



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 08:41 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

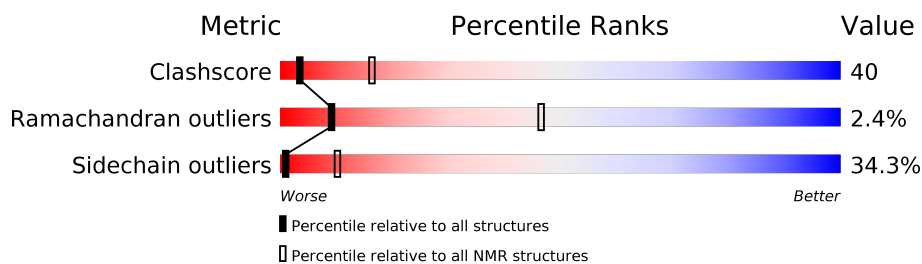
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	148	

## 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

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.

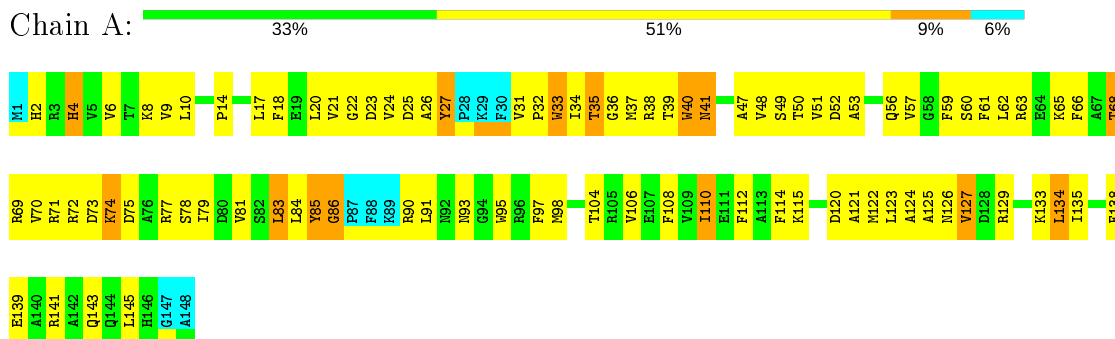
Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	148	2328	753	1152	211	207	5	0

## 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: conserved hypothetical protein

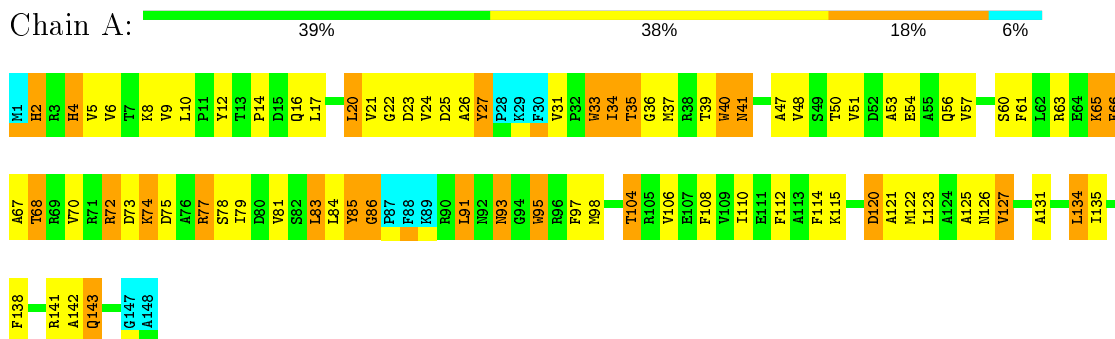


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

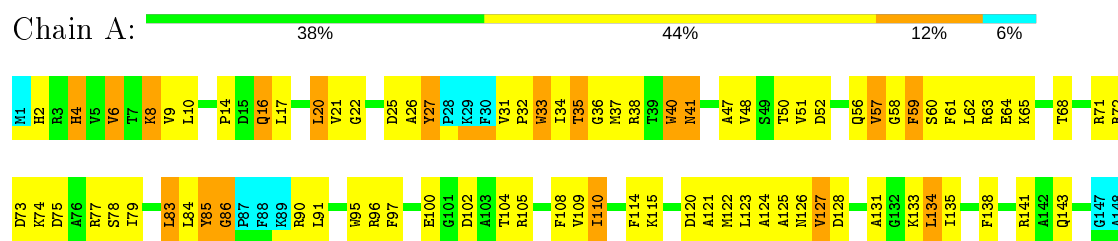
#### 4.2.1 Score per residue for model 1

- Molecule 1: conserved hypothetical protein



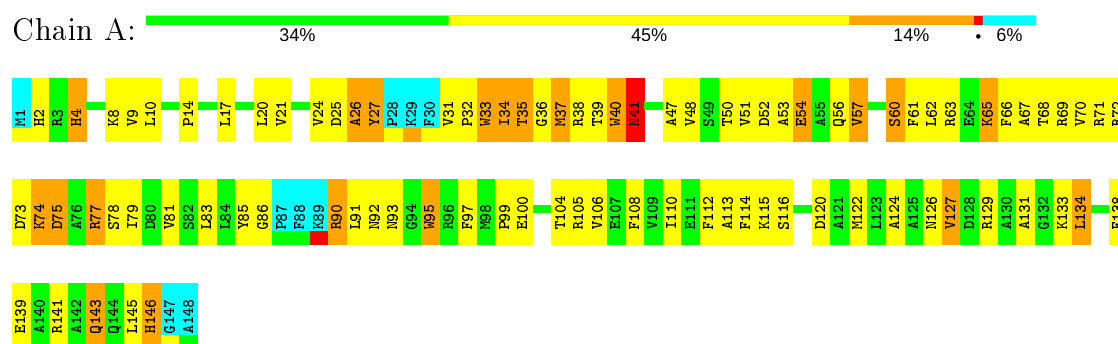
### 4.2.2 Score per residue for model 2

- Molecule 1: conserved hypothetical protein



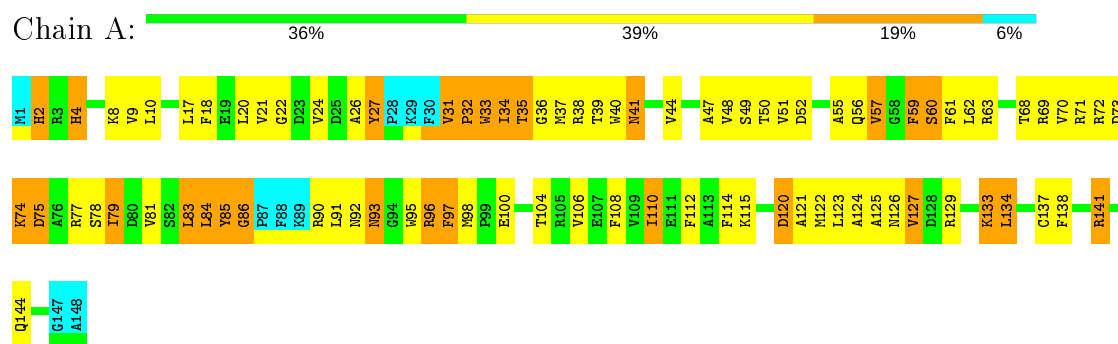
### 4.2.3 Score per residue for model 3

- Molecule 1: conserved hypothetical protein



### 4.2.4 Score per residue for model 4

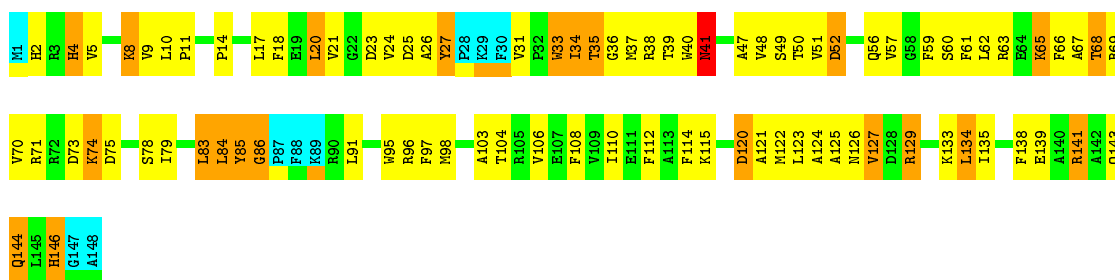
- Molecule 1: conserved hypothetical protein



### 4.2.5 Score per residue for model 5

- Molecule 1: conserved hypothetical protein

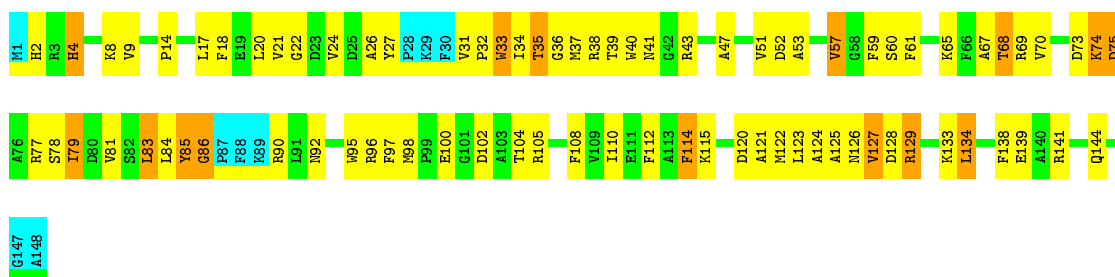




#### 4.2.6 Score per residue for model 6

- Molecule 1: conserved hypothetical protein

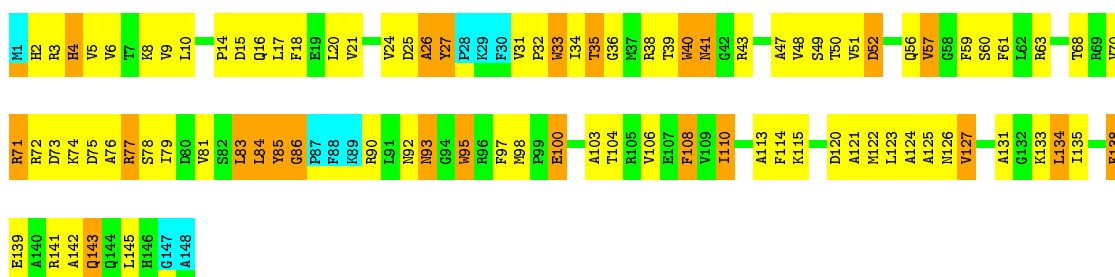
Chain A: 40% 44% 10% 6%



#### 4.2.7 Score per residue for model 7

- Molecule 1: conserved hypothetical protein

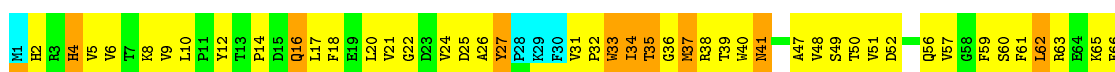
Chain A: 32% 45% 16% 6%

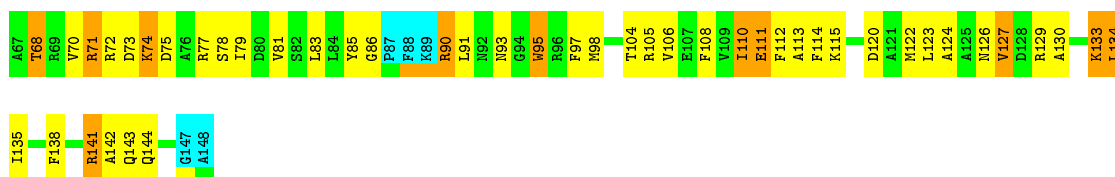


#### 4.2.8 Score per residue for model 8

- Molecule 1: conserved hypothetical protein

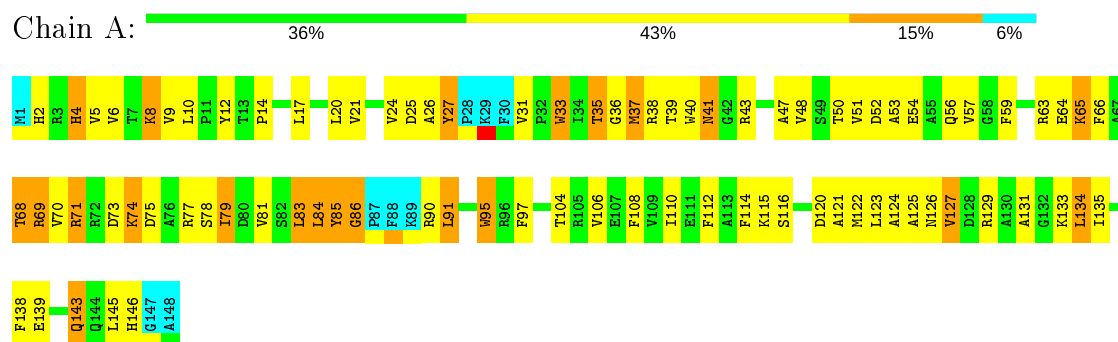
Chain A: 32% 48% 14% 6%





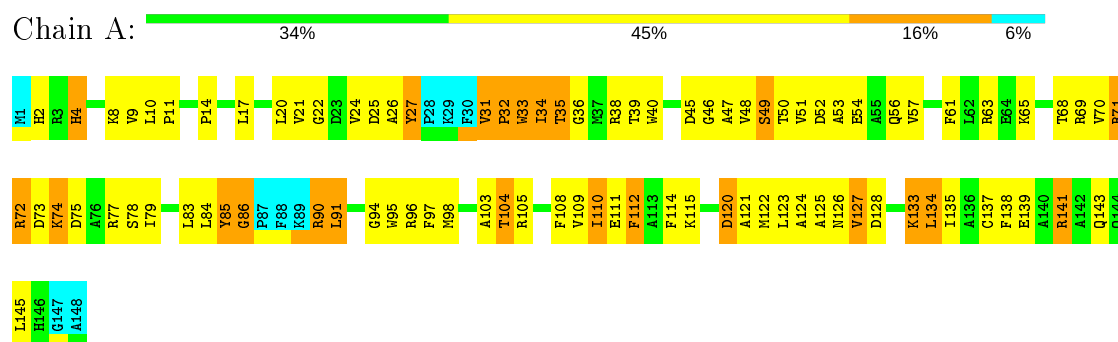
#### 4.2.9 Score per residue for model 9

- Molecule 1: conserved hypothetical protein



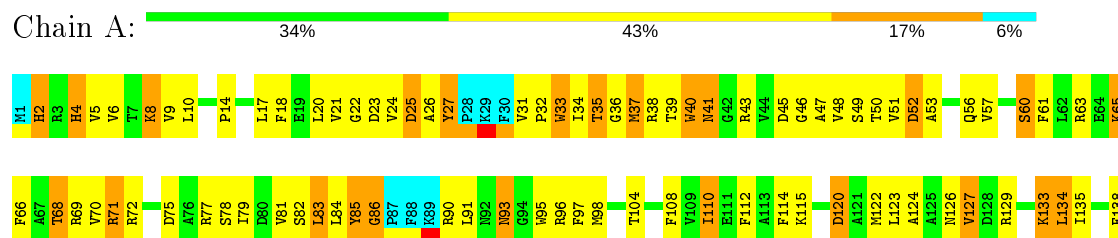
#### 4.2.10 Score per residue for model 10

- Molecule 1: conserved hypothetical protein

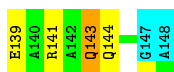


#### 4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: conserved hypothetical protein



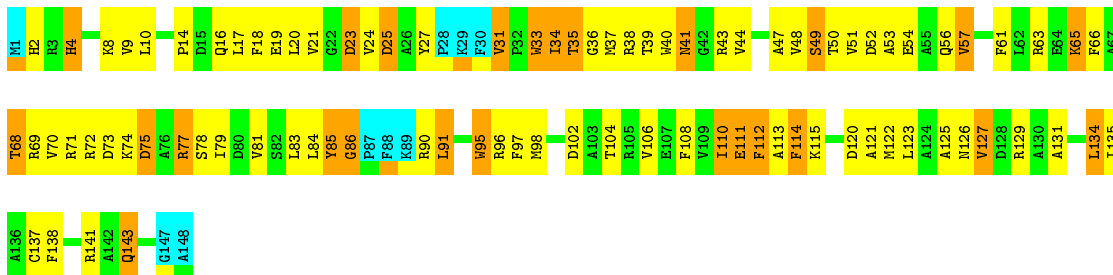




#### 4.2.12 Score per residue for model 12

- Molecule 1: conserved hypothetical protein

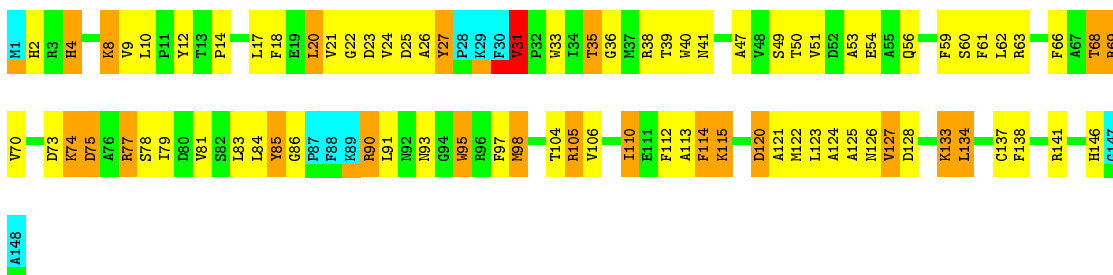
Chain A: 34% 43% 17% 6%



#### 4.2.13 Score per residue for model 13

- Molecule 1: conserved hypothetical protein

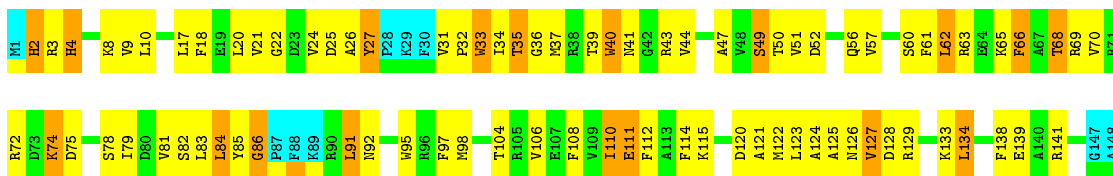
Chain A: 39% 39% 15% 6%



#### 4.2.14 Score per residue for model 14

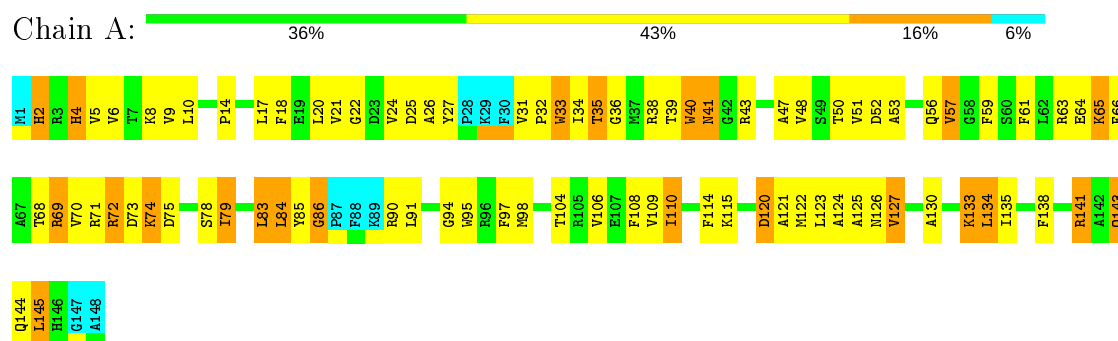
- Molecule 1: conserved hypothetical protein

Chain A: 39% 43% 12% 6%



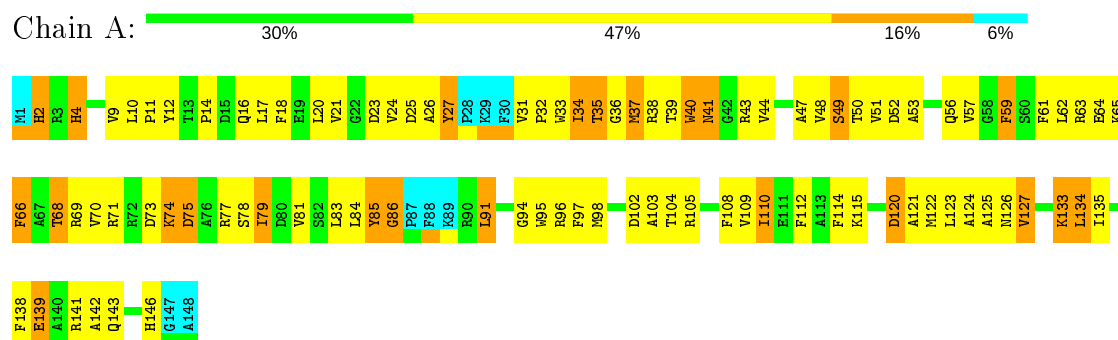
### 4.2.15 Score per residue for model 15

- Molecule 1: conserved hypothetical protein



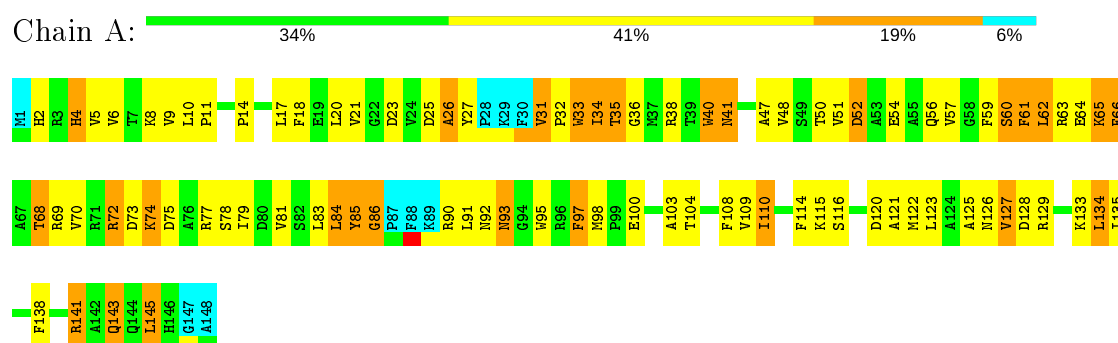
### 4.2.16 Score per residue for model 16

- Molecule 1: conserved hypothetical protein



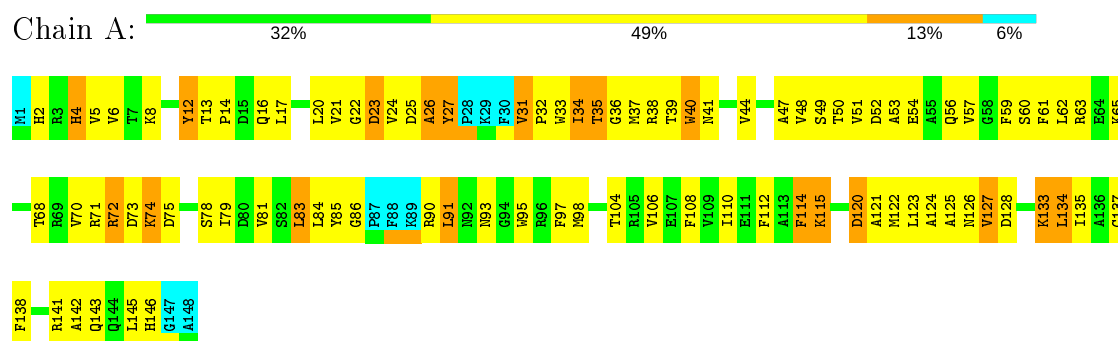
### 4.2.17 Score per residue for model 17

- Molecule 1: conserved hypothetical protein



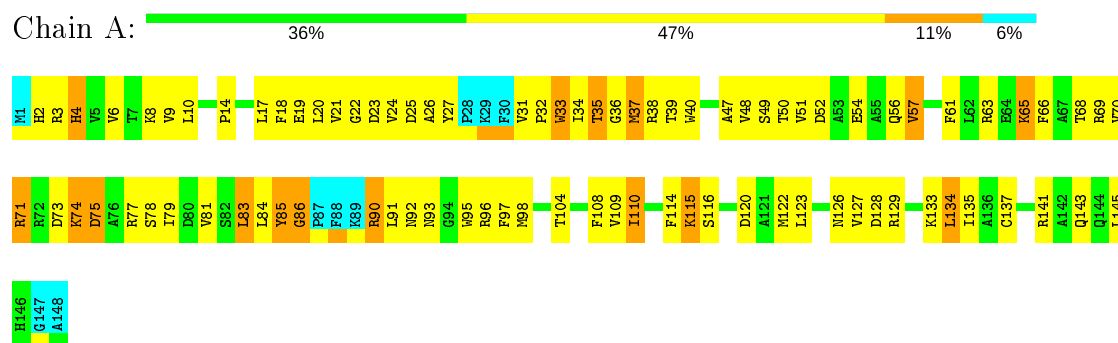
### 4.2.18 Score per residue for model 18

- Molecule 1: conserved hypothetical protein



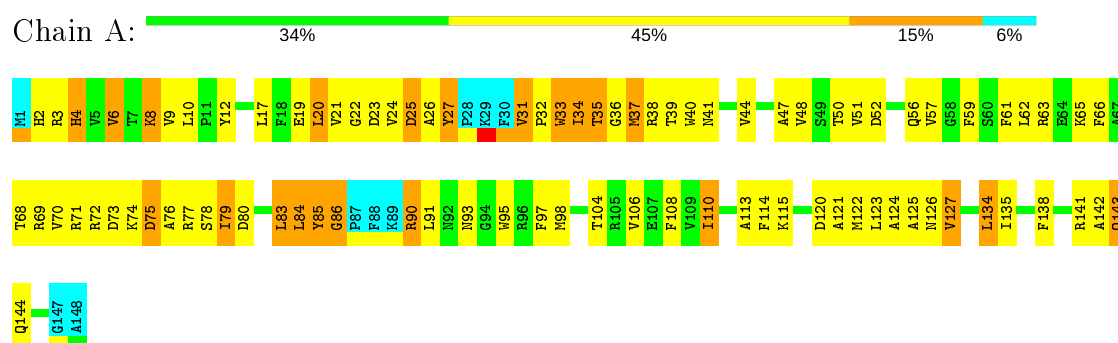
### 4.2.19 Score per residue for model 19

- Molecule 1: conserved hypothetical protein



### 4.2.20 Score per residue for model 20

- Molecule 1: conserved hypothetical protein



## 5 Refinement protocol and experimental data overview

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

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 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	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:110:ILE:O	1:A:110:ILE:HD13	0.78	1.77	2	3
1:A:21:VAL:HG13	1:A:79:ILE:HG13	0.78	1.52	4	8
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:134:LEU:C	1:A:134:LEU:HD12	0.76	2.00	16	8
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:HD12	1:A:134:LEU:C	0.75	2.01	17	7
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: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	2
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:HD12	1:A:110:ILE:O	0.72	1.84	3	4
1:A:26:ALA:C	1:A:27:TYR:CD1	0.71	2.63	14	10
1:A:14:PRO:CB	1:A:17:LEU:HD12	0.71	2.15	18	2
1:A:60:SER:C	1:A:61:PHE:CG	0.71	2.61	17	1
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:HD13	0.71	2.06	1	3
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:20:LEU:CD1	1:A:138:PHE:CE2	0.70	2.74	13	3
1:A:21:VAL:HG22	1:A:97:PHE:CD1	0.70	2.21	17	1
1:A:10:LEU:HD12	1:A:138:PHE:CE2	0.70	2.22	12	7
1:A:108:PHE:CZ	1:A:110:ILE:HG22	0.70	2.21	4	8
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: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:24:VAL:HG23	1:A:39:THR:HG21	0.69	1.63	18	6
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:51:VAL:O	1:A:70:VAL:HG12	0.69	1.88	10	15
1:A:47:ALA:HB1	1:A:74:LYS:CG	0.69	2.18	7	10
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	8
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:91:LEU:HD12	1:A:112:PHE:CB	0.66	2.21	3	2
1:A:8:LYS:HD3	1:A:135:ILE:HG23	0.66	1.66	15	3

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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:27:TYR:O	1:A:27:TYR:CD2	0.65	2.50	10	4
1:A:61:PHE:CG	1:A:61:PHE:O	0.65	2.49	4	8
1:A:31:VAL:HG13	1:A:33:TRP:CZ2	0.65	2.26	18	1
1:A:110:ILE:O	1:A:110:ILE:HD12	0.65	1.92	1	5
1:A:95:TRP:CZ3	1:A:97:PHE:CE1	0.65	2.84	6	1
1:A:25:ASP:O	1:A:27:TYR:CZ	0.65	2.49	9	1
1:A:83:LEU:HD11	1:A:91:LEU:H	0.65	1.51	14	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:27:TYR:CD2	1:A:27:TYR:O	0.63	2.51	8	3
1:A:23:ASP:O	1:A:27:TYR:CE2	0.63	2.52	16	4
1:A:134:LEU:HD12	1:A:135:ILE:N	0.63	2.08	17	5
1:A:20:LEU:HD11	1:A:138:PHE:CD2	0.63	2.29	13	5
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:12:TYR:CD2	1:A:142:ALA:HB1	0.62	2.29	1	2
1:A:111:GLU:O	1:A:112:PHE:CD1	0.62	2.53	8	3
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:VAL:CG1	1:A:33:TRP:CE3	0.61	2.80	5	2
1:A:2:HIS:CE1	1:A:120:ASP:OD1	0.61	2.54	4	2
1:A:20:LEU:HD11	1:A:138:PHE:CG	0.61	2.31	12	4
1:A:95:TRP:CH2	1:A:108:PHE:CG	0.61	2.88	4	3
1:A:2:HIS:CD2	1:A:120:ASP:OD2	0.60	2.54	13	7
1:A:21:VAL:HG22	1:A:97:PHE:CZ	0.60	2.31	19	4
1:A:2:HIS:CD2	1:A:120:ASP:OD1	0.60	2.55	20	5
1:A:4:HIS:CE1	1:A:124:ALA:O	0.60	2.54	13	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: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:84:LEU:C	1:A:84:LEU:HD13	0.59	2.18	5	1
1:A:23:ASP:O	1:A:27:TYR:CD2	0.59	2.54	17	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:25:ASP:O	1:A:27:TYR:CE2	0.59	2.55	3	1
1:A:20:LEU:CD1	1:A:138:PHE:CG	0.59	2.85	8	2
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:79:ILE:HB	1:A:95:TRP:CD1	0.58	2.34	8	3
1:A:131:ALA:O	1:A:135:ILE:HD12	0.58	1.98	12	1
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:17:LEU:HD22	1:A:97:PHE:CE1	0.58	2.32	6	1
1:A:95:TRP:CD1	1:A:95:TRP:O	0.58	2.57	9	2
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:33:TRP:HB2	1:A:130:ALA:HB1	0.58	1.76	15	2
1:A:70:VAL:HG23	1:A:81:VAL:CG2	0.58	2.29	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:LYS:HZ2	1:A:106:VAL:HB	0.58	1.59	20	1
1:A:57:VAL:HG22	1:A:64:GLU:O	0.57	1.99	9	3
1:A:108:PHE:CE2	1:A:110:ILE:CG2	0.57	2.87	20	2
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:O	1:A:27:TYR:CZ	0.57	2.56	16	4
1:A:23:ASP:OD1	1:A:27:TYR:CG	0.57	2.58	12	2
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:110:ILE:HD12	1:A:110:ILE:C	0.57	2.21	3	3
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:110:ILE:CD1	1:A:112:PHE:CD2	0.56	2.88	16	2
1:A:77:ARG:O	1:A:97:PHE:CE2	0.56	2.58	13	1
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: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:65:LYS:O	1:A:66:PHE:CD1	0.55	2.59	17	9
1:A:2:HIS:CG	1:A:120:ASP:OD1	0.55	2.60	7	4
1:A:31:VAL:CG1	1:A:33:TRP:CD2	0.55	2.90	1	2
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: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:40:TRP:CD1	1:A:41:ASN:N	0.54	2.76	16	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:84:LEU:HD13	1:A:85:TYR:HB2	0.54	1.77	15	1
1:A:2:HIS:N	1:A:2:HIS:CD2	0.54	2.76	16	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:54:GLU:CG	1:A:67:ALA:HB2	0.53	2.33	3	1
1:A:70:VAL:HG23	1:A:81:VAL:HG22	0.53	1.81	18	4
1:A:60:SER:O	1:A:61:PHE:CB	0.53	2.56	1	2
1:A:53:ALA:HB2	1:A:70:VAL:CG1	0.53	2.33	15	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:141:ARG:NH2	1:A:144:GLN:HE22	0.52	2.02	8	2
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: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:95:TRP:CH2	1:A:108:PHE:CE1	0.52	2.97	5	2
1:A:62:LEU:HD11	1:A:64:GLU:HG3	0.52	1.81	17	1
1:A:31:VAL:HG13	1:A:33:TRP:CE2	0.52	2.40	18	1
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:134:LEU:HD12	1:A:134:LEU:O	0.52	2.05	18	3
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:PHE:CD2	1:A:61:PHE:O	0.52	2.63	14	2
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:33:TRP:CE2	1:A:134:LEU:HD12	0.51	2.41	4	1
1:A:61:PHE:O	1:A:61:PHE:CD2	0.51	2.64	16	3
1:A:27:TYR:O	1:A:27:TYR:CG	0.51	2.63	13	4
1:A:26:ALA:C	1:A:27:TYR:CD2	0.51	2.84	3	1
1:A:110:ILE:O	1:A:110:ILE:CD1	0.51	2.59	10	3
1:A:17:LEU:HD21	1:A:106:VAL:CG2	0.51	2.35	4	1
1:A:110:ILE:HB	1:A:112:PHE:CZ	0.51	2.40	10	3
1:A:47:ALA:HB1	1:A:74:LYS:CD	0.51	2.36	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: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	4
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: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:17:LEU:HD13	1:A:97:PHE:HD2	0.49	1.65	3	2
1:A:84:LEU:HD13	1:A:85:TYR:N	0.49	2.22	14	2
1:A:83:LEU:C	1:A:83:LEU:CD1	0.49	2.80	2	3
1:A:95:TRP:CZ3	1:A:108:PHE:CD1	0.49	3.00	5	3
1:A:47:ALA:CB	1:A:75:ASP:OD1	0.49	2.61	4	1
1:A:84:LEU:HD13	1:A:85:TYR:CB	0.49	2.38	14	2
1:A:84:LEU:HD13	1:A:84:LEU:O	0.49	2.06	5	1
1:A:27:TYR:OH	1:A:37:MET:CE	0.49	2.61	8	1
1:A:2:HIS:CE1	1:A:124:ALA:CB	0.49	2.96	15	1
1:A:64:GLU:O	1:A:66:PHE:CE1	0.49	2.65	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:SER:O	1:A:61:PHE:CD2	0.49	2.65	17	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:17:LEU:HB3	1:A:97:PHE:CE2	0.49	2.43	6	1
1:A:95:TRP:CZ2	1:A:97:PHE:CD2	0.49	3.00	9	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:12:TYR:CE2	1:A:142:ALA:HB3	0.49	2.43	8	2
1:A:111:GLU:C	1:A:112:PHE:CD1	0.49	2.86	12	3
1:A:17:LEU:HB3	1:A:97:PHE:CZ	0.49	2.43	6	2
1:A:25:ASP:O	1:A:26:ALA:C	0.49	2.51	20	3
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: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:19:GLU:O	1:A:23:ASP:N	0.48	2.46	12	3
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:97:PHE:N	1:A:97:PHE:CD1	0.48	2.81	2	2
1:A:115:LYS:N	1:A:115:LYS:CD	0.48	2.76	13	2
1:A:27:TYR:CD2	1:A:31:VAL:HG21	0.48	2.43	13	1
1:A:65:LYS:C	1:A:66:PHE:CD1	0.48	2.87	14	1
1:A:8:LYS:HG2	1:A:9:VAL:N	0.48	2.22	15	1
1:A:131:ALA:O	1:A:135:ILE:CD1	0.48	2.61	12	1
1:A:50:THR:CG2	1:A:69:ARG:CD	0.48	2.92	15	2
1:A:27:TYR:CE1	1:A:31:VAL:HG21	0.48	2.44	1	1
1:A:81:VAL:N	1:A:93:ASN:O	0.48	2.47	13	6
1:A:12:TYR:CD2	1:A:142:ALA:CB	0.48	2.96	8	1
1:A:91:LEU:C	1:A:91:LEU:HD23	0.48	2.29	13	1
1:A:21:VAL:CG2	1:A:97:PHE:CZ	0.48	2.97	1	2
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:93:ASN:OD1	1:A:108:PHE:CE1	0.48	2.66	20	1
1:A:141:ARG:CZ	1:A:144:GLN:OE1	0.48	2.61	5	1
1:A:2:HIS:CE1	1:A:120:ASP:HB3	0.48	2.44	9	5
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
1:A:134:LEU:HD13	1:A:135:ILE:CA	0.47	2.37	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	9
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:20:LEU:HG	1:A:138:PHE:CD1	0.47	2.45	2	2
1:A:95:TRP:C	1:A:95:TRP:CD1	0.47	2.87	3	2
1:A:60:SER:O	1:A:61:PHE:HB3	0.47	2.09	2	11
1:A:68:THR:HB	1:A:81:VAL:HG12	0.47	1.86	6	2
1:A:95:TRP:CD1	1:A:95:TRP:C	0.47	2.88	7	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:33:TRP:CD2	1:A:134:LEU:HB2	0.47	2.45	20	4
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:23:ASP:HB2	1:A:27:TYR:CE1	0.47	2.44	12	1
1:A:33:TRP:CZ3	1:A:134:LEU:HB2	0.47	2.44	18	4
1:A:16:GLN:OE1	1:A:138:PHE:CE1	0.47	2.68	2	2
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:32:PRO:O	1:A:34:ILE:N	0.47	2.48	4	2
1:A:131:ALA:O	1:A:135:ILE:CG1	0.47	2.62	12	1
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:126:ASN:C	1:A:126:ASN:OD1	0.46	2.54	13	11
1:A:37:MET:N	1:A:37:MET:SD	0.46	2.88	4	5
1:A:79:ILE:CG2	1:A:95:TRP:NE1	0.46	2.77	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:HIS:NE2	1:A:120:ASP:OD2	0.46	2.49	11	2
1:A:23:ASP:O	1:A:27:TYR:CG	0.46	2.69	17	1
1:A:50:THR:HG23	1:A:71:ARG:HG2	0.46	1.86	2	1
1:A:2:HIS:CE1	1:A:124:ALA:HB2	0.46	2.45	4	1
1:A:4:HIS:CG	1:A:127:VAL:HG11	0.46	2.45	16	3
1:A:11:PRO:HB3	1:A:103:ALA:HB2	0.46	1.86	17	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:67:ALA:O	1:A:68:THR:HG23	0.45	2.11	1	3
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: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:25:ASP:C	1:A:27:TYR:CE2	0.45	2.89	3	1
1:A:21:VAL:CG1	1:A:79:ILE:CG1	0.45	2.94	20	2
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: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:48:VAL:HG22	1:A:73:ASP:OD1	0.45	2.12	12	1
1:A:95:TRP:CZ3	1:A:106:VAL:CG1	0.45	3.00	9	2
1:A:33:TRP:CE2	1:A:134:LEU:HB2	0.45	2.46	17	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
1:A:4:HIS:H	1:A:110:ILE:HD13	0.44	1.71	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:141:ARG:NH1	1:A:145:LEU:HD12	0.44	2.28	17	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:67:ALA:HB3	1:A:85:TYR:HB2	0.44	1.89	5	1
1:A:21:VAL:HG13	1:A:95:TRP:HZ2	0.44	1.73	6	1
1:A:60:SER:C	1:A:61:PHE:CD1	0.44	2.90	17	1
1:A:114:PHE:CD2	1:A:120:ASP:HA	0.44	2.47	3	1
1:A:26:ALA:C	1:A:27:TYR:O	0.44	2.55	7	2
1:A:50:THR:HG23	1:A:71:ARG:CG	0.44	2.39	11	1
1:A:115:LYS:CE	1:A:115:LYS:N	0.44	2.81	19	3
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: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:21:VAL:HG22	1:A:95:TRP:HE1	0.44	1.73	9	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: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:35:THR:CG2	1:A:57:VAL:CA	0.43	2.96	14	1
1:A:10:LEU:HD22	1:A:139:GLU:HG3	0.43	1.90	16	1
1:A:32:PRO:O	1:A:33:TRP:C	0.43	2.55	4	2
1:A:33:TRP:CE2	1:A:134:LEU:CD1	0.43	3.01	4	1
1:A:110:ILE:O	1:A:110:ILE:CG1	0.43	2.66	10	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:23:ASP:OD1	1:A:23:ASP:C	0.43	2.56	12	2
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:O	0.43	2.71	7	1
1:A:138:PHE:CD1	1:A:138:PHE:C	0.43	2.90	7	1
1:A:74:LYS:O	1:A:77:ARG:NH1	0.43	2.52	8	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:27:TYR:CD2	1:A:31:VAL:CG1	0.43	3.02	11	1
1:A:95:TRP:HB3	1:A:97:PHE:CZ	0.43	2.49	2	2
1:A:5:VAL:C	1:A:6:VAL:CG2	0.43	2.87	8	3
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:8:LYS:CD	1:A:8:LYS:N	0.43	2.81	5	1
1:A:79:ILE:HB	1:A:95:TRP:CE2	0.43	2.48	6	1
1:A:16:GLN:OE1	1:A:16:GLN:N	0.43	2.51	8	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: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: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:111:GLU:C	1:A:112:PHE:CG	0.42	2.92	8	1
1:A:8:LYS:HE2	1:A:138:PHE:CD2	0.42	2.49	20	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:83:LEU:CD1	1:A:83:LEU:C	0.42	2.79	19	1
1:A:33:TRP:CE3	1:A:134:LEU:CB	0.42	3.02	1	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: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:100:GLU:CD	1:A:105:ARG:NH1	0.42	2.72	2	1
1:A:4:HIS:HB2	1:A:110:ILE:CG1	0.42	2.45	10	2
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: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:19:GLU:O	1:A:23:ASP:CA	0.41	2.68	12	1
1:A:4:HIS:CB	1:A:110:ILE:CG1	0.41	2.98	12	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:3:ARG:HB2	1:A:111:GLU:CG	0.41	2.45	14	1
1:A:94:GLY:CA	1:A:109:VAL:HG23	0.41	2.45	15	2
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:123:LEU:HD23	1:A:126:ASN:ND2	0.41	2.28	8	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: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:35:THR:CG2	1:A:57:VAL:C	0.41	2.89	14	1
1:A:84:LEU:CD1	1:A:85:TYR:HB2	0.41	2.46	15	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: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:37:MET:SD	1:A:37:MET:C	0.41	2.99	1	1
1:A:41:ASN:O	1:A:52:ASP:OD1	0.41	2.39	17	2
1:A:79:ILE:HB	1:A:95:TRP:NE1	0.41	2.31	6	1
1:A:52:ASP:OD1	1:A:52:ASP:N	0.41	2.54	11	1
1:A:112:PHE:C	1:A:112:PHE:CD1	0.41	2.94	13	1
1:A:32:PRO:HB2	1:A:59:PHE:CE2	0.41	2.51	16	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:4:HIS:CB	1:A:110:ILE:CD1	0.40	2.99	17	1
1:A:96:ARG:C	1:A:97:PHE:CG	0.40	2.95	2	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:95:TRP:CD2	1:A:108:PHE:CE1	0.40	3.09	18	1
1:A:133:LYS:HB2	1:A:133:LYS:NZ	0.40	2.31	11	1
1:A:25:ASP:CG	1:A:39:THR:OG1	0.40	2.59	11	1
1:A:68:THR:CB	1:A:82:SER:O	0.40	2.70	14	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:23:ASP:O	1:A:25:ASP:N	0.40	2.54	12	1
1:A:46:GLY:O	1:A:48:VAL:HG23	0.40	2.16	10	1
1:A:56:GLN:HG2	1:A:65:LYS:CB	0.40	2.46	17	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%)	9	46
All	All	2780/2960 (94%)	2423 (87%)	291 (10%)	66 (2%)	9	46

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%)	<b>1</b> <b>10</b>
All	All	2260/2400 (94%)	1484 (66%)	776 (34%)	<b>1</b> <b>10</b>

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

No chemical shift data were provided