



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:44 PM BST

PDB ID : 1J7H  
Title : Solution Structure of HI0719, a Hypothetical Protein From Haemophilus Influenzae  
Authors : Parsons, L.; Bonander, N.; Eisenstein, E.; Gilson, M.; Kairys, V.; Orban, J.; Structure 2 Function Project (S2F)  
Deposited on : 2001-05-16

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

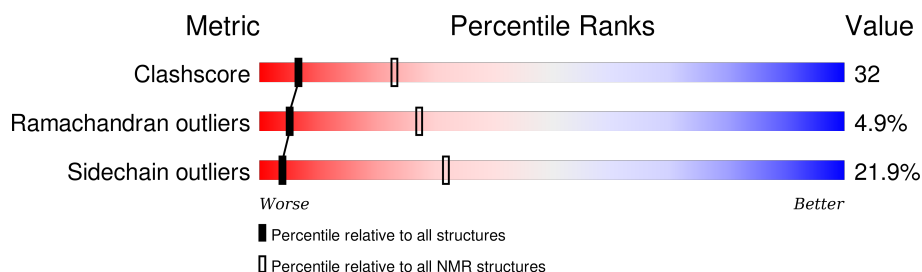
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment 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	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  $\geq 3$ , 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	130	
1	B	130	
1	C	130	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models).

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:36, A:43-A:129, B:3-B:36, B:43-B:129, C:3-C:36, C:43-C:130 (364)	0.47	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. No single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 5994 atoms, of which 3033 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HYPOTHETICAL PROTEIN HI0719.

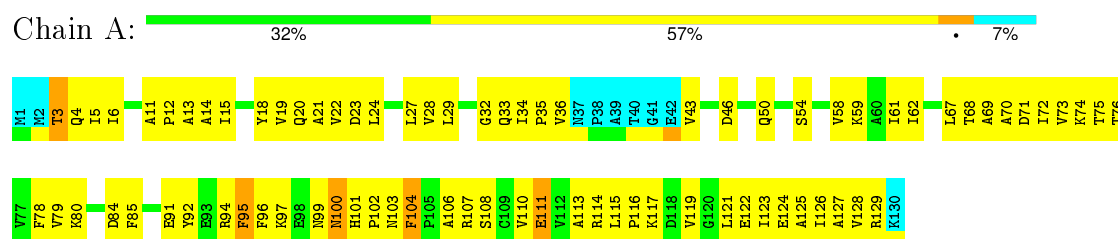
Mol	Chain	Residues	Atoms						Trace
1	A	130	Total 1998	C 626	H 1011	N 170	O 188	S 3	0
1	B	130	Total 1998	C 626	H 1011	N 170	O 188	S 3	0
1	C	130	Total 1998	C 626	H 1011	N 170	O 188	S 3	0

## 4 Residue-property plots [i](#)

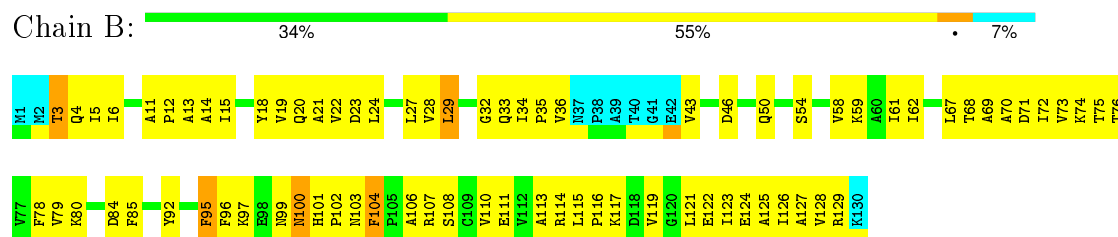
### 4.1 Average score per residue in the NMR ensemble

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.

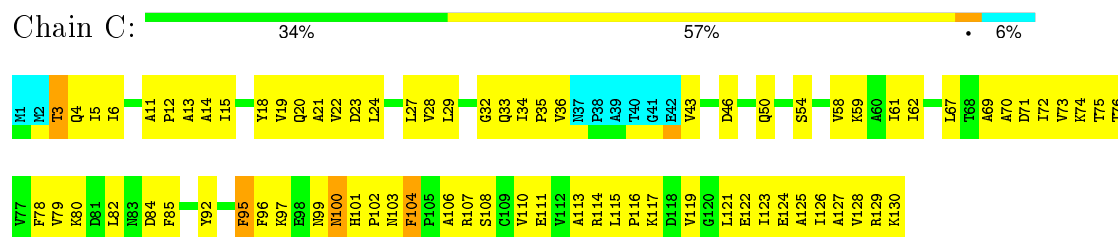
#### • Molecule 1: HYPOTHETICAL PROTEIN HI0719



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#### • Molecule 1: HYPOTHETICAL PROTEIN HI0719

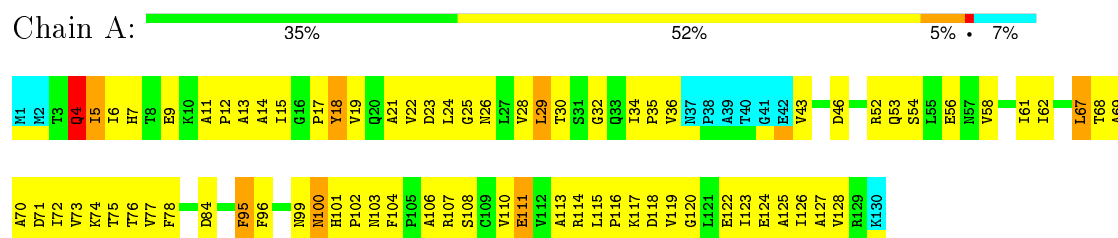


### 4.2 Scores per residue for each member of the ensemble

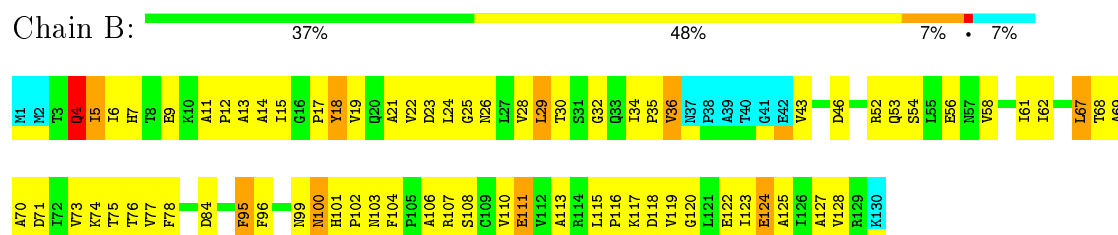
Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

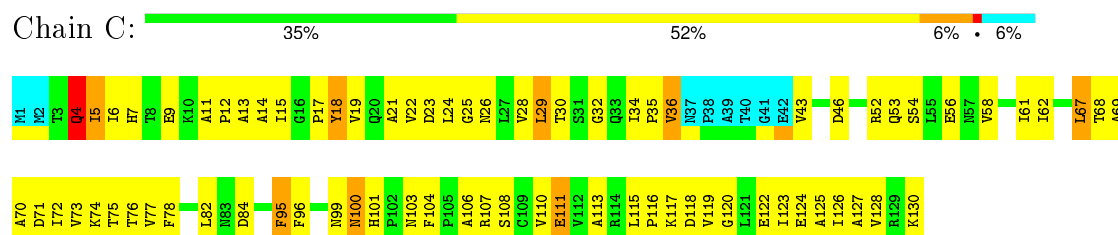
#### • Molecule 1: HYPOTHETICAL PROTEIN HI0719



#### • Molecule 1: HYPOTHETICAL PROTEIN HI0719

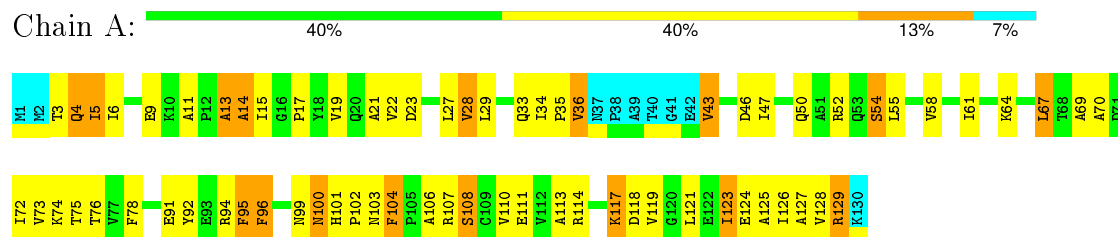


#### • Molecule 1: HYPOTHETICAL PROTEIN HI0719

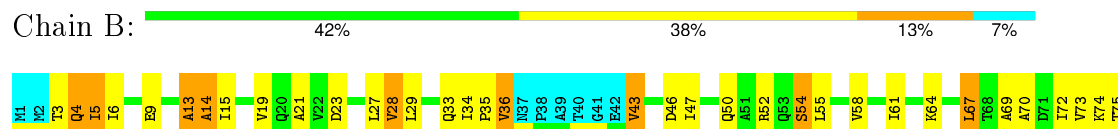


### 4.2.2 Score per residue for model 2

#### • Molecule 1: HYPOTHETICAL PROTEIN HI0719



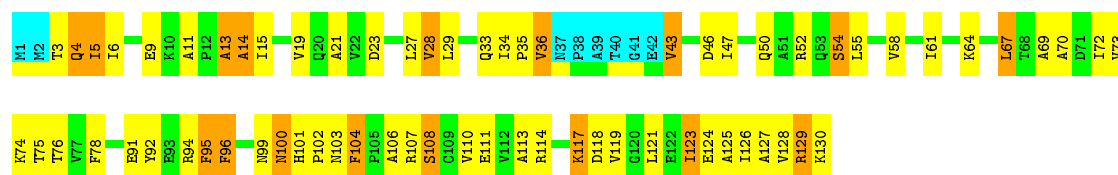
#### • Molecule 1: HYPOTHETICAL PROTEIN HI0719





• Molecule 1: HYPOTHETICAL PROTEIN HI0719

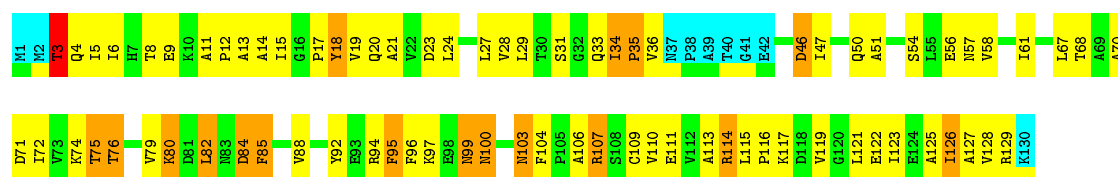
Chain C: 42% 39% 13% 6%



#### 4.2.3 Score per residue for model 3

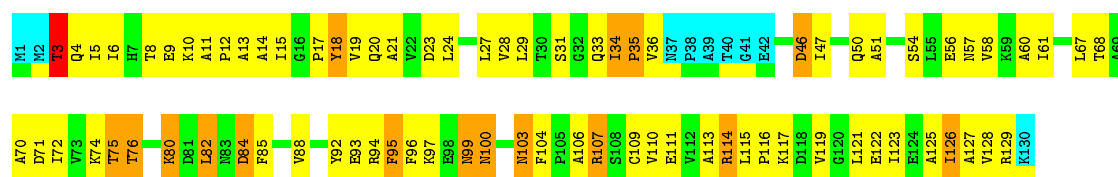
• Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain A: 34% 45% 13% 7%



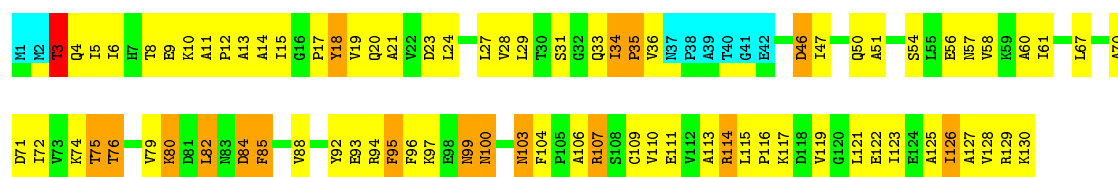
• Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain B: 32% 48% 12% 7%



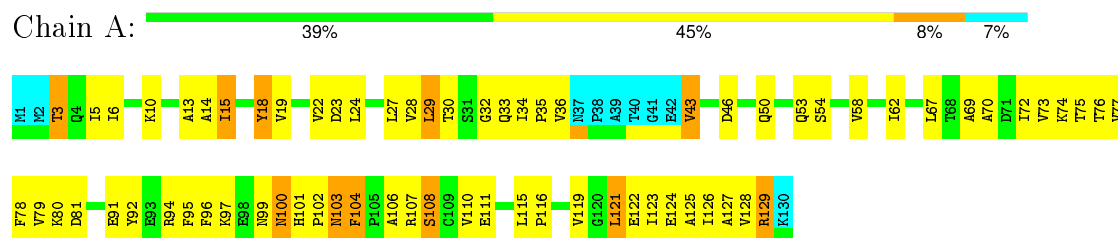
• Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain C: 32% 48% 13% 6%

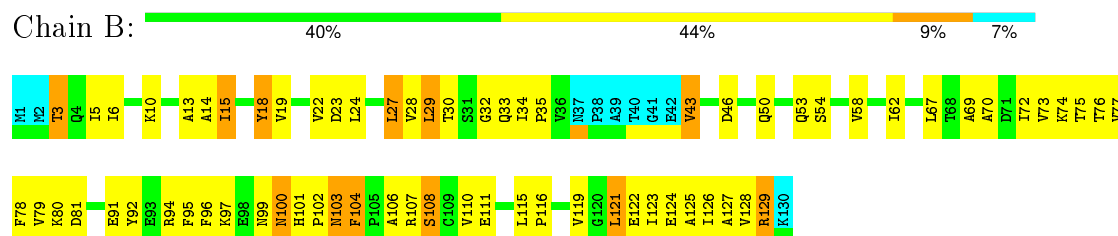


#### 4.2.4 Score per residue for model 4 (medoid)

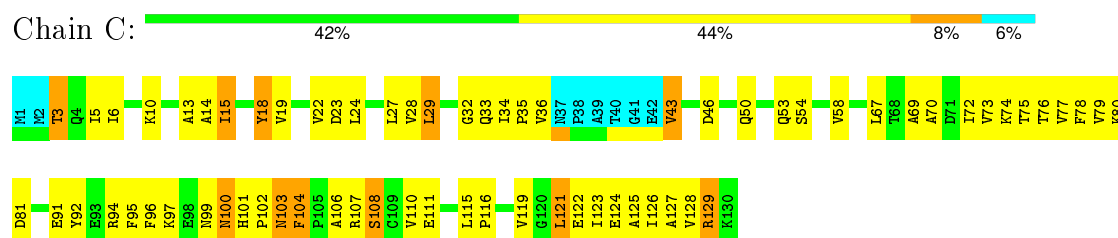
• Molecule 1: HYPOTHETICAL PROTEIN HI0719



• Molecule 1: HYPOTHETICAL PROTEIN HI0719

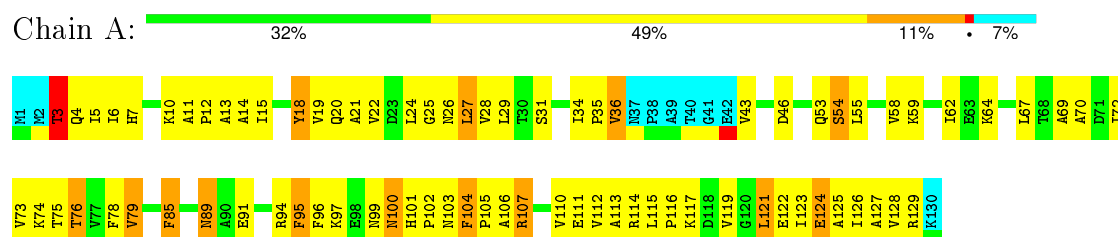


• Molecule 1: HYPOTHETICAL PROTEIN HI0719

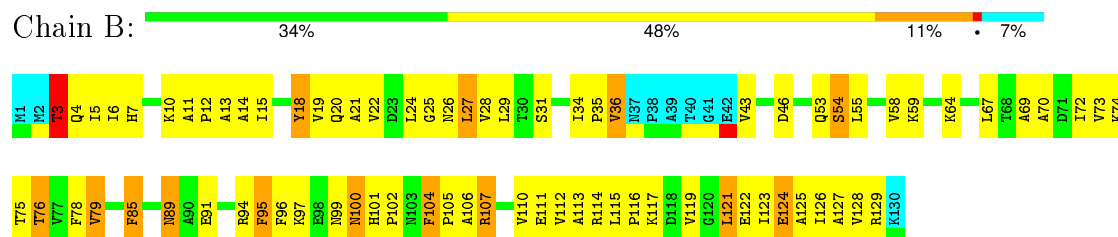


#### 4.2.5 Score per residue for model 5

• Molecule 1: HYPOTHETICAL PROTEIN HI0719

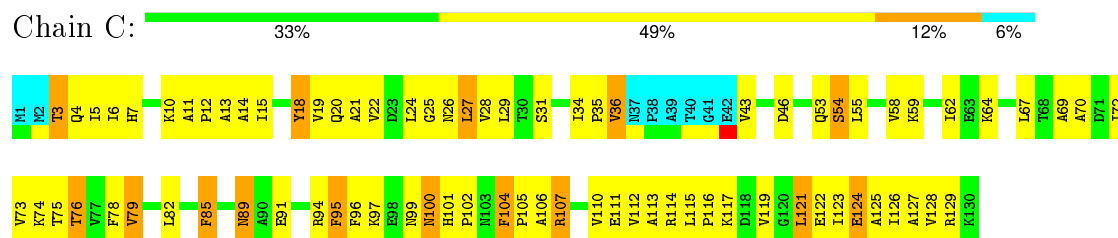


• Molecule 1: HYPOTHETICAL PROTEIN HI0719



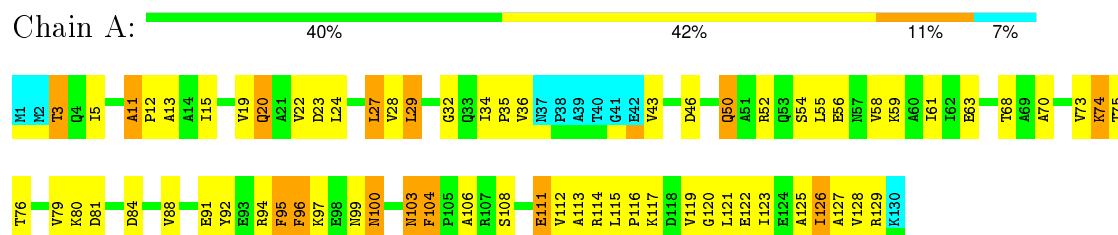
• Molecule 1: HYPOTHETICAL PROTEIN HI0719



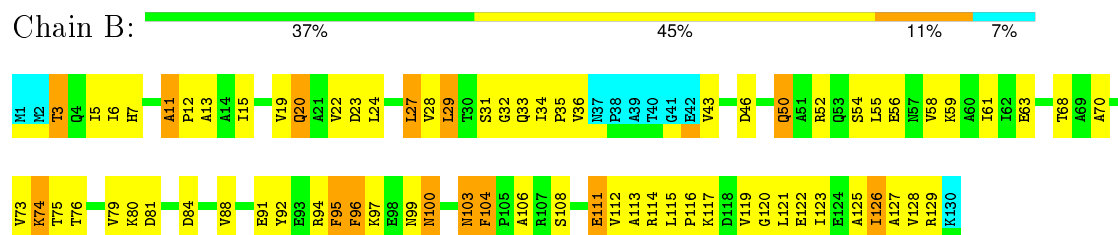


#### 4.2.6 Score per residue for model 6

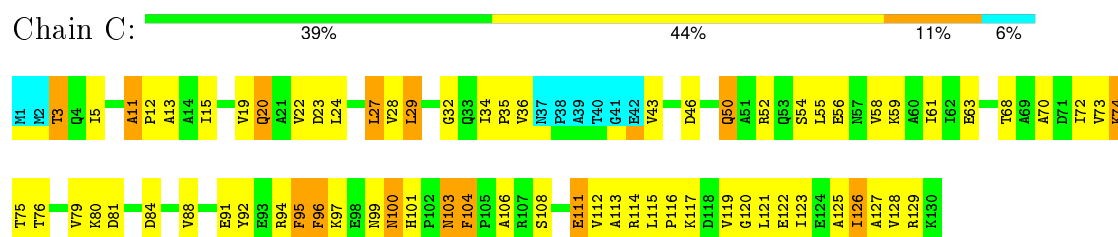
- Molecule 1: HYPOTHETICAL PROTEIN HI0719



- Molecule 1: HYPOTHETICAL PROTEIN HI0719

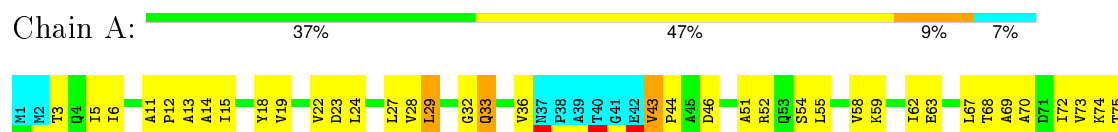


- Molecule 1: HYPOTHETICAL PROTEIN HI0719



#### 4.2.7 Score per residue for model 7

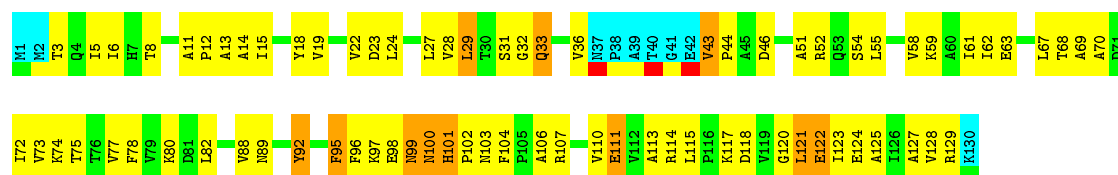
- Molecule 1: HYPOTHETICAL PROTEIN HI0719





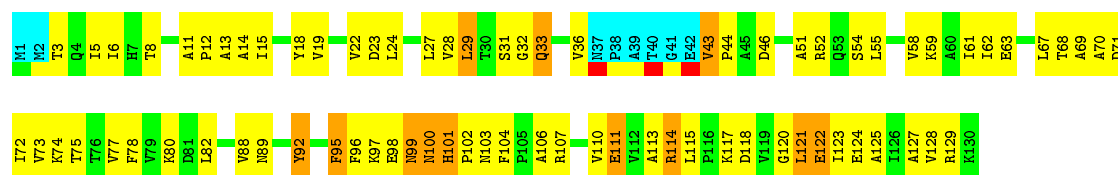
• Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain B: 35% 50% 8% 7%



• Molecule 1: HYPOTHETICAL PROTEIN HI0719

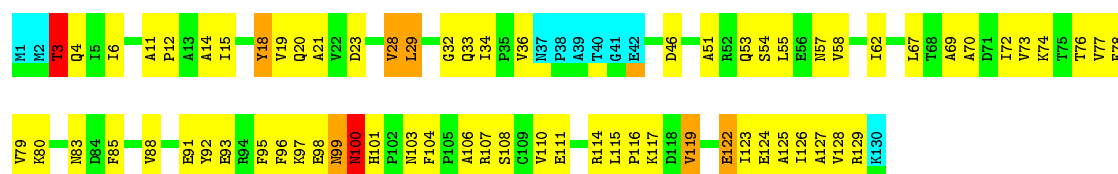
Chain C: 35% 50% 9% 6%



#### 4.2.8 Score per residue for model 8

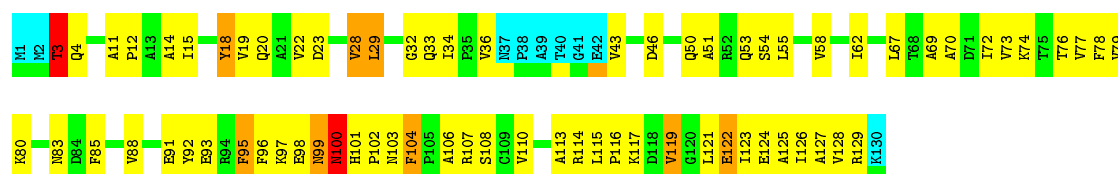
• Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain A: 39% 48% 5% 7%



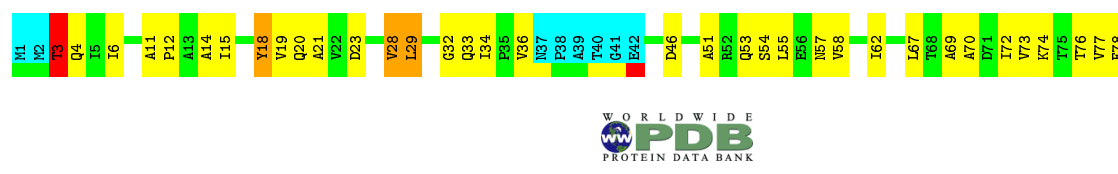
• Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain B: 38% 48% 6% 7%



• Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain C: 40% 46% 6% 6%

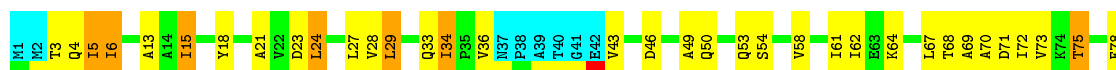




#### 4.2.9 Score per residue for model 9

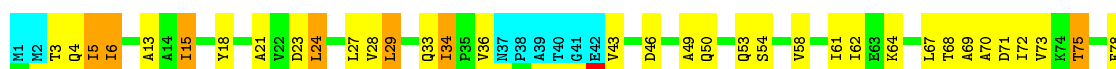
- Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain A: 42% 40% 11% 7%



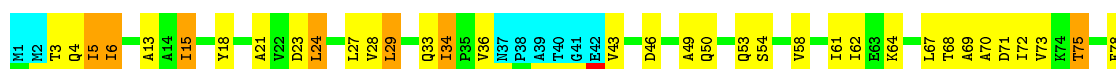
- Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain B: 42% 41% 11% 7%



- Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain C: 43% 40% 11% 6%



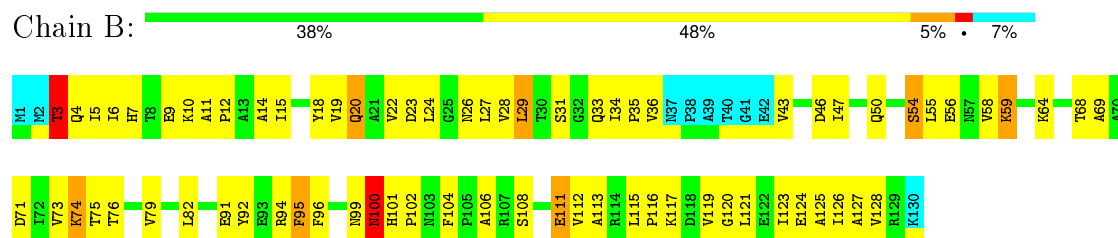
#### 4.2.10 Score per residue for model 10

- Molecule 1: HYPOTHETICAL PROTEIN HI0719

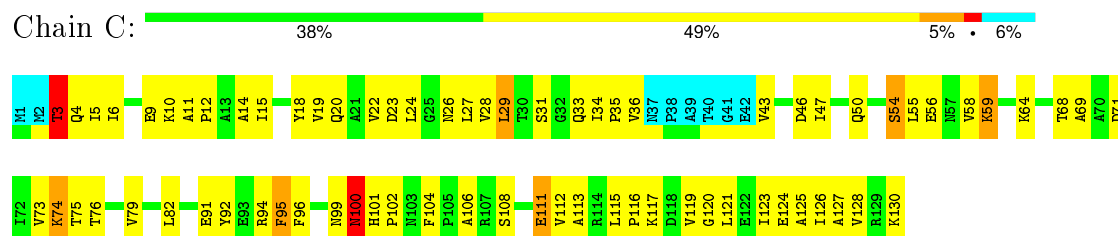
Chain A: 39% 46% 6% 7%



- Molecule 1: HYPOTHETICAL PROTEIN HI0719

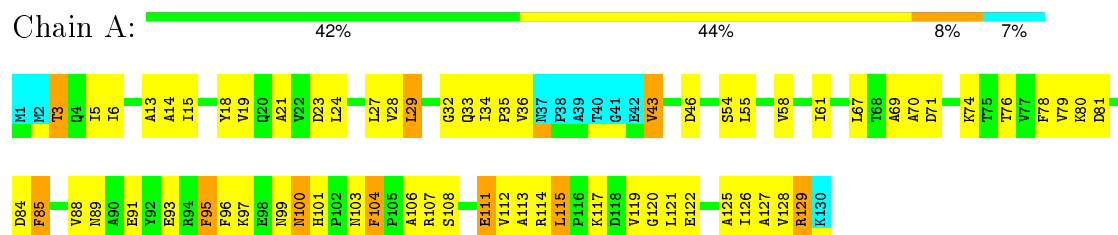


• Molecule 1: HYPOTHETICAL PROTEIN HI0719

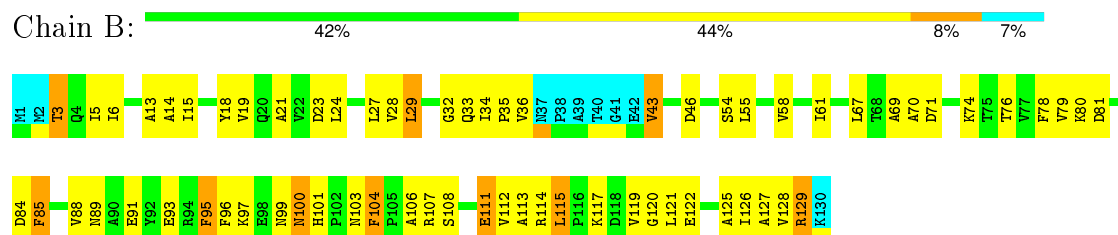


#### 4.2.11 Score per residue for model 11

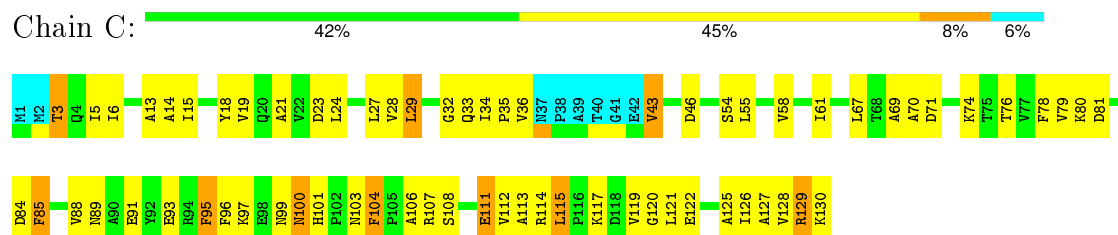
• Molecule 1: HYPOTHETICAL PROTEIN HI0719



• Molecule 1: HYPOTHETICAL PROTEIN HI0719

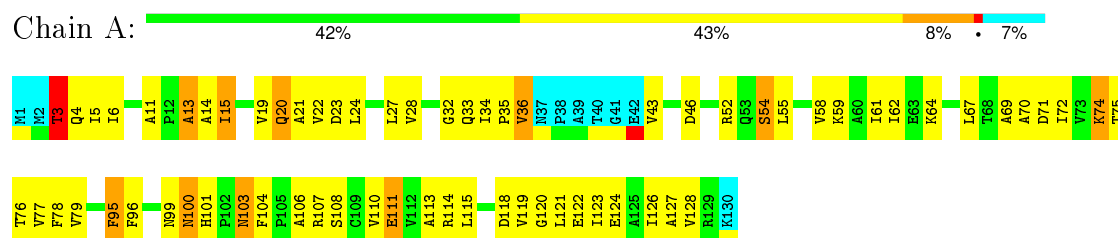


• Molecule 1: HYPOTHETICAL PROTEIN HI0719

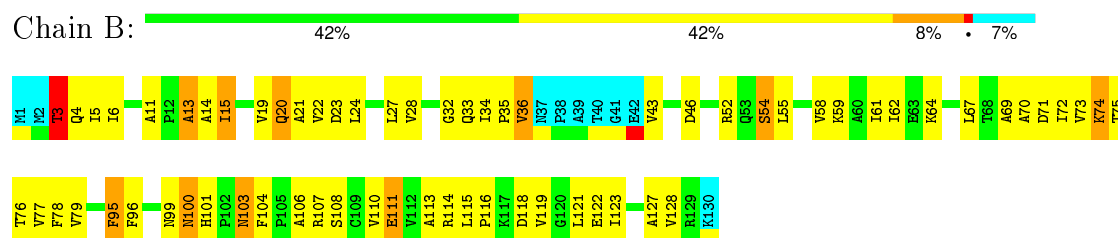


### 4.2.12 Score per residue for model 12

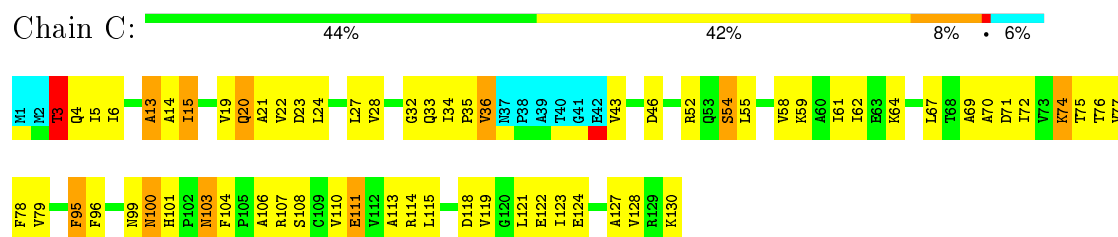
- Molecule 1: HYPOTHETICAL PROTEIN HI0719



- Molecule 1: HYPOTHETICAL PROTEIN HI0719

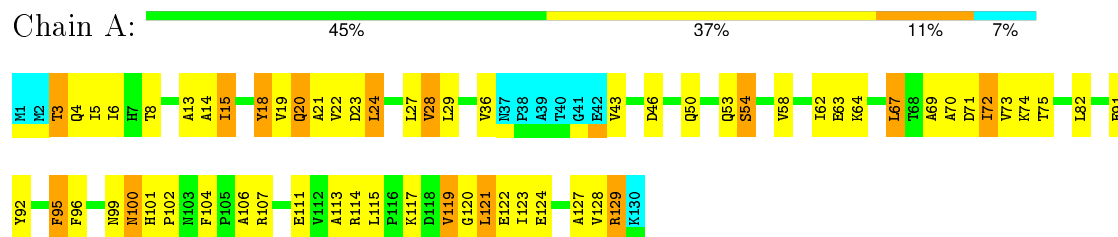


- Molecule 1: HYPOTHETICAL PROTEIN HI0719

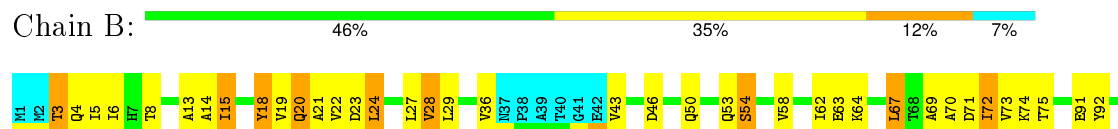


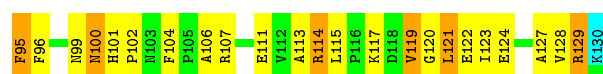
### 4.2.13 Score per residue for model 13

- Molecule 1: HYPOTHETICAL PROTEIN HI0719



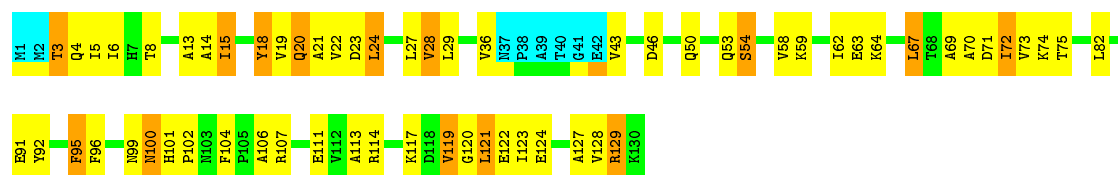
- Molecule 1: HYPOTHETICAL PROTEIN HI0719





• Molecule 1: HYPOTHETICAL PROTEIN HI0719

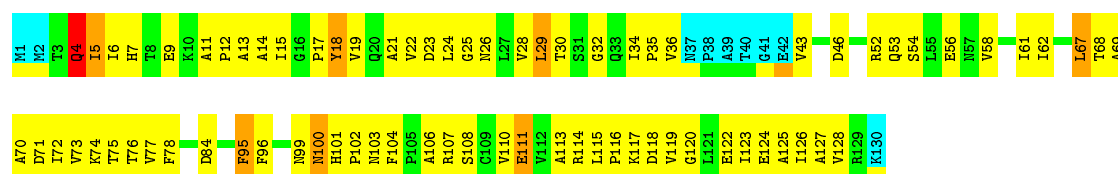
Chain C: 46% 37% 11% 6%



#### 4.2.14 Score per residue for model 14

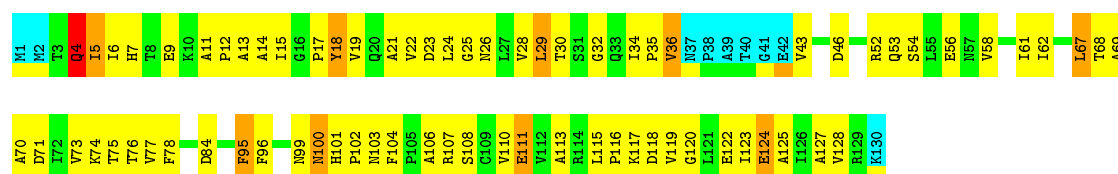
• Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain A: 35% 52% 5% 7%



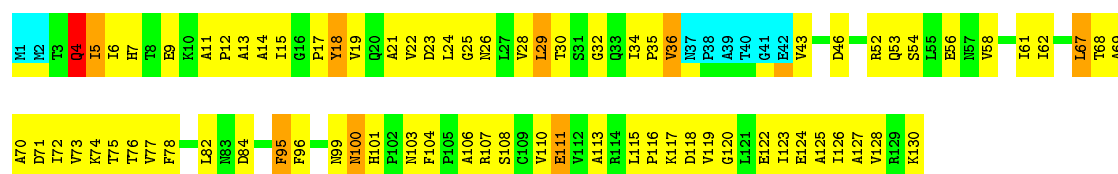
• Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain B: 37% 48% 7% 7%



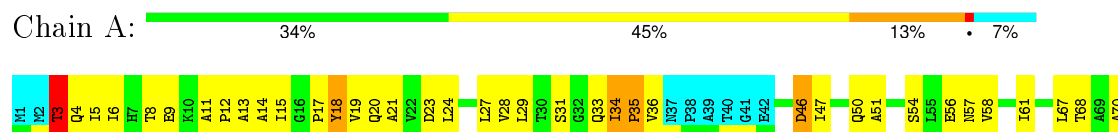
• Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain C: 35% 52% 6% 6%



#### 4.2.15 Score per residue for model 15

• Molecule 1: HYPOTHETICAL PROTEIN HI0719



• Molecule 1: HYPOTHETICAL PROTEIN HI0719



• Molecule 1: HYPOTHETICAL PROTEIN HI0719

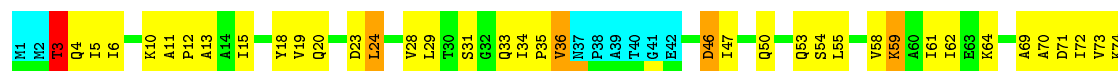


#### 4.2.16 Score per residue for model 16

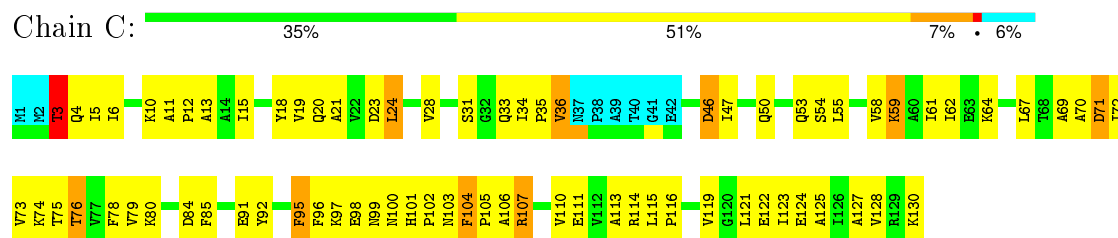
• Molecule 1: HYPOTHETICAL PROTEIN HI0719



• Molecule 1: HYPOTHETICAL PROTEIN HI0719

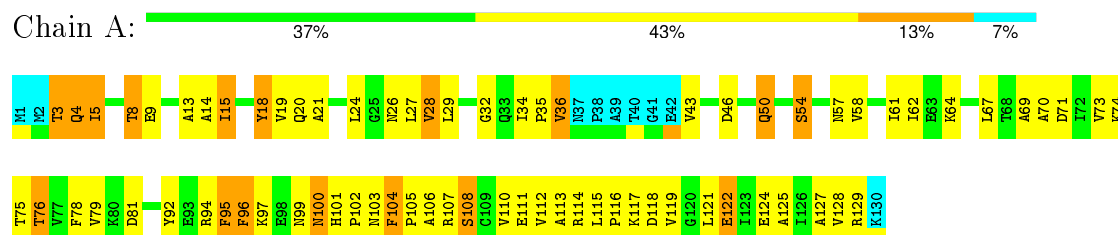


• Molecule 1: HYPOTHETICAL PROTEIN HI0719

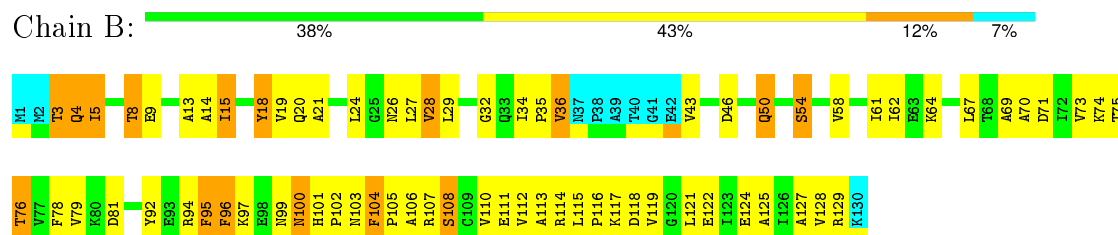


#### 4.2.17 Score per residue for model 17

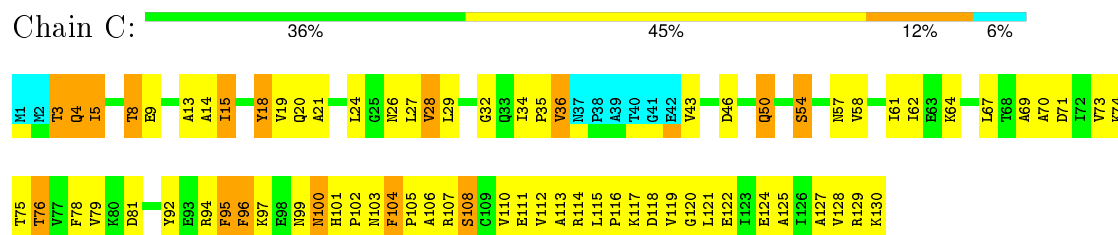
- Molecule 1: HYPOTHETICAL PROTEIN HI0719



- Molecule 1: HYPOTHETICAL PROTEIN HI0719

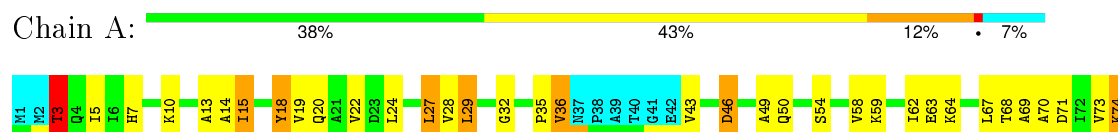


- Molecule 1: HYPOTHETICAL PROTEIN HI0719



#### 4.2.18 Score per residue for model 18

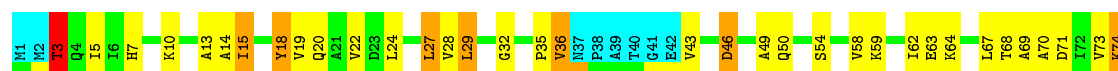
- Molecule 1: HYPOTHETICAL PROTEIN HI0719



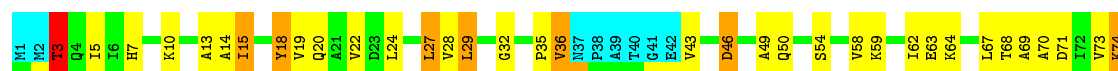




• Molecule 1: HYPOTHETICAL PROTEIN HI0719



• Molecule 1: HYPOTHETICAL PROTEIN HI0719

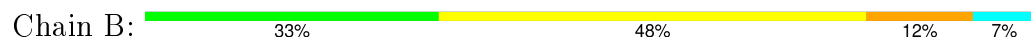


#### 4.2.19 Score per residue for model 19

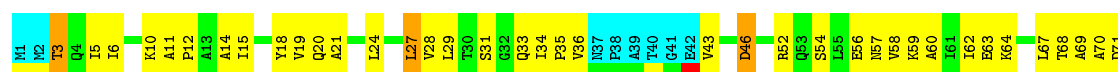
• Molecule 1: HYPOTHETICAL PROTEIN HI0719



• Molecule 1: HYPOTHETICAL PROTEIN HI0719



• Molecule 1: HYPOTHETICAL PROTEIN HI0719

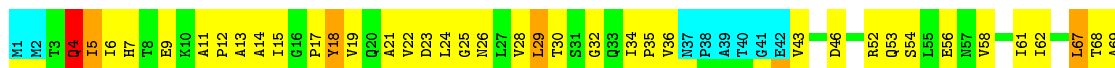




#### 4.2.20 Score per residue for model 20

- Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain A: 35% 52% 5% • 7%



- Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain B: 37% 48% 7% • 7%



- Molecule 1: HYPOTHETICAL PROTEIN HI0719

Chain C: 35% 52% 6% • 6%



## 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CNS	structure solution	1.0
CNS	refinement	1.0

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	921	944	942	68±10
1	B	921	944	942	69±10
1	C	931	957	955	69±9
All	All	55460	56900	56780	3602

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 32.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:128:VAL:HG21	1:C:3:THR:HG21	1.08	1.25	6	12
1:A:128:VAL:HG21	1:B:3:THR:HG21	1.05	1.27	6	13
1:A:3:THR:HG21	1:C:128:VAL:HG21	1.00	1.29	19	13
1:C:69:ALA:HB3	1:C:101:HIS:CE1	0.97	1.94	17	8
1:A:69:ALA:HB3	1:A:101:HIS:CE1	0.97	1.94	17	8
1:A:72:ILE:HD13	1:A:127:ALA:HB2	0.96	1.38	12	3
1:B:69:ALA:HB3	1:B:101:HIS:CE1	0.95	1.94	17	8
1:A:5:ILE:HD11	1:A:19:VAL:HG11	0.94	1.37	10	2
1:C:72:ILE:HD13	1:C:127:ALA:HB2	0.94	1.37	12	3
1:A:28:VAL:HG23	1:A:127:ALA:HB3	0.91	1.40	5	12
1:B:28:VAL:HG13	1:B:127:ALA:HB3	0.91	1.40	8	1
1:B:72:ILE:HD13	1:B:127:ALA:HB2	0.91	1.38	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:28:VAL:HG23	1:B:127:ALA:HB3	0.91	1.39	5	12
1:C:28:VAL:HG12	1:C:127:ALA:HB3	0.91	1.42	7	7
1:C:28:VAL:HG13	1:C:127:ALA:HB3	0.90	1.40	8	1
1:B:5:ILE:HD11	1:B:19:VAL:HG11	0.90	1.38	10	2
1:C:5:ILE:HD11	1:C:19:VAL:HG11	0.90	1.38	10	2
1:A:28:VAL:HG12	1:A:127:ALA:HB3	0.90	1.41	7	7
1:C:28:VAL:HG23	1:C:127:ALA:HB3	0.89	1.39	5	12
1:B:28:VAL:HG12	1:B:127:ALA:HB3	0.89	1.45	10	7
1:A:28:VAL:HG13	1:A:127:ALA:HB3	0.88	1.40	8	1
1:A:70:ALA:HB2	1:A:101:HIS:CD2	0.87	2.04	5	7
1:B:70:ALA:HB2	1:B:101:HIS:CD2	0.87	2.04	5	7
1:C:70:ALA:HB2	1:C:101:HIS:CD2	0.87	2.03	5	7
1:C:28:VAL:CG1	1:C:127:ALA:HB3	0.85	2.02	19	8
1:C:62:ILE:HD13	1:C:72:ILE:HD11	0.85	1.49	9	5
1:A:62:ILE:HD13	1:A:72:ILE:HD11	0.85	1.49	9	5
1:A:28:VAL:CG1	1:A:127:ALA:HB3	0.84	2.02	19	8
1:C:58:VAL:HG21	1:C:123:ILE:HG21	0.84	1.48	4	8
1:A:58:VAL:HG21	1:A:123:ILE:HG21	0.84	1.49	4	8
1:B:28:VAL:CG1	1:B:127:ALA:HB3	0.84	2.02	19	8
1:C:58:VAL:HG21	1:C:123:ILE:CG2	0.83	2.03	13	11
1:B:58:VAL:HG21	1:B:123:ILE:CG2	0.83	2.03	13	11
1:A:58:VAL:HG21	1:A:123:ILE:CG2	0.83	2.04	13	11
1:B:62:ILE:HD13	1:B:72:ILE:HD11	0.82	1.49	9	5
1:A:24:LEU:HD22	1:C:128:VAL:HG11	0.82	1.52	7	6
1:B:106:ALA:HB2	1:C:19:VAL:HG23	0.82	1.49	16	2
1:A:19:VAL:HG23	1:C:106:ALA:HB2	0.81	1.49	16	2
1:A:106:ALA:HB2	1:B:19:VAL:HG23	0.81	1.49	16	2
1:C:76:THR:HG23	1:C:108:SER:O	0.81	1.76	4	10
1:B:104:PHE:HB3	1:C:19:VAL:HG13	0.81	1.52	2	2
1:A:19:VAL:HG13	1:C:104:PHE:HB3	0.81	1.52	2	2
1:A:24:LEU:HD21	1:C:128:VAL:HG11	0.81	1.51	13	1
1:B:58:VAL:HG21	1:B:123:ILE:HG21	0.81	1.51	4	8
1:A:24:LEU:HD13	1:A:24:LEU:O	0.81	1.75	14	3
1:A:128:VAL:HG11	1:B:24:LEU:HD21	0.81	1.53	13	1
1:B:76:THR:HG23	1:B:108:SER:O	0.81	1.76	4	10
1:C:34:ILE:HG23	1:C:36:VAL:HG23	0.81	1.53	19	2
1:C:55:LEU:HD13	1:C:95:PHE:CE2	0.80	2.10	6	7
1:B:24:LEU:O	1:B:24:LEU:HD13	0.80	1.76	14	1
1:B:24:LEU:HD13	1:B:24:LEU:O	0.80	1.76	20	2
1:B:128:VAL:HG11	1:C:24:LEU:HD21	0.80	1.49	13	1
1:C:24:LEU:O	1:C:24:LEU:HD13	0.80	1.76	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:24:LEU:HD13	1:C:24:LEU:O	0.80	1.76	20	2
1:B:34:ILE:HG23	1:B:36:VAL:HG23	0.80	1.53	19	2
1:C:55:LEU:HD21	1:C:92:TYR:CD2	0.80	2.12	8	1
1:B:55:LEU:HD13	1:B:95:PHE:CE2	0.80	2.12	6	7
1:A:34:ILE:HG23	1:A:36:VAL:HG23	0.79	1.53	19	2
1:A:55:LEU:HD13	1:A:95:PHE:CE2	0.79	2.11	6	7
1:B:55:LEU:HD21	1:B:92:TYR:CD2	0.79	2.12	8	1
1:C:29:LEU:HD12	1:C:126:ILE:HG23	0.79	1.55	6	2
1:C:54:SER:O	1:C:58:VAL:HG23	0.79	1.78	3	20
1:A:76:THR:HG23	1:A:108:SER:O	0.79	1.76	4	10
1:A:34:ILE:HG21	1:A:119:VAL:HG21	0.79	1.54	6	1
1:C:24:LEU:HD11	1:C:29:LEU:HD12	0.79	1.53	19	2
1:C:74:LYS:CG	1:C:106:ALA:HB3	0.79	2.08	6	8
1:B:54:SER:O	1:B:58:VAL:HG23	0.79	1.78	3	20
1:A:104:PHE:HB3	1:B:19:VAL:HG13	0.79	1.53	2	2
1:A:128:VAL:HG11	1:B:24:LEU:HD22	0.79	1.53	7	4
1:B:34:ILE:HG21	1:B:119:VAL:HG21	0.79	1.54	6	1
1:C:34:ILE:HG21	1:C:119:VAL:HG21	0.78	1.52	6	1
1:A:29:LEU:HD12	1:A:126:ILE:HG23	0.78	1.55	6	2
1:B:128:VAL:HG11	1:C:24:LEU:HD22	0.78	1.54	7	5
1:A:55:LEU:HD21	1:A:92:TYR:CD2	0.78	2.13	8	1
1:A:24:LEU:HD11	1:A:29:LEU:HD12	0.78	1.53	19	2
1:A:74:LYS:CG	1:A:106:ALA:HB3	0.78	2.08	6	7
1:A:54:SER:O	1:A:58:VAL:HG23	0.78	1.78	3	20
1:B:74:LYS:CG	1:B:106:ALA:HB3	0.77	2.09	6	8
1:A:69:ALA:HB3	1:A:101:HIS:CD2	0.77	2.15	4	3
1:B:24:LEU:HD11	1:B:29:LEU:HD12	0.76	1.53	19	2
1:A:113:ALA:HB3	1:C:111:GLU:O	0.76	1.81	16	18
1:B:111:GLU:O	1:C:113:ALA:HB3	0.76	1.81	19	18
1:A:111:GLU:O	1:B:113:ALA:HB3	0.76	1.80	16	19
1:C:69:ALA:HB3	1:C:101:HIS:NE2	0.76	1.96	2	5
1:C:69:ALA:HB3	1:C:101:HIS:CD2	0.76	2.16	4	3
1:B:29:LEU:HD12	1:B:126:ILE:HG23	0.76	1.55	6	2
1:A:5:ILE:HD11	1:A:19:VAL:HG21	0.75	1.59	12	1
1:C:28:VAL:CG2	1:C:127:ALA:HB3	0.75	2.11	17	11
1:B:69:ALA:HB3	1:B:101:HIS:NE2	0.75	1.96	2	5
1:B:69:ALA:HB3	1:B:101:HIS:CD2	0.75	2.16	4	3
1:A:28:VAL:CG2	1:A:127:ALA:HB3	0.74	2.12	14	11
1:B:28:VAL:CG2	1:B:127:ALA:HB3	0.74	2.12	5	11
1:A:11:ALA:HB1	1:A:12:PRO:HD2	0.74	1.60	5	12
1:A:69:ALA:HB3	1:A:101:HIS:NE2	0.74	1.97	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:106:ALA:HB1	1:C:31:SER:HB3	0.74	1.58	19	2
1:C:29:LEU:HG	1:C:126:ILE:HG23	0.74	1.59	5	2
1:C:11:ALA:HB1	1:C:12:PRO:HD2	0.74	1.60	5	12
1:A:14:ALA:HB1	1:A:18:TYR:O	0.74	1.83	14	8
1:B:14:ALA:HB1	1:B:18:TYR:O	0.74	1.83	14	8
1:B:5:ILE:HD11	1:B:19:VAL:HG21	0.74	1.59	12	1
1:A:103:ASN:OD1	1:B:5:ILE:HD13	0.74	1.83	3	3
1:B:11:ALA:HB1	1:B:12:PRO:HD2	0.73	1.59	5	12
1:B:76:THR:HG23	1:B:107:ARG:CD	0.73	2.14	5	1
1:A:73:VAL:HG11	1:A:128:VAL:HG13	0.73	1.59	9	5
1:B:103:ASN:OD1	1:C:5:ILE:HD13	0.73	1.83	3	3
1:C:67:LEU:HD22	1:C:71:ASP:OD2	0.73	1.84	11	4
1:A:31:SER:HB3	1:C:106:ALA:HB1	0.73	1.60	19	2
1:B:128:VAL:HG21	1:C:3:THR:CG2	0.73	2.12	19	6
1:C:14:ALA:HB1	1:C:18:TYR:O	0.72	1.83	14	8
1:B:73:VAL:HG11	1:B:128:VAL:HG13	0.72	1.59	9	5
1:A:76:THR:HG23	1:A:107:ARG:CD	0.72	2.14	5	1
1:C:70:ALA:HB2	1:C:101:HIS:ND1	0.72	2.00	4	4
1:B:70:ALA:HB2	1:B:101:HIS:ND1	0.72	2.00	4	4
1:C:5:ILE:HD11	1:C:19:VAL:HG21	0.72	1.60	12	1
1:C:76:THR:HG23	1:C:107:ARG:CD	0.72	2.13	5	1
1:A:67:LEU:HD22	1:A:71:ASP:OD2	0.72	1.84	11	4
1:B:104:PHE:CB	1:C:19:VAL:HG13	0.72	2.14	2	5
1:B:67:LEU:HD22	1:B:71:ASP:OD2	0.72	1.84	11	4
1:A:104:PHE:CB	1:B:19:VAL:HG13	0.72	2.15	2	8
1:C:73:VAL:HG11	1:C:128:VAL:HG13	0.72	1.59	9	5
1:A:70:ALA:HB2	1:A:101:HIS:ND1	0.72	1.99	4	4
1:A:106:ALA:HB1	1:B:31:SER:HB3	0.72	1.60	19	2
1:A:28:VAL:HG13	1:A:127:ALA:CB	0.72	2.15	8	1
1:B:106:ALA:HB2	1:C:19:VAL:CG2	0.71	2.15	19	2
1:A:29:LEU:HG	1:A:126:ILE:HG23	0.71	1.60	5	2
1:A:19:VAL:HG13	1:C:104:PHE:CB	0.71	2.14	2	5
1:A:5:ILE:HD13	1:C:103:ASN:OD1	0.71	1.84	3	3
1:B:23:ASP:HA	1:B:28:VAL:HG12	0.71	1.62	11	2
1:A:27:LEU:HD22	1:A:128:VAL:HG12	0.71	1.62	10	2
1:A:19:VAL:CG2	1:C:106:ALA:HB2	0.71	2.16	19	2
1:C:23:ASP:HA	1:C:28:VAL:HG12	0.71	1.63	11	2
1:A:79:VAL:HG12	1:A:121:LEU:HD23	0.71	1.62	12	3
1:A:106:ALA:HB1	1:B:31:SER:HB2	0.71	1.62	5	3
1:B:79:VAL:HG12	1:B:121:LEU:HD23	0.70	1.62	12	3
1:B:29:LEU:HG	1:B:126:ILE:HG23	0.70	1.61	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:27:LEU:HD22	1:C:128:VAL:HG12	0.70	1.63	10	2
1:B:104:PHE:HB2	1:C:19:VAL:HG13	0.70	1.63	17	9
1:C:28:VAL:HG13	1:C:127:ALA:CB	0.70	2.15	8	1
1:C:74:LYS:HG2	1:C:106:ALA:HB3	0.70	1.62	12	3
1:C:112:VAL:HG21	1:C:115:LEU:HD21	0.70	1.63	5	5
1:A:23:ASP:HA	1:A:28:VAL:HG12	0.70	1.64	13	2
1:A:69:ALA:HB3	1:A:101:HIS:ND1	0.70	2.02	12	3
1:C:79:VAL:HG12	1:C:121:LEU:HD23	0.70	1.62	12	3
1:A:5:ILE:HD11	1:C:103:ASN:OD1	0.70	1.86	11	4
1:A:5:ILE:HD13	1:C:103:ASN:ND2	0.70	2.01	4	4
1:A:103:ASN:ND2	1:B:5:ILE:HD13	0.70	2.01	4	4
1:A:106:ALA:HB2	1:B:19:VAL:CG2	0.70	2.17	19	2
1:B:69:ALA:HB3	1:B:101:HIS:ND1	0.69	2.01	12	3
1:C:69:ALA:HB3	1:C:101:HIS:ND1	0.69	2.02	12	3
1:A:75:THR:HG21	1:A:92:TYR:OH	0.69	1.87	10	5
1:A:103:ASN:OD1	1:B:5:ILE:HD11	0.69	1.87	11	4
1:B:75:THR:HG21	1:B:92:TYR:OH	0.69	1.87	10	5
1:C:75:THR:HG21	1:C:92:TYR:OH	0.69	1.87	10	5
1:A:14:ALA:O	1:A:15:ILE:HD13	0.69	1.87	14	7
1:C:14:ALA:O	1:C:15:ILE:HD13	0.69	1.87	14	7
1:B:103:ASN:OD1	1:C:5:ILE:HD11	0.69	1.87	11	4
1:B:103:ASN:ND2	1:C:5:ILE:HD13	0.69	2.03	4	4
1:B:74:LYS:HG2	1:B:106:ALA:HB3	0.69	1.63	12	3
1:A:112:VAL:HG21	1:A:115:LEU:HD21	0.69	1.63	5	5
1:A:22:VAL:HG11	1:C:73:VAL:O	0.69	1.88	4	3
1:B:14:ALA:O	1:B:15:ILE:HD13	0.69	1.87	14	7
1:B:27:LEU:HD22	1:B:128:VAL:HG12	0.69	1.64	10	2
1:A:74:LYS:HG2	1:A:106:ALA:HB3	0.69	1.63	12	3
1:A:31:SER:HB2	1:C:106:ALA:HB1	0.68	1.65	5	3
1:A:11:ALA:HB3	1:A:20:GLN:OE1	0.68	1.89	5	3
1:A:115:LEU:HD22	1:A:122:GLU:HB2	0.68	1.64	11	11
1:B:33:GLN:HG2	1:B:58:VAL:HG22	0.68	1.65	3	3
1:B:104:PHE:O	1:C:19:VAL:HG13	0.67	1.88	12	3
1:B:115:LEU:HD22	1:B:122:GLU:HB2	0.67	1.64	11	11
1:B:28:VAL:HG13	1:B:127:ALA:CB	0.67	2.16	8	1
1:A:70:ALA:HB2	1:A:101:HIS:HD2	0.67	1.49	12	7
1:A:104:PHE:HB2	1:B:19:VAL:HG13	0.67	1.66	17	9
1:B:128:VAL:CG1	1:C:24:LEU:HD22	0.67	2.18	6	3
1:B:125:ALA:C	1:B:126:ILE:HD13	0.67	2.09	6	3
1:C:115:LEU:HD22	1:C:122:GLU:HB2	0.67	1.65	11	11
1:A:125:ALA:C	1:A:126:ILE:HD13	0.67	2.09	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:73:VAL:O	1:C:22:VAL:HG11	0.67	1.90	4	3
1:B:106:ALA:HB1	1:C:31:SER:HB2	0.67	1.65	3	3
1:B:70:ALA:HB2	1:B:101:HIS:HD2	0.67	1.49	17	7
1:B:112:VAL:HG21	1:B:115:LEU:HD21	0.67	1.63	5	5
1:A:104:PHE:O	1:B:19:VAL:HG13	0.67	1.90	12	3
1:A:19:VAL:HG13	1:C:104:PHE:HB2	0.67	1.65	17	9
1:B:24:LEU:HD11	1:B:29:LEU:HD13	0.67	1.66	5	2
1:A:24:LEU:HD11	1:A:29:LEU:HD13	0.67	1.66	5	2
1:C:125:ALA:C	1:C:126:ILE:HD13	0.67	2.09	6	3
1:A:33:GLN:HG2	1:A:58:VAL:HG22	0.67	1.65	3	3
1:C:76:THR:O	1:C:123:ILE:HG23	0.66	1.90	3	2
1:A:128:VAL:CG1	1:B:24:LEU:HD22	0.66	2.21	6	3
1:B:11:ALA:HB3	1:B:20:GLN:OE1	0.66	1.89	5	3
1:C:11:ALA:HB3	1:C:20:GLN:OE1	0.66	1.89	5	3
1:A:19:VAL:HG13	1:C:104:PHE:O	0.66	1.90	12	3
1:B:54:SER:HB2	1:B:123:ILE:HD13	0.66	1.65	7	1
1:A:76:THR:O	1:A:123:ILE:HG23	0.66	1.91	3	2
1:B:76:THR:O	1:B:123:ILE:HG23	0.66	1.91	3	2
1:A:29:LEU:CD2	1:A:126:ILE:HD12	0.66	2.21	5	1
1:C:70:ALA:HB2	1:C:101:HIS:HD2	0.66	1.49	12	7
1:C:74:LYS:HD3	1:C:126:ILE:HD12	0.66	1.68	19	1
1:A:67:LEU:HD11	1:A:129:ARG:HB2	0.66	1.68	17	4
1:C:34:ILE:HG13	1:C:119:VAL:HG11	0.66	1.68	19	1
1:A:34:ILE:HG13	1:A:119:VAL:HG11	0.66	1.68	19	1
1:B:29:LEU:CD2	1:B:126:ILE:HD12	0.65	2.21	5	1
1:C:24:LEU:HD11	1:C:29:LEU:HD13	0.65	1.66	5	2
1:C:33:GLN:HG2	1:C:58:VAL:HG22	0.65	1.65	3	3
1:A:73:VAL:CG1	1:A:128:VAL:HG13	0.65	2.21	9	2
1:B:74:LYS:HD3	1:B:126:ILE:HD12	0.65	1.68	19	1
1:B:24:LEU:HD11	1:B:29:LEU:CD1	0.65	2.21	19	1
1:C:67:LEU:HD11	1:C:129:ARG:HB2	0.65	1.68	11	4
1:B:73:VAL:CG1	1:B:128:VAL:HG13	0.65	2.20	9	2
1:C:73:VAL:CG1	1:C:128:VAL:HG13	0.65	2.21	9	2
1:C:3:THR:HG23	1:C:24:LEU:HA	0.65	1.69	7	2
1:A:6:ILE:HB	1:A:21:ALA:HB3	0.65	1.69	11	6
1:A:24:LEU:HD11	1:A:29:LEU:CD1	0.65	2.21	19	1
1:B:33:GLN:HG3	1:B:58:VAL:HG22	0.65	1.68	19	2
1:A:11:ALA:HB1	1:A:12:PRO:CD	0.64	2.23	7	7
1:A:70:ALA:HB2	1:A:100:ASN:O	0.64	1.92	18	6
1:A:24:LEU:HD22	1:C:128:VAL:CG1	0.64	2.22	6	2
1:A:3:THR:HG21	1:C:128:VAL:CG2	0.64	2.20	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:99:ASN:HB3	1:C:101:HIS:CE1	0.64	2.28	16	10
1:B:70:ALA:HB2	1:B:100:ASN:O	0.64	1.93	18	6
1:C:11:ALA:HB1	1:C:12:PRO:CD	0.64	2.23	7	8
1:B:99:ASN:HB3	1:B:101:HIS:CE1	0.64	2.27	5	10
1:B:67:LEU:HD11	1:B:129:ARG:HB2	0.64	1.68	11	4
1:B:11:ALA:HB1	1:B:12:PRO:CD	0.64	2.23	7	8
1:B:34:ILE:HG13	1:B:119:VAL:HG11	0.64	1.70	19	1
1:C:122:GLU:O	1:C:123:ILE:HD13	0.64	1.93	13	5
1:B:122:GLU:O	1:B:123:ILE:HD13	0.64	1.93	13	5
1:A:73:VAL:O	1:B:22:VAL:HG11	0.64	1.93	4	3
1:C:24:LEU:HD11	1:C:29:LEU:CD1	0.64	2.21	19	1
1:B:6:ILE:HB	1:B:21:ALA:HB3	0.64	1.69	11	6
1:B:128:VAL:CG2	1:C:3:THR:HG21	0.64	2.16	6	3
1:A:99:ASN:HB3	1:A:101:HIS:CE1	0.64	2.28	16	10
1:B:34:ILE:HB	1:B:119:VAL:HG11	0.64	1.69	2	10
1:C:29:LEU:CD2	1:C:126:ILE:HD12	0.64	2.22	5	1
1:A:54:SER:HB2	1:A:123:ILE:HD13	0.64	1.68	7	1
1:A:122:GLU:O	1:A:123:ILE:HD13	0.63	1.93	13	5
1:A:3:THR:HG23	1:A:24:LEU:HA	0.63	1.69	7	2
1:A:128:VAL:CG2	1:B:3:THR:HG21	0.63	2.17	6	4
1:C:22:VAL:HG23	1:C:29:LEU:HD13	0.63	1.70	18	1
1:B:74:LYS:HG3	1:B:106:ALA:HB3	0.63	1.71	18	12
1:C:77:VAL:HG13	1:C:122:GLU:O	0.63	1.94	14	4
1:C:70:ALA:HB2	1:C:100:ASN:O	0.63	1.93	18	6
1:A:74:LYS:HD3	1:A:126:ILE:HD12	0.63	1.69	19	1
1:C:33:GLN:HG3	1:C:58:VAL:HG22	0.63	1.69	19	2
1:A:33:GLN:HG3	1:A:58:VAL:HG22	0.63	1.69	19	2
1:C:74:LYS:HG3	1:C:106:ALA:HB3	0.63	1.71	18	12
1:C:34:ILE:HB	1:C:119:VAL:HG11	0.63	1.69	2	11
1:B:11:ALA:HB2	1:B:61:ILE:CG1	0.62	2.24	14	7
1:A:74:LYS:HG3	1:A:106:ALA:HB3	0.62	1.71	18	11
1:A:79:VAL:HG12	1:A:121:LEU:HD21	0.62	1.71	18	3
1:B:120:GLY:C	1:B:121:LEU:HD13	0.62	2.15	7	1
1:A:26:ASN:C	1:A:27:LEU:HD23	0.62	2.15	10	1
1:B:110:VAL:HG11	1:C:78:PHE:CD2	0.62	2.29	14	10
1:C:11:ALA:HB2	1:C:61:ILE:CG1	0.62	2.25	14	7
1:B:26:ASN:C	1:B:27:LEU:HD23	0.62	2.15	10	1
1:A:78:PHE:CD2	1:C:110:VAL:HG11	0.62	2.29	2	10
1:A:77:VAL:HG13	1:A:122:GLU:O	0.62	1.94	14	4
1:C:54:SER:HB2	1:C:123:ILE:HD13	0.62	1.69	7	1
1:A:50:GLN:OE1	1:A:121:LEU:HD12	0.62	1.95	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:77:VAL:HG13	1:B:122:GLU:O	0.62	1.95	14	4
1:B:3:THR:HG23	1:B:24:LEU:HA	0.62	1.70	7	2
1:A:3:THR:CG2	1:C:128:VAL:HG21	0.62	2.17	19	6
1:C:22:VAL:HG23	1:C:29:LEU:HD23	0.62	1.72	10	1
1:C:26:ASN:C	1:C:27:LEU:HD23	0.62	2.14	10	1
1:C:50:GLN:OE1	1:C:121:LEU:HD12	0.62	1.95	10	2
1:C:34:ILE:CG2	1:C:119:VAL:HG21	0.62	2.23	6	1
1:B:22:VAL:HG23	1:B:29:LEU:HD13	0.62	1.70	18	1
1:B:23:ASP:HA	1:B:28:VAL:HG23	0.62	1.72	10	5
1:A:27:LEU:HG	1:A:128:VAL:HG12	0.62	1.72	5	2
1:C:6:ILE:HB	1:C:21:ALA:HB3	0.62	1.69	11	6
1:A:11:ALA:HB2	1:A:61:ILE:CG1	0.61	2.25	14	7
1:C:55:LEU:HD21	1:C:92:TYR:CE2	0.61	2.30	8	1
1:C:23:ASP:HA	1:C:28:VAL:HG23	0.61	1.72	12	5
1:A:67:LEU:HD21	1:A:129:ARG:HG3	0.61	1.72	9	1
1:A:5:ILE:HD11	1:C:103:ASN:CG	0.61	2.16	11	4
1:A:22:VAL:HG23	1:A:29:LEU:HD23	0.61	1.72	10	1
1:A:22:VAL:HG23	1:A:29:LEU:HD13	0.61	1.70	18	1
1:B:79:VAL:HG12	1:B:121:LEU:HD21	0.61	1.72	18	3
1:A:34:ILE:CG1	1:A:119:VAL:HG11	0.61	2.25	19	1
1:A:110:VAL:HG11	1:B:78:PHE:CD2	0.61	2.30	14	10
1:B:103:ASN:CG	1:C:5:ILE:HD11	0.61	2.16	11	4
1:B:34:ILE:CG2	1:B:119:VAL:HG21	0.61	2.25	6	1
1:A:115:LEU:HD23	1:C:110:VAL:HG12	0.61	1.73	16	7
1:A:24:LEU:HD21	1:C:73:VAL:HG21	0.61	1.71	4	1
1:B:27:LEU:HG	1:B:128:VAL:HG12	0.61	1.72	5	2
1:C:120:GLY:C	1:C:121:LEU:HD13	0.61	2.16	7	1
1:A:84:ASP:O	1:A:88:VAL:HG23	0.61	1.96	6	5
1:A:120:GLY:C	1:A:121:LEU:HD13	0.60	2.16	7	1
1:C:43:VAL:CG2	1:C:119:VAL:HG23	0.60	2.26	10	1
1:B:29:LEU:HD12	1:B:126:ILE:HD12	0.60	1.72	10	1
1:A:103:ASN:CG	1:B:5:ILE:HD13	0.60	2.16	18	4
1:A:23:ASP:HA	1:A:28:VAL:HG23	0.60	1.72	12	5
1:B:67:LEU:HD21	1:B:129:ARG:HG3	0.60	1.72	9	1
1:C:79:VAL:HG12	1:C:121:LEU:CD2	0.60	2.26	12	4
1:A:55:LEU:HD21	1:A:92:TYR:CE2	0.60	2.31	8	1
1:C:79:VAL:HG12	1:C:121:LEU:HD21	0.60	1.72	18	3
1:A:29:LEU:HD12	1:A:126:ILE:HD12	0.60	1.72	10	1
1:B:75:THR:HG21	1:B:92:TYR:CZ	0.60	2.32	17	2
1:A:67:LEU:HD21	1:A:129:ARG:HB3	0.60	1.73	2	2
1:C:28:VAL:HG11	1:C:67:LEU:CD1	0.60	2.27	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:VAL:CG2	1:A:119:VAL:HG23	0.60	2.26	10	1
1:A:35:PRO:O	1:A:43:VAL:HA	0.60	1.97	11	9
1:A:103:ASN:CG	1:B:5:ILE:HD11	0.60	2.15	11	4
1:B:43:VAL:CG2	1:B:119:VAL:HG23	0.60	2.27	10	1
1:A:5:ILE:HD13	1:C:103:ASN:CG	0.60	2.16	18	5
1:C:84:ASP:O	1:C:88:VAL:HG23	0.60	1.96	6	5
1:B:29:LEU:N	1:B:29:LEU:HD22	0.60	2.12	10	1
1:C:62:ILE:HG22	1:C:67:LEU:HB3	0.60	1.74	13	1
1:B:26:ASN:O	1:B:27:LEU:HD23	0.60	1.97	10	1
1:A:34:ILE:CG2	1:A:119:VAL:HG21	0.60	2.26	6	1
1:B:76:THR:HG23	1:B:107:ARG:HD3	0.60	1.73	5	1
1:B:75:THR:HG22	1:B:125:ALA:CB	0.60	2.27	10	3
1:A:29:LEU:N	1:A:29:LEU:HD22	0.60	2.12	10	1
1:B:84:ASP:O	1:B:88:VAL:HG23	0.60	1.96	6	5
1:B:71:ASP:OD1	1:B:127:ALA:HB1	0.60	1.97	11	1
1:C:67:LEU:HD21	1:C:129:ARG:HG3	0.60	1.73	9	1
1:A:26:ASN:O	1:A:27:LEU:HD23	0.59	1.97	10	1
1:A:34:ILE:HB	1:A:119:VAL:HG11	0.59	1.71	2	10
1:C:67:LEU:HD21	1:C:129:ARG:HB3	0.59	1.74	2	2
1:B:28:VAL:HG11	1:B:67:LEU:CD1	0.59	2.27	8	1
1:B:55:LEU:HD21	1:B:92:TYR:CE2	0.59	2.31	8	1
1:A:128:VAL:HG21	1:B:3:THR:CG2	0.59	2.18	6	7
1:C:29:LEU:HD22	1:C:29:LEU:N	0.59	2.11	10	1
1:A:29:LEU:HD12	1:A:126:ILE:CG2	0.59	2.27	6	1
1:A:121:LEU:N	1:A:121:LEU:HD13	0.59	2.13	7	1
1:A:75:THR:HG21	1:A:92:TYR:CZ	0.59	2.33	17	2
1:C:75:THR:HG22	1:C:125:ALA:CB	0.59	2.27	10	3
1:B:5:ILE:HG21	1:B:19:VAL:HG11	0.59	1.74	18	2
1:A:76:THR:HG23	1:A:107:ARG:HD3	0.59	1.73	5	1
1:B:103:ASN:O	1:C:5:ILE:HD11	0.59	1.98	2	1
1:C:121:LEU:HD13	1:C:121:LEU:N	0.59	2.12	7	1
1:C:34:ILE:CG1	1:C:119:VAL:HG11	0.59	2.27	19	1
1:B:79:VAL:HG12	1:B:121:LEU:CD2	0.59	2.26	12	4
1:B:121:LEU:N	1:B:121:LEU:HD13	0.59	2.12	7	2
1:A:28:VAL:HG11	1:A:67:LEU:CD1	0.59	2.28	8	1
1:C:29:LEU:HD12	1:C:126:ILE:CG2	0.59	2.27	6	1
1:A:34:ILE:HG23	1:A:119:VAL:HG11	0.59	1.74	4	1
1:A:79:VAL:HG12	1:A:121:LEU:CD2	0.59	2.27	12	4
1:A:55:LEU:HD13	1:A:95:PHE:CD2	0.59	2.32	11	5
1:C:5:ILE:HG21	1:C:19:VAL:HG11	0.59	1.74	18	2
1:A:69:ALA:HB3	1:A:99:ASN:HB3	0.59	1.75	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:110:VAL:HG12	1:C:115:LEU:HD23	0.59	1.73	16	7
1:A:75:THR:HG22	1:A:125:ALA:CB	0.59	2.27	10	4
1:C:29:LEU:HD12	1:C:126:ILE:HD12	0.59	1.73	10	1
1:A:5:ILE:HG21	1:A:19:VAL:HG11	0.59	1.74	18	2
1:A:110:VAL:HG12	1:B:115:LEU:HD23	0.58	1.73	16	9
1:B:22:VAL:HG23	1:B:29:LEU:HD23	0.58	1.72	10	1
1:C:26:ASN:O	1:C:27:LEU:HD23	0.58	1.97	10	1
1:B:62:ILE:HG22	1:B:67:LEU:HB3	0.58	1.74	13	1
1:B:50:GLN:OE1	1:B:121:LEU:HD12	0.58	1.98	10	2
1:A:62:ILE:HG22	1:A:67:LEU:HB3	0.58	1.74	13	1
1:A:31:SER:CB	1:C:106:ALA:HB1	0.58	2.27	3	3
1:C:35:PRO:O	1:C:43:VAL:HA	0.58	1.98	11	9
1:C:29:LEU:HD23	1:C:126:ILE:HD12	0.58	1.76	8	3
1:B:67:LEU:HD21	1:B:129:ARG:HB3	0.58	1.74	2	2
1:C:71:ASP:OD1	1:C:127:ALA:HB1	0.58	1.98	11	1
1:A:27:LEU:HD23	1:A:127:ALA:O	0.58	1.97	19	1
1:C:27:LEU:HG	1:C:128:VAL:HG12	0.58	1.73	5	2
1:A:29:LEU:HD22	1:C:74:LYS:CE	0.58	2.29	19	1
1:C:76:THR:HG23	1:C:107:ARG:HD3	0.58	1.73	5	1
1:A:8:THR:HG22	1:A:20:GLN:OE1	0.58	1.99	13	3
1:B:62:ILE:HD12	1:B:127:ALA:CB	0.58	2.29	17	2
1:B:106:ALA:HB1	1:C:31:SER:CB	0.58	2.29	3	4
1:A:62:ILE:HD12	1:A:127:ALA:CB	0.58	2.29	17	2
1:C:27:LEU:HD23	1:C:127:ALA:O	0.58	1.99	19	1
1:C:28:VAL:HG11	1:C:67:LEU:HD13	0.58	1.75	8	1
1:C:8:THR:HG22	1:C:20:GLN:OE1	0.58	1.99	13	3
1:B:29:LEU:HD12	1:B:126:ILE:CG2	0.58	2.28	6	1
1:C:34:ILE:HG23	1:C:119:VAL:HG11	0.58	1.75	4	1
1:C:34:ILE:HD12	1:C:36:VAL:CG2	0.57	2.29	17	2
1:A:71:ASP:OD1	1:A:127:ALA:HB1	0.57	1.97	11	1
1:B:35:PRO:O	1:B:43:VAL:HA	0.57	1.98	11	9
1:C:75:THR:HG21	1:C:92:TYR:CZ	0.57	2.34	17	1
1:A:33:GLN:CG	1:A:58:VAL:HG22	0.57	2.29	3	2
1:B:27:LEU:HD21	1:C:24:LEU:HD13	0.57	1.74	18	1
1:B:59:LYS:HG3	1:B:69:ALA:HB2	0.57	1.75	16	1
1:A:34:ILE:HD12	1:A:36:VAL:CG2	0.57	2.29	17	2
1:B:34:ILE:HD12	1:B:36:VAL:CG2	0.57	2.29	17	2
1:B:13:ALA:HB1	1:B:33:GLN:OE1	0.57	1.98	2	1
1:C:36:VAL:HG21	1:C:117:LYS:HD2	0.57	1.76	7	1
1:A:79:VAL:HG12	1:A:121:LEU:HD22	0.57	1.75	11	2
1:B:34:ILE:CG1	1:B:119:VAL:HG11	0.57	2.30	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ALA:HB3	1:A:20:GLN:NE2	0.57	2.14	16	2
1:A:120:GLY:O	1:A:121:LEU:HD23	0.57	2.00	6	2
1:A:34:ILE:HG13	1:A:36:VAL:HG23	0.57	1.76	5	2
1:C:112:VAL:CG2	1:C:115:LEU:HD11	0.57	2.30	10	1
1:B:55:LEU:HD13	1:B:95:PHE:CD2	0.57	2.35	11	6
1:A:27:LEU:N	1:A:27:LEU:HD12	0.57	2.15	17	1
1:C:30:THR:HG21	1:C:62:ILE:HD11	0.57	1.76	14	3
1:C:33:GLN:CG	1:C:58:VAL:HG22	0.57	2.30	3	2
1:B:11:ALA:HB3	1:B:20:GLN:NE2	0.57	2.14	16	2
1:C:11:ALA:HB3	1:C:20:GLN:NE2	0.57	2.14	16	2
1:A:28:VAL:HG11	1:A:67:LEU:HD13	0.57	1.77	8	1
1:B:120:GLY:O	1:B:121:LEU:HD23	0.57	2.00	6	2
1:A:5:ILE:HD11	1:C:103:ASN:O	0.57	2.00	2	1
1:C:28:VAL:C	1:C:29:LEU:HD13	0.57	2.21	10	1
1:B:103:ASN:CG	1:C:5:ILE:HD13	0.57	2.20	18	5
1:A:106:ALA:HB1	1:B:31:SER:CB	0.57	2.29	3	4
1:C:6:ILE:HD12	1:C:21:ALA:CB	0.56	2.30	12	5
1:B:27:LEU:HD12	1:B:27:LEU:N	0.56	2.15	17	1
1:C:29:LEU:HD12	1:C:29:LEU:N	0.56	2.15	14	1
1:A:30:THR:HG21	1:A:62:ILE:HD11	0.56	1.76	14	4
1:C:29:LEU:N	1:C:29:LEU:HD12	0.56	2.15	20	3
1:C:59:LYS:HD3	1:C:69:ALA:HB2	0.56	1.77	10	1
1:B:27:LEU:HD23	1:B:127:ALA:O	0.56	1.99	19	1
1:B:69:ALA:HB3	1:B:99:ASN:HB3	0.56	1.76	18	2
1:C:43:VAL:HB	1:C:119:VAL:HG12	0.56	1.77	2	4
1:A:8:THR:HG21	1:A:61:ILE:CG1	0.56	2.31	17	1
1:A:73:VAL:CG1	1:A:128:VAL:HG12	0.56	2.30	2	1
1:B:29:LEU:N	1:B:29:LEU:HD12	0.56	2.15	14	3
1:B:30:THR:HG21	1:B:62:ILE:HD11	0.56	1.76	14	4
1:B:29:LEU:HD12	1:B:29:LEU:N	0.56	2.15	1	1
1:B:112:VAL:CG2	1:B:115:LEU:HD11	0.56	2.30	10	1
1:B:79:VAL:HG12	1:B:121:LEU:HD22	0.56	1.75	11	2
1:B:74:LYS:CE	1:C:29:LEU:HD22	0.56	2.30	19	1
1:B:11:ALA:HB2	1:B:61:ILE:HG12	0.56	1.78	6	7
1:B:28:VAL:HG11	1:B:67:LEU:HD13	0.56	1.76	8	1
1:A:112:VAL:CG2	1:A:115:LEU:HD11	0.56	2.30	10	1
1:C:8:THR:HG21	1:C:61:ILE:CG1	0.56	2.30	17	1
1:A:15:ILE:HG22	1:A:15:ILE:O	0.56	2.01	7	11
1:B:36:VAL:HG21	1:B:117:LYS:HD2	0.56	1.77	7	1
1:C:43:VAL:HG21	1:C:119:VAL:HG23	0.56	1.77	10	1
1:A:74:LYS:CE	1:B:29:LEU:HD22	0.56	2.30	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:62:ILE:HD12	1:C:127:ALA:CB	0.56	2.30	17	2
1:B:28:VAL:C	1:B:29:LEU:HD13	0.56	2.21	10	1
1:A:43:VAL:HG21	1:A:119:VAL:HG23	0.56	1.77	10	1
1:C:120:GLY:O	1:C:121:LEU:HD23	0.56	2.00	6	2
1:C:59:LYS:HG3	1:C:69:ALA:HB2	0.56	1.76	16	2
1:C:67:LEU:HD21	1:C:129:ARG:HB2	0.56	1.78	8	3
1:C:27:LEU:HD12	1:C:27:LEU:N	0.56	2.15	17	1
1:A:29:LEU:HD23	1:A:126:ILE:HD12	0.56	1.76	8	3
1:B:34:ILE:HG13	1:B:36:VAL:HG23	0.56	1.76	5	5
1:A:13:ALA:HB1	1:A:33:GLN:OE1	0.56	2.01	2	1
1:B:8:THR:HG21	1:B:61:ILE:CG1	0.56	2.31	17	1
1:B:29:LEU:HD23	1:B:126:ILE:HD12	0.56	1.78	8	3
1:C:11:ALA:HB2	1:C:61:ILE:HG12	0.56	1.78	6	7
1:C:115:LEU:HD22	1:C:122:GLU:CB	0.56	2.30	12	4
1:B:15:ILE:O	1:B:15:ILE:HG22	0.56	2.01	7	11
1:C:34:ILE:HG13	1:C:36:VAL:HG23	0.56	1.76	5	5
1:A:103:ASN:O	1:B:5:ILE:HD11	0.56	2.00	2	1
1:A:43:VAL:HB	1:A:119:VAL:HG12	0.56	1.76	9	4
1:A:59:LYS:HG3	1:A:69:ALA:HB2	0.56	1.77	16	1
1:B:8:THR:HG22	1:B:20:GLN:OE1	0.55	2.00	13	3
1:B:33:GLN:CG	1:B:58:VAL:HG22	0.55	2.30	3	3
1:C:99:ASN:O	1:C:100:ASN:CB	0.55	2.55	19	19
1:A:28:VAL:C	1:A:29:LEU:HD13	0.55	2.21	10	1
1:C:3:THR:HG23	1:C:24:LEU:HD23	0.55	1.77	12	1
1:A:15:ILE:O	1:A:15:ILE:HG22	0.55	2.02	17	8
1:A:73:VAL:HG21	1:B:24:LEU:HD21	0.55	1.78	4	1
1:B:73:VAL:HB	1:C:22:VAL:HG21	0.55	1.78	7	3
1:C:73:VAL:CG1	1:C:128:VAL:HG12	0.55	2.31	2	1
1:A:29:LEU:N	1:A:29:LEU:HD12	0.55	2.15	14	1
1:C:15:ILE:O	1:C:15:ILE:HG22	0.55	2.01	7	7
1:A:29:LEU:HD12	1:A:29:LEU:N	0.55	2.15	20	3
1:A:33:GLN:CB	1:A:58:VAL:HG22	0.55	2.31	3	3
1:A:79:VAL:HG11	1:A:85:PHE:CD1	0.55	2.36	18	4
1:A:75:THR:HG23	1:A:75:THR:O	0.55	2.02	19	3
1:C:43:VAL:HG11	1:C:119:VAL:HA	0.55	1.79	10	1
1:C:43:VAL:O	1:C:43:VAL:HG13	0.55	2.02	1	8
1:B:43:VAL:HB	1:B:119:VAL:HG12	0.55	1.78	9	4
1:C:43:VAL:HG13	1:C:43:VAL:O	0.55	2.02	14	4
1:A:76:THR:HG22	1:A:78:PHE:CE1	0.55	2.37	16	2
1:C:33:GLN:CB	1:C:58:VAL:HG22	0.55	2.32	3	3
1:B:79:VAL:HG11	1:B:85:PHE:CD1	0.55	2.36	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:VAL:HG13	1:A:43:VAL:O	0.55	2.01	12	4
1:A:22:VAL:HG21	1:C:73:VAL:HB	0.55	1.79	7	2
1:A:121:LEU:C	1:A:121:LEU:HD22	0.55	2.22	13	1
1:B:99:ASN:O	1:B:100:ASN:CB	0.55	2.55	6	20
1:A:74:LYS:O	1:A:75:THR:HG23	0.55	2.02	12	1
1:A:47:ILE:HG13	1:A:121:LEU:HD11	0.55	1.79	10	1
1:C:75:THR:O	1:C:75:THR:HG23	0.55	2.02	19	2
1:B:72:ILE:HG22	1:B:74:LYS:O	0.55	2.02	19	1
1:A:99:ASN:O	1:A:100:ASN:CB	0.55	2.55	6	20
1:C:5:ILE:CD1	1:C:19:VAL:HG21	0.55	2.32	12	1
1:B:15:ILE:HG22	1:B:15:ILE:O	0.55	2.02	10	8
1:A:43:VAL:O	1:A:43:VAL:HG13	0.55	2.02	20	7
1:A:110:VAL:HG12	1:B:115:LEU:CD2	0.55	2.32	5	1
1:B:73:VAL:CG1	1:B:128:VAL:HG12	0.55	2.32	2	1
1:C:75:THR:HG23	1:C:105:PRO:HB2	0.55	1.78	16	1
1:A:75:THR:HG23	1:A:105:PRO:HB2	0.55	1.78	16	1
1:C:79:VAL:HG11	1:C:85:PHE:CD1	0.55	2.37	18	4
1:B:104:PHE:O	1:C:19:VAL:HG22	0.55	2.02	10	4
1:B:43:VAL:O	1:B:43:VAL:HG13	0.55	2.01	12	7
1:C:55:LEU:HD13	1:C:95:PHE:CD2	0.55	2.37	6	6
1:C:13:ALA:HB1	1:C:33:GLN:OE1	0.55	2.01	2	1
1:B:76:THR:HG22	1:B:78:PHE:CE1	0.55	2.37	16	2
1:A:43:VAL:HG11	1:A:119:VAL:HA	0.55	1.79	10	1
1:A:23:ASP:CA	1:A:28:VAL:HG12	0.55	2.32	13	1
1:B:74:LYS:O	1:B:75:THR:HG23	0.54	2.02	12	1
1:B:72:ILE:HG23	1:B:126:ILE:O	0.54	2.02	2	6
1:C:47:ILE:HD13	1:C:84:ASP:OD2	0.54	2.02	16	1
1:A:19:VAL:HG22	1:C:104:PHE:O	0.54	2.02	10	4
1:A:59:LYS:HD3	1:A:69:ALA:HB2	0.54	1.77	10	1
1:C:121:LEU:C	1:C:121:LEU:HD22	0.54	2.22	13	1
1:C:27:LEU:HD23	1:C:28:VAL:N	0.54	2.18	3	2
1:B:75:THR:HG23	1:B:75:THR:O	0.54	2.02	19	1
1:C:76:THR:HG22	1:C:78:PHE:CE1	0.54	2.37	16	2
1:B:67:LEU:HD21	1:B:129:ARG:HB2	0.54	1.78	8	2
1:B:59:LYS:HD3	1:B:69:ALA:HB2	0.54	1.77	10	1
1:A:27:LEU:HD23	1:A:28:VAL:N	0.54	2.18	3	2
1:B:62:ILE:HG22	1:B:67:LEU:HB2	0.54	1.79	9	2
1:A:62:ILE:HG22	1:A:67:LEU:HB2	0.54	1.80	9	1
1:A:115:LEU:HD22	1:A:122:GLU:CB	0.54	2.32	12	4
1:C:15:ILE:HG22	1:C:15:ILE:O	0.54	2.02	17	12
1:A:67:LEU:HD21	1:A:129:ARG:HB2	0.54	1.78	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:73:VAL:HG21	1:C:24:LEU:HD21	0.54	1.79	4	1
1:C:69:ALA:HB3	1:C:99:ASN:HB3	0.54	1.77	18	2
1:A:35:PRO:O	1:A:36:VAL:HG12	0.54	2.03	18	2
1:C:69:ALA:HA	1:C:72:ILE:HD13	0.54	1.79	8	1
1:B:121:LEU:C	1:B:121:LEU:HD22	0.54	2.22	13	1
1:B:27:LEU:HD23	1:B:28:VAL:N	0.54	2.18	3	2
1:C:79:VAL:HG12	1:C:121:LEU:HD22	0.54	1.77	11	2
1:B:115:LEU:HD22	1:B:122:GLU:CB	0.54	2.32	12	3
1:C:72:ILE:HG23	1:C:126:ILE:O	0.54	2.02	2	9
1:B:75:THR:HG23	1:B:105:PRO:HB2	0.54	1.78	16	1
1:B:33:GLN:CB	1:B:58:VAL:HG22	0.54	2.33	3	3
1:C:47:ILE:HG13	1:C:121:LEU:HD11	0.54	1.79	10	1
1:B:23:ASP:CA	1:B:28:VAL:HG12	0.54	2.32	13	1
1:A:5:ILE:HD12	1:A:22:VAL:HG12	0.54	1.80	12	1
1:C:27:LEU:CD2	1:C:128:VAL:HG12	0.54	2.33	6	2
1:A:11:ALA:HB2	1:A:61:ILE:HG12	0.54	1.77	6	7
1:C:5:ILE:HD12	1:C:22:VAL:HG12	0.54	1.78	12	1
1:C:74:LYS:O	1:C:75:THR:HG23	0.54	2.02	12	1
1:A:43:VAL:HG23	1:A:50:GLN:HG3	0.54	1.80	17	1
1:C:75:THR:HG23	1:C:105:PRO:CB	0.54	2.33	16	2
1:A:115:LEU:CD2	1:C:110:VAL:HG12	0.54	2.32	5	1
1:B:43:VAL:HG13	1:B:43:VAL:O	0.54	2.02	14	4
1:C:23:ASP:CA	1:C:28:VAL:HG12	0.54	2.32	13	1
1:B:34:ILE:HG23	1:B:119:VAL:HG11	0.54	1.78	4	1
1:A:104:PHE:O	1:B:19:VAL:HG22	0.54	2.02	10	4
1:B:75:THR:HG22	1:B:125:ALA:HB2	0.54	1.79	10	2
1:C:62:ILE:HG22	1:C:67:LEU:HB2	0.54	1.79	9	2
1:B:43:VAL:HG11	1:B:119:VAL:HA	0.54	1.79	10	1
1:C:43:VAL:HG23	1:C:50:GLN:HG3	0.53	1.80	17	1
1:A:75:THR:HG23	1:A:105:PRO:CB	0.53	2.33	16	2
1:C:78:PHE:HB2	1:C:115:LEU:HD21	0.53	1.80	4	4
1:C:75:THR:HG22	1:C:125:ALA:HB2	0.53	1.79	10	2
1:A:75:THR:HG22	1:A:125:ALA:HB2	0.53	1.80	9	2
1:A:72:ILE:HG22	1:A:74:LYS:O	0.53	2.02	19	1
1:A:72:ILE:HG23	1:A:126:ILE:O	0.53	2.03	2	10
1:B:35:PRO:CG	1:B:43:VAL:HG23	0.53	2.33	5	2
1:B:5:ILE:CD1	1:B:19:VAL:HG21	0.53	2.31	12	1
1:A:75:THR:HG23	1:A:125:ALA:HB2	0.53	1.81	2	6
1:B:47:ILE:HD13	1:B:84:ASP:OD2	0.53	2.03	16	1
1:B:43:VAL:HG21	1:B:119:VAL:HG23	0.53	1.77	10	1
1:B:24:LEU:CD1	1:B:29:LEU:HD21	0.53	2.33	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:72:ILE:HG22	1:C:74:LYS:O	0.53	2.02	19	1
1:C:14:ALA:HA	1:C:18:TYR:CE1	0.53	2.39	18	4
1:B:75:THR:HG23	1:B:105:PRO:CB	0.53	2.34	5	2
1:B:35:PRO:HG2	1:B:43:VAL:HG23	0.53	1.80	5	1
1:B:69:ALA:HA	1:B:72:ILE:HD13	0.53	1.80	8	1
1:B:27:LEU:HD21	1:C:24:LEU:HD22	0.53	1.81	4	1
1:A:78:PHE:HB2	1:A:115:LEU:HD21	0.53	1.81	14	4
1:A:24:LEU:CD1	1:A:29:LEU:HD21	0.53	2.34	10	1
1:A:5:ILE:CD1	1:A:19:VAL:HG21	0.53	2.31	12	1
1:C:34:ILE:HG22	1:C:119:VAL:HG21	0.53	1.81	12	1
1:B:35:PRO:O	1:B:36:VAL:HG12	0.53	2.03	18	2
1:C:24:LEU:CD1	1:C:29:LEU:HD21	0.53	2.34	10	1
1:A:43:VAL:HG21	1:A:120:GLY:H	0.53	1.64	14	6
1:B:6:ILE:HD12	1:B:21:ALA:CB	0.53	2.34	12	4
1:C:35:PRO:O	1:C:36:VAL:HG12	0.53	2.03	18	2
1:A:67:LEU:HD13	1:A:71:ASP:OD2	0.53	2.04	3	2
1:B:5:ILE:HD12	1:B:22:VAL:HG12	0.53	1.80	12	1
1:C:116:PRO:O	1:C:119:VAL:HG22	0.53	2.04	4	13
1:A:36:VAL:HG21	1:A:117:LYS:HD2	0.53	1.79	7	1
1:A:69:ALA:HA	1:A:72:ILE:HD13	0.53	1.78	8	1
1:A:116:PRO:O	1:A:119:VAL:HG22	0.52	2.04	4	13
1:B:73:VAL:HG11	1:C:24:LEU:CD2	0.52	2.34	5	1
1:B:92:TYR:CE1	1:B:96:PHE:CE1	0.52	2.97	6	4
1:A:92:TYR:CE1	1:A:96:PHE:CE1	0.52	2.97	6	4
1:C:95:PHE:CZ	1:C:96:PHE:CE1	0.52	2.97	16	11
1:A:14:ALA:HA	1:A:18:TYR:CE1	0.52	2.39	18	4
1:B:75:THR:HG23	1:B:125:ALA:HB2	0.52	1.80	2	6
1:A:82:LEU:HD11	1:B:115:LEU:C	0.52	2.25	10	3
1:A:35:PRO:HG2	1:A:43:VAL:HG23	0.52	1.81	5	1
1:C:92:TYR:CE1	1:C:96:PHE:CE1	0.52	2.97	6	4
1:B:95:PHE:CZ	1:B:96:PHE:CE1	0.52	2.97	16	11
1:A:95:PHE:CZ	1:A:96:PHE:CE1	0.52	2.97	16	11
1:A:35:PRO:CG	1:A:43:VAL:HG23	0.52	2.35	5	2
1:A:47:ILE:HD13	1:A:84:ASP:OD2	0.52	2.04	16	1
1:B:47:ILE:HG13	1:B:121:LEU:HD11	0.52	1.79	10	1
1:B:43:VAL:HG23	1:B:50:GLN:HG3	0.52	1.80	17	1
1:B:110:VAL:HG12	1:C:115:LEU:CD2	0.52	2.34	5	1
1:A:15:ILE:N	1:A:15:ILE:HD12	0.52	2.20	2	2
1:B:43:VAL:HG21	1:B:120:GLY:H	0.52	1.65	14	5
1:C:67:LEU:HD13	1:C:71:ASP:OD2	0.52	2.04	3	2
1:A:6:ILE:HD12	1:A:21:ALA:CB	0.52	2.34	12	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:34:ILE:HG23	1:C:36:VAL:CG2	0.52	2.32	19	1
1:A:75:THR:HG22	1:A:105:PRO:HB2	0.52	1.81	19	1
1:C:6:ILE:HD12	1:C:21:ALA:HB3	0.52	1.82	12	4
1:C:35:PRO:CG	1:C:43:VAL:HG23	0.52	2.34	5	2
1:A:73:VAL:HG13	1:A:128:VAL:HG22	0.52	1.82	7	7
1:A:27:LEU:CD2	1:A:128:VAL:HG12	0.52	2.34	6	2
1:B:27:LEU:CD2	1:B:128:VAL:HG12	0.52	2.34	5	2
1:C:75:THR:HG23	1:C:125:ALA:HB2	0.52	1.80	2	6
1:B:116:PRO:O	1:B:119:VAL:HG22	0.51	2.04	4	14
1:B:73:VAL:CG1	1:B:128:VAL:HG22	0.51	2.35	14	3
1:C:73:VAL:CG1	1:C:128:VAL:HG22	0.51	2.35	14	3
1:B:75:THR:HG21	1:B:107:ARG:NH2	0.51	2.20	7	1
1:B:67:LEU:HD13	1:B:71:ASP:OD2	0.51	2.04	3	2
1:C:75:THR:HG22	1:C:105:PRO:HB2	0.51	1.81	19	1
1:B:14:ALA:HA	1:B:18:TYR:CE1	0.51	2.39	18	4
1:C:15:ILE:HD12	1:C:15:ILE:N	0.51	2.20	2	2
1:A:73:VAL:CG1	1:A:128:VAL:HG22	0.51	2.35	14	3
1:B:78:PHE:HB2	1:B:115:LEU:HD21	0.51	1.81	14	4
1:A:74:LYS:O	1:A:125:ALA:HB1	0.51	2.05	5	6
1:A:75:THR:HG21	1:A:107:ARG:NH2	0.51	2.20	7	1
1:A:69:ALA:CB	1:A:101:HIS:CE1	0.51	2.93	10	1
1:C:43:VAL:HG21	1:C:120:GLY:H	0.51	1.65	14	6
1:B:73:VAL:HG13	1:B:128:VAL:HG22	0.51	1.82	14	7
1:C:35:PRO:HG2	1:C:43:VAL:HG23	0.51	1.81	5	1
1:A:122:GLU:C	1:A:123:ILE:HD12	0.51	2.26	3	3
1:C:47:ILE:O	1:C:51:ALA:HB2	0.51	2.06	3	2
1:A:112:VAL:HG21	1:A:115:LEU:HD11	0.51	1.83	10	1
1:A:24:LEU:HD13	1:C:27:LEU:HD21	0.51	1.81	18	1
1:C:5:ILE:HG23	1:C:19:VAL:HG21	0.51	1.83	5	2
1:A:24:LEU:HD21	1:C:73:VAL:HG11	0.51	1.82	13	1
1:B:14:ALA:C	1:B:15:ILE:HD12	0.51	2.26	2	1
1:A:14:ALA:C	1:A:15:ILE:HD12	0.51	2.26	2	1
1:B:82:LEU:HD11	1:C:115:LEU:C	0.51	2.26	7	2
1:B:74:LYS:O	1:B:125:ALA:HB1	0.51	2.06	5	6
1:A:47:ILE:HD13	1:A:50:GLN:NE2	0.51	2.21	2	3
1:B:4:GLN:OE1	1:B:24:LEU:HD23	0.51	2.05	14	3
1:B:67:LEU:HD12	1:B:129:ARG:HG3	0.51	1.83	13	1
1:A:76:THR:O	1:A:77:VAL:HG13	0.51	2.06	18	1
1:C:73:VAL:HG13	1:C:128:VAL:HG22	0.51	1.82	14	7
1:C:14:ALA:C	1:C:15:ILE:HD12	0.51	2.26	2	1
1:C:123:ILE:HD12	1:C:123:ILE:N	0.51	2.21	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:47:ILE:O	1:B:51:ALA:HB2	0.51	2.06	3	2
1:B:75:THR:HG22	1:B:105:PRO:HB2	0.51	1.81	19	1
1:B:3:THR:HG23	1:B:24:LEU:HD23	0.50	1.84	12	1
1:C:74:LYS:O	1:C:125:ALA:HB1	0.50	2.05	5	6
1:A:99:ASN:O	1:A:100:ASN:ND2	0.50	2.44	8	1
1:C:76:THR:O	1:C:77:VAL:HG13	0.50	2.06	18	1
1:B:67:LEU:HD21	1:B:129:ARG:CG	0.50	2.36	9	1
1:A:34:ILE:HG22	1:A:119:VAL:HG21	0.50	1.83	12	1
1:A:5:ILE:HG23	1:A:19:VAL:HG21	0.50	1.83	5	2
1:B:15:ILE:N	1:B:15:ILE:HD12	0.50	2.20	2	1
1:C:47:ILE:HD13	1:C:50:GLN:NE2	0.50	2.21	2	3
1:A:4:GLN:OE1	1:A:24:LEU:HD23	0.50	2.05	14	3
1:C:122:GLU:C	1:C:123:ILE:HD12	0.50	2.26	3	3
1:B:76:THR:O	1:B:77:VAL:HG13	0.50	2.06	18	1
1:B:5:ILE:HG23	1:B:19:VAL:HG21	0.50	1.83	5	2
1:B:47:ILE:HD13	1:B:50:GLN:NE2	0.50	2.21	2	3
1:A:92:TYR:CD1	1:A:92:TYR:C	0.50	2.85	7	1
1:C:92:TYR:CZ	1:C:96:PHE:CE1	0.50	2.99	6	3
1:A:73:VAL:HB	1:B:22:VAL:HG21	0.50	1.82	7	3
1:C:95:PHE:CD1	1:C:95:PHE:C	0.50	2.85	13	8
1:B:12:PRO:O	1:B:13:ALA:HB3	0.50	2.07	16	9
1:C:75:THR:HG21	1:C:107:ARG:NH2	0.50	2.20	7	1
1:A:33:GLN:HB2	1:A:58:VAL:HG22	0.50	1.83	8	1
1:C:99:ASN:O	1:C:100:ASN:ND2	0.50	2.44	8	1
1:B:122:GLU:C	1:B:123:ILE:HD12	0.50	2.26	3	3
1:A:92:TYR:CZ	1:A:96:PHE:CE1	0.50	2.99	6	3
1:A:47:ILE:O	1:A:51:ALA:HB2	0.50	2.06	3	2
1:C:4:GLN:OE1	1:C:24:LEU:HD23	0.50	2.05	14	3
1:A:33:GLN:O	1:A:34:ILE:HG23	0.50	2.07	16	2
1:B:62:ILE:HD12	1:B:127:ALA:HB2	0.50	1.84	18	1
1:B:99:ASN:CB	1:B:101:HIS:CE1	0.50	2.95	14	9
1:C:70:ALA:CB	1:C:101:HIS:CD2	0.50	2.90	5	6
1:B:95:PHE:C	1:B:95:PHE:CD1	0.50	2.85	13	5
1:A:73:VAL:HG11	1:B:24:LEU:CD2	0.50	2.37	5	1
1:A:12:PRO:O	1:A:13:ALA:HB3	0.50	2.07	3	9
1:C:12:PRO:O	1:C:13:ALA:HB3	0.50	2.07	16	9
1:B:92:TYR:CD1	1:B:92:TYR:C	0.50	2.85	7	1
1:C:112:VAL:HG21	1:C:115:LEU:HD11	0.50	1.83	10	1
1:A:99:ASN:CB	1:A:101:HIS:CE1	0.50	2.95	14	9
1:B:123:ILE:N	1:B:123:ILE:HD12	0.50	2.21	3	3
1:C:67:LEU:HD12	1:C:129:ARG:HG3	0.50	1.83	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:34:ILE:HG23	1:B:36:VAL:CG2	0.50	2.32	19	1
1:A:34:ILE:HG23	1:A:36:VAL:CG2	0.50	2.32	19	1
1:A:95:PHE:C	1:A:95:PHE:CD1	0.49	2.85	13	7
1:B:95:PHE:CE2	1:B:96:PHE:CD1	0.49	3.00	5	6
1:C:33:GLN:O	1:C:34:ILE:HG23	0.49	2.07	11	2
1:B:128:VAL:CG1	1:C:24:LEU:HD11	0.49	2.37	16	2
1:B:92:TYR:CZ	1:B:96:PHE:CE1	0.49	2.99	6	3
1:B:6:ILE:HD11	1:B:23:ASP:HB2	0.49	1.83	16	3
1:C:58:VAL:HA	1:C:61:ILE:HD12	0.49	1.84	11	1
1:A:123:ILE:HD12	1:A:123:ILE:N	0.49	2.21	15	2
1:B:33:GLN:HB2	1:B:58:VAL:HG22	0.49	1.82	8	1
1:A:123:ILE:N	1:A:123:ILE:HD12	0.49	2.21	3	1
1:B:95:PHE:CE2	1:B:96:PHE:CE2	0.49	3.01	3	2
1:A:27:LEU:CG	1:A:128:VAL:HG12	0.49	2.37	5	1
1:B:112:VAL:HG21	1:B:115:LEU:HD11	0.49	1.83	10	1
1:C:95:PHE:CE2	1:C:96:PHE:CE2	0.49	3.01	3	2
1:A:67:LEU:HD21	1:A:129:ARG:CG	0.49	2.36	9	1
1:C:99:ASN:CB	1:C:101:HIS:CE1	0.49	2.95	14	8
1:A:79:VAL:HG11	1:A:85:PHE:CD2	0.49	2.43	9	1
1:C:3:THR:HG23	1:C:24:LEU:CD2	0.49	2.38	12	3
1:B:6:ILE:HD12	1:B:21:ALA:HB3	0.49	1.85	3	4
1:A:95:PHE:CE2	1:A:96:PHE:CD1	0.49	3.00	5	6
1:A:95:PHE:CE2	1:A:96:PHE:CE1	0.49	3.01	19	6
1:C:95:PHE:CE2	1:C:96:PHE:CD1	0.49	3.00	5	6
1:A:6:ILE:HD11	1:A:23:ASP:HB2	0.49	1.84	16	3
1:C:6:ILE:HD11	1:C:23:ASP:HB2	0.49	1.84	16	3
1:A:128:VAL:O	1:A:128:VAL:HG23	0.49	2.08	3	3
1:A:29:LEU:CD1	1:A:126:ILE:HG23	0.49	2.37	10	1
1:B:77:VAL:HG12	1:B:123:ILE:HG12	0.49	1.85	18	1
1:A:95:PHE:CD1	1:A:95:PHE:C	0.49	2.86	3	10
1:C:62:ILE:CD1	1:C:72:ILE:HD11	0.49	2.38	16	2
1:B:33:GLN:O	1:B:34:ILE:HG23	0.49	2.07	11	2
1:A:51:ALA:HB1	1:A:88:VAL:HG22	0.49	1.84	7	1
1:C:69:ALA:CB	1:C:101:HIS:CE1	0.49	2.93	10	1
1:A:6:ILE:HD12	1:A:21:ALA:HB3	0.49	1.85	3	4
1:A:24:LEU:HD11	1:C:128:VAL:CG1	0.49	2.38	16	2
1:C:92:TYR:CD1	1:C:92:TYR:C	0.49	2.85	7	1
1:B:99:ASN:O	1:B:100:ASN:ND2	0.49	2.44	8	1
1:B:128:VAL:HG11	1:C:24:LEU:CD2	0.49	2.32	13	1
1:A:67:LEU:HD12	1:A:129:ARG:HG3	0.49	1.83	13	1
1:B:50:GLN:HG3	1:B:121:LEU:HD21	0.49	1.85	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:27:LEU:CG	1:C:128:VAL:HG12	0.49	2.37	5	1
1:C:29:LEU:CD1	1:C:126:ILE:HG23	0.49	2.38	10	1
1:A:24:LEU:CD2	1:C:128:VAL:HG11	0.49	2.33	13	1
1:A:95:PHE:CE2	1:A:96:PHE:CE2	0.49	3.01	3	2
1:A:62:ILE:HD12	1:A:127:ALA:HB2	0.49	1.84	18	1
1:C:67:LEU:HD21	1:C:129:ARG:CG	0.49	2.37	9	1
1:B:79:VAL:HG11	1:B:85:PHE:CD2	0.49	2.43	9	1
1:B:95:PHE:CE2	1:B:96:PHE:CE1	0.48	3.01	5	6
1:C:95:PHE:CE2	1:C:96:PHE:CE1	0.48	3.01	5	6
1:C:103:ASN:O	1:C:104:PHE:HB2	0.48	2.08	9	2
1:C:117:LYS:HB3	1:C:119:VAL:HG13	0.48	1.85	13	2
1:B:51:ALA:HB1	1:B:88:VAL:HG13	0.48	1.85	8	1
1:B:128:VAL:O	1:B:128:VAL:HG23	0.48	2.08	3	2
1:B:59:LYS:CD	1:B:69:ALA:HB2	0.48	2.38	10	1
1:B:128:VAL:HG23	1:B:128:VAL:O	0.48	2.08	15	1
1:C:79:VAL:HG11	1:C:85:PHE:CD2	0.48	2.43	9	1
1:A:22:VAL:HG23	1:A:29:LEU:HG	0.48	1.85	4	1
1:C:99:ASN:O	1:C:100:ASN:HB2	0.48	2.09	16	4
1:A:99:ASN:O	1:A:100:ASN:HB2	0.48	2.09	16	3
1:A:33:GLN:OE1	1:A:61:ILE:HD11	0.48	2.08	16	1
1:B:33:GLN:OE1	1:B:61:ILE:HD11	0.48	2.08	16	1
1:A:82:LEU:HD12	1:B:114:ARG:HB3	0.48	1.85	3	4
1:C:35:PRO:HB2	1:C:43:VAL:HG23	0.48	1.86	19	1
1:C:62:ILE:HD12	1:C:127:ALA:HB2	0.48	1.84	18	1
1:A:73:VAL:HG11	1:A:128:VAL:CG1	0.48	2.37	9	7
1:B:28:VAL:C	1:B:29:LEU:HD12	0.48	2.29	13	5
1:B:4:GLN:HA	1:B:23:ASP:N	0.48	2.24	14	4
1:C:77:VAL:HG13	1:C:123:ILE:HD13	0.48	1.85	8	2
1:B:29:LEU:CD1	1:B:126:ILE:HG23	0.48	2.38	10	1
1:B:74:LYS:HE2	1:C:29:LEU:HD22	0.48	1.86	3	2
1:B:95:PHE:CD1	1:B:95:PHE:C	0.48	2.86	3	13
1:B:34:ILE:HG22	1:B:119:VAL:HG21	0.48	1.84	12	1
1:A:62:ILE:CD1	1:A:72:ILE:HD11	0.48	2.38	16	2
1:A:115:LEU:C	1:C:82:LEU:HD11	0.48	2.28	10	3
1:C:128:VAL:HG22	1:C:129:ARG:N	0.48	2.24	2	1
1:C:73:VAL:HG13	1:C:128:VAL:HG12	0.48	1.86	2	1
1:A:115:LEU:HB2	1:A:119:VAL:HG23	0.48	1.85	8	2
1:C:115:LEU:HB2	1:C:119:VAL:HG23	0.48	1.85	8	2
1:C:33:GLN:HB2	1:C:58:VAL:HG22	0.48	1.86	8	1
1:A:59:LYS:CD	1:A:69:ALA:HB2	0.48	2.38	10	1
1:B:67:LEU:HD21	1:B:71:ASP:CB	0.48	2.39	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:75:THR:HG21	1:B:92:TYR:HH	0.48	1.68	6	1
1:A:123:ILE:HD13	1:A:123:ILE:N	0.48	2.24	2	1
1:A:128:VAL:CG1	1:B:24:LEU:HD11	0.48	2.38	16	2
1:B:51:ALA:HB1	1:B:88:VAL:HG22	0.48	1.85	7	1
1:A:77:VAL:HG13	1:A:123:ILE:HD13	0.48	1.85	8	2
1:C:128:VAL:O	1:C:128:VAL:HG23	0.48	2.08	3	3
1:C:67:LEU:HD11	1:C:129:ARG:CB	0.48	2.39	11	1
1:A:22:VAL:HG23	1:A:29:LEU:CG	0.48	2.39	4	1
1:C:22:VAL:HG23	1:C:29:LEU:CG	0.48	2.39	4	1
1:A:77:VAL:HG12	1:A:123:ILE:HG12	0.48	1.84	18	1
1:A:28:VAL:C	1:A:29:LEU:HD12	0.48	2.29	13	5
1:C:28:VAL:C	1:C:29:LEU:HD12	0.48	2.29	13	5
1:A:128:VAL:HG22	1:A:129:ARG:N	0.48	2.24	2	1
1:C:50:GLN:HG3	1:C:121:LEU:HD21	0.48	1.84	2	2
1:C:33:GLN:OE1	1:C:61:ILE:HD11	0.48	2.09	16	1
1:C:126:ILE:N	1:C:126:ILE:HD13	0.48	2.24	3	2
1:A:74:LYS:HE2	1:B:29:LEU:HD22	0.48	1.85	3	2
1:A:14:ALA:HB3	1:A:19:VAL:HA	0.48	1.85	19	1
1:A:35:PRO:HB2	1:A:43:VAL:HG23	0.48	1.86	19	1
1:C:126:ILE:HD13	1:C:126:ILE:N	0.48	2.24	15	1
1:A:103:ASN:O	1:A:104:PHE:HB2	0.48	2.08	9	2
1:A:117:LYS:HB3	1:A:119:VAL:HG13	0.48	1.85	13	2
1:B:89:ASN:HA	1:B:92:TYR:CE2	0.48	2.44	7	1
1:C:120:GLY:O	1:C:121:LEU:HD12	0.48	2.09	19	1
1:A:3:THR:HG23	1:A:24:LEU:HD23	0.48	1.85	12	1
1:B:27:LEU:CG	1:B:128:VAL:HG12	0.48	2.37	5	1
1:A:4:GLN:NE2	1:C:73:VAL:HB	0.48	2.24	9	4
1:A:5:ILE:HD12	1:A:19:VAL:HG11	0.48	1.85	13	1
1:B:75:THR:O	1:B:75:THR:HG23	0.48	2.09	3	2
1:B:126:ILE:N	1:B:126:ILE:HD13	0.48	2.24	3	2
1:C:75:THR:HG21	1:C:92:TYR:HH	0.48	1.68	6	1
1:B:22:VAL:HG23	1:B:29:LEU:CG	0.48	2.39	4	1
1:C:95:PHE:C	1:C:95:PHE:CD1	0.48	2.86	3	10
1:C:4:GLN:HA	1:C:23:ASP:N	0.48	2.24	14	5
1:A:4:GLN:HA	1:A:23:ASP:N	0.48	2.24	14	5
1:B:70:ALA:HB2	1:B:100:ASN:OD1	0.48	2.09	13	1
1:B:34:ILE:O	1:B:35:PRO:O	0.48	2.32	3	2
1:B:99:ASN:O	1:B:100:ASN:HB2	0.47	2.09	16	3
1:C:123:ILE:N	1:C:123:ILE:HD13	0.47	2.24	2	1
1:B:117:LYS:HB3	1:B:119:VAL:HG13	0.47	1.85	13	2
1:B:73:VAL:HG11	1:C:24:LEU:HD21	0.47	1.86	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ILE:O	1:A:35:PRO:O	0.47	2.32	3	2
1:B:128:VAL:HG22	1:B:129:ARG:N	0.47	2.24	2	1
1:C:89:ASN:HA	1:C:92:TYR:CE2	0.47	2.44	7	1
1:C:34:ILE:O	1:C:35:PRO:O	0.47	2.32	3	2
1:B:103:ASN:O	1:B:104:PHE:HB2	0.47	2.08	9	2
1:C:67:LEU:HD21	1:C:128:VAL:O	0.47	2.09	14	3
1:A:67:LEU:HD21	1:A:71:ASP:CB	0.47	2.39	13	1
1:B:14:ALA:HB3	1:B:19:VAL:HA	0.47	1.85	19	1
1:A:6:ILE:CG2	1:A:61:ILE:HG22	0.47	2.39	9	1
1:B:123:ILE:HD13	1:B:123:ILE:N	0.47	2.24	2	1
1:B:73:VAL:HB	1:C:4:GLN:NE2	0.47	2.25	9	4
1:C:24:LEU:HD11	1:C:29:LEU:HD21	0.47	1.86	10	1
1:B:69:ALA:CB	1:B:101:HIS:CE1	0.47	2.93	10	1
1:C:92:TYR:CZ	1:C:96:PHE:CZ	0.47	3.03	10	2
1:A:73:VAL:HG11	1:B:24:LEU:HD21	0.47	1.86	13	1
1:C:72:ILE:CD1	1:C:72:ILE:N	0.47	2.78	13	1
1:C:115:LEU:HD22	1:C:122:GLU:OE1	0.47	2.09	6	1
1:B:58:VAL:HA	1:B:61:ILE:HD12	0.47	1.85	11	1
1:B:6:ILE:CG2	1:B:61:ILE:HG22	0.47	2.39	9	1
1:C:96:PHE:CD2	1:C:101:HIS:HB2	0.47	2.45	10	6
1:B:62:ILE:CD1	1:B:72:ILE:HD11	0.47	2.39	16	1
1:A:89:ASN:HA	1:A:92:TYR:CE2	0.47	2.44	7	1
1:B:77:VAL:HG13	1:B:123:ILE:HD13	0.47	1.86	4	2
1:C:59:LYS:CD	1:C:69:ALA:HB2	0.47	2.38	10	1
1:A:96:PHE:CZ	1:A:105:PRO:CD	0.47	2.98	18	1
1:C:29:LEU:CG	1:C:126:ILE:HG23	0.47	2.37	5	1
1:C:92:TYR:CZ	1:C:107:ARG:CZ	0.47	2.98	7	1
1:C:69:ALA:O	1:C:101:HIS:CD2	0.47	2.68	19	2
1:C:29:LEU:HD22	1:C:29:LEU:H	0.47	1.69	10	1
1:C:70:ALA:HB2	1:C:100:ASN:OD1	0.47	2.09	13	1
1:B:22:VAL:HG23	1:B:29:LEU:HG	0.47	1.85	4	1
1:C:75:THR:HG23	1:C:75:THR:O	0.47	2.09	15	1
1:A:50:GLN:HG3	1:A:121:LEU:HD21	0.47	1.87	2	2
1:A:114:ARG:HB3	1:C:82:LEU:HD12	0.47	1.85	3	6
1:B:95:PHE:CZ	1:B:96:PHE:CD1	0.47	3.03	6	3
1:B:92:TYR:CZ	1:B:96:PHE:CZ	0.47	3.02	10	2
1:A:92:TYR:CZ	1:A:96:PHE:CZ	0.47	3.02	10	2
1:B:121:LEU:HD12	1:B:121:LEU:C	0.47	2.31	3	2
1:C:14:ALA:HB3	1:C:19:VAL:HA	0.47	1.85	19	1
1:B:120:GLY:O	1:B:121:LEU:HD12	0.47	2.09	19	1
1:C:72:ILE:CD1	1:C:127:ALA:HB2	0.47	2.27	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:99:ASN:HB3	1:C:101:HIS:NE2	0.47	2.25	14	5
1:A:95:PHE:CZ	1:A:96:PHE:CD1	0.47	3.03	6	3
1:B:92:TYR:CZ	1:B:107:ARG:CZ	0.47	2.98	7	1
1:A:51:ALA:HB1	1:A:88:VAL:HG13	0.47	1.86	8	1
1:C:67:LEU:HD21	1:C:71:ASP:CB	0.47	2.39	13	1
1:C:73:VAL:HG11	1:C:128:VAL:CG1	0.47	2.36	9	7
1:A:96:PHE:CD2	1:A:101:HIS:HB2	0.47	2.45	10	6
1:B:24:LEU:HD11	1:B:29:LEU:HD21	0.47	1.86	10	1
1:B:82:LEU:HD12	1:C:114:ARG:HB3	0.47	1.86	3	3
1:A:126:ILE:HD13	1:A:126:ILE:N	0.47	2.24	3	2
1:A:120:GLY:O	1:A:121:LEU:HD12	0.47	2.09	19	1
1:C:22:VAL:HG23	1:C:29:LEU:HG	0.47	1.85	4	1
1:C:77:VAL:HG12	1:C:123:ILE:HG12	0.47	1.85	18	1
1:A:126:ILE:N	1:A:126:ILE:HD13	0.47	2.24	15	1
1:C:6:ILE:CG2	1:C:61:ILE:HG22	0.47	2.39	9	1
1:B:29:LEU:H	1:B:29:LEU:HD22	0.47	1.69	10	1
1:A:24:LEU:HD11	1:A:29:LEU:HD21	0.47	1.86	10	1
1:A:121:LEU:HD12	1:A:121:LEU:C	0.47	2.31	3	1
1:B:109:CYS:O	1:B:110:VAL:HG13	0.47	2.10	19	3
1:A:121:LEU:C	1:A:121:LEU:HD12	0.47	2.31	15	1
1:A:70:ALA:CB	1:A:101:HIS:CD2	0.46	2.93	17	7
1:A:73:VAL:HG13	1:A:128:VAL:HG12	0.46	1.86	2	1
1:B:69:ALA:O	1:B:101:HIS:CD2	0.46	2.68	19	2
1:A:72:ILE:CD1	1:A:72:ILE:N	0.46	2.78	13	1
1:A:92:TYR:CZ	1:A:107:ARG:CZ	0.46	2.98	7	1
1:A:58:VAL:HG21	1:A:123:ILE:CB	0.46	2.41	13	2
1:A:70:ALA:HB2	1:A:100:ASN:OD1	0.46	2.09	13	1
1:C:109:CYS:O	1:C:110:VAL:HG13	0.46	2.10	19	3
1:A:5:ILE:N	1:A:5:ILE:CD1	0.46	2.78	9	1
1:C:6:ILE:HG21	1:C:61:ILE:HG22	0.46	1.86	12	2
1:B:99:ASN:HB3	1:B:101:HIS:NE2	0.46	2.25	14	5
1:B:67:LEU:HD21	1:B:128:VAL:O	0.46	2.10	14	3
1:A:92:TYR:CZ	1:A:107:ARG:NE	0.46	2.83	7	1
1:A:88:VAL:HG12	1:A:92:TYR:HE1	0.46	1.70	8	1
1:A:24:LEU:CD1	1:A:29:LEU:HD11	0.46	2.41	11	1
1:A:58:VAL:HA	1:A:61:ILE:HD12	0.46	1.86	11	1
1:B:96:PHE:CZ	1:B:105:PRO:CD	0.46	2.99	18	1
1:A:67:LEU:HD11	1:A:129:ARG:CB	0.46	2.39	11	1
1:C:96:PHE:CZ	1:C:105:PRO:CD	0.46	2.98	18	1
1:A:3:THR:HG23	1:A:24:LEU:CD2	0.46	2.41	3	3
1:A:67:LEU:HD21	1:A:128:VAL:O	0.46	2.10	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:ALA:HA	1:A:101:HIS:CG	0.46	2.46	8	3
1:A:99:ASN:CB	1:A:101:HIS:NE2	0.46	2.79	13	3
1:A:121:LEU:CD1	1:A:121:LEU:N	0.46	2.78	13	1
1:C:121:LEU:HD12	1:C:121:LEU:C	0.46	2.30	3	1
1:C:121:LEU:C	1:C:121:LEU:HD12	0.46	2.30	15	1
1:C:4:GLN:O	1:C:5:ILE:HG22	0.46	2.11	17	1
1:C:36:VAL:HG22	1:C:36:VAL:O	0.46	2.11	2	2
1:A:121:LEU:O	1:A:121:LEU:HD22	0.46	2.10	7	2
1:B:92:TYR:CZ	1:B:107:ARG:NE	0.46	2.83	7	1
1:A:69:ALA:O	1:A:101:HIS:CD2	0.46	2.68	19	2
1:C:88:VAL:HG12	1:C:92:TYR:HE1	0.46	1.69	8	1
1:C:95:PHE:CZ	1:C:96:PHE:CD1	0.46	3.03	6	2
1:B:119:VAL:HG13	1:B:120:GLY:N	0.46	2.26	10	1
1:B:99:ASN:CB	1:B:101:HIS:NE2	0.46	2.79	13	3
1:B:72:ILE:CD1	1:B:72:ILE:N	0.46	2.78	13	1
1:A:29:LEU:HD22	1:C:74:LYS:HE2	0.46	1.87	3	2
1:B:24:LEU:CD1	1:B:29:LEU:HD11	0.46	2.41	11	1
1:B:22:VAL:CG2	1:B:29:LEU:HD13	0.46	2.40	18	1
1:B:8:THR:HG21	1:B:61:ILE:HG12	0.46	1.88	17	1
1:B:67:LEU:HD22	1:B:71:ASP:CB	0.46	2.41	18	4
1:B:21:ALA:HB2	1:B:61:ILE:HG21	0.46	1.87	14	3
1:B:121:LEU:HD22	1:B:121:LEU:O	0.46	2.10	7	1
1:B:115:LEU:HB2	1:B:119:VAL:HG23	0.46	1.85	8	2
1:A:29:LEU:HD22	1:A:29:LEU:H	0.46	1.69	10	1
1:C:24:LEU:CD1	1:C:29:LEU:HD11	0.46	2.41	11	1
1:B:5:ILE:N	1:B:5:ILE:CD1	0.46	2.79	9	1
1:B:36:VAL:HG22	1:B:36:VAL:O	0.46	2.11	2	1
1:A:55:LEU:HD22	1:A:92:TYR:HB2	0.46	1.88	7	1
1:C:70:ALA:HA	1:C:101:HIS:CG	0.46	2.46	8	3
1:C:92:TYR:O	1:C:95:PHE:CD2	0.46	2.69	3	4
1:B:35:PRO:HB2	1:B:43:VAL:HG23	0.46	1.86	19	1
1:B:22:VAL:HG23	1:B:29:LEU:CD1	0.46	2.41	18	1
1:A:5:ILE:HG21	1:A:19:VAL:CG1	0.46	2.41	18	1
1:A:96:PHE:CZ	1:A:105:PRO:CG	0.46	2.99	9	1
1:A:103:ASN:HD22	1:B:5:ILE:HD13	0.46	1.69	12	1
1:A:13:ALA:HB3	1:A:20:GLN:HE21	0.46	1.71	12	1
1:A:8:THR:HG21	1:A:61:ILE:HG12	0.46	1.88	17	1
1:B:96:PHE:CD2	1:B:101:HIS:HB2	0.46	2.45	10	6
1:B:58:VAL:HG21	1:B:123:ILE:HB	0.46	1.88	8	1
1:A:35:PRO:HD2	1:A:119:VAL:HG21	0.46	1.87	10	1
1:A:128:VAL:HG11	1:B:24:LEU:CD2	0.46	2.35	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:29:LEU:CD1	1:C:126:ILE:HD12	0.46	2.41	6	1
1:A:75:THR:HG21	1:A:92:TYR:HH	0.46	1.69	6	1
1:B:73:VAL:HG11	1:B:128:VAL:CG1	0.46	2.40	17	7
1:C:5:ILE:CD1	1:C:19:VAL:HG11	0.46	2.41	2	1
1:C:21:ALA:HB2	1:C:61:ILE:HG21	0.46	1.87	14	3
1:C:121:LEU:O	1:C:121:LEU:HD22	0.46	2.10	7	1
1:C:35:PRO:CD	1:C:119:VAL:HG21	0.46	2.41	10	1
1:A:115:LEU:HD22	1:A:122:GLU:OE1	0.46	2.11	6	1
1:B:70:ALA:CB	1:B:101:HIS:CD2	0.45	2.90	5	6
1:A:21:ALA:CB	1:A:61:ILE:HG21	0.45	2.41	17	1
1:B:4:GLN:O	1:B:5:ILE:HG22	0.45	2.11	17	1
1:C:92:TYR:CZ	1:C:107:ARG:NE	0.45	2.84	7	1
1:B:58:VAL:HG21	1:B:123:ILE:CB	0.45	2.41	13	2
1:C:121:LEU:N	1:C:121:LEU:CD1	0.45	2.79	13	1
1:C:5:ILE:CD1	1:C:5:ILE:N	0.45	2.79	9	1
1:C:96:PHE:CZ	1:C:105:PRO:CG	0.45	2.99	9	1
1:B:88:VAL:HG12	1:B:92:TYR:HE1	0.45	1.70	8	1
1:B:67:LEU:HD11	1:B:129:ARG:CB	0.45	2.39	11	1
1:A:24:LEU:CD2	1:C:73:VAL:HG11	0.45	2.42	5	1
1:A:67:LEU:HD22	1:A:71:ASP:CB	0.45	2.41	18	4
1:A:99:ASN:HB3	1:A:101:HIS:NE2	0.45	2.25	14	5
1:B:72:ILE:HG21	1:B:75:THR:HG22	0.45	1.88	5	1
1:A:28:VAL:HG22	1:A:67:LEU:HD13	0.45	1.89	2	1
1:B:5:ILE:CD1	1:B:19:VAL:HG11	0.45	2.42	2	1
1:B:11:ALA:CB	1:B:12:PRO:CD	0.45	2.95	16	5
1:C:34:ILE:HD12	1:C:36:VAL:HG21	0.45	1.89	16	1
1:B:92:TYR:O	1:B:95:PHE:CD2	0.45	2.69	3	5
1:B:107:ARG:CB	1:C:18:TYR:CD2	0.45	2.99	18	1
1:B:3:THR:HG23	1:B:24:LEU:CD2	0.45	2.42	3	3
1:C:72:ILE:HG21	1:C:75:THR:HG22	0.45	1.88	5	1
1:C:67:LEU:HD22	1:C:71:ASP:CB	0.45	2.41	18	5
1:B:88:VAL:O	1:B:92:TYR:CD1	0.45	2.70	8	1
1:C:35:PRO:HD2	1:C:119:VAL:HG21	0.45	1.87	10	1
1:A:34:ILE:HD12	1:A:36:VAL:HG22	0.45	1.88	12	1
1:C:13:ALA:HB3	1:C:20:GLN:HE21	0.45	1.71	12	1
1:C:21:ALA:CB	1:C:61:ILE:HG21	0.45	2.41	17	1
1:C:99:ASN:CB	1:C:101:HIS:NE2	0.45	2.79	13	3
1:B:121:LEU:CD1	1:B:121:LEU:N	0.45	2.79	13	1
1:C:47:ILE:HD11	1:C:80:LYS:HE2	0.45	1.89	3	2
1:A:95:PHE:CZ	1:A:96:PHE:CZ	0.45	3.05	3	2
1:A:22:VAL:CG2	1:A:29:LEU:HD11	0.45	2.42	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:VAL:CG2	1:A:29:LEU:HD13	0.45	2.40	18	1
1:B:5:ILE:HG21	1:B:19:VAL:CG1	0.45	2.41	18	1
1:A:6:ILE:HG21	1:A:61:ILE:HG22	0.45	1.89	12	1
1:C:5:ILE:HG22	1:C:6:ILE:N	0.45	2.27	5	2
1:A:119:VAL:HG13	1:A:120:GLY:N	0.45	2.26	10	1
1:A:92:TYR:O	1:A:95:PHE:CD2	0.45	2.69	3	5
1:B:10:LYS:HB2	1:B:60:ALA:HB1	0.45	1.89	3	3
1:A:29:LEU:CD1	1:A:126:ILE:HD12	0.45	2.42	6	1
1:A:18:TYR:CD2	1:C:107:ARG:CB	0.45	3.00	18	1
1:A:26:ASN:C	1:A:27:LEU:HD12	0.45	2.32	17	1
1:A:36:VAL:HG22	1:A:36:VAL:O	0.45	2.11	2	1
1:A:21:ALA:HB2	1:A:61:ILE:HG21	0.45	1.88	14	3
1:C:75:THR:CG2	1:C:105:PRO:CB	0.45	2.95	16	1
1:B:55:LEU:HD22	1:B:92:TYR:HB2	0.45	1.89	7	1
1:C:58:VAL:HG21	1:C:123:ILE:CB	0.45	2.41	13	2
1:B:35:PRO:CD	1:B:119:VAL:HG21	0.45	2.42	10	1
1:A:109:CYS:O	1:A:110:VAL:HG13	0.45	2.10	19	3
1:B:22:VAL:CG2	1:B:29:LEU:HD11	0.45	2.42	4	1
1:B:5:ILE:HG22	1:B:6:ILE:N	0.45	2.27	5	2
1:C:119:VAL:HG13	1:C:120:GLY:N	0.45	2.26	10	1
1:A:24:LEU:HD11	1:C:128:VAL:HG11	0.45	1.88	13	1
1:B:128:VAL:HG11	1:C:24:LEU:HD11	0.45	1.88	13	1
1:C:95:PHE:CZ	1:C:96:PHE:CZ	0.45	3.05	3	2
1:A:34:ILE:CG2	1:A:119:VAL:HG11	0.45	2.42	4	1
1:C:22:VAL:HG23	1:C:29:LEU:CD1	0.45	2.41	18	1
1:C:72:ILE:HG21	1:C:75:THR:HG23	0.45	1.89	9	1
1:C:26:ASN:C	1:C:27:LEU:HD12	0.45	2.33	17	1
1:B:21:ALA:CB	1:B:61:ILE:HG21	0.45	2.41	17	1
1:C:5:ILE:HG21	1:C:19:VAL:CG1	0.45	2.41	18	1
1:A:4:GLN:O	1:A:5:ILE:HG22	0.44	2.11	17	1
1:A:5:ILE:HG22	1:A:6:ILE:N	0.44	2.27	5	2
1:C:28:VAL:HG22	1:C:67:LEU:HD13	0.44	1.88	2	1
1:B:73:VAL:HG13	1:B:128:VAL:HG12	0.44	1.87	2	1
1:A:73:VAL:HB	1:B:4:GLN:NE2	0.44	2.26	9	4
1:A:34:ILE:HD12	1:A:36:VAL:HG21	0.44	1.88	16	1
1:B:79:VAL:HG11	1:B:85:PHE:HD1	0.44	1.72	16	1
1:A:79:VAL:HG11	1:A:85:PHE:HD1	0.44	1.72	16	1
1:C:96:PHE:CD2	1:C:101:HIS:CB	0.44	3.01	10	1
1:B:96:PHE:CZ	1:B:105:PRO:CG	0.44	3.01	9	1
1:C:73:VAL:HG23	1:C:74:LYS:N	0.44	2.28	19	7
1:C:8:THR:HG21	1:C:61:ILE:HG12	0.44	1.88	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:THR:N	1:A:107:ARG:HG3	0.44	2.27	5	1
1:B:25:GLY:O	1:B:26:ASN:CB	0.44	2.65	5	4
1:C:88:VAL:O	1:C:92:TYR:CD1	0.44	2.70	8	1
1:B:72:ILE:CD1	1:B:127:ALA:HB2	0.44	2.27	12	1
1:C:77:VAL:HG22	1:C:123:ILE:HG22	0.44	1.89	12	1
1:B:96:PHE:CG	1:B:101:HIS:HB2	0.44	2.48	17	2
1:A:72:ILE:HG21	1:A:75:THR:HG22	0.44	1.88	5	1
1:C:25:GLY:O	1:C:26:ASN:CB	0.44	2.66	14	4
1:A:100:ASN:CG	1:A:100:ASN:O	0.44	2.56	8	1
1:C:121:LEU:HD22	1:C:121:LEU:O	0.44	2.13	13	1
1:A:103:ASN:O	1:B:19:VAL:HG13	0.44	2.12	18	3
1:A:72:ILE:HG21	1:A:75:THR:HG23	0.44	1.89	9	1
1:B:73:VAL:HG23	1:B:74:LYS:N	0.44	2.28	19	7
1:B:34:ILE:HD12	1:B:36:VAL:HG21	0.44	1.88	16	1
1:A:75:THR:CG2	1:A:105:PRO:CB	0.44	2.95	16	1
1:A:88:VAL:O	1:A:92:TYR:CD1	0.44	2.70	8	1
1:B:70:ALA:HA	1:B:101:HIS:CG	0.44	2.46	8	3
1:C:24:LEU:CG	1:C:29:LEU:HD21	0.44	2.43	10	1
1:A:96:PHE:CD2	1:A:101:HIS:CB	0.44	3.01	10	1
1:B:5:ILE:HD12	1:B:19:VAL:HG11	0.44	1.88	13	1
1:C:121:LEU:HD12	1:C:121:LEU:O	0.44	2.13	3	1
1:B:30:THR:CG2	1:B:62:ILE:HD11	0.44	2.43	4	1
1:C:121:LEU:O	1:C:121:LEU:HD12	0.44	2.13	15	1
1:B:75:THR:N	1:B:107:ARG:HG3	0.44	2.28	5	1
1:A:25:GLY:O	1:A:26:ASN:CB	0.44	2.66	14	4
1:A:5:ILE:CD1	1:A:19:VAL:HG11	0.44	2.42	2	1
1:B:55:LEU:HD22	1:B:95:PHE:CE2	0.44	2.47	2	2
1:C:4:GLN:NE2	1:C:22:VAL:HB	0.44	2.28	14	3
1:C:51:ALA:HB1	1:C:88:VAL:HG13	0.44	1.87	8	1
1:A:35:PRO:CD	1:A:119:VAL:HG21	0.44	2.41	10	1
1:B:115:LEU:HD22	1:B:122:GLU:OE1	0.44	2.12	6	1
1:C:34:ILE:HD12	1:C:36:VAL:HG22	0.44	1.88	12	1
1:B:34:ILE:HD12	1:B:36:VAL:HG22	0.44	1.88	12	1
1:B:13:ALA:HB3	1:B:20:GLN:HE21	0.44	1.71	12	1
1:C:96:PHE:CG	1:C:101:HIS:HB2	0.44	2.47	17	2
1:A:112:VAL:HG21	1:A:115:LEU:CD2	0.44	2.41	5	1
1:A:19:VAL:HG11	1:C:103:ASN:O	0.44	2.13	16	1
1:B:96:PHE:CD2	1:B:101:HIS:CB	0.44	3.01	10	1
1:A:76:THR:N	1:A:107:ARG:HG2	0.44	2.28	3	2
1:B:95:PHE:CZ	1:B:96:PHE:CZ	0.44	3.05	3	2
1:C:22:VAL:CG2	1:C:29:LEU:HD11	0.44	2.42	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:VAL:HG22	1:A:123:ILE:HG22	0.44	1.88	12	1
1:A:73:VAL:HG23	1:A:74:LYS:N	0.44	2.28	17	7
1:A:4:GLN:NE2	1:A:22:VAL:HB	0.44	2.28	14	3
1:B:75:THR:CG2	1:B:105:PRO:CB	0.44	2.95	16	1
1:A:58:VAL:HG21	1:A:123:ILE:HB	0.44	1.88	8	1
1:A:62:ILE:HG21	1:A:72:ILE:HD11	0.44	1.89	8	1
1:C:79:VAL:O	1:C:111:GLU:HA	0.44	2.13	19	1
1:A:5:ILE:HD12	1:A:5:ILE:N	0.44	2.27	9	1
1:B:5:ILE:N	1:B:5:ILE:HD12	0.44	2.27	9	1
1:B:26:ASN:C	1:B:27:LEU:HD12	0.44	2.32	17	1
1:B:103:ASN:O	1:C:19:VAL:HG11	0.44	2.13	16	1
1:C:5:ILE:HD12	1:C:19:VAL:HG11	0.44	1.87	13	1
1:B:121:LEU:O	1:B:121:LEU:HD22	0.44	2.13	13	1
1:B:5:ILE:HD11	1:B:19:VAL:CG2	0.44	2.39	12	1
1:A:96:PHE:CG	1:A:101:HIS:HB2	0.44	2.47	17	2
1:A:128:VAL:CG2	1:A:129:ARG:N	0.44	2.81	2	1
1:A:103:ASN:O	1:B:19:VAL:HG11	0.44	2.13	16	1
1:C:8:THR:HG21	1:C:61:ILE:HA	0.44	1.90	7	1
1:B:62:ILE:HG21	1:B:72:ILE:HD11	0.44	1.89	8	1
1:A:24:LEU:CG	1:A:29:LEU:HD21	0.44	2.43	10	1
1:B:128:VAL:CG2	1:B:129:ARG:N	0.43	2.81	2	1
1:A:92:TYR:O	1:A:96:PHE:CD2	0.43	2.71	8	2
1:C:100:ASN:CG	1:C:100:ASN:O	0.43	2.56	8	1
1:A:19:VAL:HG13	1:C:103:ASN:O	0.43	2.13	18	3
1:B:79:VAL:O	1:B:111:GLU:HA	0.43	2.13	19	1
1:B:35:PRO:HD2	1:B:119:VAL:HG21	0.43	1.88	10	1
1:C:23:ASP:CB	1:C:28:VAL:HG12	0.43	2.43	13	1
1:C:67:LEU:HD22	1:C:71:ASP:HB3	0.43	1.90	19	1
1:A:79:VAL:O	1:A:111:GLU:HA	0.43	2.13	19	1
1:B:72:ILE:HG21	1:B:75:THR:HG23	0.43	1.89	9	1
1:B:6:ILE:HG21	1:B:61:ILE:HG22	0.43	1.89	12	2
1:C:76:THR:HG22	1:C:108:SER:O	0.43	2.13	17	1
1:B:28:VAL:HG22	1:B:67:LEU:HD13	0.43	1.90	2	1
1:B:76:THR:N	1:B:124:GLU:O	0.43	2.51	19	2
1:C:76:THR:N	1:C:124:GLU:O	0.43	2.51	19	2
1:B:92:TYR:O	1:B:96:PHE:CD2	0.43	2.71	8	2
1:B:34:ILE:HG22	1:B:121:LEU:O	0.43	2.13	3	2
1:C:76:THR:HG23	1:C:107:ARG:NH1	0.43	2.29	19	1
1:C:22:VAL:CG2	1:C:29:LEU:HD13	0.43	2.40	18	1
1:A:5:ILE:HD13	1:C:103:ASN:HD22	0.43	1.69	12	1
1:B:77:VAL:HG22	1:B:123:ILE:HG22	0.43	1.89	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:100:ASN:CG	1:B:100:ASN:O	0.43	2.56	8	1
1:B:121:LEU:HD12	1:B:121:LEU:O	0.43	2.13	3	2
1:A:121:LEU:HD12	1:A:121:LEU:O	0.43	2.13	3	2
1:B:76:THR:HG23	1:B:107:ARG:NH1	0.43	2.28	19	1
1:B:76:THR:HG22	1:B:108:SER:O	0.43	2.13	17	1
1:C:128:VAL:CG2	1:C:129:ARG:N	0.43	2.81	2	1
1:A:5:ILE:HD11	1:A:19:VAL:CG1	0.43	2.35	16	1
1:C:79:VAL:HG11	1:C:85:PHE:HD1	0.43	1.72	16	1
1:B:47:ILE:HD11	1:B:80:LYS:HE2	0.43	1.90	3	2
1:C:5:ILE:HD12	1:C:5:ILE:N	0.43	2.28	9	1
1:C:75:THR:N	1:C:107:ARG:HG3	0.43	2.28	5	1
1:A:100:ASN:C	1:A:102:PRO:HD3	0.43	2.34	2	1
1:B:104:PHE:CD1	1:C:17:PRO:HA	0.43	2.49	14	3
1:A:11:ALA:CB	1:A:12:PRO:CD	0.43	2.95	16	2
1:B:24:LEU:HD11	1:B:29:LEU:HD11	0.43	1.90	11	1
1:B:36:VAL:O	1:B:36:VAL:HG22	0.43	2.14	18	1
1:A:101:HIS:N	1:A:102:PRO:CD	0.43	2.81	17	8
1:B:101:HIS:N	1:B:102:PRO:CD	0.43	2.81	17	9
1:A:76:THR:HG22	1:A:108:SER:O	0.43	2.13	17	1
1:B:4:GLN:NE2	1:B:22:VAL:HB	0.43	2.28	14	3
1:A:104:PHE:CD1	1:B:17:PRO:HA	0.43	2.49	14	3
1:B:15:ILE:HD12	1:B:15:ILE:N	0.43	2.29	16	1
1:B:51:ALA:CB	1:B:88:VAL:HG22	0.43	2.44	7	1
1:B:33:GLN:O	1:B:34:ILE:HD13	0.43	2.14	10	1
1:A:23:ASP:CB	1:A:28:VAL:HG12	0.43	2.44	13	1
1:B:29:LEU:CD1	1:B:126:ILE:HD12	0.43	2.42	6	1
1:A:24:LEU:HD11	1:A:29:LEU:HD11	0.43	1.90	11	1
1:B:29:LEU:HD23	1:B:126:ILE:HG12	0.43	1.91	19	1
1:A:62:ILE:CD1	1:A:127:ALA:CB	0.43	2.97	17	2
1:B:54:SER:HB3	1:B:123:ILE:HD12	0.43	1.90	2	1
1:A:115:LEU:HD13	1:A:120:GLY:C	0.43	2.34	10	1
1:B:23:ASP:CB	1:B:28:VAL:HG12	0.43	2.43	13	1
1:A:18:TYR:CG	1:C:107:ARG:NH1	0.43	2.87	13	1
1:B:46:ASP:HB3	1:B:49:ALA:HB3	0.43	1.91	18	1
1:C:101:HIS:N	1:C:102:PRO:CD	0.43	2.81	17	6
1:C:112:VAL:HG21	1:C:115:LEU:CD2	0.43	2.41	5	1
1:A:5:ILE:HD11	1:C:103:ASN:ND2	0.43	2.28	2	1
1:C:92:TYR:O	1:C:96:PHE:CD2	0.43	2.72	13	2
1:B:103:ASN:O	1:C:19:VAL:HG13	0.43	2.14	18	3
1:C:24:LEU:HD11	1:C:29:LEU:HD11	0.43	1.90	11	1
1:A:71:ASP:O	1:A:128:VAL:HG22	0.43	2.14	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LEU:CG	1:A:126:ILE:HG23	0.43	2.37	5	1
1:A:54:SER:HB3	1:A:123:ILE:HD12	0.43	1.90	2	1
1:A:17:PRO:HA	1:C:104:PHE:CD1	0.43	2.49	14	3
1:B:76:THR:N	1:B:107:ARG:HG2	0.43	2.28	3	2
1:A:47:ILE:HD11	1:A:80:LYS:HE2	0.43	1.89	3	2
1:B:74:LYS:O	1:B:75:THR:HB	0.43	2.14	3	2
1:A:72:ILE:CD1	1:A:127:ALA:HB2	0.42	2.28	12	2
1:C:14:ALA:HB1	1:C:18:TYR:CD1	0.42	2.50	5	1
1:B:24:LEU:CG	1:B:29:LEU:HD21	0.42	2.43	10	1
1:A:116:PRO:O	1:A:119:VAL:HG12	0.42	2.14	10	1
1:C:76:THR:N	1:C:107:ARG:HG2	0.42	2.28	3	2
1:A:29:LEU:HD23	1:A:126:ILE:HG12	0.42	1.91	19	1
1:A:76:THR:HG23	1:A:107:ARG:NH1	0.42	2.28	19	1
1:B:62:ILE:CD1	1:B:127:ALA:CB	0.42	2.97	17	2
1:B:100:ASN:C	1:B:102:PRO:HD3	0.42	2.34	2	1
1:C:55:LEU:HD22	1:C:95:PHE:CE2	0.42	2.48	2	1
1:C:55:LEU:HD22	1:C:92:TYR:HB2	0.42	1.90	7	1
1:A:114:ARG:HD3	1:C:82:LEU:HD12	0.42	1.90	7	1
1:C:115:LEU:HD13	1:C:120:GLY:C	0.42	2.34	10	1
1:B:107:ARG:NH1	1:C:18:TYR:CG	0.42	2.88	13	1
1:C:26:ASN:HB2	1:C:27:LEU:HD12	0.42	1.91	17	1
1:B:78:PHE:CE2	1:B:124:GLU:OE2	0.42	2.73	5	4
1:A:103:ASN:ND2	1:B:5:ILE:HD11	0.42	2.28	2	1
1:C:54:SER:HB3	1:C:123:ILE:HD12	0.42	1.90	2	1
1:C:75:THR:CG2	1:C:105:PRO:HB2	0.42	2.45	16	1
1:B:75:THR:O	1:B:107:ARG:CB	0.42	2.68	16	2
1:C:11:ALA:CB	1:C:12:PRO:CD	0.42	2.95	10	3
1:C:58:VAL:HG21	1:C:123:ILE:HB	0.42	1.90	8	1
1:A:22:VAL:HG23	1:A:29:LEU:CD1	0.42	2.41	18	1
1:B:71:ASP:O	1:B:128:VAL:HG22	0.42	2.13	9	1
1:C:115:LEU:HD22	1:C:122:GLU:HB3	0.42	1.91	12	1
1:C:35:PRO:CB	1:C:50:GLN:CG	0.42	2.97	17	1
1:B:14:ALA:HB1	1:B:18:TYR:CD1	0.42	2.50	5	1
1:A:75:THR:O	1:A:107:ARG:CB	0.42	2.68	16	1
1:B:116:PRO:O	1:B:119:VAL:HG12	0.42	2.14	10	1
1:B:47:ILE:HD12	1:B:50:GLN:NE2	0.42	2.29	10	1
1:C:74:LYS:O	1:C:75:THR:HB	0.42	2.14	3	2
1:B:28:VAL:HG12	1:B:127:ALA:CB	0.42	2.42	6	1
1:A:36:VAL:O	1:A:36:VAL:HG22	0.42	2.14	18	1
1:A:27:LEU:HD21	1:B:24:LEU:HD13	0.42	1.91	18	1
1:C:71:ASP:O	1:C:128:VAL:HG22	0.42	2.14	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:73:VAL:HG12	1:C:4:GLN:CG	0.42	2.45	9	1
1:A:5:ILE:HD11	1:A:19:VAL:CG2	0.42	2.39	12	1
1:B:103:ASN:ND2	1:C:5:ILE:HD11	0.42	2.29	2	1
1:B:99:ASN:O	1:B:100:ASN:CG	0.42	2.58	2	1
1:B:4:GLN:N	1:B:4:GLN:OE1	0.42	2.53	14	2
1:B:4:GLN:OE1	1:B:4:GLN:N	0.42	2.53	20	1
1:C:51:ALA:HB1	1:C:88:VAL:HG22	0.42	1.89	7	1
1:A:29:LEU:HD13	1:C:74:LYS:HD2	0.42	1.92	19	1
1:B:67:LEU:HD22	1:B:71:ASP:HB3	0.42	1.91	19	1
1:B:74:LYS:HD2	1:C:29:LEU:HD13	0.42	1.92	19	1
1:A:76:THR:N	1:A:124:GLU:O	0.42	2.51	19	1
1:B:107:ARG:HB3	1:C:18:TYR:CD2	0.42	2.49	18	1
1:A:107:ARG:CB	1:B:18:TYR:CD2	0.42	3.03	18	1
1:B:29:LEU:CG	1:B:126:ILE:HG23	0.42	2.37	5	1
1:A:5:ILE:HD13	1:A:19:VAL:HG11	0.42	1.92	2	1
1:A:99:ASN:O	1:A:100:ASN:CG	0.42	2.58	2	1
1:C:4:GLN:N	1:C:4:GLN:OE1	0.42	2.53	14	3
1:B:103:ASN:O	1:C:19:VAL:CG1	0.42	2.67	8	2
1:A:47:ILE:HD12	1:A:50:GLN:NE2	0.42	2.29	10	1
1:A:74:LYS:O	1:A:75:THR:HB	0.42	2.14	3	2
1:A:26:ASN:HB2	1:A:27:LEU:HD12	0.42	1.92	17	1
1:C:102:PRO:O	1:C:104:PHE:CD2	0.42	2.73	5	2
1:A:76:THR:CG2	1:A:78:PHE:CE1	0.42	3.03	2	1
1:A:73:VAL:HG12	1:B:4:GLN:CG	0.42	2.45	9	1
1:C:62:ILE:CD1	1:C:127:ALA:CB	0.42	2.98	18	2
1:C:6:ILE:HG22	1:C:7:HIS:N	0.42	2.30	5	1
1:A:19:VAL:HG23	1:A:21:ALA:O	0.42	2.15	14	3
1:C:62:ILE:HG21	1:C:72:ILE:HD11	0.42	1.90	8	1
1:B:99:ASN:HB2	1:B:101:HIS:CE1	0.42	2.50	10	1
1:C:99:ASN:HB2	1:C:101:HIS:CE1	0.42	2.50	10	1
1:A:33:GLN:O	1:A:34:ILE:HD13	0.42	2.14	10	1
1:A:128:VAL:HG11	1:B:24:LEU:HD11	0.42	1.91	13	1
1:C:28:VAL:O	1:C:126:ILE:HG22	0.42	2.14	3	2
1:A:17:PRO:HA	1:C:104:PHE:CG	0.42	2.50	3	2
1:C:92:TYR:O	1:C:95:PHE:CE2	0.42	2.73	4	2
1:B:75:THR:CB	1:B:125:ALA:HB2	0.42	2.45	17	1
1:C:28:VAL:O	1:C:29:LEU:HD12	0.42	2.15	5	1
1:B:19:VAL:HG23	1:B:21:ALA:O	0.42	2.14	14	3
1:A:75:THR:CG2	1:A:105:PRO:HB2	0.42	2.45	16	1
1:A:88:VAL:HG12	1:A:92:TYR:CE1	0.42	2.50	8	1
1:C:102:PRO:O	1:C:104:PHE:CE2	0.42	2.73	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:102:PRO:O	1:B:104:PHE:CD2	0.42	2.73	5	2
1:A:73:VAL:CG1	1:A:128:VAL:CG1	0.42	2.98	2	1
1:A:55:LEU:HD22	1:A:95:PHE:CE2	0.42	2.50	2	2
1:C:75:THR:O	1:C:107:ARG:CB	0.42	2.68	16	1
1:A:51:ALA:CB	1:A:88:VAL:HG22	0.42	2.44	7	1
1:A:103:ASN:O	1:B:19:VAL:CG1	0.42	2.68	8	2
1:C:101:HIS:O	1:C:101:HIS:CD2	0.42	2.73	8	1
1:C:116:PRO:O	1:C:119:VAL:HG12	0.42	2.14	10	1
1:B:71:ASP:OD2	1:B:127:ALA:HB1	0.42	2.15	3	2
1:B:28:VAL:HG21	1:B:67:LEU:HD12	0.42	1.91	11	1
1:B:102:PRO:O	1:B:104:PHE:CE2	0.42	2.73	18	2
1:A:102:PRO:O	1:A:104:PHE:CE2	0.42	2.73	18	2
1:C:69:ALA:CB	1:C:101:HIS:CD2	0.42	2.99	4	1
1:A:46:ASP:HB3	1:A:49:ALA:HB3	0.42	1.91	18	1
1:A:103:ASN:HB3	1:B:5:ILE:HD11	0.41	1.90	5	1
1:C:85:PHE:CE2	1:C:89:ASN:OD1	0.41	2.73	5	1
1:C:76:THR:CG2	1:C:78:PHE:CE1	0.41	3.03	2	1
1:A:99:ASN:HB2	1:A:101:HIS:CE1	0.41	2.50	10	1
1:C:33:GLN:O	1:C:34:ILE:HD13	0.41	2.14	10	1
1:A:107:ARG:NH1	1:B:18:TYR:CG	0.41	2.88	13	1
1:C:10:LYS:HB2	1:C:60:ALA:HB1	0.41	1.92	3	3
1:A:104:PHE:CG	1:B:17:PRO:HA	0.41	2.50	3	2
1:A:92:TYR:O	1:A:95:PHE:CE2	0.41	2.73	4	2
1:B:92:TYR:O	1:B:95:PHE:CE2	0.41	2.73	4	2
1:C:100:ASN:C	1:C:102:PRO:HD3	0.41	2.34	2	1
1:B:76:THR:CG2	1:B:78:PHE:CE1	0.41	3.03	2	1
1:C:19:VAL:HG23	1:C:21:ALA:O	0.41	2.15	14	3
1:A:19:VAL:CG1	1:C:103:ASN:O	0.41	2.69	7	2
1:B:24:LEU:HG	1:B:29:LEU:HD21	0.41	1.91	10	1
1:C:55:LEU:HD23	1:C:123:ILE:HD13	0.41	1.92	10	1
1:C:34:ILE:CG2	1:C:119:VAL:HG11	0.41	2.42	4	1
1:B:85:PHE:CE2	1:B:89:ASN:OD1	0.41	2.73	5	1
1:C:78:PHE:CE2	1:C:124:GLU:OE2	0.41	2.73	5	1
1:A:78:PHE:CE2	1:A:124:GLU:OE2	0.41	2.72	5	1
1:C:99:ASN:O	1:C:100:ASN:CG	0.41	2.58	2	1
1:B:82:LEU:HD12	1:C:114:ARG:HD3	0.41	1.91	7	1
1:C:88:VAL:HG12	1:C:92:TYR:CE1	0.41	2.50	8	1
1:B:104:PHE:CG	1:C:17:PRO:HA	0.41	2.51	3	2
1:B:67:LEU:HD11	1:B:129:ARG:HG2	0.41	1.92	2	1
1:B:8:THR:HG21	1:B:61:ILE:HA	0.41	1.92	7	1
1:C:24:LEU:HG	1:C:29:LEU:HD21	0.41	1.91	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:115:LEU:HD13	1:B:120:GLY:C	0.41	2.35	10	1
1:C:71:ASP:OD2	1:C:127:ALA:HB1	0.41	2.15	3	2
1:A:34:ILE:O	1:A:36:VAL:N	0.41	2.53	19	1
1:C:46:ASP:HB3	1:C:49:ALA:HB3	0.41	1.91	18	1
1:A:11:ALA:CB	1:A:61:ILE:CG1	0.41	2.98	2	2
1:A:96:PHE:CE2	1:A:105:PRO:HD3	0.41	2.50	17	1
1:B:26:ASN:HB2	1:B:27:LEU:HD12	0.41	1.92	17	1
1:B:28:VAL:O	1:B:29:LEU:HD12	0.41	2.15	5	1
1:A:102:PRO:O	1:A:104:PHE:CD2	0.41	2.73	5	2
1:B:6:ILE:HG22	1:B:7:HIS:N	0.41	2.30	5	2
1:C:73:VAL:CG1	1:C:128:VAL:CG1	0.41	2.98	2	1
1:B:55:LEU:HD23	1:B:123:ILE:HD13	0.41	1.92	10	1
1:A:29:LEU:HD22	1:C:74:LYS:NZ	0.41	2.31	19	1
1:A:74:LYS:HD2	1:B:29:LEU:HD13	0.41	1.93	19	1
1:B:11:ALA:CB	1:B:61:ILE:CG1	0.41	2.98	12	1
1:A:14:ALA:HB1	1:A:18:TYR:CD1	0.41	2.50	5	1
1:C:6:ILE:HG13	1:C:21:ALA:HB3	0.41	1.92	16	1
1:A:67:LEU:HD22	1:A:71:ASP:CG	0.41	2.36	16	1
1:C:67:LEU:HD22	1:C:71:ASP:CG	0.41	2.36	16	1
1:A:3:THR:HA	1:A:23:ASP:O	0.41	2.16	7	1
1:A:101:HIS:O	1:A:101:HIS:CD2	0.41	2.73	8	1
1:A:68:THR:O	1:A:71:ASP:OD1	0.41	2.39	3	2
1:B:68:THR:O	1:B:71:ASP:OD1	0.41	2.38	3	2
1:B:35:PRO:CB	1:B:50:GLN:CG	0.41	2.98	17	1
1:A:6:ILE:HG22	1:A:7:HIS:N	0.41	2.30	5	1
1:C:47:ILE:HD12	1:C:50:GLN:NE2	0.41	2.29	10	1
1:C:34:ILE:HG22	1:C:121:LEU:O	0.41	2.16	3	2
1:A:34:ILE:CD1	1:A:36:VAL:CG2	0.41	2.99	12	2
1:B:104:PHE:HB2	1:C:19:VAL:CG1	0.41	2.43	17	1
1:A:85:PHE:CE2	1:A:89:ASN:OD1	0.41	2.73	5	1
1:A:17:PRO:HA	1:C:104:PHE:CE2	0.41	2.51	2	1
1:B:75:THR:HG21	1:B:92:TYR:CE2	0.41	2.51	2	1
1:B:102:PRO:O	1:B:104:PHE:CZ	0.41	2.74	8	1
1:A:92:TYR:OH	1:A:96:PHE:CZ	0.41	2.74	10	1
1:C:72:ILE:O	1:C:101:HIS:NE2	0.41	2.53	6	1
1:A:4:GLN:CG	1:C:73:VAL:HG12	0.41	2.45	9	1
1:C:46:ASP:HB2	1:C:49:ALA:HB3	0.41	1.92	9	1
1:B:43:VAL:O	1:B:43:VAL:CG1	0.41	2.69	12	1
1:C:78:PHE:CE2	1:C:124:GLU:OE1	0.41	2.74	12	2
1:A:78:PHE:CE2	1:A:124:GLU:OE1	0.41	2.74	9	2
1:B:96:PHE:CE2	1:B:105:PRO:HD3	0.41	2.50	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:75:THR:CB	1:C:125:ALA:HB2	0.41	2.45	17	1
1:B:27:LEU:N	1:B:27:LEU:CD1	0.41	2.84	17	1
1:A:35:PRO:CB	1:A:50:GLN:CG	0.41	2.98	17	1
1:A:57:ASN:OD1	1:A:58:VAL:N	0.41	2.54	17	1
1:C:5:ILE:O	1:C:5:ILE:CG2	0.41	2.69	17	1
1:B:5:ILE:O	1:B:5:ILE:CG2	0.41	2.69	17	1
1:A:28:VAL:O	1:A:29:LEU:HD12	0.41	2.15	5	1
1:C:75:THR:HG21	1:C:92:TYR:CE2	0.41	2.51	2	1
1:C:11:ALA:CB	1:C:61:ILE:CG1	0.41	2.99	2	1
1:A:4:GLN:NE2	1:A:22:VAL:CG2	0.41	2.84	14	3
1:A:4:GLN:N	1:A:4:GLN:OE1	0.41	2.53	14	2
1:B:4:GLN:NE2	1:B:22:VAL:CG2	0.41	2.84	14	3
1:B:75:THR:CG2	1:B:105:PRO:HB2	0.41	2.45	16	1
1:A:4:GLN:OE1	1:A:4:GLN:N	0.41	2.53	20	1
1:C:75:THR:CG2	1:C:107:ARG:NH2	0.41	2.84	7	1
1:C:54:SER:O	1:C:57:ASN:OD1	0.41	2.39	8	1
1:B:101:HIS:O	1:B:101:HIS:CD2	0.41	2.73	8	1
1:A:91:GLU:HA	1:A:94:ARG:HG2	0.41	1.93	10	1
1:A:72:ILE:HD12	1:A:127:ALA:CB	0.41	2.46	13	1
1:A:71:ASP:OD2	1:A:127:ALA:HB1	0.41	2.16	3	2
1:B:85:PHE:CD2	1:B:89:ASN:OD1	0.41	2.74	11	1
1:A:85:PHE:CD2	1:A:89:ASN:OD1	0.41	2.74	11	1
1:A:18:TYR:CD2	1:C:107:ARG:HB3	0.41	2.51	18	1
1:C:6:ILE:HG22	1:C:61:ILE:HG22	0.41	1.93	9	1
1:B:88:VAL:O	1:B:92:TYR:N	0.41	2.52	9	1
1:A:46:ASP:HB2	1:A:49:ALA:HB3	0.41	1.92	9	1
1:B:34:ILE:CD1	1:B:36:VAL:CG2	0.41	2.99	5	2
1:C:96:PHE:CE2	1:C:105:PRO:HD3	0.41	2.51	17	1
1:C:5:ILE:HD13	1:C:19:VAL:HG11	0.41	1.91	2	1
1:B:3:THR:HA	1:B:23:ASP:O	0.41	2.16	7	1
1:A:23:ASP:CG	1:A:28:VAL:HG12	0.41	2.37	9	1
1:B:73:VAL:CG1	1:B:128:VAL:CG1	0.40	2.99	2	1
1:B:93:GLU:HG3	1:B:104:PHE:CE1	0.40	2.51	16	1
1:B:29:LEU:CD2	1:B:29:LEU:N	0.40	2.81	10	1
1:C:121:LEU:N	1:C:121:LEU:HD13	0.40	2.31	13	1
1:B:93:GLU:CG	1:B:104:PHE:CZ	0.40	3.04	3	2
1:C:28:VAL:HG21	1:C:67:LEU:HD12	0.40	1.92	11	1
1:A:75:THR:CB	1:A:125:ALA:HB2	0.40	2.46	17	1
1:C:57:ASN:OD1	1:C:58:VAL:N	0.40	2.54	17	1
1:A:5:ILE:CG2	1:A:5:ILE:O	0.40	2.69	17	1
1:C:101:HIS:CD2	1:C:101:HIS:N	0.40	2.90	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:67:LEU:HD11	1:C:129:ARG:HG2	0.40	1.92	2	1
1:C:4:GLN:NE2	1:C:22:VAL:CG2	0.40	2.84	14	3
1:A:54:SER:O	1:A:57:ASN:OD1	0.40	2.39	8	1
1:C:102:PRO:O	1:C:104:PHE:CE1	0.40	2.74	8	1
1:C:102:PRO:O	1:C:104:PHE:CZ	0.40	2.74	8	1
1:A:24:LEU:HG	1:A:29:LEU:HD21	0.40	1.91	10	1
1:C:93:GLU:CG	1:C:104:PHE:CZ	0.40	3.04	3	2
1:C:78:PHE:CE2	1:C:122:GLU:OE1	0.40	2.74	4	1
1:B:34:ILE:CG2	1:B:119:VAL:HG11	0.40	2.45	4	1
1:B:72:ILE:O	1:B:101:HIS:CE1	0.40	2.74	9	1
1:B:6:ILE:HG22	1:B:61:ILE:HG22	0.40	1.92	9	1
1:B:78:PHE:CE2	1:B:124:GLU:OE1	0.40	2.74	9	1
1:C:34:ILE:CD1	1:C:36:VAL:CG2	0.40	2.99	12	2
1:C:85:PHE:CD2	1:C:89:ASN:OD1	0.40	2.74	11	2
1:B:5:ILE:HD13	1:B:19:VAL:HG11	0.40	1.91	2	1
1:A:74:LYS:HD2	1:B:29:LEU:HD22	0.40	1.94	16	1
1:A:5:ILE:HA	1:A:22:VAL:HG12	0.40	1.94	7	1
1:B:7:HIS:CD2	1:B:20:GLN:OE1	0.40	2.74	10	1
1:C:4:GLN:O	1:C:5:ILE:HB	0.40	2.17	9	1
1:B:46:ASP:HB2	1:B:49:ALA:HB3	0.40	1.91	9	1
1:B:103:ASN:HD22	1:C:5:ILE:HD13	0.40	1.72	12	1
1:C:73:VAL:CG2	1:C:74:LYS:N	0.40	2.85	17	1
1:C:5:ILE:H	1:C:5:ILE:HD12	0.40	1.76	5	1
1:A:5:ILE:H	1:A:5:ILE:HD12	0.40	1.76	5	1
1:A:6:ILE:HD11	1:A:22:VAL:C	0.40	2.37	2	1
1:A:93:GLU:HG3	1:A:104:PHE:CE1	0.40	2.51	16	1
1:C:3:THR:HA	1:C:23:ASP:O	0.40	2.16	7	1
1:C:103:ASN:O	1:C:104:PHE:CB	0.40	2.69	8	1
1:B:47:ILE:HG21	1:B:84:ASP:HB3	0.40	1.93	3	2
1:B:93:GLU:HG3	1:B:104:PHE:CZ	0.40	2.52	3	2
1:A:67:LEU:HD22	1:A:71:ASP:HB3	0.40	1.92	19	1
1:C:35:PRO:O	1:C:36:VAL:CG1	0.40	2.69	18	1
1:A:72:ILE:O	1:A:101:HIS:CE1	0.40	2.75	9	1
1:B:23:ASP:CG	1:B:28:VAL:HG12	0.40	2.37	9	1
1:A:6:ILE:HG22	1:A:61:ILE:HG22	0.40	1.93	9	1
1:A:78:PHE:CD2	1:A:122:GLU:OE1	0.40	2.75	17	1
1:B:5:ILE:H	1:B:5:ILE:HD12	0.40	1.76	5	1
1:B:103:ASN:ND2	1:C:4:GLN:NE2	0.40	2.69	2	1
1:B:75:THR:CG2	1:B:107:ARG:NH2	0.40	2.84	7	1
1:C:50:GLN:CD	1:C:121:LEU:HD12	0.40	2.37	10	1
1:A:72:ILE:CG2	1:A:74:LYS:O	0.40	2.70	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:72:ILE:HD12	1:C:127:ALA:CB	0.40	2.46	13	1
1:B:72:ILE:HD12	1:B:127:ALA:CB	0.40	2.46	13	1
1:A:75:THR:HG22	1:A:125:ALA:HB1	0.40	1.93	6	1
1:B:75:THR:H	1:B:107:ARG:HB2	0.40	1.77	19	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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	121/130 (93%)	97±3 (80±2%)	18±3 (15±2%)	6±1 (5±1%)	5	26
1	B	121/130 (93%)	97±3 (80±2%)	19±3 (15±2%)	6±1 (5±1%)	5	27
1	C	121/130 (93%)	97±3 (80±2%)	19±3 (15±2%)	6±1 (5±1%)	5	27
All	All	7260/7800 (93%)	5792 (80%)	1110 (15%)	358 (5%)	5	27

All 60 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	100	ASN	20
1	B	100	ASN	19
1	C	100	ASN	19
1	B	36	VAL	14
1	C	3	THR	14
1	C	36	VAL	14
1	A	3	THR	14
1	A	36	VAL	14
1	B	3	THR	14
1	B	104	PHE	12
1	C	104	PHE	12
1	A	104	PHE	12
1	B	32	GLY	11
1	C	32	GLY	11
1	A	32	GLY	11

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Mol	Chain	Res	Type	Models (Total)
1	C	13	ALA	8
1	B	13	ALA	8
1	A	13	ALA	8
1	C	15	ILE	7
1	B	15	ILE	7
1	A	15	ILE	7
1	A	5	ILE	6
1	C	5	ILE	6
1	B	5	ILE	6
1	B	46	ASP	4
1	A	43	VAL	4
1	B	43	VAL	4
1	C	4	GLN	4
1	A	4	GLN	4
1	A	46	ASP	4
1	C	46	ASP	4
1	B	4	GLN	4
1	C	43	VAL	4
1	A	119	VAL	3
1	B	14	ALA	3
1	C	75	THR	3
1	C	14	ALA	3
1	B	119	VAL	3
1	B	75	THR	3
1	C	119	VAL	3
1	A	14	ALA	3
1	A	75	THR	3
1	A	35	PRO	2
1	C	35	PRO	2
1	B	35	PRO	2
1	A	129	ARG	1
1	A	106	ALA	1
1	A	111	GLU	1
1	B	111	GLU	1
1	C	106	ALA	1
1	A	6	ILE	1
1	A	11	ALA	1
1	B	129	ARG	1
1	B	11	ALA	1
1	C	6	ILE	1
1	C	111	GLU	1
1	B	106	ALA	1

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Mol	Chain	Res	Type	Models (Total)
1	B	6	ILE	1
1	C	11	ALA	1
1	C	129	ARG	1

### 6.3.2 Protein sidechains ⓘ

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	98/105 (93%)	77±3 (78±3%)	21±3 (22±3%)	4	32
1	B	98/105 (93%)	77±3 (78±3%)	21±3 (22±3%)	4	32
1	C	99/105 (94%)	77±3 (78±3%)	22±3 (22±3%)	4	31
All	All	5900/6300 (94%)	4605 (78%)	1295 (22%)	4	32

All 202 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	B	46	ASP	19
1	C	95	PHE	19
1	C	46	ASP	19
1	B	95	PHE	19
1	A	46	ASP	19
1	A	95	PHE	19
1	A	107	ARG	16
1	B	107	ARG	16
1	C	107	ARG	16
1	C	18	TYR	15
1	A	18	TYR	15
1	B	18	TYR	15
1	C	29	LEU	13
1	B	117	LYS	13
1	B	29	LEU	13
1	B	114	ARG	13
1	A	114	ARG	13
1	C	124	GLU	13
1	C	114	ARG	13
1	A	117	LYS	13

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Mol	Chain	Res	Type	Models (Total)
1	C	130	LYS	13
1	B	124	GLU	13
1	C	117	LYS	13
1	A	124	GLU	13
1	A	29	LEU	13
1	B	4	GLN	12
1	C	4	GLN	12
1	A	4	GLN	12
1	A	97	LYS	11
1	B	97	LYS	11
1	C	97	LYS	11
1	C	64	LYS	10
1	C	94	ARG	10
1	B	111	GLU	10
1	B	64	LYS	10
1	A	80	LYS	10
1	B	3	THR	10
1	A	64	LYS	10
1	C	80	LYS	10
1	C	91	GLU	10
1	A	111	GLU	10
1	B	27	LEU	10
1	B	94	ARG	10
1	C	27	LEU	10
1	C	3	THR	10
1	B	91	GLU	10
1	B	80	LYS	10
1	A	3	THR	10
1	C	111	GLU	10
1	A	94	ARG	10
1	A	27	LEU	10
1	A	91	GLU	10
1	B	103	ASN	9
1	B	68	THR	9
1	C	103	ASN	9
1	A	103	ASN	9
1	A	68	THR	9
1	C	53	GLN	9
1	A	53	GLN	9
1	B	53	GLN	9
1	C	68	THR	9
1	B	9	GLU	8

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Mol	Chain	Res	Type	Models (Total)
1	A	56	GLU	8
1	A	118	ASP	8
1	C	59	LYS	8
1	C	52	ARG	8
1	B	52	ARG	8
1	C	56	GLU	8
1	A	52	ARG	8
1	B	20	GLN	8
1	C	20	GLN	8
1	A	59	LYS	8
1	A	9	GLU	8
1	B	59	LYS	8
1	A	20	GLN	8
1	B	56	GLU	8
1	B	118	ASP	8
1	C	9	GLU	8
1	C	118	ASP	8
1	B	121	LEU	7
1	B	129	ARG	7
1	A	121	LEU	7
1	C	121	LEU	7
1	C	129	ARG	7
1	A	129	ARG	7
1	C	96	PHE	6
1	A	54	SER	6
1	B	76	THR	6
1	C	50	GLN	6
1	C	85	PHE	6
1	A	96	PHE	6
1	A	76	THR	6
1	A	50	GLN	6
1	B	96	PHE	6
1	B	50	GLN	6
1	A	85	PHE	6
1	C	54	SER	6
1	C	76	THR	6
1	B	85	PHE	6
1	B	54	SER	6
1	C	99	ASN	5
1	B	67	LEU	5
1	A	10	LYS	5
1	C	67	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	99	ASN	5
1	A	63	GLU	5
1	B	99	ASN	5
1	B	63	GLU	5
1	B	10	LYS	5
1	B	84	ASP	5
1	C	84	ASP	5
1	C	10	LYS	5
1	A	67	LEU	5
1	C	63	GLU	5
1	A	84	ASP	5
1	A	98	GLU	4
1	A	81	ASP	4
1	C	74	LYS	4
1	A	108	SER	4
1	B	81	ASP	4
1	B	74	LYS	4
1	C	28	VAL	4
1	A	7	HIS	4
1	A	122	GLU	4
1	B	98	GLU	4
1	B	7	HIS	4
1	B	108	SER	4
1	C	7	HIS	4
1	C	81	ASP	4
1	C	122	GLU	4
1	A	74	LYS	4
1	B	122	GLU	4
1	C	108	SER	4
1	A	28	VAL	4
1	C	98	GLU	4
1	B	28	VAL	4
1	C	57	ASN	3
1	B	33	GLN	3
1	A	57	ASN	3
1	B	82	LEU	3
1	A	34	ILE	3
1	B	71	ASP	3
1	A	126	ILE	3
1	C	34	ILE	3
1	C	24	LEU	3
1	C	93	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	B	34	ILE	3
1	B	126	ILE	3
1	A	71	ASP	3
1	C	82	LEU	3
1	A	33	GLN	3
1	A	82	LEU	3
1	A	93	GLU	3
1	C	33	GLN	3
1	B	93	GLU	3
1	C	71	ASP	3
1	A	24	LEU	3
1	B	57	ASN	3
1	C	126	ILE	3
1	B	24	LEU	3
1	C	79	VAL	2
1	C	100	ASN	2
1	B	100	ASN	2
1	A	79	VAL	2
1	B	31	SER	2
1	B	75	THR	2
1	A	75	THR	2
1	B	79	VAL	2
1	A	100	ASN	2
1	C	75	THR	2
1	A	123	ILE	1
1	A	83	ASN	1
1	A	92	TYR	1
1	B	101	HIS	1
1	B	89	ASN	1
1	A	72	ILE	1
1	A	8	THR	1
1	B	115	LEU	1
1	C	22	VAL	1
1	C	31	SER	1
1	C	83	ASN	1
1	B	8	THR	1
1	C	123	ILE	1
1	A	115	LEU	1
1	C	23	ASP	1
1	B	92	TYR	1
1	A	22	VAL	1
1	B	72	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	B	22	VAL	1
1	B	23	ASP	1
1	C	89	ASN	1
1	C	115	LEU	1
1	C	101	HIS	1
1	A	31	SER	1
1	C	92	TYR	1
1	A	23	ASP	1
1	B	83	ASN	1
1	C	72	ILE	1
1	A	89	ASN	1
1	C	8	THR	1
1	A	101	HIS	1
1	B	123	ILE	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