Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 05:10 PM BST

PDB ID	:	1T17
Title	:	Solution Structure of the 18 kDa Protein CC1736 from Caulobacter crescentus: The Northeast Structural Genomics Consortium Target CcR19
Authors	:	Shen, Y.; Atreya, H.S.; Acton, T.; Xiao, R.; Montelione, G.T.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2004-04-15

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

http://wwpdb.org/validation/2016/NMRValidationReportHelp

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:
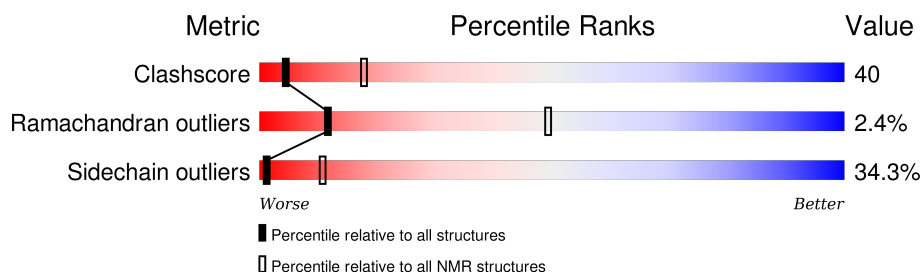
1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 83%.

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		40
Ramachandran outliers		2.4%
Sidechain outliers		34.3%

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	148	33% 51% 9% 6%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations,lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:27, A:31-A:86, A:90-A:146 (139)	0.35	11

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 8 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2328 atoms, of which 1152 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called conserved hypothetical protein.

Mol	Chain	Residues	Atoms						Trace
1	A	148	Total	C	H	N	O	S	0
			2328	753	1152	211	207	5	

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: conserved hypothetical protein
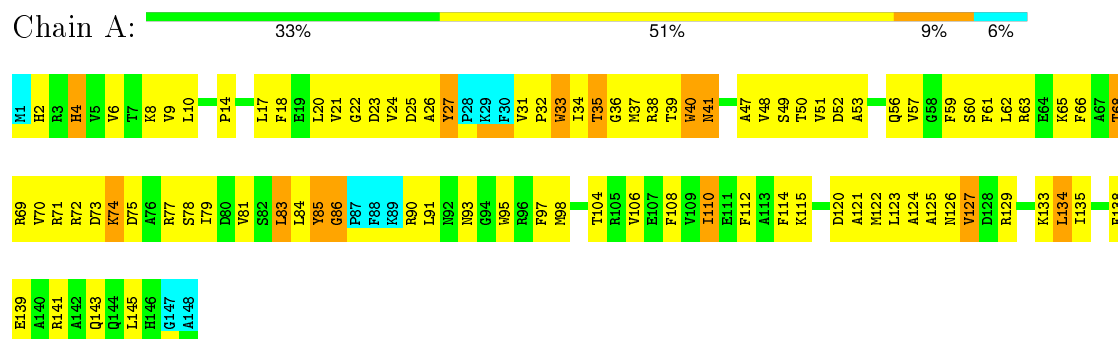
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: conserved hypothetical protein
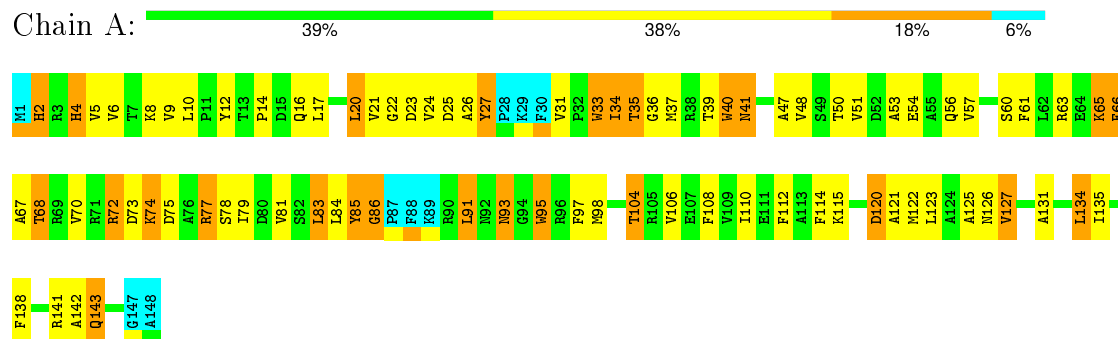
4.2.2 Score per residue for model 2

• Molecule 1: conserved hypothetical protein

4.2.3 Score per residue for model 3

• Molecule 1: conserved hypothetical protein

4.2.4 Score per residue for model 4

• Molecule 1: conserved hypothetical protein

4.2.5 Score per residue for model 5

• Molecule 1: conserved hypothetical protein

4.2.6 Score per residue for model 6

- Molecule 1: conserved hypothetical protein

Chain A:

4.2.7 Score per residue for model 7

- Molecule 1: conserved hypothetical protein

Chain A:

4.2.8 Score per residue for model 8

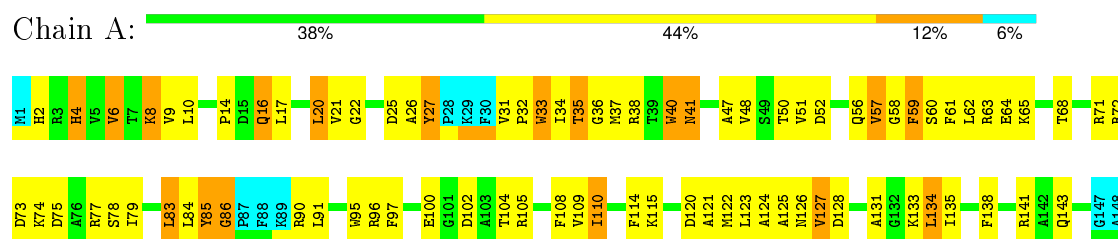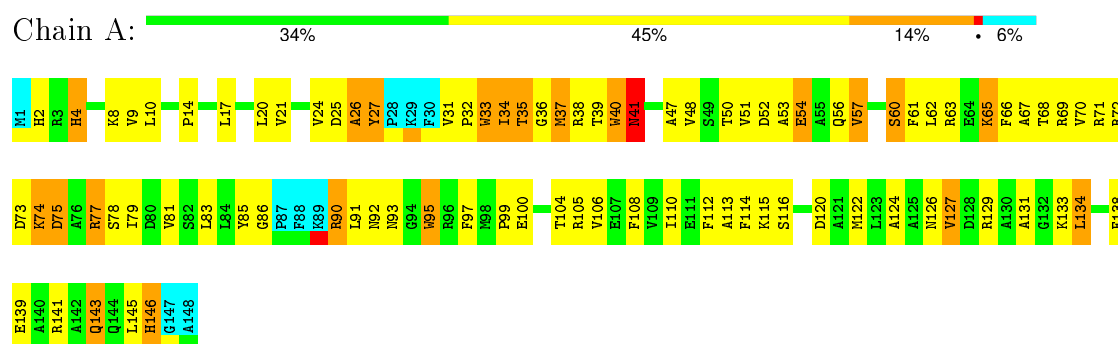- Molecule 1: conserved hypothetical protein

Chain A:
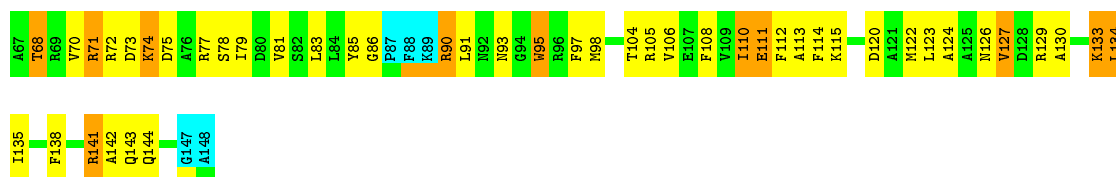
4.2.9 Score per residue for model 9

• Molecule 1: conserved hypothetical protein

Chain A:

4.2.10 Score per residue for model 10

• Molecule 1: conserved hypothetical protein

Chain A:

4.2.11 Score per residue for model 11 (medoid)

• Molecule 1: conserved hypothetical protein

Chain A:

E139 A140 R141 A142 Q143 Q144 G147 A148

4.2.12 Score per residue for model 12

• Molecule 1: conserved hypothetical protein

Chain A:

34% 43% 17% 6%

M1 H2 R3 H4 K8 V9 L10 P14 D15 Q16 L17 F18 E19 L20 V21 G22 D23 V24 D25 A26 Y27 P28 K29 F30 V31 P32 W33 I34 T35 G36 M37 R38 T39 W40 N41 G42 R43 V44 A47 V48 S49 T50 V51 D52 A53 E54 A55 Q56 V57 F61 L62 R63 E64 K65 F66 A67

T68 R69 V70 R71 R72 D73 K74 D75 A76 R77 S78 I79 D80 V81 S82 L83 L84 Y85 G86 P87 F88 K89 R90 L91 W95 R96 F97 M98 D102 A103 T104 R105 V106 E107 F108 V109 I110 E111 F112 A113 F114 K115 D120 A121 M122 L123 A124 A125 N126 V127 D128 R129 A130 A131 L134 I135

A136 C137 F138 R141 A142 Q143 G147 A148

4.2.13 Score per residue for model 13

• Molecule 1: conserved hypothetical protein

Chain A:

39% 39% 15% • 6%

M1 H2 R3 H4 K8 V9 L10 P11 Y12 T13 P14 L17 F18 E19 L20 V21 G22 D23 V24 D25 A26 Y27 P28 K29 F30 V31 P32 W33 I34 T35 G36 M37 R38 T39 W40 N41 A47 V48 S49 T50 V51 D52 A53 E54 A55 Q56 F59 S60 F61 L62 R63 F66 A67 T68 R69

V70 D73 K74 D75 A76 R77 S78 I79 D80 V81 S82 L83 L84 Y85 G86 P87 F88 K89 R90 L91 N92 N93 G94 W95 R96 F97 M98 T104 R105 V106 I110 E111 F112 A113 F114 K115 D120 A121 M122 L123 A124 A125 N126 V127 D128 K133 L134 C137 F138 R141 H146 G147

A148

4.2.14 Score per residue for model 14

• Molecule 1: conserved hypothetical protein

Chain A:

39% 43% 12% 6%

M1 H2 R3 H4 K8 V9 L10 L17 F18 E19 L20 V21 G22 D23 V24 D25 A26 Y27 P28 K29 F30 V31 P32 W33 I34 T35 G36 M37 R38 T39 W40 N41 G42 R43 V44 A47 V48 S49 T50 V51 D52 Q56 V57 S60 F61 L62 R63 E64 K65 F66 A67 T68 R69 V70 R71

R72 D73 K74 D75 S78 I79 D80 V81 S82 L83 L84 Y85 G86 P87 F88 K89 R90 L91 N92 W95 R96 F97 M98 T104 R105 V106 E107 F108 V109 I110 E111 F112 A113 F114 K115 D120 A121 M122 L123 A124 A125 N126 V127 D128 R129 K133 L134 F138 E139 A140 R141 G147 A148

4.2.15　Score per residue for model 15

• Molecule 1: conserved hypothetical protein

Chain A:
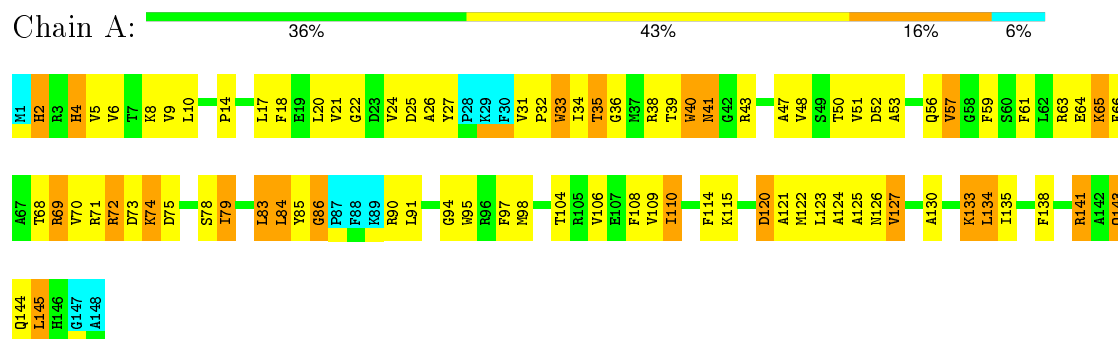
4.2.16　Score per residue for model 16
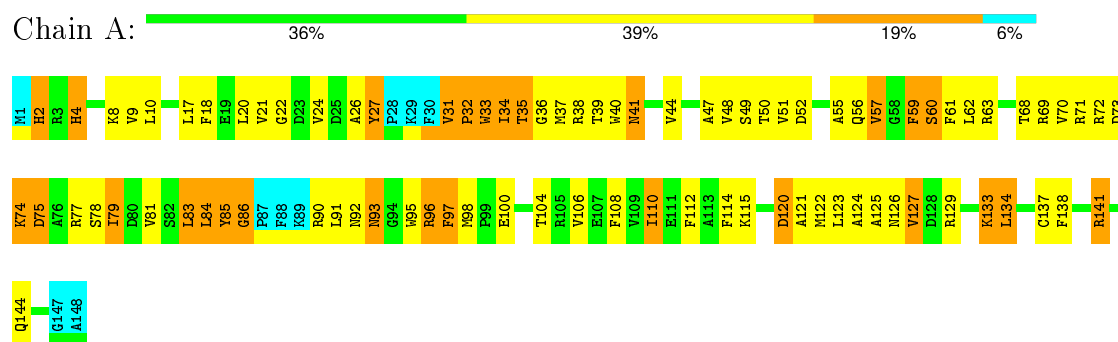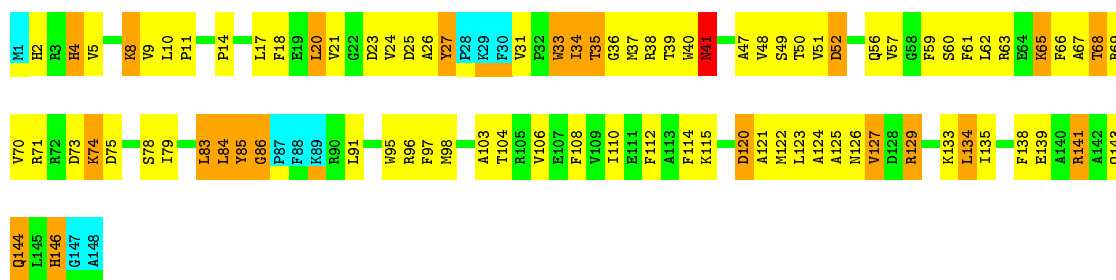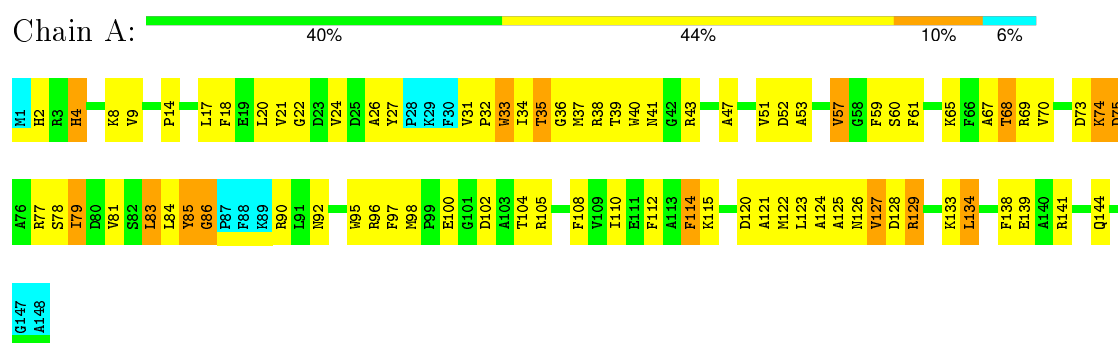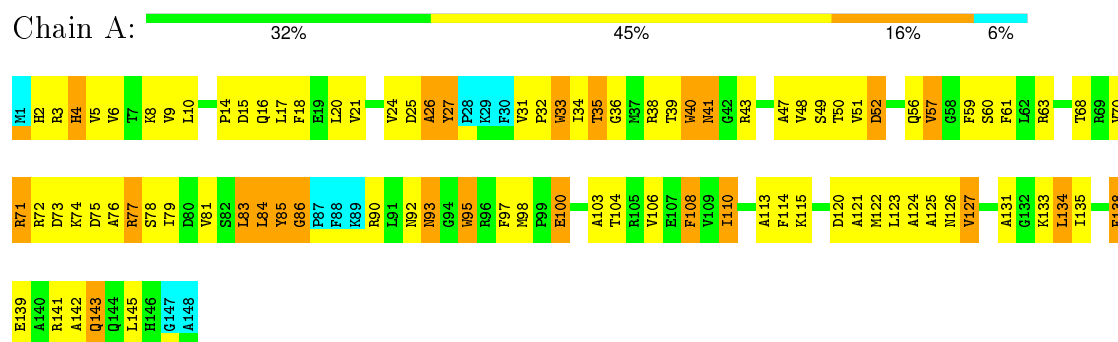
• Molecule 1: conserved hypothetical protein

Chain A:
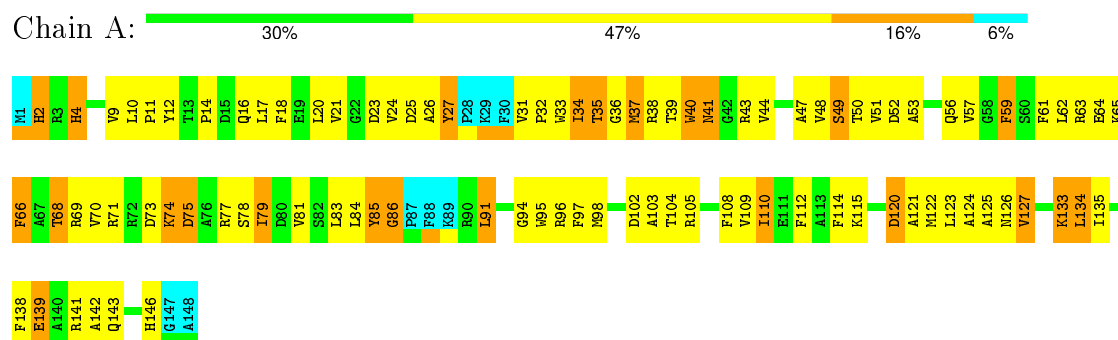
4.2.17　Score per residue for model 17

• Molecule 1: conserved hypothetical protein

Chain A:
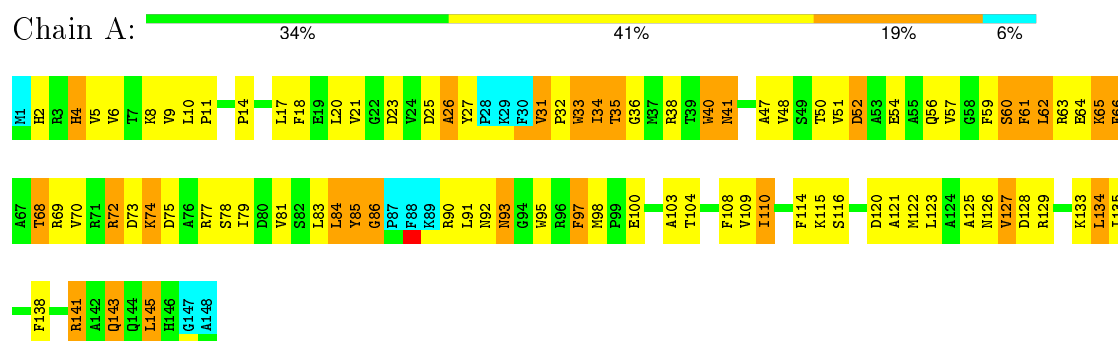
4.2.18 Score per residue for model 18

• Molecule 1: conserved hypothetical protein
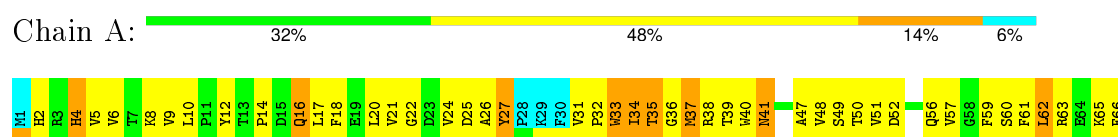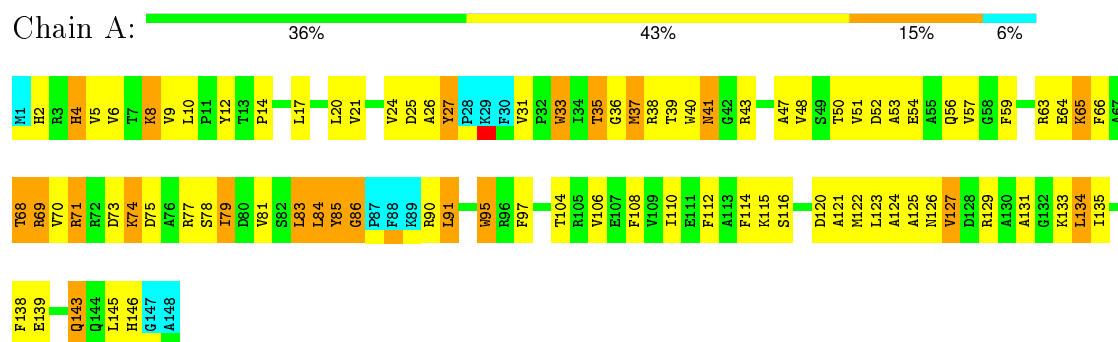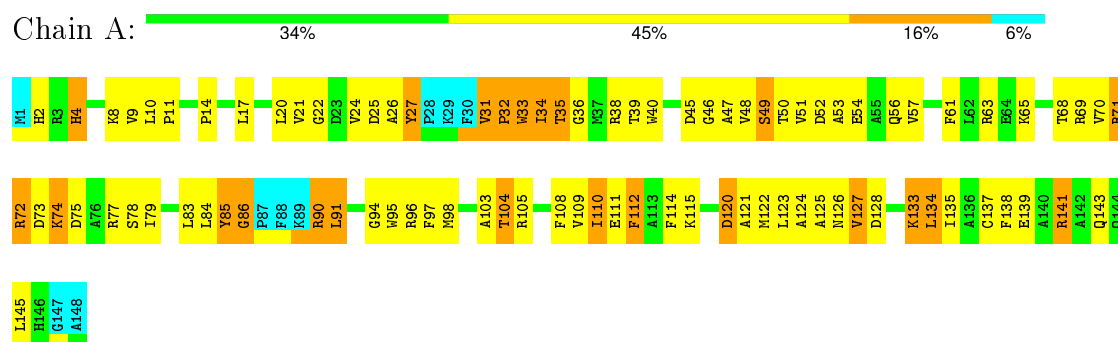
Chain A:

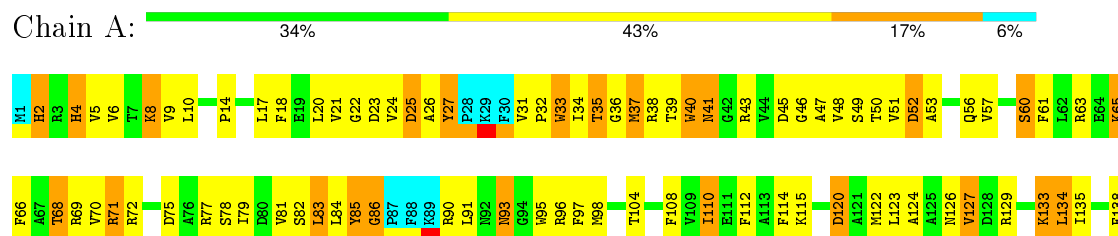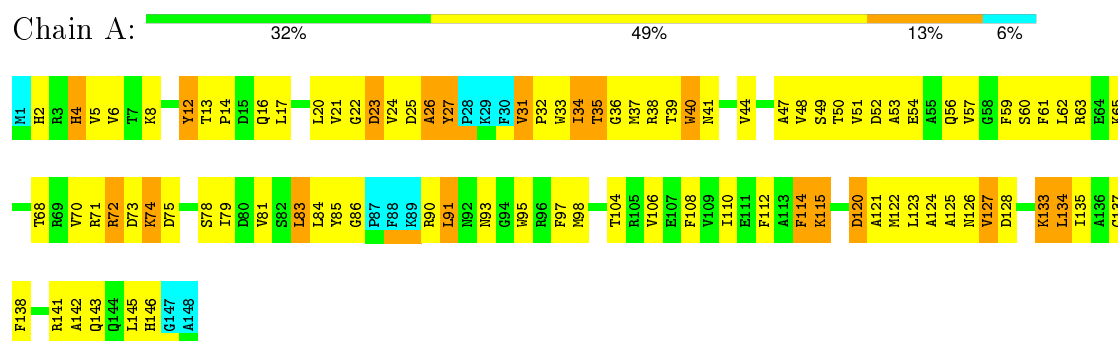#### 4.2.19 Score per residue for model 19

• Molecule 1: conserved hypothetical protein

Chain A:
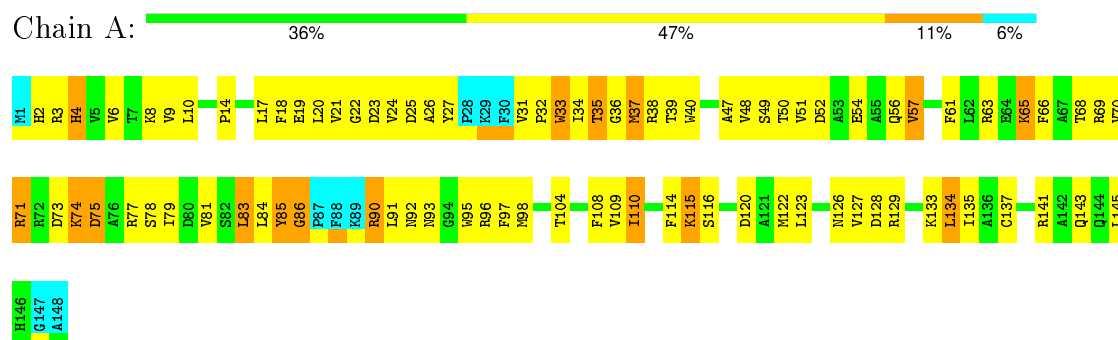
4.2.20 Score per residue for model 20

• Molecule 1: conserved hypothetical protein

Chain A:
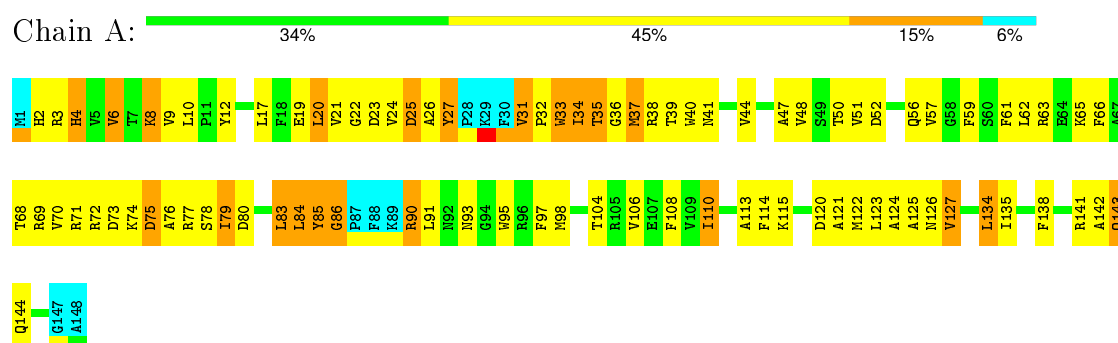
5 Refinement protocol and experimental data overview (i)

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

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

Software name	Classification	Version
DYANA	structure solution	1.5
DYANA	refinement	1.5

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)	BMRB entry 6120
Number of chemical shift lists	1
Total number of shifts	1705
Number of shifts mapped to atoms	1705
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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	1105	1079	1092	88±8
All	All	22100	21580	21840	1753

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 40.

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:114:PHE:CZ	1:A:123:LEU:HD13	1.10	1.81	1	19
1:A:21:VAL:HG22	1:A:97:PHE:CE2	1.01	1.90	10	7
1:A:31:VAL:HG12	1:A:33:TRP:CH2	0.97	1.94	13	1
1:A:114:PHE:CE1	1:A:123:LEU:HD13	0.96	1.94	19	16
1:A:134:LEU:HD13	1:A:135:ILE:N	0.96	1.75	19	1
1:A:31:VAL:HG13	1:A:33:TRP:CE3	0.95	1.96	5	2
1:A:21:VAL:HG13	1:A:79:ILE:HD11	0.94	1.37	7	6
1:A:83:LEU:HD22	1:A:84:LEU:N	0.92	1.80	9	6
1:A:9:VAL:O	1:A:10:LEU:HD23	0.90	1.66	1	18
1:A:84:LEU:HD22	1:A:84:LEU:C	0.90	1.87	15	2
1:A:141:ARG:HH21	1:A:145:LEU:HD12	0.89	1.26	15	1
1:A:110:ILE:HD13	1:A:112:PHE:CE2	0.89	2.03	3	9
1:A:83:LEU:HD12	1:A:84:LEU:N	0.88	1.83	7	4
1:A:21:VAL:HG13	1:A:79:ILE:CG1	0.87	1.98	16	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:TRP:CH2	1:A:106:VAL:HG11	0.87	2.05	12	4
1:A:134:LEU:O	1:A:134:LEU:HD12	0.86	1.68	15	6
1:A:33:TRP:CZ2	1:A:134:LEU:HD22	0.86	2.04	15	3
1:A:12:TYR:CE2	1:A:142:ALA:HB1	0.86	2.05	1	2
1:A:33:TRP:CE2	1:A:134:LEU:HD22	0.85	2.06	10	2
1:A:31:VAL:HG12	1:A:33:TRP:CZ2	0.84	2.06	17	2
1:A:14:PRO:HA	1:A:17:LEU:HD12	0.83	1.49	1	15
1:A:24:VAL:CG2	1:A:39:THR:HG21	0.83	2.03	20	12
1:A:95:TRP:CZ2	1:A:108:PHE:CE1	0.81	2.68	2	7
1:A:95:TRP:CZ2	1:A:108:PHE:CZ	0.81	2.69	18	4
1:A:31:VAL:HG12	1:A:33:TRP:CZ3	0.81	2.10	9	12
1:A:26:ALA:O	1:A:27:TYR:CG	0.80	2.34	3	10
1:A:97:PHE:CD1	1:A:106:VAL:HG13	0.80	2.11	20	6
1:A:47:ALA:HB1	1:A:74:LYS:HG3	0.80	1.51	14	9
1:A:21:VAL:HG13	1:A:79:ILE:CD1	0.80	2.06	19	9
1:A:95:TRP:CH2	1:A:108:PHE:CE2	0.80	2.70	5	5
1:A:17:LEU:HD22	1:A:97:PHE:CD1	0.79	2.12	11	5
1:A:95:TRP:CH2	1:A:108:PHE:CZ	0.79	2.71	5	4
1:A:95:TRP:CH2	1:A:97:PHE:CZ	0.78	2.71	6	1
1:A:21:VAL:HG13	1:A:79:ILE:HG13	0.78	1.52	4	8
1:A:110:ILE:O	1:A:110:ILE:HD13	0.78	1.77	2	3
1:A:47:ALA:HB1	1:A:74:LYS:HG2	0.77	1.55	13	10
1:A:110:ILE:HD13	1:A:110:ILE:O	0.77	1.79	20	2
1:A:21:VAL:HG22	1:A:95:TRP:CZ2	0.76	2.15	6	1
1:A:17:LEU:HD13	1:A:97:PHE:CD2	0.76	2.15	7	3
1:A:21:VAL:HG22	1:A:97:PHE:CD2	0.76	2.15	10	2
1:A:95:TRP:CZ3	1:A:108:PHE:CG	0.76	2.74	4	10
1:A:21:VAL:CG1	1:A:79:ILE:HD11	0.76	2.10	12	5
1:A:134:LEU:C	1:A:134:LEU:HD12	0.76	2.00	16	9
1:A:95:TRP:CE2	1:A:108:PHE:CE1	0.75	2.75	18	5
1:A:35:THR:HG23	1:A:36:GLY:H	0.75	1.39	18	4
1:A:84:LEU:HD23	1:A:85:TYR:HB2	0.74	1.59	12	9
1:A:21:VAL:HG13	1:A:79:ILE:HD13	0.74	1.58	13	1
1:A:95:TRP:CH2	1:A:97:PHE:CE2	0.74	2.75	6	1
1:A:68:THR:HG22	1:A:83:LEU:HA	0.74	1.60	9	18
1:A:70:VAL:HA	1:A:81:VAL:HG22	0.74	1.57	12	8
1:A:134:LEU:HD12	1:A:134:LEU:C	0.74	2.02	12	6
1:A:26:ALA:O	1:A:27:TYR:O	0.73	2.06	7	10
1:A:84:LEU:C	1:A:84:LEU:HD12	0.73	2.03	7	1
1:A:83:LEU:C	1:A:83:LEU:HD23	0.73	2.04	15	1
1:A:20:LEU:HD12	1:A:138:PHE:CZ	0.73	2.18	11	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:LEU:HD22	1:A:84:LEU:O	0.72	1.83	15	2
1:A:33:TRP:CZ3	1:A:134:LEU:HD23	0.72	2.19	19	1
1:A:83:LEU:HD13	1:A:83:LEU:C	0.72	2.05	19	3
1:A:95:TRP:CE2	1:A:108:PHE:CD1	0.72	2.78	20	2
1:A:17:LEU:HD22	1:A:97:PHE:CG	0.72	2.18	7	2
1:A:110:ILE:O	1:A:110:ILE:HD12	0.72	1.84	3	5
1:A:26:ALA:C	1:A:27:TYR:CD1	0.71	2.63	14	10
1:A:60:SER:C	1:A:61:PHE:CG	0.71	2.61	17	1
1:A:14:PRO:CB	1:A:17:LEU:HD12	0.71	2.15	18	2
1:A:95:TRP:CE3	1:A:108:PHE:CD1	0.71	2.78	18	4
1:A:83:LEU:C	1:A:83:LEU:HD12	0.71	2.05	7	2
1:A:95:TRP:CZ3	1:A:106:VAL:HG11	0.71	2.21	13	3
1:A:95:TRP:CH2	1:A:108:PHE:CD2	0.71	2.79	4	5
1:A:21:VAL:HG22	1:A:97:PHE:CD1	0.70	2.21	17	1
1:A:20:LEU:CD1	1:A:138:PHE:CE2	0.70	2.74	13	3
1:A:108:PHE:CZ	1:A:110:ILE:HG22	0.70	2.21	4	8
1:A:10:LEU:HD12	1:A:138:PHE:CE2	0.70	2.22	12	7
1:A:72:ARG:HA	1:A:79:ILE:HD13	0.70	1.64	11	6
1:A:4:HIS:CD2	1:A:127:VAL:CG1	0.70	2.74	4	16
1:A:26:ALA:O	1:A:27:TYR:CD1	0.69	2.45	7	11
1:A:50:THR:HG23	1:A:71:ARG:HG3	0.69	1.63	11	13
1:A:110:ILE:HD12	1:A:110:ILE:O	0.69	1.87	8	4
1:A:24:VAL:HG23	1:A:39:THR:HG21	0.69	1.63	18	6
1:A:20:LEU:HD13	1:A:95:TRP:CH2	0.69	2.23	9	3
1:A:79:ILE:CG2	1:A:95:TRP:CD1	0.69	2.75	6	2
1:A:17:LEU:HD22	1:A:97:PHE:HB3	0.69	1.62	17	6
1:A:17:LEU:HD13	1:A:97:PHE:CD1	0.69	2.23	9	1
1:A:47:ALA:HB1	1:A:74:LYS:CG	0.69	2.18	7	10
1:A:51:VAL:O	1:A:70:VAL:HG12	0.69	1.88	10	15
1:A:95:TRP:CZ3	1:A:108:PHE:CD2	0.69	2.80	18	6
1:A:121:ALA:O	1:A:125:ALA:HB2	0.68	1.88	15	16
1:A:21:VAL:HG22	1:A:97:PHE:CE1	0.67	2.23	2	3
1:A:95:TRP:CZ3	1:A:97:PHE:CZ	0.67	2.82	6	1
1:A:110:ILE:C	1:A:110:ILE:HD12	0.67	2.09	11	9
1:A:60:SER:O	1:A:123:LEU:HD21	0.67	1.90	18	1
1:A:84:LEU:CD2	1:A:84:LEU:C	0.67	2.63	15	2
1:A:9:VAL:C	1:A:10:LEU:HD23	0.67	2.11	16	8
1:A:31:VAL:HG13	1:A:33:TRP:CH2	0.66	2.25	18	1
1:A:131:ALA:HA	1:A:134:LEU:HD23	0.66	1.66	9	4
1:A:8:LYS:HD3	1:A:135:ILE:HG23	0.66	1.66	15	3
1:A:91:LEU:HD12	1:A:112:PHE:CB	0.66	2.21	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:ARG:NH2	1:A:145:LEU:HD12	0.66	2.04	10	2
1:A:95:TRP:CD2	1:A:108:PHE:CD1	0.66	2.83	18	3
1:A:114:PHE:CE1	1:A:123:LEU:CD1	0.66	2.79	8	7
1:A:6:VAL:HG11	1:A:131:ALA:HB1	0.66	1.68	1	1
1:A:79:ILE:HG22	1:A:95:TRP:CD1	0.66	2.26	6	3
1:A:61:PHE:CG	1:A:61:PHE:O	0.65	2.49	4	8
1:A:27:TYR:O	1:A:27:TYR:CD2	0.65	2.50	10	6
1:A:31:VAL:HG13	1:A:33:TRP:CZ2	0.65	2.26	18	1
1:A:95:TRP:CZ3	1:A:97:PHE:CE1	0.65	2.84	6	1
1:A:83:LEU:HD11	1:A:91:LEU:H	0.65	1.51	14	1
1:A:25:ASP:O	1:A:27:TYR:CZ	0.65	2.49	9	1
1:A:66:PHE:CD1	1:A:66:PHE:N	0.64	2.65	16	1
1:A:61:PHE:O	1:A:61:PHE:CG	0.64	2.50	5	6
1:A:8:LYS:CD	1:A:135:ILE:HG23	0.64	2.23	15	1
1:A:95:TRP:CZ2	1:A:108:PHE:CD1	0.64	2.85	2	2
1:A:31:VAL:HB	1:A:34:ILE:HG22	0.64	1.70	3	2
1:A:91:LEU:HD12	1:A:112:PHE:HB3	0.64	1.69	8	3
1:A:114:PHE:CZ	1:A:123:LEU:CD1	0.64	2.78	9	10
1:A:108:PHE:CE1	1:A:110:ILE:HG22	0.63	2.28	4	3
1:A:95:TRP:CE3	1:A:108:PHE:CG	0.63	2.86	18	1
1:A:20:LEU:HD11	1:A:138:PHE:CD2	0.63	2.29	13	5
1:A:134:LEU:HD12	1:A:135:ILE:N	0.63	2.08	17	5
1:A:23:ASP:O	1:A:27:TYR:CE2	0.63	2.52	16	4
1:A:33:TRP:CZ3	1:A:134:LEU:HD13	0.63	2.28	10	1
1:A:24:VAL:HB	1:A:39:THR:HG21	0.63	1.68	15	10
1:A:31:VAL:CG1	1:A:33:TRP:CZ2	0.62	2.82	17	2
1:A:23:ASP:OD2	1:A:27:TYR:CD1	0.62	2.53	16	2
1:A:72:ARG:HD2	1:A:79:ILE:HD11	0.62	1.70	15	1
1:A:17:LEU:HD11	1:A:104:THR:HG21	0.62	1.70	10	2
1:A:2:HIS:CD2	1:A:120:ASP:CG	0.62	2.73	7	11
1:A:33:TRP:CZ2	1:A:134:LEU:HD12	0.62	2.30	4	1
1:A:31:VAL:HG23	1:A:31:VAL:O	0.62	1.94	16	1
1:A:111:GLU:O	1:A:112:PHE:CD1	0.62	2.53	8	3
1:A:12:TYR:CD2	1:A:142:ALA:HB1	0.62	2.29	1	2
1:A:68:THR:HG21	1:A:91:LEU:HD23	0.61	1.70	8	4
1:A:23:ASP:CG	1:A:27:TYR:CD2	0.61	2.74	18	1
1:A:48:VAL:HG22	1:A:73:ASP:CG	0.61	2.16	8	15
1:A:31:VAL:CG1	1:A:33:TRP:CH2	0.61	2.80	13	1
1:A:61:PHE:CD1	1:A:61:PHE:N	0.61	2.68	17	1
1:A:31:VAL:CG1	1:A:33:TRP:CE3	0.61	2.80	5	2
1:A:20:LEU:HD11	1:A:138:PHE:CG	0.61	2.31	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:TRP:CH2	1:A:108:PHE:CG	0.61	2.88	4	3
1:A:2:HIS:CE1	1:A:120:ASP:OD1	0.61	2.54	4	2
1:A:2:HIS:CD2	1:A:120:ASP:OD2	0.60	2.54	13	7
1:A:4:HIS:CE1	1:A:124:ALA:O	0.60	2.54	13	4
1:A:2:HIS:CD2	1:A:120:ASP:OD1	0.60	2.55	20	5
1:A:21:VAL:HG22	1:A:97:PHE:CZ	0.60	2.31	19	4
1:A:110:ILE:CD1	1:A:112:PHE:CE2	0.60	2.85	5	9
1:A:26:ALA:O	1:A:27:TYR:CD2	0.60	2.54	3	1
1:A:23:ASP:OD1	1:A:27:TYR:CE1	0.60	2.54	1	1
1:A:77:ARG:O	1:A:97:PHE:CZ	0.60	2.54	3	5
1:A:110:ILE:HD11	1:A:112:PHE:CE2	0.60	2.32	11	2
1:A:12:TYR:CE2	1:A:142:ALA:CB	0.60	2.85	20	3
1:A:83:LEU:C	1:A:83:LEU:HD13	0.60	2.17	5	2
1:A:62:LEU:HD23	1:A:62:LEU:O	0.60	1.96	5	1
1:A:84:LEU:O	1:A:84:LEU:HD12	0.60	1.96	7	1
1:A:14:PRO:CA	1:A:17:LEU:HD12	0.60	2.26	13	8
1:A:31:VAL:HG13	1:A:33:TRP:CD2	0.59	2.30	1	2
1:A:134:LEU:HD13	1:A:134:LEU:C	0.59	2.16	19	1
1:A:23:ASP:O	1:A:27:TYR:CD2	0.59	2.54	17	1
1:A:84:LEU:C	1:A:84:LEU:HD13	0.59	2.18	5	1
1:A:23:ASP:OD2	1:A:27:TYR:CE2	0.59	2.55	20	1
1:A:84:LEU:C	1:A:84:LEU:CD1	0.59	2.71	5	2
1:A:77:ARG:O	1:A:97:PHE:CE1	0.59	2.55	1	2
1:A:83:LEU:O	1:A:83:LEU:HD13	0.59	1.97	1	3
1:A:20:LEU:CD1	1:A:138:PHE:CG	0.59	2.85	8	2
1:A:25:ASP:O	1:A:27:TYR:CE2	0.59	2.55	3	1
1:A:108:PHE:CZ	1:A:110:ILE:CG2	0.59	2.86	4	1
1:A:35:THR:OG1	1:A:36:GLY:N	0.59	2.35	14	19
1:A:131:ALA:O	1:A:135:ILE:HD12	0.58	1.98	12	1
1:A:79:ILE:HB	1:A:95:TRP:CD1	0.58	2.34	8	3
1:A:26:ALA:C	1:A:27:TYR:CG	0.58	2.76	14	9
1:A:34:ILE:HG23	1:A:35:THR:N	0.58	2.14	18	17
1:A:83:LEU:HD22	1:A:84:LEU:H	0.58	1.58	19	5
1:A:95:TRP:CD1	1:A:95:TRP:O	0.58	2.57	9	2
1:A:17:LEU:HD22	1:A:97:PHE:CE1	0.58	2.32	6	1
1:A:20:LEU:CD1	1:A:138:PHE:CZ	0.58	2.86	13	4
1:A:123:LEU:HD23	1:A:126:ASN:HD21	0.58	1.57	8	4
1:A:23:ASP:CG	1:A:27:TYR:CE1	0.58	2.77	11	4
1:A:70:VAL:HG23	1:A:81:VAL:CG2	0.58	2.29	17	3
1:A:33:TRP:HB2	1:A:130:ALA:HB1	0.58	1.76	15	2
1:A:8:LYS:HZ2	1:A:106:VAL:HB	0.58	1.59	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:PHE:CE2	1:A:110:ILE:CG2	0.57	2.87	20	2
1:A:57:VAL:HG22	1:A:64:GLU:O	0.57	1.99	9	3
1:A:31:VAL:HG12	1:A:33:TRP:HZ3	0.57	1.54	14	4
1:A:110:ILE:HD13	1:A:112:PHE:HE2	0.57	1.55	1	6
1:A:108:PHE:CE2	1:A:110:ILE:HG22	0.57	2.34	20	2
1:A:23:ASP:OD1	1:A:27:TYR:CG	0.57	2.58	12	2
1:A:23:ASP:O	1:A:27:TYR:CZ	0.57	2.56	16	4
1:A:53:ALA:HB2	1:A:70:VAL:HB	0.57	1.76	13	3
1:A:12:TYR:CE1	1:A:146:HIS:CD2	0.57	2.93	13	1
1:A:17:LEU:O	1:A:21:VAL:HG23	0.57	2.00	8	5
1:A:95:TRP:CZ2	1:A:106:VAL:HG11	0.56	2.35	12	3
1:A:21:VAL:HG13	1:A:79:ILE:HG12	0.56	1.77	10	6
1:A:23:ASP:OD1	1:A:27:TYR:CD1	0.56	2.58	17	2
1:A:77:ARG:O	1:A:97:PHE:CE2	0.56	2.58	13	1
1:A:110:ILE:CD1	1:A:112:PHE:CD2	0.56	2.88	16	2
1:A:68:THR:HG21	1:A:91:LEU:HD21	0.56	1.76	10	1
1:A:85:TYR:O	1:A:86:GLY:O	0.56	2.24	20	13
1:A:12:TYR:CD1	1:A:12:TYR:C	0.56	2.77	18	1
1:A:24:VAL:HG21	1:A:39:THR:HG21	0.55	1.76	20	1
1:A:85:TYR:O	1:A:86:GLY:C	0.55	2.44	1	6
1:A:35:THR:HG21	1:A:57:VAL:C	0.55	2.22	14	11
1:A:2:HIS:CG	1:A:120:ASP:OD2	0.55	2.59	18	3
1:A:133:LYS:HG3	1:A:134:LEU:N	0.55	2.16	13	7
1:A:4:HIS:CD2	1:A:127:VAL:HG12	0.55	2.36	15	7
1:A:138:PHE:O	1:A:142:ALA:HB2	0.55	2.02	18	1
1:A:44:VAL:HG23	1:A:49:SER:OG	0.55	2.01	4	5
1:A:27:TYR:CD2	1:A:27:TYR:O	0.55	2.60	6	1
1:A:23:ASP:OD2	1:A:27:TYR:CE1	0.55	2.59	16	1
1:A:33:TRP:CH2	1:A:134:LEU:HD23	0.55	2.36	19	1
1:A:61:PHE:CD1	1:A:61:PHE:O	0.55	2.60	4	1
1:A:2:HIS:CG	1:A:120:ASP:OD1	0.55	2.60	7	4
1:A:65:LYS:O	1:A:66:PHE:CD1	0.55	2.59	17	9
1:A:26:ALA:O	1:A:27:TYR:C	0.55	2.44	9	7
1:A:31:VAL:HG12	1:A:33:TRP:CE2	0.55	2.37	17	1
1:A:60:SER:O	1:A:61:PHE:CG	0.55	2.59	17	1
1:A:31:VAL:CG1	1:A:33:TRP:CD2	0.55	2.90	1	2
1:A:47:ALA:HB3	1:A:75:ASP:HB2	0.54	1.79	16	3
1:A:22:GLY:O	1:A:26:ALA:N	0.54	2.40	8	13
1:A:33:TRP:CE3	1:A:134:LEU:HB2	0.54	2.37	1	13
1:A:21:VAL:HG22	1:A:97:PHE:HE2	0.54	1.56	8	2
1:A:68:THR:HG21	1:A:91:LEU:CD2	0.54	2.32	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:40:TRP:CD1	1:A:41:ASN:N	0.54	2.76	16	6
1:A:83:LEU:HD12	1:A:83:LEU:C	0.54	2.21	20	1
1:A:65:LYS:C	1:A:66:PHE:CG	0.54	2.80	17	7
1:A:6:VAL:HG12	1:A:135:ILE:HD11	0.54	1.79	8	2
1:A:134:LEU:CD1	1:A:134:LEU:C	0.54	2.75	16	4
1:A:69:ARG:HG3	1:A:84:LEU:HD12	0.54	1.80	13	1
1:A:134:LEU:C	1:A:134:LEU:CD1	0.54	2.76	17	6
1:A:2:HIS:N	1:A:2:HIS:CD2	0.54	2.76	16	1
1:A:84:LEU:HD13	1:A:85:TYR:HB2	0.54	1.77	15	1
1:A:134:LEU:HD22	1:A:134:LEU:O	0.54	2.03	19	1
1:A:93:ASN:ND2	1:A:95:TRP:CZ2	0.54	2.76	11	1
1:A:69:ARG:CG	1:A:84:LEU:HD12	0.53	2.32	13	1
1:A:35:THR:CG2	1:A:57:VAL:N	0.53	2.72	14	15
1:A:21:VAL:HG22	1:A:97:PHE:HZ	0.53	1.63	4	1
1:A:35:THR:CG2	1:A:56:GLN:C	0.53	2.77	11	17
1:A:70:VAL:HG23	1:A:81:VAL:HG22	0.53	1.81	18	4
1:A:54:GLU:CG	1:A:67:ALA:HB2	0.53	2.33	3	1
1:A:53:ALA:HB2	1:A:70:VAL:CG1	0.53	2.33	15	2
1:A:60:SER:O	1:A:61:PHE:CB	0.53	2.56	1	2
1:A:20:LEU:HD13	1:A:95:TRP:CZ3	0.53	2.38	9	1
1:A:33:TRP:CB	1:A:133:LYS:CE	0.53	2.87	19	2
1:A:124:ALA:O	1:A:127:VAL:HG12	0.53	2.04	3	8
1:A:21:VAL:HG22	1:A:95:TRP:CH2	0.53	2.39	6	1
1:A:121:ALA:O	1:A:125:ALA:CB	0.53	2.57	7	15
1:A:4:HIS:HB2	1:A:110:ILE:HD11	0.52	1.80	9	13
1:A:40:TRP:CG	1:A:41:ASN:N	0.52	2.77	16	8
1:A:59:PHE:O	1:A:59:PHE:CD1	0.52	2.62	7	1
1:A:6:VAL:CG1	1:A:135:ILE:HD11	0.52	2.34	8	5
1:A:141:ARG:NH2	1:A:144:GLN:HE22	0.52	2.02	8	2
1:A:97:PHE:CD1	1:A:97:PHE:N	0.52	2.78	1	3
1:A:31:VAL:CG1	1:A:33:TRP:CZ3	0.52	2.92	2	3
1:A:62:LEU:HD11	1:A:64:GLU:HG3	0.52	1.81	17	1
1:A:95:TRP:CH2	1:A:108:PHE:CE1	0.52	2.97	5	2
1:A:31:VAL:HG13	1:A:33:TRP:CE2	0.52	2.40	18	1
1:A:134:LEU:HD12	1:A:134:LEU:O	0.52	2.05	18	3
1:A:22:GLY:O	1:A:26:ALA:CB	0.52	2.58	15	5
1:A:31:VAL:HG13	1:A:33:TRP:CZ3	0.52	2.40	18	2
1:A:33:TRP:CH2	1:A:134:LEU:HD13	0.52	2.40	11	2
1:A:120:ASP:O	1:A:124:ALA:CB	0.52	2.57	3	14
1:A:20:LEU:CD1	1:A:138:PHE:CD2	0.52	2.93	12	3
1:A:61:PHE:O	1:A:61:PHE:CD2	0.52	2.63	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:TRP:CZ3	1:A:97:PHE:CE2	0.51	2.98	6	1
1:A:23:ASP:OD1	1:A:27:TYR:CD2	0.51	2.62	20	2
1:A:68:THR:HG21	1:A:91:LEU:HD22	0.51	1.82	19	1
1:A:27:TYR:O	1:A:27:TYR:CG	0.51	2.63	13	4
1:A:33:TRP:CE2	1:A:134:LEU:HD12	0.51	2.41	4	1
1:A:110:ILE:O	1:A:110:ILE:CD1	0.51	2.59	10	4
1:A:26:ALA:C	1:A:27:TYR:CD2	0.51	2.84	3	1
1:A:110:ILE:HD12	1:A:110:ILE:C	0.51	2.25	1	2
1:A:110:ILE:HB	1:A:112:PHE:CZ	0.51	2.40	10	3
1:A:17:LEU:HD21	1:A:106:VAL:CG2	0.51	2.35	4	1
1:A:25:ASP:O	1:A:27:TYR:CE1	0.51	2.64	7	2
1:A:114:PHE:C	1:A:115:LYS:CE	0.51	2.79	18	3
1:A:47:ALA:HB1	1:A:74:LYS:CD	0.51	2.36	4	1
1:A:17:LEU:HD21	1:A:106:VAL:HG21	0.51	1.82	4	2
1:A:37:MET:O	1:A:37:MET:CE	0.51	2.59	8	3
1:A:6:VAL:HG12	1:A:8:LYS:HE3	0.51	1.83	2	1
1:A:58:GLY:O	1:A:59:PHE:CB	0.50	2.58	2	1
1:A:21:VAL:CG2	1:A:97:PHE:CE2	0.50	2.82	10	2
1:A:24:VAL:CB	1:A:39:THR:HG21	0.50	2.36	15	3
1:A:110:ILE:CD1	1:A:110:ILE:O	0.50	2.58	12	3
1:A:6:VAL:HG11	1:A:135:ILE:HD11	0.50	1.81	7	1
1:A:31:VAL:CG1	1:A:33:TRP:CE2	0.50	2.94	18	1
1:A:20:LEU:HG	1:A:138:PHE:CE1	0.50	2.41	15	8
1:A:48:VAL:CG2	1:A:73:ASP:CG	0.50	2.80	3	5
1:A:93:ASN:OD1	1:A:95:TRP:CZ2	0.50	2.64	17	1
1:A:50:THR:HG22	1:A:69:ARG:CD	0.50	2.37	9	1
1:A:40:TRP:NE1	1:A:41:ASN:ND2	0.50	2.60	7	1
1:A:61:PHE:CD2	1:A:61:PHE:O	0.50	2.65	10	1
1:A:20:LEU:HD12	1:A:138:PHE:CE1	0.50	2.42	18	2
1:A:8:LYS:NZ	1:A:106:VAL:CG2	0.50	2.74	20	1
1:A:10:LEU:CD1	1:A:138:PHE:CE2	0.50	2.95	9	2
1:A:84:LEU:HD13	1:A:85:TYR:N	0.49	2.22	14	2
1:A:17:LEU:HD13	1:A:97:PHE:HD2	0.49	1.65	3	2
1:A:83:LEU:C	1:A:83:LEU:CD1	0.49	2.80	2	2
1:A:95:TRP:CZ3	1:A:108:PHE:CD1	0.49	3.00	5	3
1:A:84:LEU:HD13	1:A:85:TYR:CB	0.49	2.38	14	2
1:A:47:ALA:CB	1:A:75:ASP:OD1	0.49	2.61	4	1
1:A:60:SER:O	1:A:61:PHE:CD2	0.49	2.65	17	1
1:A:84:LEU:HD13	1:A:84:LEU:O	0.49	2.06	5	1
1:A:64:GLU:O	1:A:66:PHE:CE1	0.49	2.65	16	1
1:A:2:HIS:CE1	1:A:124:ALA:CB	0.49	2.96	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:27:TYR:OH	1:A:37:MET:CE	0.49	2.61	8	1
1:A:25:ASP:C	1:A:27:TYR:CE1	0.49	2.85	7	1
1:A:83:LEU:C	1:A:83:LEU:HD22	0.49	2.26	9	1
1:A:95:TRP:CZ2	1:A:97:PHE:CD2	0.49	3.00	9	1
1:A:17:LEU:HB3	1:A:97:PHE:CE2	0.49	2.43	6	1
1:A:83:LEU:C	1:A:83:LEU:CD2	0.49	2.78	15	1
1:A:24:VAL:O	1:A:37:MET:CG	0.49	2.61	1	4
1:A:97:PHE:CE1	1:A:106:VAL:HG13	0.49	2.43	20	1
1:A:73:ASP:HB3	1:A:76:ALA:HB3	0.49	1.85	7	2
1:A:111:GLU:C	1:A:112:PHE:CD1	0.49	2.86	12	3
1:A:12:TYR:CE2	1:A:142:ALA:HB3	0.49	2.43	8	2
1:A:25:ASP:O	1:A:26:ALA:C	0.49	2.51	20	3
1:A:17:LEU:HB3	1:A:97:PHE:CZ	0.49	2.43	6	2
1:A:115:LYS:CD	1:A:115:LYS:N	0.48	2.76	19	1
1:A:95:TRP:CE3	1:A:108:PHE:HB2	0.48	2.43	19	1
1:A:19:GLU:O	1:A:23:ASP:N	0.48	2.46	12	3
1:A:25:ASP:CA	1:A:27:TYR:CE2	0.48	2.96	9	1
1:A:4:HIS:CG	1:A:127:VAL:CG1	0.48	2.96	13	1
1:A:20:LEU:HD12	1:A:138:PHE:CE2	0.48	2.43	16	5
1:A:20:LEU:CD1	1:A:138:PHE:CD1	0.48	2.96	8	1
1:A:65:LYS:C	1:A:66:PHE:CD1	0.48	2.87	14	1
1:A:131:ALA:O	1:A:135:ILE:CD1	0.48	2.61	12	1
1:A:97:PHE:N	1:A:97:PHE:CD1	0.48	2.81	2	2
1:A:83:LEU:CD1	1:A:83:LEU:C	0.48	2.79	1	2
1:A:27:TYR:CD2	1:A:31:VAL:HG21	0.48	2.43	13	1
1:A:115:LYS:N	1:A:115:LYS:CD	0.48	2.76	13	2
1:A:8:LYS:HG2	1:A:9:VAL:N	0.48	2.22	15	1
1:A:50:THR:CG2	1:A:69:ARG:CD	0.48	2.92	15	2
1:A:81:VAL:N	1:A:93:ASN:O	0.48	2.47	13	6
1:A:27:TYR:CE1	1:A:31:VAL:HG21	0.48	2.44	1	1
1:A:91:LEU:C	1:A:91:LEU:HD23	0.48	2.29	13	1
1:A:12:TYR:CD2	1:A:142:ALA:CB	0.48	2.96	8	1
1:A:110:ILE:HB	1:A:112:PHE:CE2	0.48	2.44	12	3
1:A:50:THR:HG22	1:A:69:ARG:HD3	0.48	1.86	9	1
1:A:21:VAL:CG2	1:A:97:PHE:CZ	0.48	2.97	1	2
1:A:93:ASN:OD1	1:A:108:PHE:CE1	0.48	2.66	20	1
1:A:2:HIS:CE1	1:A:120:ASP:HB3	0.48	2.44	9	5
1:A:141:ARG:CZ	1:A:144:GLN:OE1	0.48	2.61	5	1
1:A:21:VAL:CG2	1:A:97:PHE:CD2	0.48	2.93	10	1
1:A:17:LEU:O	1:A:20:LEU:N	0.47	2.47	6	16
1:A:32:PRO:C	1:A:34:ILE:N	0.47	2.66	4	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:LEU:HD13	1:A:135:ILE:CA	0.47	2.37	19	1
1:A:8:LYS:HZ2	1:A:106:VAL:CB	0.47	2.22	20	1
1:A:95:TRP:CZ3	1:A:108:PHE:HB2	0.47	2.44	2	4
1:A:8:LYS:NZ	1:A:135:ILE:HD11	0.47	2.24	2	2
1:A:34:ILE:HD11	1:A:55:ALA:HB1	0.47	1.85	4	1
1:A:126:ASN:OD1	1:A:126:ASN:C	0.47	2.53	18	10
1:A:51:VAL:O	1:A:70:VAL:CG1	0.47	2.63	13	2
1:A:35:THR:HG23	1:A:36:GLY:N	0.47	2.19	18	1
1:A:95:TRP:C	1:A:95:TRP:CD1	0.47	2.87	3	2
1:A:20:LEU:HG	1:A:138:PHE:CD1	0.47	2.45	2	2
1:A:68:THR:HB	1:A:81:VAL:HG12	0.47	1.86	6	2
1:A:60:SER:O	1:A:61:PHE:HB3	0.47	2.09	2	11
1:A:95:TRP:CD1	1:A:95:TRP:C	0.47	2.88	7	1
1:A:33:TRP:CD2	1:A:134:LEU:HB2	0.47	2.45	20	4
1:A:23:ASP:HB2	1:A:27:TYR:CE1	0.47	2.44	12	1
1:A:96:ARG:C	1:A:97:PHE:CD1	0.47	2.88	2	3
1:A:77:ARG:HB3	1:A:97:PHE:CE1	0.47	2.45	9	1
1:A:8:LYS:HE2	1:A:10:LEU:HD11	0.47	1.86	13	1
1:A:4:HIS:CD2	1:A:127:VAL:HG11	0.47	2.44	16	1
1:A:16:GLN:OE1	1:A:138:PHE:CE1	0.47	2.68	2	2
1:A:33:TRP:CZ3	1:A:134:LEU:HB2	0.47	2.44	18	4
1:A:25:ASP:HA	1:A:27:TYR:CE2	0.47	2.45	9	1
1:A:77:ARG:HB3	1:A:97:PHE:CE2	0.47	2.45	13	1
1:A:50:THR:OG1	1:A:71:ARG:CG	0.47	2.63	20	2
1:A:126:ASN:O	1:A:129:ARG:N	0.47	2.48	11	11
1:A:131:ALA:O	1:A:135:ILE:CG1	0.47	2.62	12	1
1:A:32:PRO:O	1:A:34:ILE:N	0.47	2.48	4	2
1:A:95:TRP:CH2	1:A:108:PHE:CD1	0.46	3.03	2	2
1:A:14:PRO:HA	1:A:17:LEU:CD1	0.46	2.39	5	2
1:A:84:LEU:HD23	1:A:85:TYR:CB	0.46	2.41	1	1
1:A:95:TRP:C	1:A:95:TRP:CE3	0.46	2.88	6	1
1:A:95:TRP:CZ3	1:A:97:PHE:CD1	0.46	3.03	6	1
1:A:110:ILE:CD1	1:A:110:ILE:C	0.46	2.78	11	1
1:A:71:ARG:O	1:A:79:ILE:HD13	0.46	2.10	15	1
1:A:8:LYS:HZ2	1:A:106:VAL:CG2	0.46	2.22	20	1
1:A:12:TYR:CD1	1:A:146:HIS:CD2	0.46	3.03	16	2
1:A:23:ASP:O	1:A:27:TYR:CD1	0.46	2.68	13	1
1:A:64:GLU:CB	1:A:66:PHE:CZ	0.46	2.99	15	1
1:A:23:ASP:OD1	1:A:23:ASP:O	0.46	2.33	20	2
1:A:2:HIS:NE2	1:A:120:ASP:OD2	0.46	2.49	11	2
1:A:126:ASN:C	1:A:126:ASN:OD1	0.46	2.54	13	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:37:MET:N	1:A:37:MET:SD	0.46	2.88	4	5
1:A:23:ASP:O	1:A:27:TYR:CG	0.46	2.69	17	1
1:A:79:ILE:CG2	1:A:95:TRP:NE1	0.46	2.77	6	1
1:A:50:THR:HG23	1:A:71:ARG:HG2	0.46	1.86	2	1
1:A:11:PRO:HB3	1:A:103:ALA:HB2	0.46	1.86	17	1
1:A:4:HIS:CG	1:A:127:VAL:HG11	0.46	2.45	16	3
1:A:2:HIS:CE1	1:A:124:ALA:HB2	0.46	2.45	4	1
1:A:126:ASN:OD1	1:A:127:VAL:N	0.46	2.49	15	7
1:A:4:HIS:NE2	1:A:124:ALA:O	0.46	2.49	15	5
1:A:134:LEU:HD22	1:A:134:LEU:C	0.46	2.31	19	1
1:A:14:PRO:HB3	1:A:17:LEU:HD12	0.46	1.85	18	1
1:A:20:LEU:HG	1:A:138:PHE:CZ	0.46	2.45	14	2
1:A:2:HIS:CE1	1:A:124:ALA:HB1	0.46	2.46	15	1
1:A:23:ASP:OD2	1:A:27:TYR:CZ	0.46	2.68	20	1
1:A:97:PHE:CB	1:A:106:VAL:HG22	0.45	2.41	1	3
1:A:53:ALA:N	1:A:68:THR:O	0.45	2.49	13	9
1:A:67:ALA:O	1:A:68:THR:HG23	0.45	2.11	1	3
1:A:98:MET:N	1:A:105:ARG:O	0.45	2.48	13	1
1:A:32:PRO:HB2	1:A:59:PHE:CD2	0.45	2.46	16	1
1:A:23:ASP:HB2	1:A:27:TYR:CE2	0.45	2.45	18	1
1:A:21:VAL:CG1	1:A:79:ILE:CG1	0.45	2.94	20	2
1:A:25:ASP:C	1:A:27:TYR:CE2	0.45	2.89	3	1
1:A:77:ARG:O	1:A:97:PHE:CD2	0.45	2.69	4	1
1:A:72:ARG:CD	1:A:79:ILE:HD11	0.45	2.40	15	1
1:A:8:LYS:HE2	1:A:138:PHE:CE2	0.45	2.46	20	1
1:A:48:VAL:HG22	1:A:73:ASP:OD1	0.45	2.12	12	1
1:A:112:PHE:CE1	1:A:114:PHE:CE2	0.45	3.05	11	1
1:A:64:GLU:HB3	1:A:66:PHE:CZ	0.45	2.46	15	1
1:A:33:TRP:CE2	1:A:134:LEU:HB2	0.45	2.46	17	2
1:A:95:TRP:CZ3	1:A:106:VAL:CG1	0.45	3.00	9	2
1:A:138:PHE:O	1:A:142:ALA:CB	0.45	2.64	18	1
1:A:23:ASP:C	1:A:25:ASP:N	0.45	2.69	12	3
1:A:31:VAL:HA	1:A:33:TRP:CZ3	0.45	2.47	13	1
1:A:13:THR:OG1	1:A:146:HIS:NE2	0.45	2.49	18	1
1:A:31:VAL:CG2	1:A:34:ILE:HG22	0.45	2.42	20	2
1:A:99:PRO:O	1:A:100:GLU:CG	0.45	2.65	3	1
1:A:52:ASP:OD2	1:A:52:ASP:N	0.45	2.49	7	1
1:A:72:ARG:CB	1:A:79:ILE:HD11	0.44	2.42	14	1
1:A:127:VAL:CG1	1:A:128:ASP:N	0.44	2.80	10	6
1:A:57:VAL:HG23	1:A:62:LEU:O	0.44	2.12	14	2
1:A:134:LEU:CD1	1:A:135:ILE:N	0.44	2.64	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:HIS:H	1:A:110:ILE:HD13	0.44	1.71	17	3
1:A:141:ARG:NH1	1:A:145:LEU:HD12	0.44	2.28	17	1
1:A:110:ILE:C	1:A:110:ILE:CD1	0.44	2.86	10	1
1:A:23:ASP:OD2	1:A:23:ASP:O	0.44	2.35	11	1
1:A:23:ASP:CG	1:A:27:TYR:CD1	0.44	2.91	11	1
1:A:47:ALA:CB	1:A:75:ASP:OD2	0.44	2.65	20	1
1:A:33:TRP:CA	1:A:133:LYS:HE3	0.44	2.43	2	7
1:A:60:SER:C	1:A:61:PHE:CD1	0.44	2.90	17	1
1:A:21:VAL:HG13	1:A:95:TRP:HZ2	0.44	1.73	6	1
1:A:67:ALA:HB3	1:A:85:TYR:HB2	0.44	1.89	5	1
1:A:26:ALA:C	1:A:27:TYR:O	0.44	2.55	7	2
1:A:114:PHE:CD2	1:A:120:ASP:HA	0.44	2.47	3	1
1:A:115:LYS:CE	1:A:115:LYS:N	0.44	2.81	19	3
1:A:50:THR:HG23	1:A:71:ARG:CG	0.44	2.39	11	1
1:A:37:MET:SD	1:A:37:MET:N	0.44	2.91	3	4
1:A:79:ILE:HG21	1:A:95:TRP:CD1	0.44	2.47	6	1
1:A:50:THR:CG2	1:A:69:ARG:HD3	0.44	2.43	15	1
1:A:21:VAL:HG22	1:A:95:TRP:HE1	0.44	1.73	9	1
1:A:22:GLY:C	1:A:24:VAL:N	0.44	2.71	1	1
1:A:47:ALA:HB1	1:A:74:LYS:HD2	0.44	1.88	4	1
1:A:4:HIS:HB2	1:A:110:ILE:CD1	0.43	2.43	17	5
1:A:97:PHE:HB3	1:A:106:VAL:HG22	0.43	1.89	3	2
1:A:45:ASP:O	1:A:48:VAL:O	0.43	2.35	10	2
1:A:8:LYS:HB2	1:A:135:ILE:HD13	0.43	1.89	15	1
1:A:16:GLN:OE1	1:A:142:ALA:HB1	0.43	2.13	7	1
1:A:97:PHE:O	1:A:97:PHE:CD1	0.43	2.71	9	1
1:A:8:LYS:HD3	1:A:135:ILE:CG2	0.43	2.41	15	1
1:A:35:THR:CG2	1:A:57:VAL:CA	0.43	2.96	14	1
1:A:9:VAL:HG13	1:A:9:VAL:O	0.43	2.13	6	1
1:A:35:THR:HG23	1:A:56:GLN:CB	0.43	2.44	19	2
1:A:10:LEU:HD22	1:A:139:GLU:HG3	0.43	1.90	16	1
1:A:23:ASP:C	1:A:23:ASP:OD1	0.43	2.56	12	1
1:A:32:PRO:O	1:A:33:TRP:C	0.43	2.55	4	2
1:A:110:ILE:O	1:A:110:ILE:CG1	0.43	2.66	10	1
1:A:33:TRP:CE2	1:A:134:LEU:CD1	0.43	3.01	4	1
1:A:31:VAL:CG2	1:A:31:VAL:O	0.43	2.65	16	1
1:A:33:TRP:CZ3	1:A:34:ILE:HD12	0.43	2.49	16	1
1:A:138:PHE:CD1	1:A:138:PHE:O	0.43	2.71	7	1
1:A:20:LEU:HD22	1:A:95:TRP:CH2	0.43	2.49	1	1
1:A:8:LYS:NZ	1:A:135:ILE:CD1	0.43	2.82	5	1
1:A:138:PHE:CD1	1:A:138:PHE:C	0.43	2.90	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:LYS:CG	1:A:134:LEU:N	0.43	2.82	17	1
1:A:74:LYS:O	1:A:77:ARG:NH1	0.43	2.52	8	1
1:A:27:TYR:CD2	1:A:31:VAL:CG1	0.43	3.02	11	1
1:A:5:VAL:C	1:A:6:VAL:CG2	0.43	2.87	8	3
1:A:95:TRP:HB3	1:A:97:PHE:CZ	0.43	2.49	2	2
1:A:95:TRP:NE1	1:A:108:PHE:CE1	0.43	2.87	20	1
1:A:54:GLU:HG2	1:A:67:ALA:HB2	0.43	1.90	3	1
1:A:79:ILE:HB	1:A:95:TRP:CE2	0.43	2.48	6	1
1:A:8:LYS:CD	1:A:8:LYS:N	0.43	2.81	5	1
1:A:2:HIS:CE1	1:A:110:ILE:HD11	0.43	2.49	15	1
1:A:35:THR:CG2	1:A:36:GLY:H	0.43	2.18	18	1
1:A:97:PHE:CD1	1:A:106:VAL:CG1	0.43	2.95	20	1
1:A:16:GLN:OE1	1:A:16:GLN:N	0.43	2.51	8	1
1:A:120:ASP:O	1:A:124:ALA:HB3	0.42	2.14	7	2
1:A:15:ASP:O	1:A:18:PHE:CB	0.42	2.67	7	1
1:A:133:LYS:HG2	1:A:134:LEU:N	0.42	2.29	5	2
1:A:20:LEU:HD13	1:A:95:TRP:CZ2	0.42	2.49	3	1
1:A:8:LYS:HE2	1:A:138:PHE:CD2	0.42	2.49	20	1
1:A:111:GLU:C	1:A:112:PHE:CG	0.42	2.92	8	1
1:A:31:VAL:O	1:A:31:VAL:HG23	0.42	2.13	6	1
1:A:68:THR:CG2	1:A:91:LEU:HD21	0.42	2.42	10	1
1:A:8:LYS:HD2	1:A:8:LYS:N	0.42	2.29	2	1
1:A:21:VAL:CG1	1:A:79:ILE:HG13	0.42	2.44	20	2
1:A:33:TRP:CE3	1:A:134:LEU:CB	0.42	3.02	1	1
1:A:23:ASP:OD2	1:A:27:TYR:CG	0.42	2.71	11	1
1:A:23:ASP:CB	1:A:27:TYR:CD2	0.42	3.02	18	1
1:A:50:THR:C	1:A:51:VAL:CG1	0.42	2.88	19	18
1:A:23:ASP:HA	1:A:26:ALA:HB3	0.42	1.91	5	2
1:A:73:ASP:OD1	1:A:75:ASP:N	0.42	2.50	13	3
1:A:34:ILE:CG2	1:A:35:THR:N	0.42	2.83	18	1
1:A:45:ASP:O	1:A:48:VAL:N	0.42	2.47	11	2
1:A:20:LEU:HD21	1:A:138:PHE:CD1	0.42	2.49	20	1
1:A:33:TRP:CB	1:A:133:LYS:HE3	0.42	2.45	2	4
1:A:12:TYR:CE2	1:A:16:GLN:HB2	0.42	2.49	18	1
1:A:2:HIS:CE1	1:A:120:ASP:OD2	0.42	2.73	13	2
1:A:83:LEU:CB	1:A:91:LEU:O	0.42	2.68	19	1
1:A:4:HIS:HB2	1:A:110:ILE:CG1	0.42	2.45	10	2
1:A:100:GLU:CD	1:A:105:ARG:NH1	0.42	2.72	2	1
1:A:46:GLY:O	1:A:47:ALA:C	0.42	2.58	11	2
1:A:20:LEU:HD13	1:A:138:PHE:CE2	0.42	2.49	13	1
1:A:48:VAL:CG2	1:A:73:ASP:OD1	0.42	2.68	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:77:ARG:O	1:A:95:TRP:CZ3	0.42	2.73	6	1
1:A:5:VAL:HG13	1:A:109:VAL:HG12	0.41	1.92	17	1
1:A:27:TYR:CG	1:A:27:TYR:O	0.41	2.72	4	2
1:A:48:VAL:HG22	1:A:73:ASP:CB	0.41	2.44	3	1
1:A:49:SER:HB3	1:A:72:ARG:CG	0.41	2.46	10	1
1:A:2:HIS:NE2	1:A:120:ASP:CG	0.41	2.73	20	1
1:A:4:HIS:CB	1:A:110:ILE:CG1	0.41	2.98	12	1
1:A:19:GLU:O	1:A:23:ASP:CA	0.41	2.68	12	1
1:A:94:GLY:O	1:A:109:VAL:HG22	0.41	2.16	10	1
1:A:95:TRP:CE3	1:A:106:VAL:CG1	0.41	3.04	13	1
1:A:94:GLY:O	1:A:95:TRP:CE3	0.41	2.74	15	2
1:A:3:ARG:HB2	1:A:111:GLU:CG	0.41	2.45	14	1
1:A:6:VAL:CG1	1:A:8:LYS:HE3	0.41	2.45	2	1
1:A:11:PRO:HA	1:A:103:ALA:CB	0.41	2.45	16	3
1:A:94:GLY:CA	1:A:109:VAL:HG23	0.41	2.45	15	2
1:A:23:ASP:OD1	1:A:23:ASP:C	0.41	2.57	18	1
1:A:143:GLN:HA	1:A:146:HIS:CD2	0.41	2.50	5	1
1:A:112:PHE:CD1	1:A:112:PHE:C	0.41	2.93	16	1
1:A:71:ARG:N	1:A:80:ASP:O	0.41	2.51	20	1
1:A:25:ASP:OD1	1:A:39:THR:OG1	0.41	2.38	14	1
1:A:109:VAL:O	1:A:109:VAL:HG23	0.41	2.15	19	1
1:A:123:LEU:HD23	1:A:126:ASN:ND2	0.41	2.28	8	1
1:A:35:THR:CG2	1:A:57:VAL:C	0.41	2.89	14	1
1:A:62:LEU:CD1	1:A:64:GLU:HG3	0.41	2.45	17	1
1:A:23:ASP:O	1:A:27:TYR:CE1	0.41	2.73	17	1
1:A:66:PHE:N	1:A:66:PHE:CD1	0.41	2.89	1	1
1:A:47:ALA:O	1:A:73:ASP:OD2	0.41	2.39	10	2
1:A:84:LEU:CD1	1:A:85:TYR:HB2	0.41	2.46	15	1
1:A:115:LYS:N	1:A:115:LYS:HD2	0.41	2.31	18	1
1:A:25:ASP:O	1:A:27:TYR:O	0.41	2.39	20	1
1:A:41:ASN:O	1:A:52:ASP:OD1	0.41	2.39	17	2
1:A:37:MET:SD	1:A:37:MET:C	0.41	2.99	1	1
1:A:79:ILE:HB	1:A:95:TRP:NE1	0.41	2.31	6	1
1:A:112:PHE:C	1:A:112:PHE:CD1	0.41	2.94	13	1
1:A:52:ASP:OD1	1:A:52:ASP:N	0.41	2.54	11	1
1:A:32:PRO:HB2	1:A:59:PHE:CE2	0.41	2.51	16	1
1:A:4:HIS:CB	1:A:110:ILE:CD1	0.40	2.99	17	1
1:A:70:VAL:CG2	1:A:79:ILE:HD11	0.40	2.46	6	1
1:A:8:LYS:CD	1:A:135:ILE:HG12	0.40	2.47	10	1
1:A:93:ASN:ND2	1:A:95:TRP:CH2	0.40	2.89	11	1
1:A:100:GLU:O	1:A:103:ALA:O	0.40	2.39	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:ARG:C	1:A:97:PHE:CG	0.40	2.95	2	1
1:A:95:TRP:CD2	1:A:108:PHE:CE1	0.40	3.09	18	1
1:A:68:THR:CB	1:A:82:SER:O	0.40	2.70	14	1
1:A:25:ASP:CG	1:A:39:THR:OG1	0.40	2.59	11	1
1:A:133:LYS:HB2	1:A:133:LYS:NZ	0.40	2.31	11	1
1:A:23:ASP:O	1:A:25:ASP:N	0.40	2.54	12	1
1:A:35:THR:HG23	1:A:56:GLN:C	0.40	2.37	2	1
1:A:33:TRP:CH2	1:A:134:LEU:HD12	0.40	2.51	4	1
1:A:56:GLN:HG2	1:A:65:LYS:CB	0.40	2.46	17	1
1:A:46:GLY:O	1:A:48:VAL:HG23	0.40	2.16	10	1
1:A:31:VAL:HG23	1:A:34:ILE:HG22	0.40	1.92	20	1
1:A:44:VAL:HG13	1:A:44:VAL:O	0.40	2.17	20	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	139/148 (94%)	121±2 (87±1%)	15±2 (10±1%)	3±1 (2±1%)	12	49
All	All	2780/2960 (94%)	2423 (87%)	291 (10%)	66 (2%)	12	49

All 8 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	86	GLY	20
1	A	27	TYR	14
1	A	41	ASN	12
1	A	90	ARG	9
1	A	26	ALA	4
1	A	31	VAL	3
1	A	32	PRO	2
1	A	59	PHE	2

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/120 (94%)	74±3 (66±3%)	39±3 (34±3%)	1	11
All	All	2260/2400 (94%)	1484 (66%)	776 (34%)	1	11

All 81 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	127	VAL	20
1	A	115	LYS	20
1	A	104	THR	20
1	A	134	LEU	20
1	A	122	MET	20
1	A	75	ASP	20
1	A	35	THR	20
1	A	78	SER	20
1	A	40	TRP	20
1	A	4	HIS	20
1	A	63	ARG	19
1	A	52	ASP	18
1	A	85	TYR	18
1	A	38	ARG	18
1	A	141	ARG	18
1	A	33	TRP	17
1	A	98	MET	17
1	A	8	LYS	17
1	A	74	LYS	15
1	A	69	ARG	15
1	A	110	ILE	14
1	A	65	LYS	14
1	A	90	ARG	13
1	A	83	LEU	12
1	A	77	ARG	12
1	A	18	PHE	12
1	A	91	LEU	12
1	A	25	ASP	12
1	A	68	THR	11

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Mol	Chain	Res	Type	Models (Total)
1	A	34	ILE	11
1	A	143	GLN	11
1	A	57	VAL	11
1	A	72	ARG	11
1	A	59	PHE	11
1	A	62	LEU	10
1	A	41	ASN	10
1	A	49	SER	10
1	A	37	MET	9
1	A	139	GLU	9
1	A	54	GLU	9
1	A	120	ASP	9
1	A	84	LEU	9
1	A	133	LYS	8
1	A	43	ARG	8
1	A	95	TRP	7
1	A	92	ASN	7
1	A	145	LEU	7
1	A	93	ASN	7
1	A	79	ILE	7
1	A	96	ARG	7
1	A	2	HIS	6
1	A	71	ARG	6
1	A	105	ARG	6
1	A	20	LEU	6
1	A	66	PHE	5
1	A	6	VAL	5
1	A	31	VAL	5
1	A	5	VAL	5
1	A	108	PHE	5
1	A	60	SER	5
1	A	144	GLN	4
1	A	102	ASP	4
1	A	16	GLN	4
1	A	114	PHE	4
1	A	116	SER	4
1	A	100	GLU	4
1	A	111	GLU	3
1	A	112	PHE	3
1	A	3	ARG	3
1	A	97	PHE	2
1	A	129	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	23	ASP	2
1	A	146	HIS	2
1	A	128	ASP	2
1	A	138	PHE	1
1	A	12	TYR	1
1	A	109	VAL	1
1	A	61	PHE	1
1	A	27	TYR	1
1	A	137	CYS	1
1	A	82	SER	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 83% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6120

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	1705
Number of shifts mapped to atoms	1705
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	144	0.08 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	136	0.07 ± 0.18	None needed (< 0.5 ppm)
$^{13}C'$	133	0.24 ± 0.19	None needed (< 0.5 ppm)
^{15}N	135	-0.23 ± 0.26	None needed (< 0.5 ppm)

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 83%, i.e. 1438 atoms were assigned a chemical shift out of a possible 1737. 22 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	663/687 (97%)	271/274 (99%)	262/278 (94%)	130/135 (96%)
Sidechain	675/888 (76%)	418/516 (81%)	251/320 (78%)	6/52 (12%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	100/162 (62%)	61/87 (70%)	36/69 (52%)	3/6 (50%)
Overall	1438/1737 (83%)	750/877 (86%)	549/667 (82%)	139/193 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1528 atoms were assigned a chemical shift out of a possible 1856. 22 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	696/728 (96%)	284/290 (98%)	277/296 (94%)	135/142 (95%)
Sidechain	721/948 (76%)	449/554 (81%)	266/340 (78%)	6/54 (11%)
Aromatic	111/180 (62%)	69/97 (71%)	39/77 (51%)	3/6 (50%)
Overall	1528/1856 (82%)	802/941 (85%)	582/713 (82%)	144/202 (71%)

7.1.4 Statistically unusual chemical shifts ⓘ

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
1	A	52	ASP	HB3	0.67	4.07 − 1.27	-7.1
1	A	52	ASP	HB2	0.88	4.07 − 1.37	-6.8
1	A	107	GLU	CG	28.20	42.24 − 29.94	-6.4
1	A	21	VAL	HG21	-0.65	2.20 − -0.60	-5.2
1	A	21	VAL	HG23	-0.65	2.20 − -0.60	-5.2
1	A	21	VAL	HG22	-0.65	2.20 − -0.60	-5.2
1	A	14	PRO	CG	32.80	32.66 − 21.76	5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A: