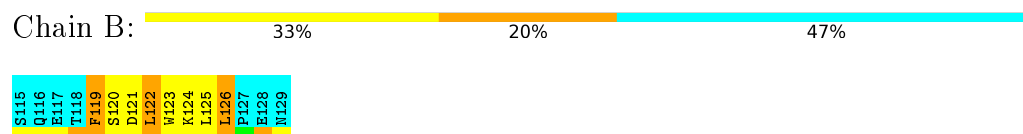
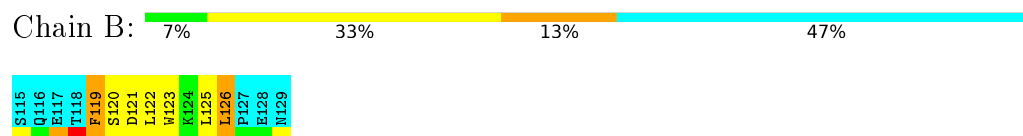

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Protein Mdm4

- Molecule 2: Cellular tumor antigen p53

Chain B: 7% 33% 13% 47%

S115 Q116 E117 T118 F119 S120 D121 L122 W123 K124 L125 L126 P127 E128 N129

4.2.2 Score per residue for model 2

• Molecule 1: Protein Mdm4

Chain A: 24% 46% 22% 7%

Q1 I2 N3 Q4 V5 R6 P7 K8 L9 P10 I11 L12 L15 H16 A17 A18 G19 A20 Q21 M24 F25 T26 V27 K28 E29 V30 N31 H32 Y33 I34 G35 Q36 M39 V40 K41 Q42 L43 Y44 D45 Q46 Q47 E48 Q49 H50 M51 V52 Y53 C54 G55 G56 D57 L58 L59 G60 L63

Q66 S67 F68 S69 V70 K71 D72 P73 S74 P75 D78 M79 L80 R81 K82 N83 L84 V85 T86 L87 A88 T89

• Molecule 2: Cellular tumor antigen p53

Chain B: 13% 20% 20% 47%

S115 Q116 E117 T118 F119 S120 D121 L122 W123 K124 L125 L126 P127 E128 N129
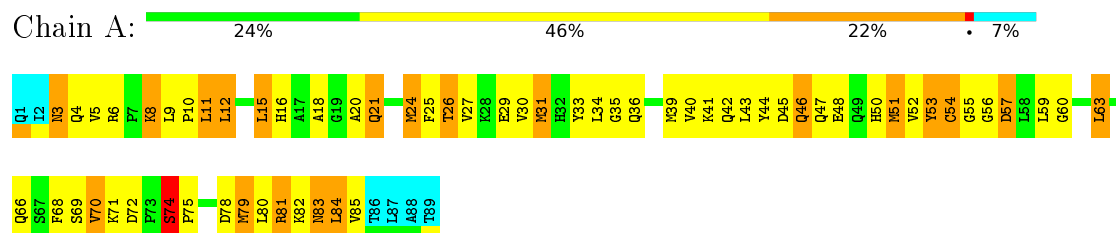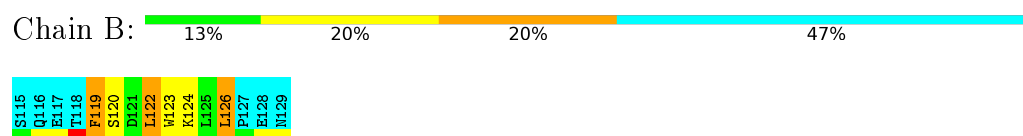
4.2.3 Score per residue for model 3

• Molecule 1: Protein Mdm4

Chain A: 28% 42% 21% 7%

Q1 I2 N3 Q4 V5 R6 P7 K8 L9 P10 I11 L12 K13 I14 L15 H16 A17 A18 G19 A20 Q21 Q22 E23 M24 F25 T26 V27 K28 E29 V30 N31 H32 Y33 L34 G35 Q36 M39 V40 K41 Q42 L43 Q46 Q47 E48 Q49 H50 M51 V52 Y53 C54 G55 G56 D57 L58 L59 L62 L63

G64 R65 Q66 S67 F68 S69 V70 K71 S74 P75 D78 M79 L80 R81 K82 N83 L84 V85 T86 L87 A88 T89

• Molecule 2: Cellular tumor antigen p53

Chain B: 7% 40% 7% 47%

S115 Q116 E117 T118 F119 S120 D121 L122 W123 K124 L125 L126 P127 E128 N129
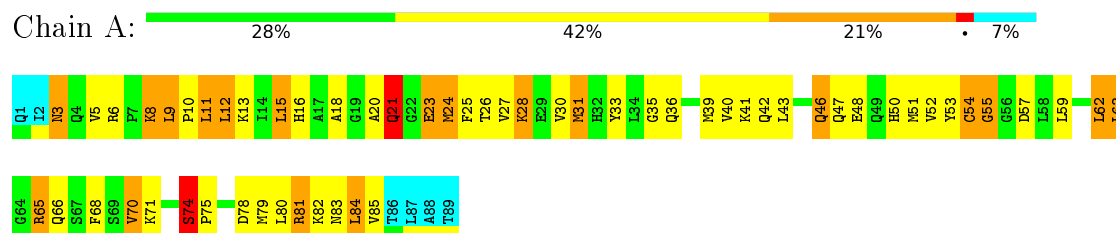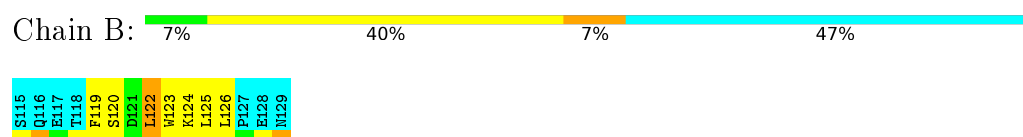
4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Protein Mdm4

Chain A: 19% 57% 15% 7%

Q1 I2 N3 Q4 V5 R6 P7 K8 L9 P10 L11 L12 K13 I14 L15 A18 G19 A20 Q21 M24 F25 T26 V27 K28 E29 V30 M31 H32 Y33 L34 G35 Q36 M39 V40 K41 Q42 L43 Y44 D45 Q46 Q47 E48 Q49 H50 M51 V52 Y53 C54 G55 G56 D57 L58 L59 G60 E61 L62 L63

G64 R65 Q66 S67 F68 S69 V70 K71 S74 P75 L76 M79 L80 R81 K82 N83 L84 V85 T86 L87 A88 T89

• Molecule 2: Cellular tumor antigen p53

Chain B: 20% 20% 13% 47%

S115 Q116 E117 T118 F119 L122 W123 K124 L125 L126 P127 E128 N129
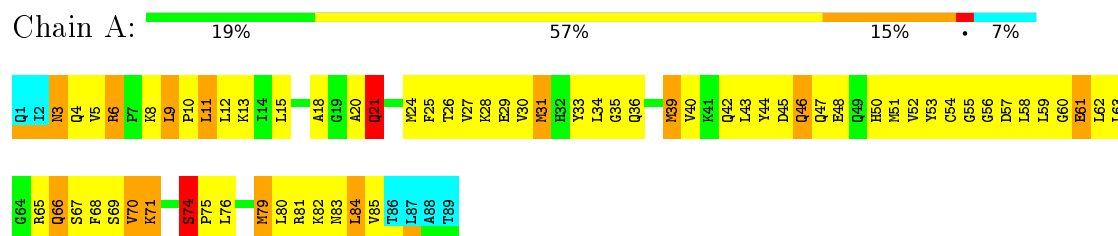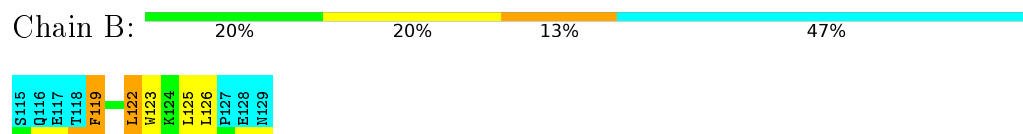
4.2.5 Score per residue for model 5

• Molecule 1: Protein Mdm4

Chain A: 28% 39% 25% 7%

Q1 I2 N3 Q4 V5 R6 L9 P10 L11 L12 K13 I14 L15 H16 A17 A18 G19 A20 Q21 G22 E23 M24 F25 V27 K28 E29 V30 M31 H32 Y33 L34 G35 Q36 M39 V40 K41 Q42 L43 Y44 D45 Q46 Q47 E48 Q49 H50 M51 V52 Y53 C54 G55 G56 D57 L58 L59 G60 E61 L62

L63 F68 S69 V70 K71 S74 P75 L76 Y77 D78 M79 L80 R81 K82 N83 L84 V85 T86 L87 A88 T89

• Molecule 2: Cellular tumor antigen p53

Chain B: 33% 20% 47%

S115 Q116 E117 T118 F119 S120 D121 L122 W123 K124 L125 L126 P127 E128 N129
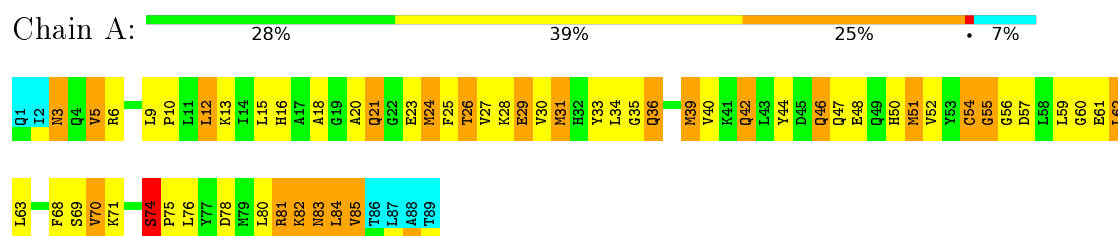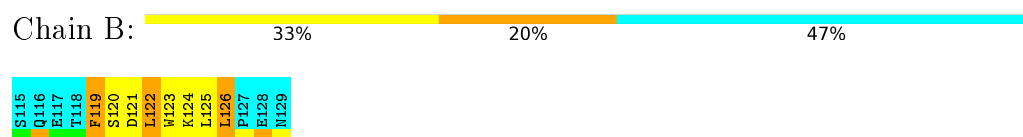
4.2.6 Score per residue for model 6

• Molecule 1: Protein Mdm4

Chain A: 29% 43% 19% 7%

Q1 I2 N3 Q4 V5 R6 P7 K8 L9 P10 L11 L12 K13 I14 L15 H16 A20 Q21 M24 F25 T26 V27 K28 E29 V30 M31 H32 Y33 Q36 M39 V40 K41 Q42 L43 Y44 D45 Q46 Q47 E48 Q49 H50 M51 V52 Y53 C54 G55 G56 D57 L58 L59 G60 E61 L62 L63 Q66

S67 F68 S69 V70 K71 S74 P75 M79 L80 R81 K82 N83 L84 V85 T86 L87 A88 T89

• Molecule 2: Cellular tumor antigen p53

Chain B: 33% 20% 47%

S115 Q116 E117 T118 F119 S120 D121 L122 W123 K124 L125 L126 P127 E128 N129
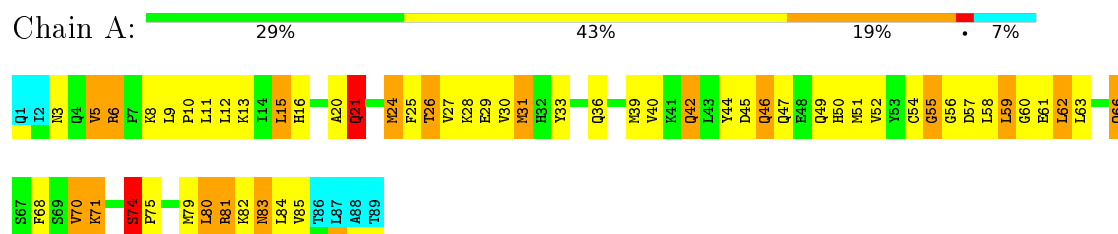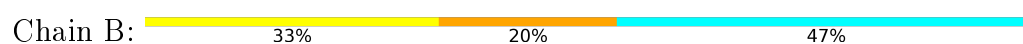
4.2.7 Score per residue for model 7

• Molecule 1: Protein Mdm4

Chain A: 24% 49% 18% 7%

Q1 I2 N3 Q4 V5 R6 P7 K8 L9 P10 L11 L12 L13 I14 L15 H16 A17 A18 G19 A20 Q21 M24 F25 T26 V27 K28 E29 V30 M31 H32 Y33 L34 G35 Q36 Y37 I38 M39 V40 K41 Q42 L43 Y44 D45 Q46 Q47 E48 Q49 H50 M51 V52 Y53 C54 D57 L58 L59 G60 E61 L62

L63 G64 R65 F68 S69 V70 K71 S74 P75 L76 Y77 D78 M79 L80 R81 K82 N83 L84 V85 T86 L87 A88 T89

• Molecule 2: Cellular tumor antigen p53

Chain B: 7% 27% 20% 47%

S115 Q116 E117 T118 F119 S120 D121 L122 W123 K124 L125 L126 P127 E128 N129

4.2.8 Score per residue for model 8

• Molecule 1: Protein Mdm4

Chain A: 21% 48% 22% 7%

Q1 I2 N3 Q4 V5 R6 P7 K8 L9 P10 L11 L12 K13 I14 L15 H16 A17 A18 G19 A20 Q21 M24 F25 T26 V27 K28 E29 V30 M31 H32 Y33 L34 G35 Q36 M39 V40 K41 Q42 L43 Y44 D45 Q46 Q47 E48 Q49 H50 M51 V52 Y53 C54 G55 D56 D57 L58 L59 L62 L63

G64 R65 Q66 S67 F68 S69 V70 K71 S74 P75 L76 M79 L80 R81 K82 N83 L84 V85 T86 L87 A88 T89

• Molecule 2: Cellular tumor antigen p53

Chain B: 7% 27% 20% 47%

S115 Q116 E117 T118 F119 S120 D121 L122 W123 K124 L125 L126 P127 E128 N129
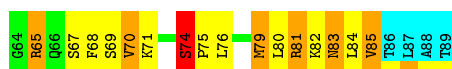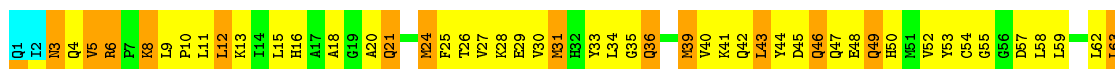
4.2.9 Score per residue for model 9

• Molecule 1: Protein Mdm4

Chain A: 22% 48% 20% 7%

• Molecule 2: Cellular tumor antigen p53

Chain B:
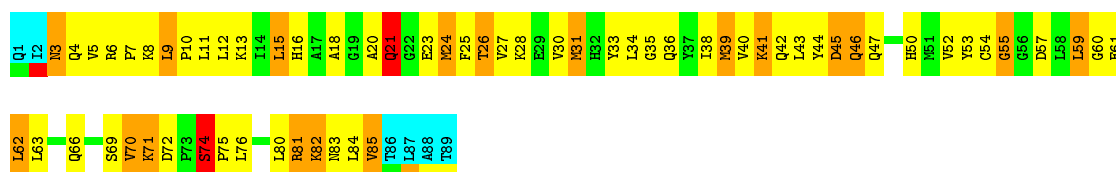
4.2.10 Score per residue for model 10

• Molecule 1: Protein Mdm4

Chain A:

• Molecule 2: Cellular tumor antigen p53

Chain B:

4.2.11 Score per residue for model 11
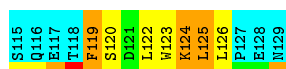
• Molecule 1: Protein Mdm4

Chain A:

• Molecule 2: Cellular tumor antigen p53

Chain B:

`S115 Q116 E117 T118 F119 S120 D121 L122 W123 K124 L125 L126 P127 E128 N129`

4.2.12 Score per residue for model 12

• Molecule 1: Protein Mdm4

Chain A: 25%   49%   16%   •   7%

`Q1 I2 N3 Q4 V5 R6 P7 K8 L9 P10 L11 L12 K13 I14 L15 H16 A17 A18 G19 A20 Q21 G22 E23 M24 F25 T26 V27 K28 E29 V30 M31 H32 Y33 L34 G35 Q36 Y37 I38 M39 V40 K41 Q42 L43 Y44 D45 Q46 Q47 E48 Q49 H50 M51 C54 G55 G56 D57 L58 L59 G60 E61`

`L62 L63 Q66 S67 F68 S69 V70 K71 S74 P75 L76 Y77 D78 M79 L80 R81 K82 N83 L84 V85 T86 L87 A88 T89`

• Molecule 2: Cellular tumor antigen p53

Chain B: 7%   40%   7%   47%

`S115 Q116 E117 T118 F119 S120 D121 L122 W123 K124 L125 L126 P127 E128 N129`

4.2.13 Score per residue for model 13

• Molecule 1: Protein Mdm4

Chain A: 24%   42%   26%   •   7%

`Q1 I2 N3 Q4 V5 K8 L9 P10 L11 L12 K13 I14 L15 H16 A17 A18 G19 A20 Q21 G22 E23 M24 F25 T26 V27 K28 E29 V30 M31 H32 Y33 L34 G35 Q36 M39 V40 K41 Q42 L43 Y44 D45 Q46 Q47 E48 Q49 H50 M51 V52 Y53 C54 G55 G56 D57 L58 L59 G60 E61 L62`

`L63 Q66 S67 F68 S69 V70 K71 S74 P75 L76 L80 R81 K82 N83 L84 V85 T86 L87 A88 T89`

• Molecule 2: Cellular tumor antigen p53

Chain B: 7%   27%   20%   47%

`S115 Q116 E117 T118 F119 S120 D121 L122 W123 K124 L125 L126 P127 E128 N129`

4.2.14 Score per residue for model 14

• Molecule 1: Protein Mdm4

Chain A: 24%   49%   19%   •   7%

● Molecule 2: Cellular tumor antigen p53

Chain B:

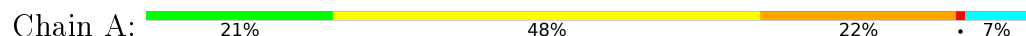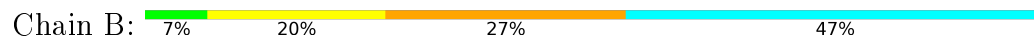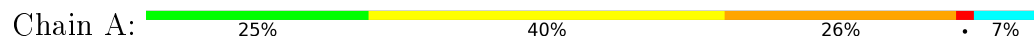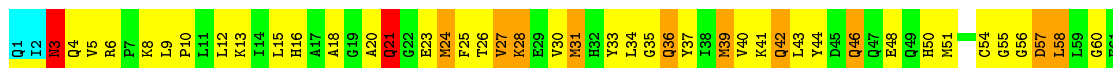### 4.2.15 Score per residue for model 15

● Molecule 1: Protein Mdm4

Chain A:

● Molecule 2: Cellular tumor antigen p53

Chain B:
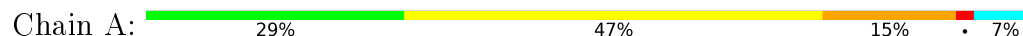
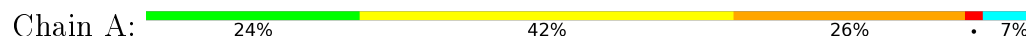### 4.2.16 Score per residue for model 16

● Molecule 1: Protein Mdm4

Chain A:

● Molecule 2: Cellular tumor antigen p53

Chain B:

S115 Q116 E117 T118 F119 S120 D121 L122 W123 K124 L125 L126 P127 E128 N129
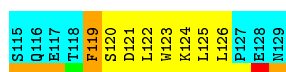
4.2.17 Score per residue for model 17

• Molecule 1: Protein Mdm4

Chain A: 28% 47% 16% · 7%

Q1 I2 N3 Q4 V5 R6 P7 K8 L9 P10 L11 L12 K13 I14 L15 H16 A17 A18 G19 A20 Q21 M24 F25 T26 V27 K28 E29 V30 M31 H32 Y33 L34 G35 Q36 M39 V40 K41 Q42 L43 Y44 D45 Q46 Q47 E48 Q49 H50 M51 V52 Y53 C54 D57 L58 L59 G60 E61 L62 L63

F68 S69 V70 S74 P75 L76 M79 L80 R81 K82 N83 L84 V85 T86 L87 A88 T89

• Molecule 2: Cellular tumor antigen p53

Chain B: 13% 27% 13% 47%

S115 Q116 E117 T118 F119 S120 D121 L122 W123 K124 L125 L126 P127 E128 N129
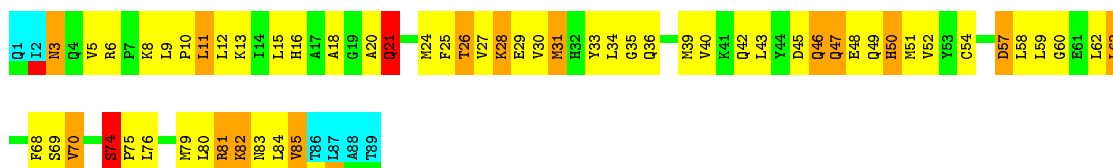
4.2.18 Score per residue for model 18

• Molecule 1: Protein Mdm4

Chain A: 22% 42% 28% · 7%

Q1 I2 N3 Q4 V5 R6 P7 K8 L9 P10 L11 L12 K13 I14 L15 H16 A17 A18 G19 A20 Q21 M24 F25 T26 V27 K28 E29 V30 M31 H32 Y33 L34 G35 Q36 M39 V40 K41 Q42 L43 Y44 D45 Q46 Q47 E48 Q49 H50 M51 V52 Y53 C54 G55 D56 D57 L58 L59 G60 E61 L62

L63 Q66 S67 F68 S69 V70 K71 S74 P75 L76 M79 L80 R81 K82 N83 L84 V85 T86 L87 A88 T89

• Molecule 2: Cellular tumor antigen p53

Chain B: 7% 27% 20% 47%

S115 Q116 E117 T118 F119 S120 D121 L122 W123 K124 L125 L126 P127 E128 N129
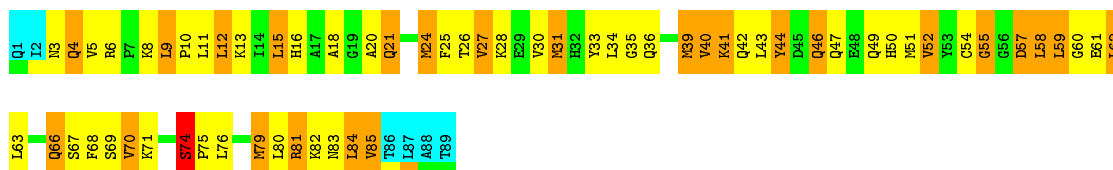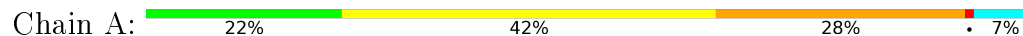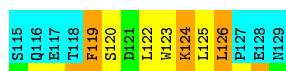
4.2.19 Score per residue for model 19

• Molecule 1: Protein Mdm4
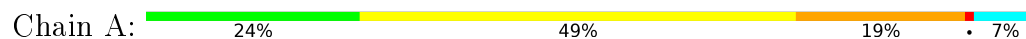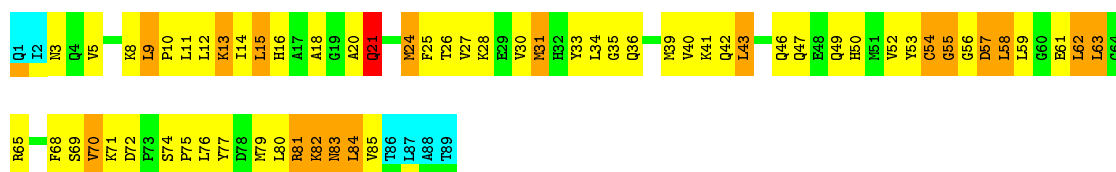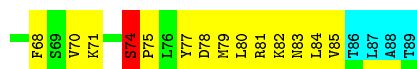
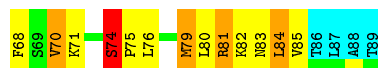Chain A: 19% 47% 26% · 7%

• Molecule 2: Cellular tumor antigen p53

Chain B:
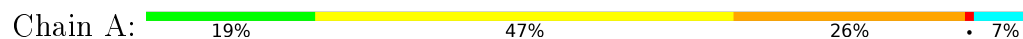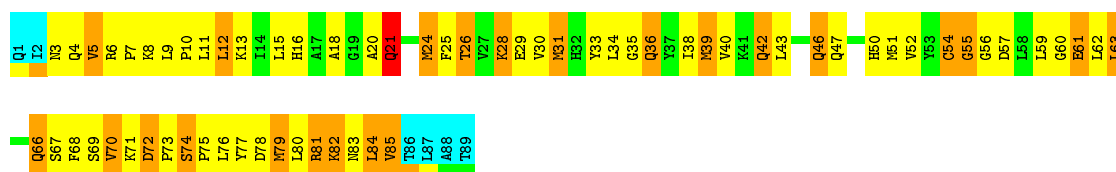
4.2.20 Score per residue for model 20
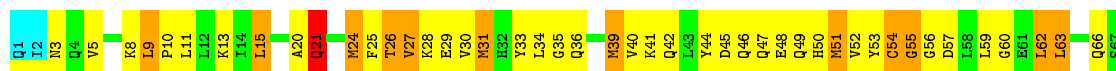
• Molecule 1: Protein Mdm4

Chain A:

• Molecule 2: Cellular tumor antigen p53

Chain B:
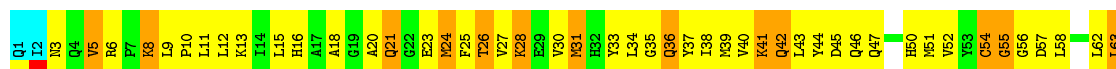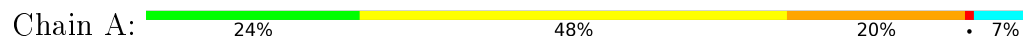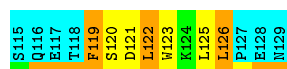
5 Refinement protocol and experimental data overview ⓘ

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	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)	2mwy_cs.cif
Number of chemical shift lists	1
Total number of shifts	585
Number of shifts mapped to atoms	585
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	34%

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	666	681	681	78±6
2	B	72	74	74	16±2
All	All	14760	15100	15100	1703

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 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:50:HIS:CE1	2:B:122:LEU:HD21	1.03	1.89	15	1
1:A:30:VAL:HG11	1:A:84:LEU:HD21	1.01	1.10	15	10
1:A:5:VAL:HG11	1:A:84:LEU:HD12	1.01	1.27	14	3
1:A:30:VAL:HG11	1:A:84:LEU:HD11	0.96	1.38	11	5
1:A:30:VAL:HG11	1:A:84:LEU:CD2	0.94	1.92	15	11
1:A:18:ALA:HB1	1:A:36:GLN:CG	0.93	1.93	8	3
1:A:30:VAL:CG1	1:A:84:LEU:HD21	0.92	1.95	15	10
1:A:5:VAL:HG22	1:A:25:PHE:O	0.92	1.63	11	13
1:A:26:THR:O	1:A:30:VAL:HG23	0.91	1.64	15	12
1:A:5:VAL:HG21	1:A:30:VAL:CG2	0.91	1.94	18	9
1:A:80:LEU:HD23	1:A:83:ASN:OD1	0.91	1.64	8	1
1:A:5:VAL:HG11	1:A:84:LEU:CD1	0.91	1.95	14	2
1:A:84:LEU:HD23	1:A:84:LEU:O	0.91	1.64	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:LEU:HD22	1:A:84:LEU:CD2	0.90	1.96	5	2
1:A:80:LEU:HD23	1:A:83:ASN:ND2	0.89	1.81	2	5
1:A:20:ALA:HB2	1:A:33:TYR:CE1	0.88	2.02	5	18
1:A:52:VAL:HG11	1:A:68:PHE:CZ	0.88	2.03	5	14
1:A:5:VAL:HG11	1:A:84:LEU:HD22	0.88	1.43	4	2
1:A:80:LEU:HD22	1:A:84:LEU:HD23	0.86	1.47	5	6
1:A:5:VAL:HG21	1:A:30:VAL:HG21	0.86	1.44	2	17
1:A:31:MET:CE	2:B:126:LEU:HD23	0.86	2.00	6	4
2:B:123:TRP:O	2:B:126:LEU:HD12	0.84	1.71	2	3
1:A:31:MET:HE1	2:B:126:LEU:HD23	0.84	1.47	8	6
1:A:80:LEU:CD2	1:A:84:LEU:HD23	0.84	2.02	18	7
1:A:43:LEU:HD13	1:A:59:LEU:HD21	0.84	1.48	7	2
1:A:50:HIS:CE1	2:B:122:LEU:HD11	0.84	2.08	15	1
1:A:50:HIS:ND1	2:B:122:LEU:HD21	0.84	1.86	15	1
1:A:18:ALA:HB1	1:A:36:GLN:HB2	0.83	1.51	14	15
1:A:20:ALA:HB2	1:A:33:TYR:CZ	0.82	2.09	6	15
1:A:30:VAL:HG11	1:A:84:LEU:CG	0.82	2.05	18	7
1:A:52:VAL:HG23	1:A:70:VAL:HG12	0.81	1.51	2	15
1:A:80:LEU:HD22	1:A:84:LEU:HD13	0.81	1.53	13	2
1:A:31:MET:HE1	2:B:126:LEU:HD22	0.80	1.52	2	6
1:A:38:ILE:HD13	1:A:52:VAL:HG21	0.80	1.53	19	2
1:A:52:VAL:HG11	1:A:68:PHE:CD1	0.79	2.13	18	1
1:A:11:LEU:HD11	1:A:83:ASN:O	0.79	1.78	6	3
1:A:18:ALA:HB1	1:A:36:GLN:HG3	0.79	1.55	15	3
1:A:30:VAL:HG11	1:A:84:LEU:CD1	0.78	2.08	17	6
1:A:30:VAL:HG11	1:A:84:LEU:HD13	0.77	1.57	17	1
2:B:123:TRP:CE3	2:B:126:LEU:HD11	0.77	2.14	2	2
1:A:50:HIS:HB3	2:B:122:LEU:HD13	0.77	1.56	6	7
1:A:30:VAL:HG21	1:A:84:LEU:HD11	0.76	1.56	10	5
1:A:59:LEU:HD23	1:A:60:GLY:N	0.76	1.96	9	9
1:A:80:LEU:HD22	1:A:84:LEU:HD12	0.76	1.58	15	2
1:A:30:VAL:HG11	1:A:84:LEU:HG	0.75	1.58	18	3
1:A:52:VAL:HG11	1:A:68:PHE:CE1	0.74	2.17	18	3
1:A:59:LEU:HD12	1:A:68:PHE:CZ	0.74	2.17	17	4
2:B:123:TRP:CZ3	2:B:126:LEU:HD11	0.74	2.18	15	2
1:A:70:VAL:O	2:B:126:LEU:HD11	0.74	1.83	19	5
1:A:43:LEU:HD13	1:A:59:LEU:CD2	0.73	2.13	17	2
1:A:62:LEU:HD12	1:A:62:LEU:O	0.73	1.84	6	1
1:A:71:LYS:CE	2:B:122:LEU:HD22	0.73	2.14	12	4
1:A:80:LEU:HB3	1:A:84:LEU:HD22	0.73	1.60	13	1
1:A:12:LEU:HD11	1:A:16:HIS:NE2	0.72	1.99	17	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:122:LEU:HD23	2:B:122:LEU:N	0.72	1.99	8	1
1:A:6:ARG:CB	1:A:85:VAL:HG11	0.72	2.14	3	5
2:B:119:PHE:CE1	2:B:123:TRP:CE3	0.71	2.78	18	17
1:A:59:LEU:HD23	1:A:60:GLY:H	0.71	1.46	9	9
1:A:31:MET:CE	2:B:126:LEU:HD13	0.71	2.15	15	2
1:A:80:LEU:HG	1:A:84:LEU:HD23	0.71	1.63	14	1
1:A:70:VAL:CG2	2:B:122:LEU:HD23	0.71	2.15	16	1
1:A:31:MET:CE	1:A:76:LEU:HD21	0.70	2.16	18	7
1:A:70:VAL:HG21	2:B:122:LEU:HD12	0.70	1.61	14	2
1:A:52:VAL:HG21	1:A:68:PHE:CE1	0.70	2.21	7	4
1:A:71:LYS:CD	2:B:122:LEU:HD22	0.70	2.16	6	1
1:A:15:LEU:C	1:A:20:ALA:HB3	0.70	2.07	8	20
1:A:11:LEU:O	1:A:15:LEU:HD22	0.70	1.87	18	8
1:A:63:LEU:HD21	1:A:75:PRO:O	0.69	1.87	19	5
1:A:70:VAL:CG2	2:B:122:LEU:HD12	0.69	2.16	5	2
1:A:12:LEU:HD22	1:A:16:HIS:NE2	0.69	2.02	18	6
1:A:85:VAL:HG12	1:A:85:VAL:O	0.69	1.87	8	3
1:A:62:LEU:C	1:A:62:LEU:HD12	0.69	2.08	6	1
1:A:80:LEU:HD22	1:A:84:LEU:CD1	0.69	2.18	4	3
1:A:5:VAL:HG21	1:A:84:LEU:CD1	0.69	2.17	9	3
1:A:52:VAL:HG23	1:A:70:VAL:CG1	0.69	2.18	10	8
1:A:50:HIS:HB3	2:B:122:LEU:HD23	0.69	1.62	11	1
1:A:12:LEU:HD22	1:A:16:HIS:CD2	0.68	2.23	5	10
1:A:5:VAL:HG22	1:A:85:VAL:O	0.68	1.89	5	1
1:A:85:VAL:O	1:A:85:VAL:HG22	0.68	1.87	5	1
1:A:62:LEU:HD21	1:A:83:ASN:CG	0.68	2.09	11	1
1:A:80:LEU:HD22	1:A:84:LEU:CG	0.68	2.19	4	1
1:A:71:LYS:HD3	2:B:122:LEU:HD11	0.68	1.66	16	1
1:A:5:VAL:HG12	1:A:85:VAL:O	0.68	1.89	14	6
1:A:43:LEU:CD1	1:A:59:LEU:HD21	0.67	2.20	7	2
1:A:46:GLN:N	1:A:46:GLN:HE21	0.67	1.88	5	3
1:A:54:CYS:HA	1:A:59:LEU:HD21	0.67	1.66	16	8
1:A:5:VAL:CG1	1:A:84:LEU:HD21	0.67	2.19	7	1
1:A:84:LEU:HD23	1:A:84:LEU:C	0.66	2.10	20	1
1:A:52:VAL:CG1	1:A:68:PHE:CD1	0.66	2.77	18	1
1:A:76:LEU:HD22	2:B:126:LEU:CD2	0.66	2.20	1	4
1:A:50:HIS:CE1	2:B:122:LEU:CD2	0.66	2.75	15	1
1:A:43:LEU:O	1:A:52:VAL:HG13	0.66	1.89	8	3
1:A:76:LEU:HD22	2:B:126:LEU:HD21	0.65	1.65	8	5
1:A:58:LEU:HD13	1:A:61:GLU:OE2	0.65	1.92	13	1
1:A:85:VAL:O	1:A:85:VAL:HG13	0.65	1.90	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ALA:HB2	1:A:33:TYR:CD1	0.65	2.27	4	15
1:A:20:ALA:CB	1:A:33:TYR:CZ	0.65	2.80	11	15
1:A:74:SER:CB	1:A:75:PRO:CD	0.65	2.75	10	20
1:A:63:LEU:HD22	1:A:79:MET:HG3	0.64	1.69	12	2
1:A:15:LEU:N	1:A:15:LEU:HD13	0.64	2.07	14	4
1:A:63:LEU:HD13	1:A:68:PHE:CD2	0.64	2.27	19	4
1:A:71:LYS:HE2	2:B:122:LEU:HD22	0.64	1.67	18	4
1:A:6:ARG:O	1:A:85:VAL:HG21	0.64	1.92	5	1
1:A:6:ARG:O	1:A:85:VAL:HG11	0.64	1.92	17	2
1:A:31:MET:CE	2:B:126:LEU:HD22	0.64	2.23	18	7
1:A:70:VAL:O	2:B:126:LEU:HD13	0.64	1.93	17	5
1:A:50:HIS:O	1:A:50:HIS:CD2	0.63	2.51	17	3
1:A:20:ALA:CB	1:A:33:TYR:CE1	0.63	2.82	5	10
1:A:5:VAL:HG21	1:A:84:LEU:HD11	0.63	1.68	10	1
1:A:6:ARG:HB2	1:A:85:VAL:HG11	0.63	1.70	3	1
1:A:6:ARG:HB3	1:A:85:VAL:HG11	0.63	1.69	6	2
1:A:5:VAL:HG21	1:A:84:LEU:HD12	0.63	1.70	9	1
2:B:119:PHE:CZ	2:B:123:TRP:CE3	0.63	2.86	3	2
1:A:54:CYS:CB	1:A:59:LEU:HD11	0.63	2.23	18	1
1:A:18:ALA:HB1	1:A:36:GLN:CB	0.62	2.24	14	3
1:A:5:VAL:HG13	1:A:6:ARG:N	0.62	2.09	5	2
1:A:3:ASN:N	1:A:27:VAL:HG23	0.62	2.10	15	2
1:A:8:LYS:HE2	1:A:85:VAL:HG21	0.62	1.71	1	1
1:A:31:MET:HE2	2:B:126:LEU:HD23	0.61	1.70	6	1
1:A:80:LEU:HD23	1:A:83:ASN:HD22	0.61	1.56	17	4
1:A:8:LYS:CE	1:A:85:VAL:HG21	0.61	2.25	1	1
1:A:70:VAL:HG22	2:B:122:LEU:HD23	0.61	1.70	16	1
1:A:50:HIS:HE1	2:B:122:LEU:HD11	0.61	1.54	15	1
1:A:15:LEU:HD13	1:A:15:LEU:N	0.61	2.10	16	5
1:A:31:MET:HE3	2:B:126:LEU:HD23	0.61	1.70	11	1
1:A:41:LYS:O	1:A:42:GLN:NE2	0.61	2.34	13	1
1:A:29:GLU:O	1:A:33:TYR:CD2	0.61	2.54	16	11
1:A:9:LEU:N	1:A:10:PRO:HD2	0.61	2.11	9	18
1:A:31:MET:SD	2:B:123:TRP:CZ2	0.61	2.94	12	8
1:A:24:MET:C	1:A:25:PHE:CD1	0.61	2.75	15	18
1:A:72:ASP:CG	1:A:72:ASP:O	0.61	2.38	19	1
1:A:52:VAL:CG2	1:A:70:VAL:HG12	0.60	2.26	10	7
1:A:3:ASN:O	1:A:27:VAL:HG23	0.60	1.96	2	5
2:B:123:TRP:CZ3	2:B:126:LEU:CD2	0.60	2.85	17	2
1:A:48:GLU:CD	1:A:50:HIS:CE1	0.60	2.75	4	1
1:A:31:MET:CE	2:B:126:LEU:CD2	0.60	2.80	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:20:ALA:HB2	1:A:33:TYR:CE2	0.60	2.32	10	5
1:A:31:MET:HE2	1:A:76:LEU:HD21	0.60	1.73	14	1
1:A:50:HIS:CD2	1:A:50:HIS:O	0.59	2.55	20	1
1:A:62:LEU:HD11	1:A:83:ASN:HB2	0.59	1.72	8	1
1:A:44:TYR:CE1	1:A:46:GLN:OE1	0.59	2.54	13	1
1:A:5:VAL:CG1	1:A:84:LEU:HD22	0.59	2.25	4	1
1:A:48:GLU:OE1	1:A:50:HIS:CE1	0.59	2.55	4	1
1:A:79:MET:O	1:A:83:ASN:CB	0.59	2.51	19	8
1:A:59:LEU:HD12	1:A:68:PHE:HZ	0.59	1.56	17	1
1:A:38:ILE:HD13	1:A:52:VAL:CG2	0.59	2.28	19	2
1:A:15:LEU:O	1:A:20:ALA:HB3	0.58	1.97	17	10
1:A:80:LEU:HG	1:A:84:LEU:HD22	0.58	1.75	6	1
1:A:30:VAL:HG21	1:A:84:LEU:HD21	0.58	1.74	4	1
2:B:123:TRP:CZ3	2:B:126:LEU:HD22	0.58	2.32	17	2
1:A:31:MET:HE2	2:B:126:LEU:HD13	0.58	1.76	2	2
1:A:31:MET:CE	2:B:126:LEU:HD11	0.58	2.28	13	1
1:A:43:LEU:HD13	1:A:59:LEU:HD22	0.58	1.75	17	1
1:A:80:LEU:HD23	1:A:84:LEU:HD23	0.57	1.76	10	2
1:A:63:LEU:CD2	1:A:79:MET:CE	0.57	2.82	12	3
1:A:4:GLN:OE1	1:A:26:THR:HG23	0.57	1.99	10	3
1:A:63:LEU:HD12	1:A:79:MET:SD	0.57	2.40	2	4
1:A:46:GLN:H	1:A:46:GLN:NE2	0.57	1.98	11	2
1:A:9:LEU:HD23	1:A:9:LEU:N	0.57	2.14	16	1
1:A:50:HIS:CE1	1:A:71:LYS:HE2	0.57	2.35	15	1
2:B:125:LEU:O	2:B:125:LEU:HD23	0.57	2.00	12	1
1:A:35:GLY:N	2:B:123:TRP:CZ2	0.56	2.73	18	18
1:A:24:MET:O	1:A:25:PHE:CG	0.56	2.58	14	19
1:A:44:TYR:CZ	1:A:46:GLN:OE1	0.56	2.59	13	6
1:A:24:MET:O	1:A:25:PHE:CD1	0.56	2.59	11	13
1:A:50:HIS:HA	1:A:70:VAL:HG22	0.56	1.77	19	14
1:A:11:LEU:HD22	1:A:85:VAL:HG23	0.56	1.76	17	1
1:A:72:ASP:OD2	1:A:75:PRO:CD	0.56	2.53	19	1
1:A:50:HIS:CE1	2:B:122:LEU:CD1	0.56	2.88	15	1
1:A:80:LEU:HD22	1:A:84:LEU:HG	0.56	1.76	4	1
1:A:63:LEU:CD2	1:A:79:MET:HE2	0.56	2.31	17	3
1:A:37:TYR:OH	1:A:58:LEU:HD23	0.56	2.01	12	2
1:A:80:LEU:HD22	1:A:84:LEU:HD22	0.56	1.77	1	2
1:A:31:MET:SD	2:B:123:TRP:CE2	0.55	2.99	19	6
1:A:54:CYS:SG	1:A:68:PHE:CE2	0.55	2.99	12	3
1:A:12:LEU:CD1	1:A:16:HIS:NE2	0.55	2.70	9	4
1:A:41:LYS:HB3	1:A:43:LEU:HD12	0.55	1.78	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:123:TRP:O	2:B:126:LEU:HD23	0.55	2.02	14	2
1:A:80:LEU:CD2	1:A:84:LEU:HD13	0.55	2.31	1	2
1:A:45:ASP:OD1	1:A:53:TYR:CZ	0.55	2.60	9	1
1:A:71:LYS:NZ	2:B:122:LEU:HD22	0.55	2.17	12	3
2:B:124:LYS:CD	2:B:125:LEU:N	0.55	2.70	11	2
1:A:46:GLN:CB	1:A:47:GLN:NE2	0.55	2.71	5	4
1:A:9:LEU:CB	1:A:10:PRO:CD	0.55	2.85	1	18
1:A:15:LEU:HD13	1:A:33:TYR:CD2	0.55	2.37	20	1
1:A:29:GLU:O	1:A:33:TYR:CE2	0.54	2.60	7	1
2:B:122:LEU:N	2:B:122:LEU:CD1	0.54	2.70	11	1
1:A:5:VAL:HG12	1:A:25:PHE:O	0.54	2.03	5	2
1:A:42:GLN:N	1:A:42:GLN:HE21	0.54	2.01	10	3
2:B:123:TRP:CE3	2:B:126:LEU:CD1	0.54	2.87	2	2
1:A:50:HIS:CD2	1:A:71:LYS:HB2	0.54	2.38	15	1
1:A:54:CYS:HB3	1:A:59:LEU:HD11	0.54	1.78	18	1
1:A:47:GLN:N	1:A:47:GLN:NE2	0.54	2.55	5	6
1:A:49:GLN:O	1:A:70:VAL:HG11	0.54	2.03	18	2
1:A:27:VAL:HG13	1:A:28:LYS:N	0.54	2.18	17	2
1:A:50:HIS:CD2	1:A:71:LYS:CE	0.54	2.91	2	1
1:A:50:HIS:CD2	1:A:71:LYS:HE3	0.54	2.37	2	2
1:A:52:VAL:HG13	1:A:68:PHE:O	0.54	2.02	18	1
1:A:52:VAL:CG1	1:A:68:PHE:CZ	0.54	2.88	5	3
1:A:81:ARG:CG	1:A:82:LYS:N	0.54	2.71	7	10
1:A:42:GLN:C	1:A:43:LEU:HD22	0.54	2.22	11	2
1:A:5:VAL:HG22	1:A:25:PHE:C	0.54	2.22	11	2
1:A:31:MET:HE1	2:B:126:LEU:CD2	0.53	2.32	17	4
1:A:50:HIS:CD2	1:A:50:HIS:C	0.53	2.81	16	1
1:A:71:LYS:CD	2:B:122:LEU:HD11	0.53	2.31	16	1
1:A:47:GLN:NE2	1:A:47:GLN:H	0.53	2.01	17	2
1:A:54:CYS:SG	1:A:68:PHE:CD2	0.53	2.94	13	3
1:A:52:VAL:CG2	1:A:68:PHE:CE1	0.53	2.92	7	2
1:A:18:ALA:HB1	1:A:33:TYR:O	0.53	2.02	5	1
1:A:46:GLN:NE2	1:A:46:GLN:N	0.53	2.57	5	3
1:A:74:SER:CB	1:A:75:PRO:HD3	0.53	2.34	11	19
1:A:3:ASN:O	1:A:27:VAL:HG12	0.53	2.03	12	1
1:A:43:LEU:HD21	1:A:57:ASP:CG	0.53	2.24	12	1
1:A:42:GLN:HE21	1:A:42:GLN:N	0.53	2.01	6	2
2:B:122:LEU:CD2	2:B:122:LEU:N	0.53	2.70	8	1
2:B:119:PHE:O	2:B:123:TRP:CB	0.53	2.57	18	18
1:A:41:LYS:HB3	1:A:43:LEU:HD21	0.53	1.79	9	2
1:A:31:MET:HE3	2:B:126:LEU:HD12	0.53	1.80	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:50:HIS:CG	1:A:71:LYS:CE	0.52	2.93	19	1
1:A:11:LEU:HD21	1:A:83:ASN:O	0.52	2.04	3	1
1:A:45:ASP:CG	1:A:53:TYR:CZ	0.52	2.83	9	1
1:A:5:VAL:CG1	1:A:85:VAL:O	0.52	2.57	14	5
1:A:30:VAL:CG1	1:A:84:LEU:HD11	0.52	2.25	1	4
1:A:18:ALA:HB1	1:A:36:GLN:CD	0.52	2.23	1	2
1:A:50:HIS:CD2	1:A:71:LYS:CB	0.52	2.92	15	1
1:A:50:HIS:CD2	1:A:71:LYS:HG3	0.52	2.40	15	1
1:A:43:LEU:HD23	1:A:53:TYR:O	0.52	2.05	10	1
1:A:54:CYS:CB	1:A:59:LEU:CD1	0.52	2.87	18	2
1:A:52:VAL:HG21	1:A:68:PHE:CZ	0.52	2.40	18	1
2:B:119:PHE:O	2:B:123:TRP:N	0.52	2.43	18	15
1:A:73:PRO:HB2	1:A:77:TYR:CE2	0.52	2.40	19	1
1:A:42:GLN:C	1:A:43:LEU:HD12	0.52	2.25	12	1
1:A:63:LEU:HD21	1:A:75:PRO:HB2	0.52	1.80	8	1
1:A:47:GLN:N	1:A:47:GLN:CD	0.52	2.63	9	4
1:A:52:VAL:HB	1:A:68:PHE:CE1	0.51	2.41	13	4
1:A:54:CYS:CB	1:A:59:LEU:HD12	0.51	2.36	3	1
1:A:52:VAL:CG1	1:A:53:TYR:N	0.51	2.73	16	2
1:A:63:LEU:HD22	1:A:79:MET:CG	0.51	2.35	12	2
1:A:9:LEU:N	1:A:10:PRO:CD	0.51	2.74	9	1
1:A:12:LEU:CD2	1:A:16:HIS:NE2	0.51	2.74	11	4
1:A:65:ARG:CA	1:A:65:ARG:NE	0.51	2.73	8	3
1:A:69:SER:O	1:A:72:ASP:OD1	0.51	2.29	19	1
2:B:123:TRP:O	2:B:126:LEU:CD1	0.50	2.60	5	1
1:A:30:VAL:CG1	1:A:84:LEU:CD2	0.50	2.88	10	3
1:A:27:VAL:CG1	1:A:28:LYS:N	0.50	2.75	11	1
1:A:50:HIS:CD2	1:A:51:MET:HG2	0.50	2.41	5	1
1:A:63:LEU:HD21	1:A:79:MET:CE	0.50	2.36	17	3
1:A:72:ASP:O	1:A:72:ASP:CG	0.50	2.50	10	1
1:A:3:ASN:O	1:A:26:THR:HG22	0.50	2.05	11	2
1:A:50:HIS:CG	1:A:71:LYS:HE2	0.50	2.41	19	2
1:A:70:VAL:O	2:B:126:LEU:CD1	0.50	2.60	7	6
1:A:11:LEU:CD1	1:A:83:ASN:O	0.50	2.59	14	2
1:A:85:VAL:CG1	1:A:85:VAL:O	0.50	2.60	10	1
1:A:43:LEU:CD1	1:A:53:TYR:O	0.50	2.59	8	3
1:A:47:GLN:NE2	1:A:47:GLN:N	0.50	2.60	13	4
1:A:43:LEU:HD11	1:A:57:ASP:CG	0.50	2.27	14	2
1:A:11:LEU:HD13	1:A:83:ASN:O	0.50	2.06	9	1
1:A:42:GLN:N	1:A:42:GLN:NE2	0.50	2.60	5	1
1:A:48:GLU:OE1	1:A:51:MET:CG	0.50	2.59	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:5:VAL:HG12	1:A:84:LEU:HD21	0.50	1.81	7	1
1:A:31:MET:SD	2:B:126:LEU:HD22	0.50	2.47	7	2
1:A:14:ILE:CD1	1:A:58:LEU:HD13	0.50	2.37	14	1
1:A:62:LEU:CD1	1:A:83:ASN:OD1	0.50	2.60	16	4
1:A:63:LEU:CD1	1:A:79:MET:SD	0.50	3.00	2	2
1:A:52:VAL:HG12	1:A:53:TYR:N	0.50	2.22	2	2
1:A:43:LEU:HD23	1:A:54:CYS:HA	0.50	1.84	10	1
1:A:63:LEU:HD21	1:A:79:MET:HE3	0.49	1.84	12	2
1:A:76:LEU:O	1:A:80:LEU:CD1	0.49	2.60	11	2
1:A:41:LYS:HB3	1:A:43:LEU:HD23	0.49	1.83	11	1
1:A:65:ARG:CD	1:A:65:ARG:N	0.49	2.73	3	2
1:A:20:ALA:CA	1:A:33:TYR:CE1	0.49	2.95	14	4
1:A:12:LEU:HG	1:A:16:HIS:CE1	0.49	2.42	17	1
1:A:79:MET:O	1:A:82:LYS:HD2	0.49	2.07	19	3
1:A:5:VAL:HG11	1:A:84:LEU:HD21	0.49	1.82	7	1
1:A:29:GLU:OE1	1:A:33:TYR:CE2	0.49	2.65	5	2
1:A:45:ASP:OD1	1:A:47:GLN:N	0.49	2.46	8	4
1:A:73:PRO:HB3	2:B:126:LEU:HD11	0.49	1.84	10	2
1:A:24:MET:SD	1:A:24:MET:N	0.49	2.85	3	4
1:A:45:ASP:CG	1:A:53:TYR:CE1	0.49	2.86	9	1
1:A:12:LEU:HD11	1:A:16:HIS:CD2	0.49	2.41	20	1
1:A:46:GLN:N	1:A:46:GLN:NE2	0.49	2.61	13	4
1:A:39:MET:HA	1:A:44:TYR:CE1	0.49	2.43	20	10
1:A:51:MET:CE	1:A:52:VAL:O	0.49	2.60	16	2
1:A:63:LEU:CD2	1:A:75:PRO:O	0.49	2.60	14	2
1:A:39:MET:O	1:A:39:MET:HE3	0.49	2.07	9	1
1:A:41:LYS:CB	1:A:43:LEU:CD2	0.49	2.90	20	1
1:A:45:ASP:OD1	1:A:47:GLN:CB	0.49	2.61	8	1
1:A:71:LYS:HD3	2:B:122:LEU:HD21	0.49	1.85	16	1
1:A:62:LEU:HD12	1:A:83:ASN:OD1	0.49	2.08	15	3
1:A:43:LEU:CD2	1:A:53:TYR:O	0.49	2.60	10	1
1:A:50:HIS:CG	1:A:71:LYS:HE3	0.49	2.43	15	2
2:B:119:PHE:CD1	2:B:123:TRP:HB2	0.49	2.43	4	11
1:A:8:LYS:O	1:A:12:LEU:N	0.49	2.46	7	15
1:A:48:GLU:HB2	1:A:50:HIS:CE1	0.49	2.42	8	1
1:A:61:GLU:CG	1:A:62:LEU:N	0.49	2.76	5	4
1:A:7:PRO:HG3	1:A:15:LEU:HD12	0.49	1.83	19	1
1:A:43:LEU:HD12	1:A:53:TYR:C	0.49	2.28	8	1
1:A:74:SER:OG	1:A:75:PRO:CD	0.49	2.61	13	1
1:A:69:SER:OG	1:A:71:LYS:CG	0.48	2.61	10	1
1:A:12:LEU:CD1	1:A:16:HIS:CD2	0.48	2.96	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:ASN:N	1:A:27:VAL:CG2	0.48	2.75	15	3
1:A:71:LYS:HD2	2:B:122:LEU:HD22	0.48	1.80	6	1
1:A:52:VAL:CB	1:A:68:PHE:CE1	0.48	2.96	7	3
1:A:48:GLU:OE2	1:A:50:HIS:CE1	0.48	2.66	17	1
1:A:6:ARG:O	1:A:85:VAL:CG1	0.48	2.61	17	1
2:B:123:TRP:CH2	2:B:126:LEU:CD2	0.48	2.97	17	1
1:A:36:GLN:N	1:A:36:GLN:NE2	0.48	2.61	10	1
1:A:4:GLN:O	1:A:5:VAL:CG1	0.48	2.61	15	2
1:A:3:ASN:O	1:A:27:VAL:N	0.48	2.47	9	2
1:A:76:LEU:HD22	2:B:126:LEU:HD23	0.48	1.85	19	1
1:A:62:LEU:HD21	1:A:83:ASN:ND2	0.48	2.23	11	3
1:A:84:LEU:CD2	1:A:84:LEU:C	0.48	2.78	20	1
1:A:15:LEU:HB3	1:A:33:TYR:CD2	0.48	2.44	18	14
1:A:6:ARG:H	1:A:85:VAL:HG12	0.48	1.68	11	1
1:A:39:MET:O	1:A:42:GLN:NE2	0.48	2.46	9	1
1:A:73:PRO:HB2	1:A:77:TYR:CD2	0.48	2.44	19	1
1:A:5:VAL:CB	1:A:85:VAL:O	0.48	2.61	9	4
1:A:15:LEU:HD22	1:A:15:LEU:N	0.48	2.23	5	1
1:A:48:GLU:HG2	1:A:50:HIS:CE1	0.48	2.44	16	2
1:A:85:VAL:HG13	1:A:85:VAL:O	0.48	2.09	19	1
1:A:65:ARG:N	1:A:65:ARG:CD	0.48	2.75	15	1
1:A:5:VAL:N	1:A:25:PHE:O	0.47	2.47	5	3
1:A:70:VAL:CG2	1:A:71:LYS:N	0.47	2.77	18	5
1:A:24:MET:C	1:A:25:PHE:CG	0.47	2.87	10	16
1:A:47:GLN:CD	1:A:47:GLN:N	0.47	2.68	20	3
1:A:48:GLU:HB3	1:A:50:HIS:CE1	0.47	2.44	5	3
2:B:122:LEU:O	2:B:125:LEU:N	0.47	2.47	14	16
1:A:45:ASP:OD1	1:A:45:ASP:C	0.47	2.52	16	2
1:A:50:HIS:C	1:A:50:HIS:CD2	0.47	2.87	18	3
1:A:30:VAL:HG21	1:A:84:LEU:CD1	0.47	2.39	9	1
1:A:5:VAL:CG2	1:A:25:PHE:O	0.47	2.63	14	3
1:A:5:VAL:CG1	1:A:84:LEU:CD2	0.47	2.92	7	1
1:A:80:LEU:N	1:A:80:LEU:CD1	0.47	2.77	6	2
1:A:45:ASP:C	1:A:45:ASP:OD1	0.47	2.51	20	1
1:A:30:VAL:CG2	1:A:84:LEU:HD21	0.47	2.38	4	1
1:A:63:LEU:HD22	1:A:65:ARG:HD3	0.47	1.86	20	1
2:B:122:LEU:O	2:B:125:LEU:CB	0.47	2.62	3	1
1:A:55:GLY:N	1:A:66:GLN:O	0.47	2.48	10	7
1:A:11:LEU:O	1:A:15:LEU:CD2	0.47	2.62	14	4
1:A:3:ASN:O	1:A:27:VAL:CG2	0.47	2.61	2	3
2:B:122:LEU:O	2:B:123:TRP:C	0.47	2.53	7	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LEU:O	1:A:20:ALA:CB	0.47	2.63	20	5
1:A:76:LEU:O	1:A:80:LEU:HD13	0.47	2.10	20	5
1:A:39:MET:CE	1:A:39:MET:O	0.47	2.63	19	2
1:A:28:LYS:HD3	1:A:29:GLU:N	0.47	2.25	17	1
1:A:48:GLU:HB3	1:A:50:HIS:CD2	0.47	2.45	2	1
1:A:83:ASN:OD1	1:A:84:LEU:N	0.47	2.48	6	1
1:A:4:GLN:OE1	1:A:26:THR:CG2	0.46	2.63	15	2
1:A:37:TYR:OH	1:A:58:LEU:CB	0.46	2.63	20	1
1:A:58:LEU:O	1:A:61:GLU:CG	0.46	2.64	14	2
1:A:58:LEU:HD22	1:A:58:LEU:H	0.46	1.69	7	1
1:A:39:MET:O	1:A:39:MET:CE	0.46	2.63	9	1
1:A:42:GLN:O	1:A:43:LEU:HD13	0.46	2.11	20	1
1:A:8:LYS:O	1:A:11:LEU:N	0.46	2.48	13	3
1:A:48:GLU:OE2	1:A:50:HIS:ND1	0.46	2.48	17	1
1:A:54:CYS:CA	1:A:59:LEU:HD21	0.46	2.40	6	2
1:A:51:MET:HE1	1:A:68:PHE:O	0.46	2.11	18	1
1:A:43:LEU:HD12	1:A:53:TYR:O	0.46	2.10	13	2
1:A:5:VAL:CG2	1:A:85:VAL:O	0.46	2.61	5	1
1:A:68:PHE:CD1	1:A:68:PHE:C	0.46	2.88	10	1
1:A:31:MET:CE	2:B:126:LEU:HD12	0.46	2.40	9	1
1:A:45:ASP:OD1	1:A:48:GLU:N	0.46	2.49	8	1
1:A:31:MET:C	1:A:31:MET:SD	0.46	2.93	6	8
1:A:52:VAL:HG21	1:A:68:PHE:HE1	0.46	1.64	7	1
1:A:15:LEU:HD12	1:A:33:TYR:CD2	0.46	2.46	5	1
1:A:20:ALA:O	1:A:21:GLN:NE2	0.46	2.49	20	19
1:A:72:ASP:O	1:A:75:PRO:HD2	0.46	2.10	19	2
1:A:54:CYS:O	1:A:56:GLY:N	0.46	2.48	19	13
1:A:26:THR:OG1	1:A:28:LYS:CD	0.46	2.64	11	1
1:A:62:LEU:O	1:A:82:LYS:NZ	0.46	2.49	14	1
1:A:30:VAL:HG21	1:A:84:LEU:CD2	0.46	2.39	4	1
1:A:76:LEU:CD2	2:B:126:LEU:HD21	0.46	2.39	8	1
2:B:123:TRP:O	2:B:126:LEU:CD2	0.46	2.64	13	1
1:A:9:LEU:HB2	1:A:10:PRO:CD	0.46	2.41	1	5
1:A:31:MET:SD	2:B:123:TRP:NE1	0.46	2.89	9	5
1:A:50:HIS:CB	2:B:122:LEU:HD13	0.45	2.40	5	1
1:A:26:THR:OG1	1:A:28:LYS:CE	0.45	2.65	17	1
1:A:31:MET:SD	1:A:31:MET:C	0.45	2.95	8	9
1:A:18:ALA:O	1:A:36:GLN:NE2	0.45	2.49	15	3
1:A:68:PHE:C	1:A:68:PHE:CD1	0.45	2.89	12	1
1:A:46:GLN:HB2	1:A:47:GLN:NE2	0.45	2.25	5	5
1:A:74:SER:HB3	1:A:75:PRO:CD	0.45	2.41	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:123:TRP:O	2:B:126:LEU:N	0.45	2.49	10	2
1:A:31:MET:SD	2:B:126:LEU:CD2	0.45	3.04	7	1
1:A:54:CYS:SG	1:A:55:GLY:N	0.45	2.89	9	6
1:A:79:MET:SD	1:A:83:ASN:ND2	0.45	2.89	17	1
1:A:52:VAL:CG1	1:A:68:PHE:CE1	0.45	2.99	6	2
1:A:50:HIS:CD2	1:A:71:LYS:CG	0.45	3.00	15	1
1:A:27:VAL:HG22	1:A:28:LYS:N	0.45	2.25	12	1
1:A:48:GLU:CD	1:A:50:HIS:NE2	0.45	2.70	3	1
1:A:49:GLN:O	1:A:70:VAL:CG1	0.45	2.65	18	1
1:A:12:LEU:HD21	1:A:22:GLY:O	0.45	2.12	13	1
2:B:123:TRP:CE3	2:B:126:LEU:HD13	0.45	2.46	1	1
1:A:48:GLU:CG	1:A:50:HIS:CE1	0.45	3.00	16	2
1:A:50:HIS:CE1	1:A:51:MET:HG2	0.45	2.47	13	1
1:A:79:MET:SD	1:A:80:LEU:N	0.45	2.90	15	2
1:A:45:ASP:OD2	1:A:48:GLU:N	0.45	2.49	13	2
1:A:62:LEU:C	1:A:62:LEU:CD1	0.45	2.80	6	1
1:A:64:GLY:C	1:A:65:ARG:NE	0.45	2.70	7	1
1:A:59:LEU:CD2	1:A:60:GLY:N	0.45	2.76	9	1
1:A:31:MET:O	2:B:123:TRP:NE1	0.45	2.49	4	3
1:A:50:HIS:CE1	1:A:71:LYS:CE	0.45	2.99	15	1
1:A:54:CYS:HB2	1:A:59:LEU:HD12	0.45	1.89	3	1
1:A:44:TYR:O	1:A:46:GLN:NE2	0.45	2.50	18	4
1:A:5:VAL:HG11	1:A:84:LEU:HD11	0.45	1.89	19	1
1:A:15:LEU:O	1:A:20:ALA:N	0.45	2.50	15	1
1:A:6:ARG:N	1:A:85:VAL:HG12	0.45	2.27	11	1
1:A:28:LYS:CD	1:A:29:GLU:N	0.45	2.80	13	1
1:A:80:LEU:O	1:A:81:ARG:C	0.45	2.55	20	10
1:A:5:VAL:HG23	1:A:7:PRO:HD3	0.45	1.89	9	1
1:A:61:GLU:CD	1:A:62:LEU:N	0.45	2.70	15	1
1:A:83:ASN:ND2	1:A:83:ASN:C	0.45	2.69	8	1
1:A:5:VAL:CB	1:A:25:PHE:O	0.44	2.64	5	2
1:A:70:VAL:O	2:B:126:LEU:HD12	0.44	2.12	7	1
1:A:79:MET:O	1:A:83:ASN:HB3	0.44	2.12	20	4
1:A:41:LYS:HB3	1:A:43:LEU:CD2	0.44	2.42	20	1
1:A:5:VAL:HB	1:A:84:LEU:HD12	0.44	1.89	18	1
2:B:125:LEU:O	2:B:126:LEU:C	0.44	2.56	14	6
1:A:34:LEU:HB3	2:B:123:TRP:CZ2	0.44	2.47	15	1
1:A:54:CYS:HB3	1:A:60:GLY:CA	0.44	2.43	12	1
1:A:15:LEU:CD1	1:A:15:LEU:N	0.44	2.80	2	3
2:B:121:ASP:N	2:B:121:ASP:OD1	0.44	2.50	14	2
1:A:76:LEU:CD2	2:B:126:LEU:CD2	0.44	2.96	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:LEU:O	1:A:84:LEU:N	0.44	2.48	12	5
1:A:3:ASN:OD1	1:A:4:GLN:NE2	0.44	2.50	12	1
1:A:15:LEU:HD22	1:A:33:TYR:CD2	0.44	2.48	19	1
1:A:58:LEU:N	1:A:58:LEU:CD1	0.44	2.81	18	1
1:A:8:LYS:CE	1:A:85:VAL:CG2	0.44	2.95	1	1
1:A:15:LEU:HD13	1:A:33:TYR:HD2	0.44	1.69	20	1
1:A:49:GLN:OE1	2:B:119:PHE:N	0.44	2.50	8	1
1:A:3:ASN:C	1:A:4:GLN:NE2	0.44	2.71	15	1
1:A:50:HIS:N	2:B:122:LEU:HD12	0.44	2.28	8	1
1:A:26:THR:OG1	1:A:28:LYS:NZ	0.44	2.50	20	1
1:A:71:LYS:CG	2:B:125:LEU:HD13	0.44	2.42	1	1
1:A:72:ASP:OD1	1:A:72:ASP:O	0.44	2.36	19	1
1:A:43:LEU:HD12	1:A:59:LEU:HD21	0.44	1.90	3	1
1:A:31:MET:CE	1:A:76:LEU:CD2	0.44	2.92	18	1
1:A:30:VAL:O	1:A:34:LEU:HD23	0.44	2.13	8	1
1:A:41:LYS:HB3	1:A:43:LEU:CD1	0.43	2.43	12	1
1:A:8:LYS:O	1:A:9:LEU:C	0.43	2.56	4	3
1:A:43:LEU:HD21	1:A:57:ASP:OD1	0.43	2.13	18	1
1:A:12:LEU:CD2	1:A:16:HIS:CD2	0.43	2.99	5	1
1:A:5:VAL:CG2	1:A:84:LEU:HD12	0.43	2.44	5	1
1:A:74:SER:HB2	1:A:75:PRO:CD	0.43	2.43	11	8
1:A:63:LEU:HB3	1:A:65:ARG:CD	0.43	2.43	20	1
1:A:59:LEU:HD23	1:A:59:LEU:N	0.43	2.28	13	1
1:A:46:GLN:NE2	1:A:46:GLN:H	0.43	2.12	14	4
1:A:11:LEU:HD22	1:A:85:VAL:CG2	0.43	2.44	17	1
1:A:50:HIS:N	2:B:122:LEU:HD23	0.43	2.28	20	1
1:A:16:HIS:CE1	1:A:21:GLN:OE1	0.43	2.71	18	1
1:A:31:MET:O	1:A:31:MET:HE2	0.43	2.13	8	1
1:A:5:VAL:CG1	1:A:25:PHE:O	0.43	2.67	5	1
2:B:125:LEU:HD23	2:B:125:LEU:O	0.43	2.13	5	1
1:A:9:LEU:HG	1:A:10:PRO:CD	0.43	2.44	3	7
1:A:83:ASN:OD1	1:A:83:ASN:C	0.43	2.56	14	2
1:A:30:VAL:HG12	1:A:84:LEU:HD21	0.43	1.86	6	1
1:A:71:LYS:HE3	2:B:122:LEU:HD22	0.43	1.90	9	1
1:A:9:LEU:CB	1:A:10:PRO:HD3	0.43	2.44	1	1
1:A:5:VAL:CG2	1:A:30:VAL:HG21	0.43	2.40	12	3
1:A:57:ASP:HB3	1:A:59:LEU:CD2	0.43	2.43	13	1
1:A:6:ARG:O	1:A:85:VAL:CG2	0.43	2.64	5	1
1:A:54:CYS:SG	1:A:60:GLY:CA	0.43	3.07	17	5
1:A:36:GLN:N	1:A:36:GLN:CD	0.43	2.72	10	1
1:A:32:HIS:CE1	2:B:124:LYS:HE2	0.43	2.49	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:122:LEU:N	2:B:122:LEU:HD13	0.43	2.28	11	1
1:A:53:TYR:O	1:A:55:GLY:N	0.43	2.51	3	1
1:A:59:LEU:HD12	1:A:68:PHE:CE2	0.43	2.48	17	2
1:A:81:ARG:HG2	1:A:82:LYS:N	0.43	2.29	17	6
1:A:50:HIS:CG	1:A:50:HIS:O	0.43	2.70	17	2
1:A:81:ARG:HG3	1:A:82:LYS:N	0.43	2.28	7	1
1:A:3:ASN:H	1:A:27:VAL:HG23	0.43	1.73	4	2
1:A:68:PHE:CB	1:A:75:PRO:CG	0.43	2.96	10	1
1:A:5:VAL:HG23	1:A:6:ARG:N	0.43	2.28	19	4
2:B:124:LYS:O	2:B:125:LEU:C	0.43	2.58	6	2
1:A:71:LYS:HE2	2:B:122:LEU:CD2	0.43	2.44	9	1
1:A:44:TYR:CD1	1:A:44:TYR:N	0.42	2.87	5	3
1:A:29:GLU:OE1	1:A:33:TYR:CZ	0.42	2.72	11	1
1:A:15:LEU:HB3	1:A:20:ALA:CB	0.42	2.45	15	2
1:A:62:LEU:HD12	1:A:82:LYS:HD3	0.42	1.89	14	1
1:A:38:ILE:HG21	1:A:52:VAL:HG22	0.42	1.90	19	1
1:A:70:VAL:HG11	2:B:119:PHE:CE1	0.42	2.49	7	5
1:A:6:ARG:O	1:A:85:VAL:CB	0.42	2.67	4	1
2:B:119:PHE:O	2:B:123:TRP:HB2	0.42	2.13	18	4
1:A:9:LEU:HB2	1:A:10:PRO:HD3	0.42	1.91	1	7
1:A:38:ILE:HD13	1:A:52:VAL:HG11	0.42	1.91	20	1
1:A:15:LEU:N	1:A:15:LEU:CD1	0.42	2.79	14	1
1:A:41:LYS:O	1:A:42:GLN:CD	0.42	2.57	13	1
1:A:31:MET:CE	2:B:126:LEU:CD1	0.42	2.96	9	1
1:A:36:GLN:C	1:A:36:GLN:CD	0.42	2.77	15	1
1:A:80:LEU:HD22	1:A:84:LEU:HB2	0.42	1.89	12	1
1:A:31:MET:SD	1:A:31:MET:O	0.42	2.78	14	3
1:A:18:ALA:CB	1:A:33:TYR:O	0.42	2.67	5	1
1:A:83:ASN:C	1:A:83:ASN:OD1	0.42	2.58	13	3
1:A:5:VAL:HB	1:A:84:LEU:CD1	0.42	2.44	19	1
1:A:24:MET:C	1:A:25:PHE:CD2	0.42	2.92	9	1
1:A:8:LYS:HE3	1:A:85:VAL:CG2	0.42	2.44	1	1
1:A:54:CYS:HB2	1:A:60:GLY:CA	0.42	2.43	19	2
1:A:79:MET:C	1:A:79:MET:SD	0.42	2.98	12	1
1:A:54:CYS:HB3	1:A:59:LEU:CD1	0.42	2.45	3	1
1:A:10:PRO:HA	1:A:13:LYS:CD	0.42	2.44	14	1
2:B:119:PHE:CE1	2:B:123:TRP:CZ3	0.42	3.08	18	1
1:A:30:VAL:HG11	1:A:84:LEU:HD22	0.42	1.91	10	1
1:A:63:LEU:CD1	1:A:68:PHE:CD2	0.42	3.02	19	1
1:A:58:LEU:HD23	1:A:58:LEU:O	0.42	2.15	20	1
2:B:122:LEU:HA	2:B:125:LEU:CD1	0.41	2.45	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:GLN:CD	1:A:36:GLN:C	0.41	2.78	8	1
1:A:36:GLN:OE1	1:A:36:GLN:C	0.41	2.59	8	1
1:A:68:PHE:HB2	1:A:75:PRO:CG	0.41	2.45	10	1
1:A:15:LEU:HD11	1:A:30:VAL:HG13	0.41	1.92	12	1
1:A:6:ARG:CB	1:A:85:VAL:CG1	0.41	2.93	3	1
1:A:3:ASN:N	1:A:27:VAL:CG1	0.41	2.83	12	1
1:A:58:LEU:HD13	1:A:58:LEU:N	0.41	2.29	12	1
1:A:14:ILE:CD1	1:A:58:LEU:CD1	0.41	2.98	14	1
1:A:50:HIS:CE1	1:A:71:LYS:HZ1	0.41	2.32	4	1
1:A:20:ALA:HB2	1:A:33:TYR:CD2	0.41	2.49	10	1
2:B:124:LYS:O	2:B:126:LEU:N	0.41	2.54	3	1
2:B:124:LYS:HD2	2:B:125:LEU:HD23	0.41	1.91	18	1
1:A:54:CYS:O	1:A:55:GLY:C	0.41	2.58	6	3
1:A:6:ARG:HB3	1:A:85:VAL:CG1	0.41	2.43	6	1
2:B:123:TRP:O	2:B:124:LYS:C	0.41	2.58	8	1
1:A:61:GLU:CD	1:A:61:GLU:C	0.41	2.79	19	3
1:A:4:GLN:C	1:A:5:VAL:HG13	0.41	2.36	15	1
2:B:119:PHE:CD1	2:B:123:TRP:CE3	0.41	3.09	18	1
1:A:45:ASP:O	1:A:48:GLU:N	0.41	2.54	1	1
1:A:53:TYR:O	1:A:54:CYS:C	0.41	2.58	9	5
1:A:65:ARG:HA	1:A:65:ARG:NE	0.41	2.30	15	2
1:A:43:LEU:HD11	1:A:57:ASP:OD2	0.41	2.14	14	1
1:A:71:LYS:CD	2:B:122:LEU:HD21	0.41	2.45	16	1
1:A:50:HIS:CD2	1:A:71:LYS:HZ2	0.41	2.33	10	1
1:A:31:MET:O	1:A:31:MET:SD	0.41	2.79	9	2
1:A:61:GLU:C	1:A:61:GLU:CD	0.41	2.79	4	1
1:A:40:VAL:CG1	1:A:41:LYS:N	0.41	2.84	18	1
2:B:124:LYS:O	2:B:126:LEU:O	0.41	2.39	8	1
1:A:18:ALA:O	1:A:36:GLN:CB	0.41	2.69	5	1
1:A:43:LEU:HD11	1:A:53:TYR:O	0.41	2.15	2	1
1:A:43:LEU:CD2	1:A:57:ASP:HB2	0.41	2.46	2	2
1:A:79:MET:O	1:A:83:ASN:N	0.41	2.54	19	1
1:A:5:VAL:HG11	1:A:30:VAL:CG2	0.41	2.46	6	1
2:B:123:TRP:O	2:B:126:LEU:CB	0.41	2.69	7	1
1:A:36:GLN:C	1:A:36:GLN:OE1	0.41	2.59	15	2
1:A:54:CYS:CB	1:A:60:GLY:CA	0.41	2.99	12	1
1:A:80:LEU:N	1:A:80:LEU:HD12	0.41	2.31	14	1
1:A:54:CYS:HG	1:A:66:GLN:C	0.41	2.18	4	1
1:A:79:MET:CE	1:A:80:LEU:HG	0.41	2.46	18	1
1:A:4:GLN:NE2	1:A:4:GLN:H	0.41	2.14	18	1
1:A:54:CYS:SG	1:A:66:GLN:O	0.41	2.79	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:31:MET:HE1	2:B:126:LEU:CD1	0.41	2.45	14	1
1:A:71:LYS:HE2	2:B:122:LEU:HD21	0.40	1.92	16	1
2:B:124:LYS:C	2:B:126:LEU:N	0.40	2.74	19	1
1:A:68:PHE:CD1	1:A:68:PHE:O	0.40	2.74	6	1
1:A:6:ARG:HB2	1:A:85:VAL:CG1	0.40	2.43	3	1
1:A:84:LEU:O	1:A:85:VAL:C	0.40	2.59	3	3
1:A:46:GLN:CA	1:A:46:GLN:NE2	0.40	2.84	17	1
1:A:79:MET:O	1:A:83:ASN:HB2	0.40	2.17	19	1
1:A:54:CYS:SG	1:A:65:ARG:O	0.40	2.80	20	1
1:A:41:LYS:CB	1:A:43:LEU:CD1	0.40	3.00	12	1
1:A:3:ASN:HD22	1:A:4:GLN:N	0.40	2.15	8	1
1:A:51:MET:HE2	1:A:51:MET:C	0.40	2.37	16	1
1:A:54:CYS:HB3	1:A:68:PHE:CE2	0.40	2.51	6	1
1:A:74:SER:HB3	1:A:75:PRO:HD3	0.40	1.94	14	1
1:A:18:ALA:CB	1:A:36:GLN:CD	0.40	2.89	1	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	83/89 (93%)	69±2 (83±3%)	11±2 (13±3%)	3±1 (4±1%)	7	35
2	B	8/15 (53%)	5±1 (60±13%)	3±1 (40±13%)	0±0 (0±0%)	100	100
All	All	1820/2080 (88%)	1480 (81%)	277 (15%)	63 (3%)	8	37

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	74	SER	18
1	A	55	GLY	17
1	A	21	GLN	12
1	A	8	LYS	5
1	A	85	VAL	3
1	A	23	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	3	ASN	2
1	A	57	ASP	2
1	A	84	LEU	1
1	A	54	CYS	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	73/78 (94%)	44±3 (60±4%)	29±3 (40±4%)	0	5
2	B	8/15 (53%)	4±1 (49±15%)	4±1 (51±15%)	0	1
All	All	1620/1860 (87%)	949 (59%)	671 (41%)	0	4

All 65 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	31	MET	20
1	A	82	LYS	20
1	A	40	VAL	20
1	A	74	SER	19
1	A	42	GLN	19
1	A	13	LYS	19
1	A	21	GLN	19
1	A	26	THR	19
1	A	63	LEU	19
1	A	57	ASP	18
1	A	3	ASN	18
1	A	70	VAL	18
2	B	119	PHE	18
2	B	120	SER	18
1	A	39	MET	18
1	A	28	LYS	17
1	A	34	LEU	16
1	A	46	GLN	16
1	A	24	MET	15
1	A	81	ARG	15

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Mol	Chain	Res	Type	Models (Total)
1	A	62	LEU	14
1	A	51	MET	13
1	A	69	SER	13
2	B	122	LEU	12
1	A	84	LEU	12
2	B	126	LEU	11
1	A	36	GLN	11
2	B	124	LYS	10
1	A	12	LEU	10
1	A	41	LYS	10
1	A	79	MET	9
1	A	83	ASN	9
1	A	11	LEU	9
1	A	15	LEU	9
1	A	9	LEU	9
1	A	58	LEU	9
2	B	125	LEU	9
1	A	78	ASP	9
1	A	66	GLN	8
1	A	45	ASP	7
1	A	54	CYS	7
1	A	59	LEU	7
1	A	65	ARG	7
1	A	71	LYS	7
1	A	6	ARG	7
1	A	8	LYS	6
1	A	5	VAL	6
1	A	85	VAL	6
1	A	67	SER	6
1	A	27	VAL	5
1	A	61	GLU	5
1	A	43	LEU	5
1	A	47	GLN	5
2	B	121	ASP	4
1	A	23	GLU	4
1	A	29	GLU	4
1	A	72	ASP	4
1	A	50	HIS	3
1	A	4	GLN	2
1	A	44	TYR	2
1	A	80	LEU	1
1	A	49	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	53	TYR	1
1	A	48	GLU	1
1	A	52	VAL	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 (i)

The completeness of assignment taking into account all chemical shift lists is 34% for the well-defined parts and 33% for the entire structure.

7.1 Chemical shift list 1

File name: 2mwy_cs.cif

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

7.1.1 Bookkeeping (i)

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	585
Number of shifts mapped to atoms	585
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

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 34%, i.e. 400 atoms were assigned a chemical shift out of a possible 1175. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/447 (0%)	0/178 (0%)	0/182 (0%)	0/87 (0%)
Sidechain	353/628 (56%)	353/370 (95%)	0/232 (0%)	0/26 (0%)
Aromatic	47/100 (47%)	47/53 (89%)	0/43 (0%)	0/4 (0%)
Overall	400/1175 (34%)	400/601 (67%)	0/457 (0%)	0/117 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 33%, i.e. 441 atoms were assigned a chemical shift out of a possible 1323. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/510 (0%)	0/203 (0%)	0/208 (0%)	0/99 (0%)
Sidechain	394/713 (55%)	394/419 (94%)	0/265 (0%)	0/29 (0%)
Aromatic	47/100 (47%)	47/53 (89%)	0/43 (0%)	0/4 (0%)
Overall	441/1323 (33%)	441/675 (65%)	0/516 (0%)	0/132 (0%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.