



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 01:01 am GMT

PDB ID : 2MHF
Title : Solution structure of the cyclic-nucleotide binding homology domain of a KCNH channel
Authors : Li, Q.; Ng, H.
Deposited on : 2013-11-21

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

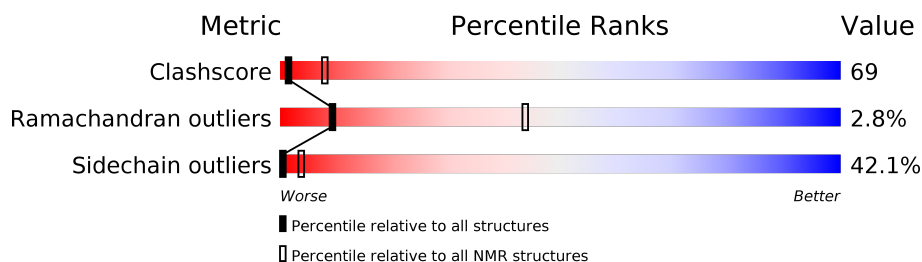
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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

Mol	Chain	Length	Quality of chain
1	A	143	

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:10-A:135 (126)	0.39	15

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

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

The models can be grouped into 5 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2151 atoms, of which 1093 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
1	A	135	Total	C	H	N	O	S	0
			2151	676	1093	176	200	6	

There are 9 discrepancies between the modelled and reference sequences:

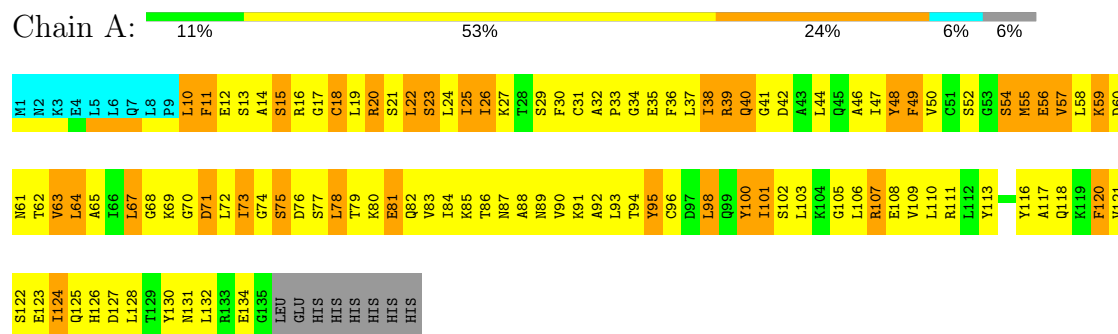
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP F1QQX6
A	136	LEU	-	EXPRESSION TAG	UNP F1QQX6
A	137	GLU	-	EXPRESSION TAG	UNP F1QQX6
A	138	HIS	-	EXPRESSION TAG	UNP F1QQX6
A	139	HIS	-	EXPRESSION TAG	UNP F1QQX6
A	140	HIS	-	EXPRESSION TAG	UNP F1QQX6
A	141	HIS	-	EXPRESSION TAG	UNP F1QQX6
A	142	HIS	-	EXPRESSION TAG	UNP F1QQX6
A	143	HIS	-	EXPRESSION TAG	UNP F1QQX6

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Uncharacterized protein

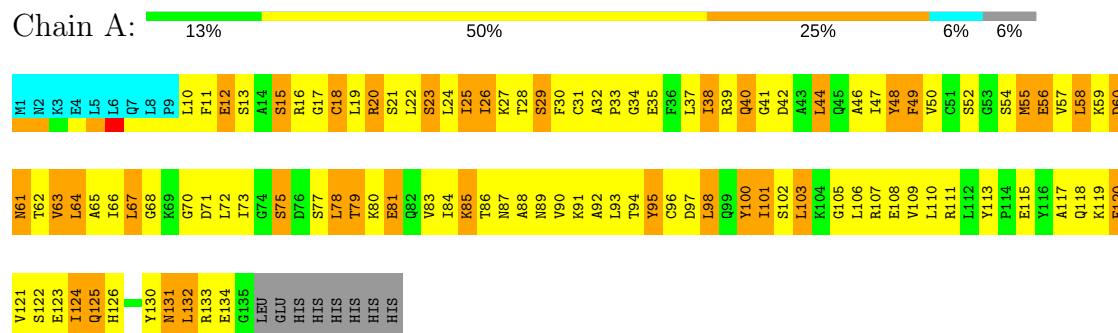


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

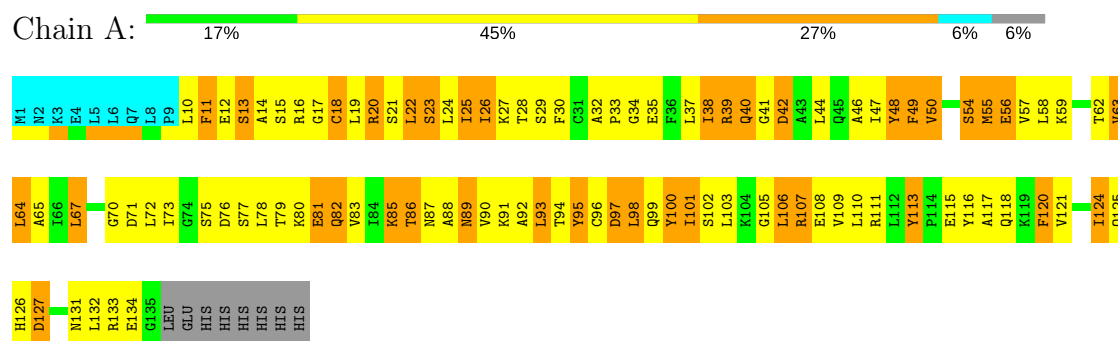
4.2.1 Score per residue for model 1

- Molecule 1: Uncharacterized protein



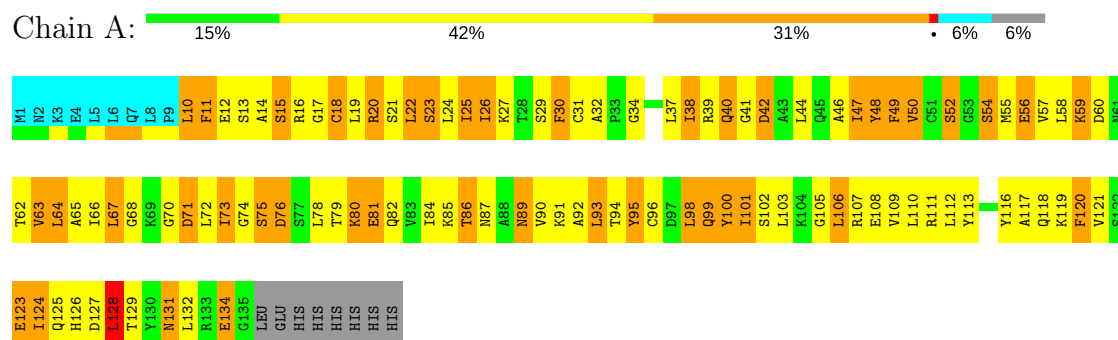
4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized protein



4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein



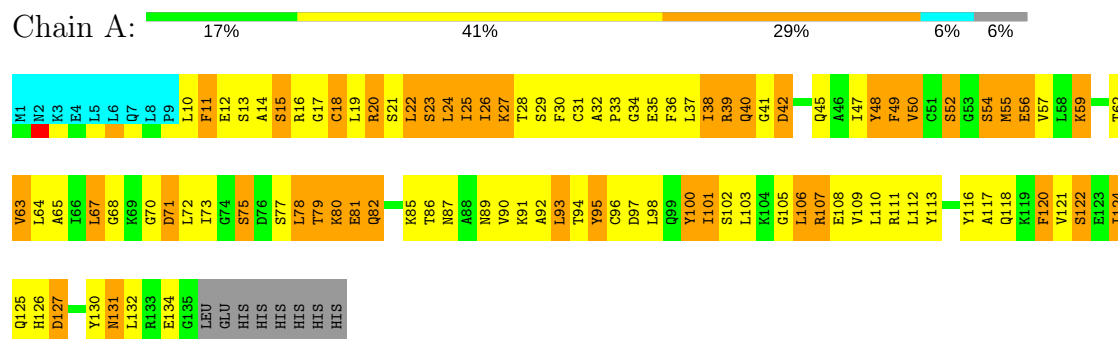
4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein



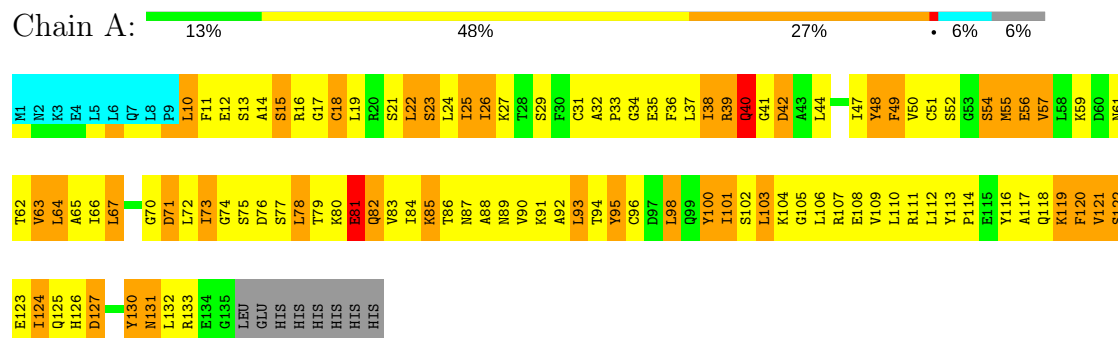
4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein



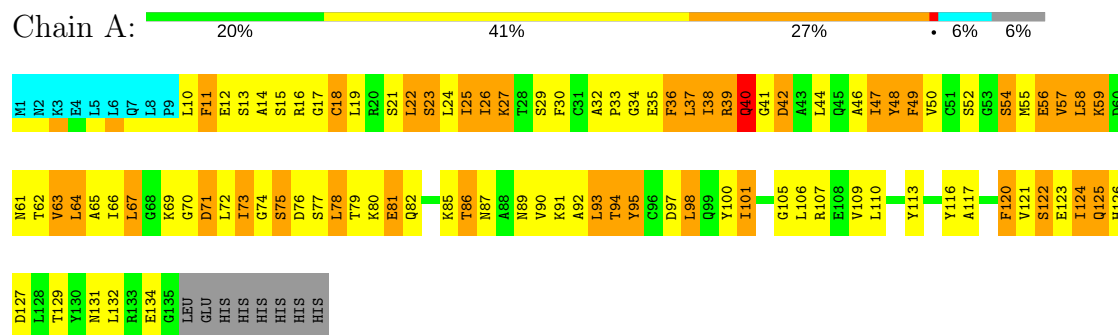
4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein



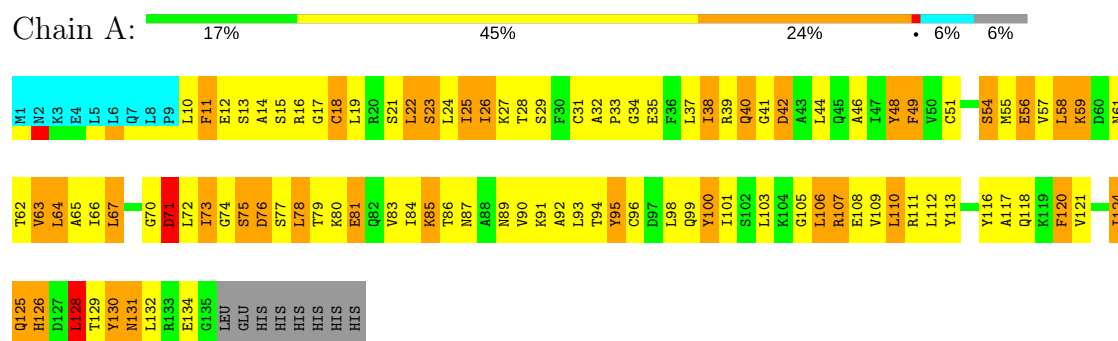
4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein



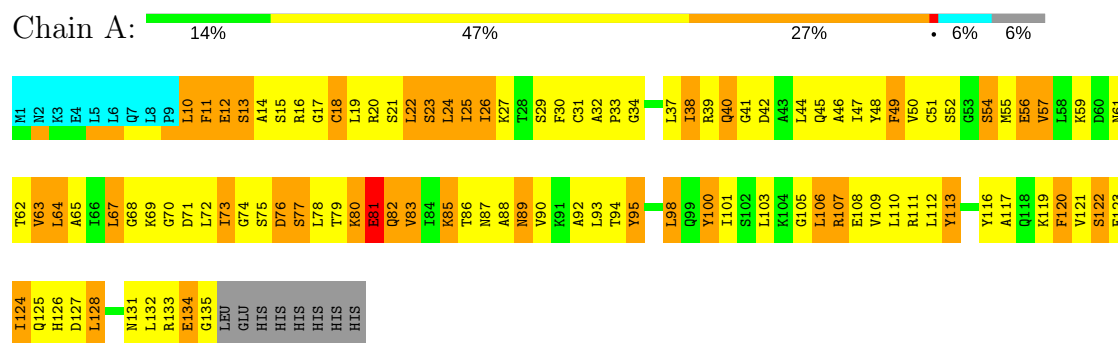
4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein



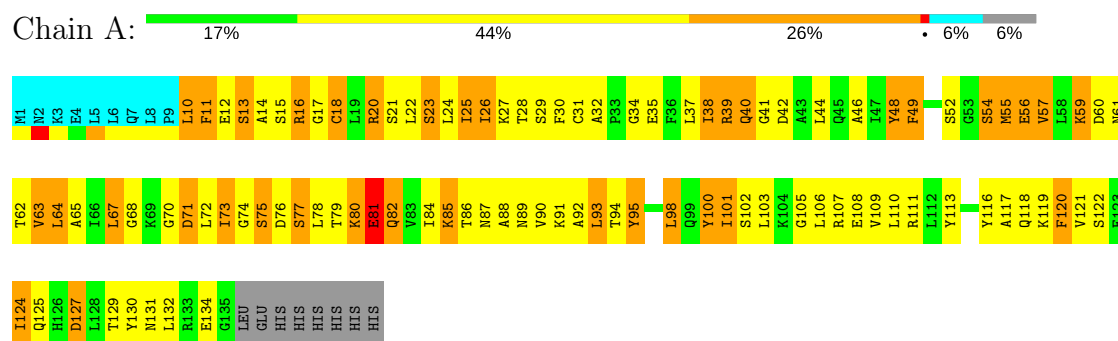
4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein



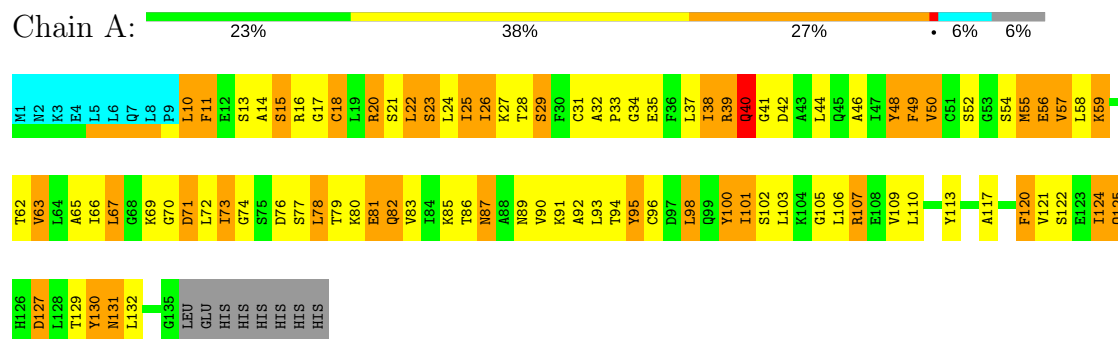
4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein



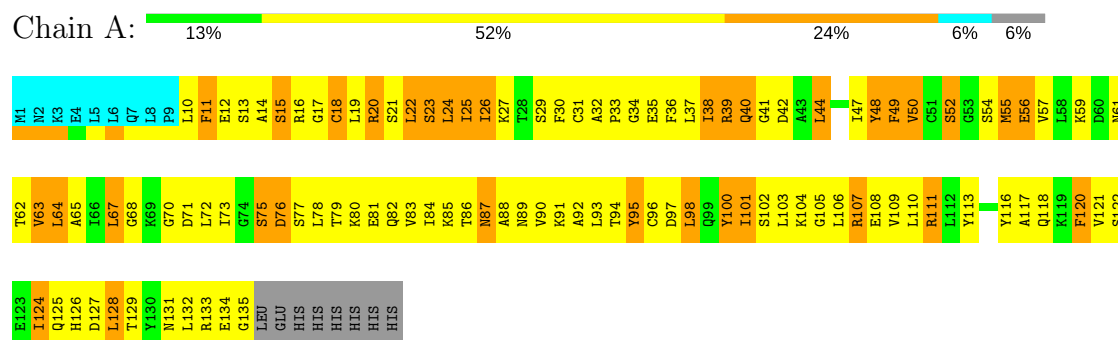
4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein



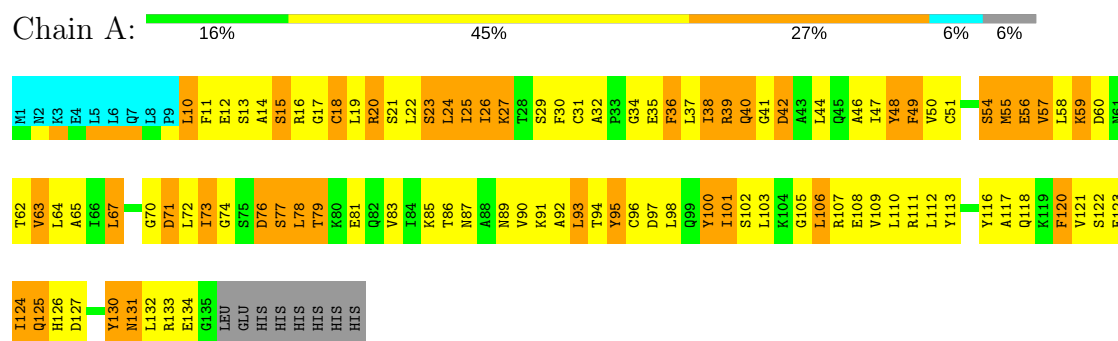
4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein




4.2.13 Score per residue for model 13

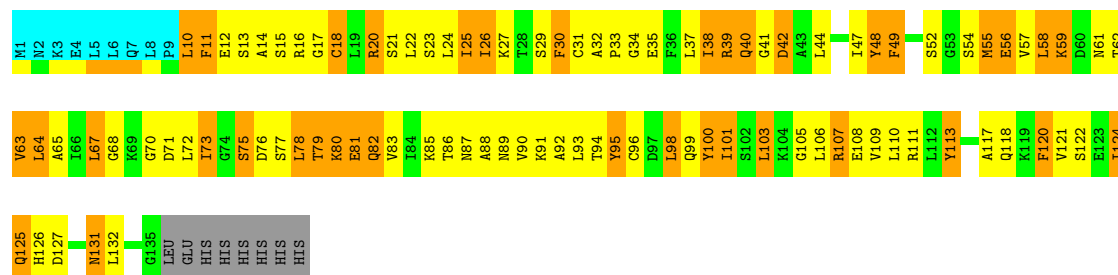
- Molecule 1: Uncharacterized protein



4.2.14 Score per residue for model 14


- Molecule 1: Uncharacterized protein

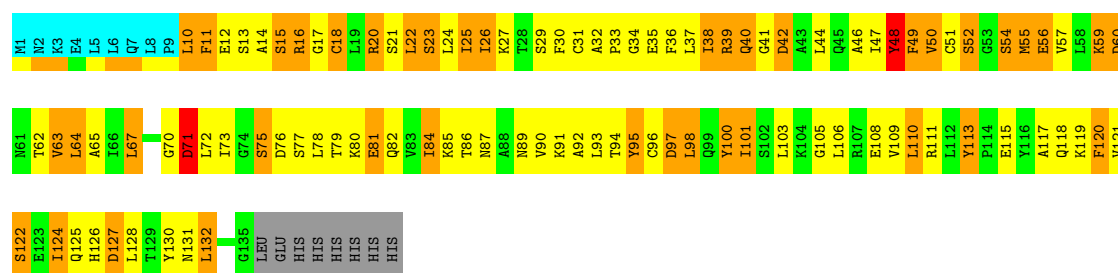
Chain A: 



4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Uncharacterized protein

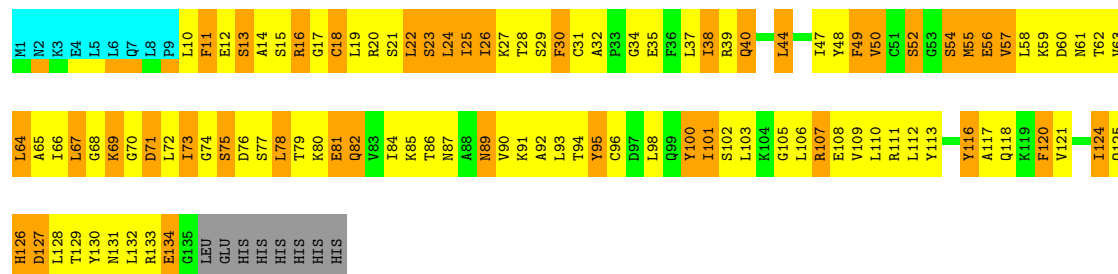
Chain A: 



4.2.16 Score per residue for model 16

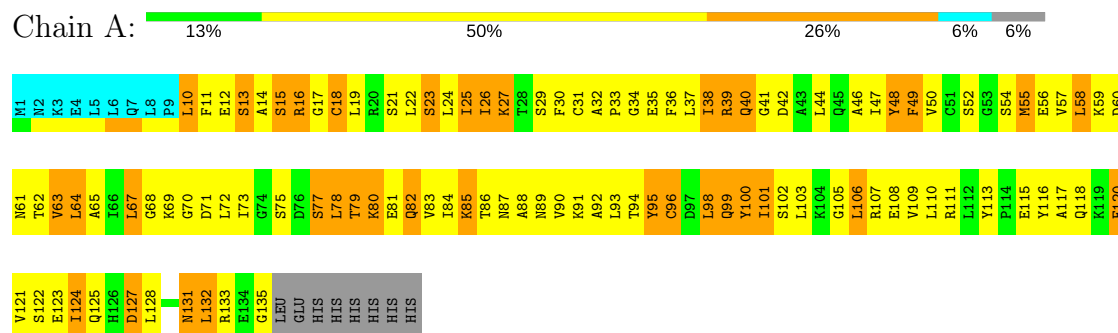
- Molecule 1: Uncharacterized protein

Chain A: 



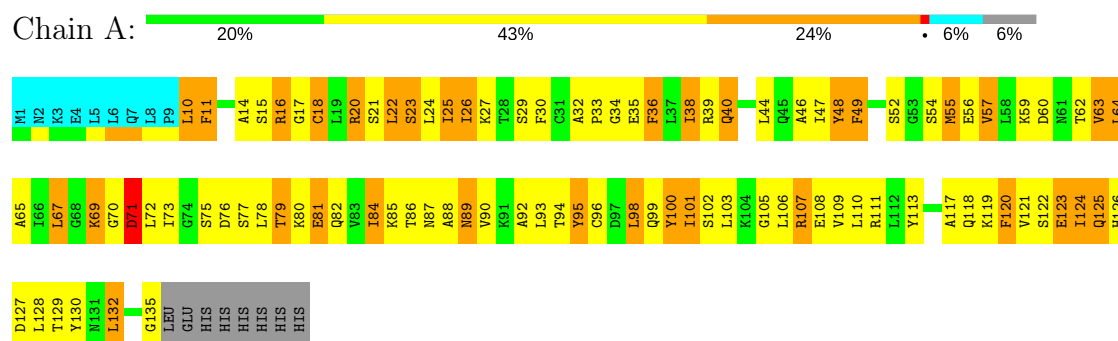
4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized protein



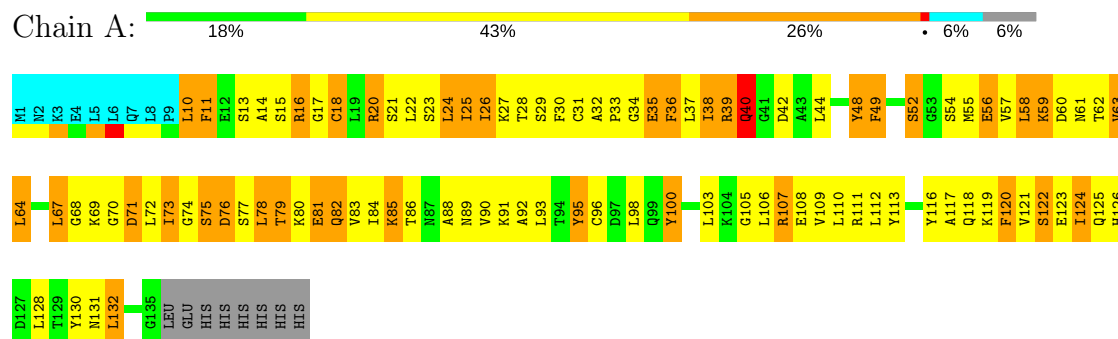
4.2.18 Score per residue for model 18

- Molecule 1: Uncharacterized protein



4.2.19 Score per residue for model 19

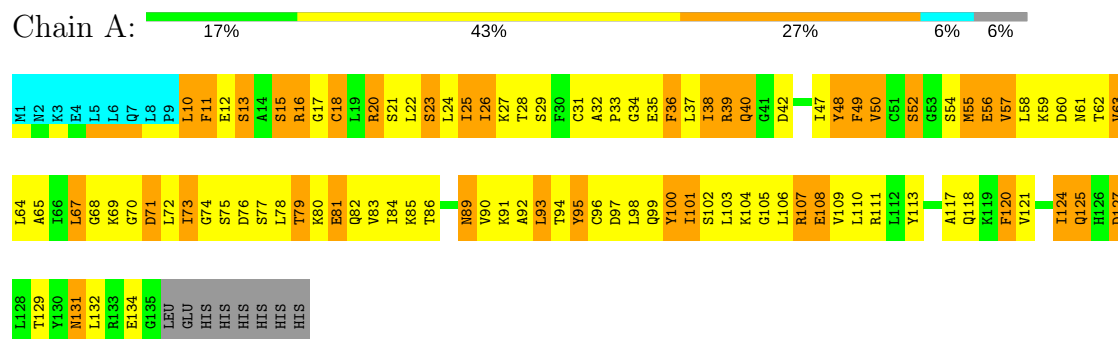
- Molecule 1: Uncharacterized protein



4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 60 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
X-PLOR-NIH	structure solution	
X-PLOR-NIH	refinement	

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

Chemical shift file(s)	2mhf_cs.str
Number of chemical shift lists	1
Total number of shifts	1524
Number of shifts mapped to atoms	1524
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.63±0.00	0±0/997 (0.0±0.0%)	0.80±0.01	0±0/1343 (0.0±0.0%)
All	All	0.63	0/19940 (0.0%)	0.80	4/26860 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	48	TYR	CB-CG-CD2	-6.91	116.85	121.00	10	4

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	984	1011	1010	137±9
All	All	19680	20220	20200	2739

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 69.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:PHE:CD2	1:A:19:LEU:HD13	0.98	1.94	6	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:CYS:SG	1:A:98:LEU:HD21	0.98	1.98	2	1
1:A:73:ILE:HD12	1:A:74:GLY:N	0.95	1.74	7	11
1:A:79:THR:OG1	1:A:121:VAL:HG11	0.94	1.62	8	3
1:A:22:LEU:HD12	1:A:109:VAL:HG21	0.92	1.42	14	20
1:A:10:LEU:HD22	1:A:120:PHE:CE1	0.91	2.00	13	2
1:A:97:ASP:C	1:A:98:LEU:HD23	0.90	1.85	2	1
1:A:31:CYS:SG	1:A:37:LEU:HD13	0.87	2.10	19	16
1:A:110:LEU:HD11	1:A:120:PHE:CD2	0.86	2.05	6	2
1:A:73:ILE:HD12	1:A:73:ILE:C	0.84	1.92	3	7
1:A:57:VAL:HG13	1:A:65:ALA:HB3	0.83	1.49	7	17
1:A:48:TYR:O	1:A:72:LEU:HD12	0.83	1.74	9	12
1:A:81:GLU:O	1:A:82:GLN:O	0.83	1.97	16	2
1:A:98:LEU:N	1:A:98:LEU:HD12	0.82	1.89	7	8
1:A:11:PHE:CD1	1:A:12:GLU:N	0.82	2.48	8	14
1:A:105:GLY:O	1:A:109:VAL:HG22	0.82	1.73	13	20
1:A:75:SER:OG	1:A:84:ILE:HG21	0.81	1.75	16	2
1:A:83:VAL:C	1:A:84:ILE:HD12	0.80	1.97	12	2
1:A:101:ILE:O	1:A:101:ILE:HD13	0.80	1.76	6	10
1:A:72:LEU:C	1:A:72:LEU:HD13	0.80	1.97	6	1
1:A:54:SER:N	1:A:96:CYS:SG	0.80	2.55	8	1
1:A:32:ALA:O	1:A:92:ALA:HB3	0.79	1.78	18	20
1:A:95:TYR:N	1:A:95:TYR:CD1	0.79	2.50	15	6
1:A:101:ILE:HD13	1:A:101:ILE:O	0.78	1.78	15	6
1:A:78:LEU:HD22	1:A:124:ILE:HD12	0.78	1.54	10	15
1:A:32:ALA:HB3	1:A:35:GLU:OE1	0.78	1.78	6	4
1:A:57:VAL:HG12	1:A:90:VAL:HG22	0.77	1.56	14	4
1:A:49:PHE:CE2	1:A:72:LEU:HD13	0.77	2.15	1	14
1:A:86:THR:OG1	1:A:132:LEU:HD21	0.77	1.77	14	4
1:A:18:CYS:SG	1:A:113:TYR:CD1	0.77	2.77	8	2
1:A:95:TYR:CD1	1:A:95:TYR:N	0.77	2.51	10	10
1:A:54:SER:CB	1:A:94:THR:HG1	0.76	1.92	12	2
1:A:55:MET:O	1:A:67:LEU:HD12	0.76	1.81	1	20
1:A:13:SER:CB	1:A:116:TYR:CZ	0.75	2.68	16	1
1:A:21:SER:O	1:A:109:VAL:HG11	0.75	1.82	19	20
1:A:39:ARG:CD	1:A:39:ARG:N	0.75	2.49	13	5
1:A:58:LEU:HD13	1:A:58:LEU:C	0.74	2.02	20	1
1:A:110:LEU:HD11	1:A:120:PHE:CE2	0.74	2.17	6	2
1:A:106:LEU:O	1:A:110:LEU:HD13	0.74	1.81	13	2
1:A:73:ILE:C	1:A:73:ILE:HD12	0.74	2.03	16	1
1:A:55:MET:SD	1:A:56:GLU:N	0.74	2.60	7	1
1:A:39:ARG:H	1:A:39:ARG:CD	0.74	1.96	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:ILE:HD13	1:A:101:ILE:C	0.73	2.03	3	3
1:A:22:LEU:HD12	1:A:109:VAL:CG2	0.73	2.13	16	20
1:A:39:ARG:NH1	1:A:89:ASN:ND2	0.73	2.36	9	2
1:A:79:THR:OG1	1:A:121:VAL:HG21	0.73	1.84	7	8
1:A:31:CYS:SG	1:A:37:LEU:HD22	0.73	2.24	5	12
1:A:39:ARG:N	1:A:39:ARG:CD	0.73	2.49	19	5
1:A:39:ARG:HH11	1:A:89:ASN:ND2	0.73	1.82	9	3
1:A:39:ARG:CD	1:A:39:ARG:H	0.73	1.96	6	5
1:A:107:ARG:NH2	1:A:118:GLN:HE22	0.72	1.83	1	6
1:A:83:VAL:HG23	1:A:83:VAL:O	0.71	1.85	17	8
1:A:47:ILE:HD11	1:A:72:LEU:HD21	0.71	1.60	4	4
1:A:107:ARG:HH12	1:A:111:ARG:NH1	0.71	1.84	20	1
1:A:107:ARG:NH1	1:A:111:ARG:NH1	0.71	2.39	20	1
1:A:34:GLY:N	1:A:92:ALA:O	0.71	2.24	19	20
1:A:48:TYR:CE2	1:A:100:TYR:CD2	0.71	2.79	16	13
1:A:49:PHE:CD2	1:A:72:LEU:HD13	0.71	2.20	13	19
1:A:125:GLN:NE2	1:A:125:GLN:H	0.71	1.83	9	1
1:A:13:SER:O	1:A:116:TYR:CE1	0.70	2.45	17	8
1:A:48:TYR:O	1:A:72:LEU:HD22	0.70	1.86	6	1
1:A:11:PHE:CD1	1:A:11:PHE:N	0.70	2.58	20	3
1:A:126:HIS:ND1	1:A:126:HIS:O	0.70	2.25	16	2
1:A:89:ASN:N	1:A:89:ASN:OD1	0.70	2.25	9	4
1:A:10:LEU:HD12	1:A:11:PHE:CG	0.70	2.22	15	5
1:A:48:TYR:CB	1:A:73:ILE:HG23	0.70	2.17	19	3
1:A:76:ASP:H	1:A:131:ASN:ND2	0.70	1.85	3	2
1:A:13:SER:O	1:A:116:TYR:CZ	0.70	2.45	9	8
1:A:39:ARG:NE	1:A:42:ASP:OD1	0.70	2.25	4	7
1:A:48:TYR:CD1	1:A:48:TYR:N	0.69	2.60	2	11
1:A:13:SER:O	1:A:116:TYR:CE2	0.69	2.45	2	3
1:A:39:ARG:CD	1:A:89:ASN:ND2	0.69	2.56	1	1
1:A:49:PHE:CD2	1:A:72:LEU:CD1	0.69	2.75	1	15
1:A:106:LEU:CD2	1:A:120:PHE:CE1	0.69	2.75	5	5
1:A:125:GLN:OE1	1:A:125:GLN:N	0.69	2.25	13	1
1:A:106:LEU:CD2	1:A:120:PHE:CZ	0.69	2.76	14	11
1:A:78:LEU:HD23	1:A:120:PHE:CZ	0.69	2.23	2	10
1:A:101:ILE:C	1:A:101:ILE:HD13	0.69	2.07	6	9
1:A:132:LEU:HD12	1:A:132:LEU:O	0.69	1.88	8	1
1:A:38:ILE:HG22	1:A:90:VAL:N	0.69	2.02	15	13
1:A:52:SER:O	1:A:96:CYS:SG	0.68	2.51	16	6
1:A:122:SER:O	1:A:125:GLN:NE2	0.68	2.26	13	2
1:A:58:LEU:HD13	1:A:59:LYS:N	0.68	2.04	7	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:GLU:CD	1:A:93:LEU:HD22	0.68	2.08	18	2
1:A:83:VAL:O	1:A:83:VAL:HG23	0.68	1.87	14	4
1:A:86:THR:HG23	1:A:132:LEU:HD11	0.68	1.63	18	2
1:A:40:GLN:OE1	1:A:59:LYS:NZ	0.68	2.27	8	1
1:A:41:GLY:N	1:A:86:THR:O	0.68	2.27	12	16
1:A:78:LEU:HD23	1:A:120:PHE:CE1	0.68	2.24	17	13
1:A:131:ASN:ND2	1:A:131:ASN:O	0.68	2.27	9	2
1:A:131:ASN:O	1:A:131:ASN:ND2	0.68	2.27	4	6
1:A:48:TYR:N	1:A:48:TYR:CD1	0.67	2.62	17	8
1:A:39:ARG:N	1:A:42:ASP:OD1	0.67	2.26	9	2
1:A:107:ARG:NH1	1:A:118:GLN:HE22	0.67	1.86	2	2
1:A:69:LYS:H	1:A:69:LYS:CD	0.67	2.01	16	2
1:A:107:ARG:NH2	1:A:118:GLN:NE2	0.67	2.42	1	1
1:A:37:LEU:O	1:A:37:LEU:HD12	0.67	1.90	7	1
1:A:125:GLN:NE2	1:A:126:HIS:N	0.67	2.43	7	2
1:A:78:LEU:HD13	1:A:124:ILE:HG21	0.67	1.64	14	1
1:A:40:GLN:NE2	1:A:87:ASN:O	0.67	2.28	15	3
1:A:11:PHE:CG	1:A:19:LEU:HD13	0.66	2.24	4	3
1:A:11:PHE:CD1	1:A:11:PHE:C	0.66	2.68	4	2
1:A:38:ILE:HD11	1:A:88:ALA:O	0.66	1.90	12	7
1:A:40:GLN:CG	1:A:87:ASN:O	0.66	2.44	5	11
1:A:59:LYS:HB3	1:A:64:LEU:HD13	0.66	1.66	17	14
1:A:110:LEU:O	1:A:113:TYR:N	0.66	2.29	11	20
1:A:107:ARG:NH1	1:A:111:ARG:HH11	0.66	1.89	20	1
1:A:56:GLU:OE1	1:A:63:VAL:CG1	0.66	2.44	13	6
1:A:20:ARG:O	1:A:24:LEU:HD23	0.66	1.91	16	4
1:A:89:ASN:OD1	1:A:90:VAL:N	0.66	2.29	5	2
1:A:18:CYS:O	1:A:21:SER:OG	0.65	2.11	1	7
1:A:94:THR:O	1:A:96:CYS:SG	0.65	2.49	8	2
1:A:54:SER:N	1:A:94:THR:OG1	0.65	2.29	2	8
1:A:110:LEU:HD21	1:A:120:PHE:CB	0.65	2.22	6	3
1:A:123:GLU:N	1:A:123:GLU:OE1	0.65	2.30	18	1
1:A:113:TYR:O	1:A:117:ALA:HB2	0.65	1.91	2	18
1:A:47:ILE:O	1:A:100:TYR:CB	0.65	2.44	7	1
1:A:118:GLN:O	1:A:121:VAL:HG22	0.65	1.92	20	9
1:A:99:GLN:O	1:A:99:GLN:NE2	0.65	2.30	3	1
1:A:106:LEU:O	1:A:109:VAL:HG23	0.65	1.92	20	20
1:A:63:VAL:CG1	1:A:65:ALA:O	0.65	2.45	16	1
1:A:11:PHE:CE1	1:A:19:LEU:HD22	0.65	2.27	4	2
1:A:77:SER:O	1:A:81:GLU:N	0.64	2.31	13	1
1:A:103:LEU:O	1:A:103:LEU:HD23	0.64	1.92	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ARG:CD	1:A:42:ASP:OD1	0.64	2.45	20	6
1:A:132:LEU:C	1:A:132:LEU:HD13	0.64	2.13	2	3
1:A:39:ARG:CZ	1:A:42:ASP:OD1	0.64	2.46	6	3
1:A:40:GLN:OE1	1:A:40:GLN:N	0.64	2.31	4	1
1:A:20:ARG:CD	1:A:20:ARG:C	0.63	2.67	20	10
1:A:42:ASP:O	1:A:85:LYS:CB	0.63	2.46	19	6
1:A:99:GLN:C	1:A:99:GLN:NE2	0.63	2.51	3	1
1:A:40:GLN:H	1:A:89:ASN:ND2	0.63	1.91	15	1
1:A:40:GLN:NE2	1:A:40:GLN:O	0.63	2.31	7	1
1:A:38:ILE:HD12	1:A:39:ARG:N	0.63	2.08	10	7
1:A:116:TYR:N	1:A:116:TYR:CD1	0.63	2.64	6	1
1:A:42:ASP:CB	1:A:86:THR:OG1	0.63	2.46	4	1
1:A:98:LEU:H	1:A:98:LEU:HD12	0.63	1.54	7	2
1:A:20:ARG:C	1:A:20:ARG:CD	0.62	2.67	10	4
1:A:80:LYS:O	1:A:82:GLN:NE2	0.62	2.31	10	2
1:A:126:HIS:CD2	1:A:126:HIS:O	0.62	2.52	8	1
1:A:59:LYS:O	1:A:60:ASP:OD1	0.62	2.17	15	1
1:A:39:ARG:CD	1:A:89:ASN:HD21	0.62	2.07	1	1
1:A:75:SER:OG	1:A:84:ILE:HD13	0.62	1.95	6	2
1:A:47:ILE:CG1	1:A:72:LEU:HD21	0.62	2.23	6	1
1:A:38:ILE:O	1:A:89:ASN:ND2	0.62	2.32	6	1
1:A:48:TYR:HB3	1:A:73:ILE:HG23	0.62	1.72	19	3
1:A:48:TYR:HB2	1:A:73:ILE:HG23	0.62	1.69	8	3
1:A:87:ASN:ND2	1:A:135:GLY:C	0.62	2.53	4	3
1:A:67:LEU:HD22	1:A:71:ASP:HB2	0.62	1.71	13	3
1:A:29:SER:O	1:A:98:LEU:O	0.62	2.17	16	20
1:A:56:GLU:OE2	1:A:91:LYS:O	0.62	2.18	13	18
1:A:59:LYS:NZ	1:A:87:ASN:OD1	0.62	2.32	18	2
1:A:39:ARG:N	1:A:42:ASP:OD2	0.62	2.32	20	2
1:A:122:SER:C	1:A:125:GLN:NE2	0.62	2.53	9	1
1:A:30:PHE:CD1	1:A:30:PHE:O	0.62	2.53	15	4
1:A:39:ARG:O	1:A:40:GLN:C	0.61	2.39	19	20
1:A:40:GLN:N	1:A:89:ASN:OD1	0.61	2.32	3	7
1:A:83:VAL:CG2	1:A:83:VAL:O	0.61	2.48	1	8
1:A:60:ASP:OD2	1:A:60:ASP:O	0.61	2.18	15	1
1:A:28:THR:HG22	1:A:99:GLN:OE1	0.61	1.95	20	1
1:A:11:PHE:N	1:A:11:PHE:CD1	0.61	2.67	11	4
1:A:77:SER:O	1:A:81:GLU:O	0.61	2.19	17	2
1:A:37:LEU:HD12	1:A:37:LEU:C	0.61	2.15	7	1
1:A:98:LEU:HD23	1:A:98:LEU:N	0.61	2.11	2	1
1:A:11:PHE:CG	1:A:12:GLU:N	0.61	2.68	1	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:THR:OG1	1:A:121:VAL:CG2	0.61	2.49	11	4
1:A:57:VAL:CG1	1:A:65:ALA:HB3	0.61	2.25	8	6
1:A:78:LEU:HD21	1:A:103:LEU:HD21	0.61	1.73	4	2
1:A:106:LEU:HD11	1:A:120:PHE:CE1	0.61	2.31	6	1
1:A:14:ALA:HB1	1:A:18:CYS:HB2	0.60	1.73	18	15
1:A:60:ASP:O	1:A:60:ASP:OD1	0.60	2.19	3	1
1:A:39:ARG:O	1:A:42:ASP:OD1	0.60	2.19	9	6
1:A:29:SER:OG	1:A:98:LEU:HD22	0.60	1.95	8	1
1:A:76:ASP:HB3	1:A:128:LEU:HD21	0.60	1.74	8	1
1:A:39:ARG:O	1:A:40:GLN:O	0.60	2.20	13	19
1:A:120:PHE:CE2	1:A:121:VAL:HG23	0.60	2.31	8	2
1:A:94:THR:HG22	1:A:95:TYR:CD1	0.60	2.32	14	3
1:A:27:LYS:O	1:A:100:TYR:O	0.60	2.19	12	20
1:A:72:LEU:HD13	1:A:73:ILE:N	0.60	2.10	6	1
1:A:38:ILE:HG21	1:A:86:THR:HG21	0.60	1.73	11	8
1:A:98:LEU:HD12	1:A:98:LEU:N	0.60	2.12	14	5
1:A:18:CYS:SG	1:A:110:LEU:HD12	0.60	2.37	16	3
1:A:80:LYS:O	1:A:81:GLU:O	0.60	2.20	16	7
1:A:31:CYS:SG	1:A:98:LEU:CD1	0.59	2.90	16	4
1:A:83:VAL:O	1:A:83:VAL:CG2	0.59	2.50	8	4
1:A:55:MET:SD	1:A:71:ASP:OD2	0.59	2.60	6	1
1:A:15:SER:C	1:A:17:GLY:N	0.59	2.53	13	20
1:A:121:VAL:CG2	1:A:122:SER:N	0.59	2.65	6	5
1:A:68:GLY:O	1:A:71:ASP:OD2	0.59	2.21	19	10
1:A:76:ASP:N	1:A:76:ASP:OD1	0.59	2.35	19	2
1:A:71:ASP:HA	1:A:129:THR:HG21	0.59	1.74	11	2
1:A:106:LEU:O	1:A:109:VAL:CG2	0.59	2.50	8	20
1:A:33:PRO:CG	1:A:95:TYR:CD2	0.59	2.85	2	9
1:A:17:GLY:O	1:A:21:SER:OG	0.59	2.18	13	8
1:A:82:GLN:O	1:A:84:ILE:HD12	0.59	1.98	10	2
1:A:59:LYS:O	1:A:62:THR:O	0.59	2.21	3	18
1:A:121:VAL:O	1:A:125:GLN:OE1	0.59	2.20	6	3
1:A:49:PHE:CE1	1:A:70:GLY:O	0.59	2.56	5	19
1:A:38:ILE:O	1:A:89:ASN:OD1	0.59	2.21	5	2
1:A:130:TYR:CD1	1:A:130:TYR:C	0.59	2.75	11	3
1:A:83:VAL:O	1:A:84:ILE:HD12	0.59	1.97	17	1
1:A:122:SER:O	1:A:125:GLN:OE1	0.58	2.21	10	8
1:A:82:GLN:CD	1:A:82:GLN:O	0.58	2.41	12	1
1:A:57:VAL:HG22	1:A:65:ALA:HB3	0.58	1.75	14	2
1:A:75:SER:CB	1:A:131:ASN:ND2	0.58	2.66	8	1
1:A:131:ASN:O	1:A:131:ASN:OD1	0.58	2.20	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LYS:O	1:A:60:ASP:OD2	0.58	2.21	3	1
1:A:56:GLU:O	1:A:56:GLU:OE1	0.58	2.21	7	9
1:A:81:GLU:CG	1:A:82:GLN:H	0.58	2.10	17	2
1:A:54:SER:OG	1:A:94:THR:OG1	0.58	2.21	2	12
1:A:131:ASN:OD1	1:A:131:ASN:O	0.58	2.21	13	3
1:A:56:GLU:O	1:A:56:GLU:OE2	0.58	2.21	8	1
1:A:18:CYS:O	1:A:21:SER:N	0.58	2.37	1	5
1:A:56:GLU:OE2	1:A:56:GLU:O	0.58	2.20	13	2
1:A:36:PHE:N	1:A:36:PHE:CD1	0.58	2.71	13	5
1:A:76:ASP:OD2	1:A:128:LEU:HD22	0.58	1.97	15	1
1:A:75:SER:OG	1:A:132:LEU:O	0.58	2.21	14	9
1:A:49:PHE:CD2	1:A:72:LEU:HD23	0.58	2.33	6	1
1:A:72:LEU:C	1:A:72:LEU:CD1	0.58	2.72	6	1
1:A:80:LYS:O	1:A:81:GLU:C	0.58	2.42	8	17
1:A:68:GLY:O	1:A:71:ASP:OD1	0.58	2.21	3	1
1:A:71:ASP:OD1	1:A:71:ASP:N	0.58	2.35	3	1
1:A:114:PRO:O	1:A:118:GLN:OE1	0.58	2.22	6	1
1:A:31:CYS:SG	1:A:37:LEU:CD1	0.58	2.91	10	10
1:A:56:GLU:OE1	1:A:56:GLU:O	0.57	2.23	19	5
1:A:121:VAL:O	1:A:125:GLN:NE2	0.57	2.36	5	2
1:A:131:ASN:CG	1:A:131:ASN:O	0.57	2.43	2	6
1:A:64:LEU:O	1:A:130:TYR:OH	0.57	2.21	19	4
1:A:122:SER:O	1:A:125:GLN:CG	0.57	2.53	18	4
1:A:119:LYS:O	1:A:123:GLU:OE1	0.57	2.22	3	3
1:A:40:GLN:NE2	1:A:59:LYS:NZ	0.57	2.52	20	2
1:A:73:ILE:HD12	1:A:74:GLY:CA	0.57	2.30	7	3
1:A:56:GLU:HG3	1:A:93:LEU:HD13	0.57	1.76	16	17
1:A:64:LEU:HD12	1:A:64:LEU:N	0.57	2.13	20	1
1:A:82:GLN:O	1:A:82:GLN:CD	0.57	2.42	17	1
1:A:15:SER:O	1:A:17:GLY:N	0.57	2.38	17	20
1:A:30:PHE:C	1:A:30:PHE:CD1	0.57	2.78	2	4
1:A:126:HIS:O	1:A:126:HIS:CD2	0.57	2.58	4	3
1:A:38:ILE:O	1:A:89:ASN:CG	0.57	2.43	5	1
1:A:25:ILE:O	1:A:25:ILE:HG23	0.57	1.99	19	11
1:A:59:LYS:O	1:A:60:ASP:CG	0.57	2.43	3	1
1:A:110:LEU:O	1:A:113:TYR:C	0.57	2.43	17	20
1:A:56:GLU:CD	1:A:56:GLU:O	0.57	2.43	12	8
1:A:77:SER:O	1:A:79:THR:N	0.57	2.38	16	8
1:A:79:THR:O	1:A:107:ARG:NH2	0.57	2.38	17	1
1:A:73:ILE:CD1	1:A:73:ILE:C	0.57	2.62	3	4
1:A:12:GLU:OE1	1:A:12:GLU:O	0.57	2.22	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:SER:CB	1:A:132:LEU:O	0.57	2.53	14	10
1:A:123:GLU:C	1:A:125:GLN:OE1	0.57	2.43	18	4
1:A:132:LEU:CD1	1:A:132:LEU:O	0.57	2.53	8	1
1:A:56:GLU:OE2	1:A:93:LEU:CD1	0.56	2.52	17	6
1:A:97:ASP:OD1	1:A:97:ASP:O	0.56	2.23	20	1
1:A:82:GLN:NE2	1:A:82:GLN:O	0.56	2.39	12	1
1:A:117:ALA:O	1:A:120:PHE:N	0.56	2.36	6	7
1:A:20:ARG:HD2	1:A:24:LEU:HD23	0.56	1.77	13	1
1:A:103:LEU:C	1:A:103:LEU:HD23	0.56	2.21	8	2
1:A:40:GLN:O	1:A:40:GLN:OE1	0.56	2.22	16	1
1:A:89:ASN:OD1	1:A:89:ASN:N	0.56	2.38	16	2
1:A:97:ASP:O	1:A:98:LEU:HD23	0.56	1.99	2	1
1:A:56:GLU:C	1:A:56:GLU:OE1	0.56	2.44	7	10
1:A:56:GLU:OE2	1:A:93:LEU:HD13	0.56	2.00	14	12
1:A:56:GLU:O	1:A:56:GLU:CD	0.56	2.44	16	6
1:A:85:LYS:HZ3	1:A:85:LYS:N	0.56	1.98	17	1
1:A:78:LEU:HD13	1:A:124:ILE:HD12	0.56	1.77	19	1
1:A:80:LYS:O	1:A:82:GLN:N	0.56	2.39	6	6
1:A:122:SER:C	1:A:125:GLN:OE1	0.56	2.45	13	4
1:A:103:LEU:HD23	1:A:103:LEU:O	0.56	2.00	11	1
1:A:115:GLU:N	1:A:115:GLU:OE1	0.56	2.39	17	1
1:A:40:GLN:CG	1:A:89:ASN:OD1	0.56	2.54	9	2
1:A:21:SER:C	1:A:109:VAL:HG11	0.55	2.22	19	20
1:A:71:ASP:O	1:A:71:ASP:OD1	0.55	2.24	9	2
1:A:48:TYR:O	1:A:72:LEU:CD1	0.55	2.55	19	5
1:A:108:GLU:O	1:A:111:ARG:CB	0.55	2.55	18	17
1:A:39:ARG:HH11	1:A:89:ASN:HD21	0.55	1.44	14	1
1:A:55:MET:SD	1:A:67:LEU:HD11	0.55	2.41	5	3
1:A:81:GLU:O	1:A:82:GLN:OE1	0.55	2.25	15	2
1:A:113:TYR:O	1:A:117:ALA:CB	0.55	2.55	2	17
1:A:56:GLU:OE1	1:A:56:GLU:C	0.55	2.45	6	5
1:A:39:ARG:HD3	1:A:39:ARG:H	0.55	1.62	5	6
1:A:69:LYS:CB	1:A:69:LYS:NZ	0.55	2.69	17	1
1:A:71:ASP:OD1	1:A:71:ASP:C	0.55	2.45	6	8
1:A:56:GLU:CG	1:A:93:LEU:HD13	0.55	2.32	17	17
1:A:40:GLN:CD	1:A:40:GLN:O	0.55	2.45	12	1
1:A:107:ARG:CZ	1:A:118:GLN:NE2	0.55	2.70	1	1
1:A:106:LEU:HD22	1:A:120:PHE:CZ	0.55	2.37	15	8
1:A:57:VAL:HG22	1:A:65:ALA:N	0.55	2.17	2	12
1:A:40:GLN:O	1:A:40:GLN:CD	0.55	2.45	16	1
1:A:38:ILE:C	1:A:38:ILE:HD12	0.55	2.22	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:ASN:O	1:A:131:ASN:CG	0.55	2.45	1	6
1:A:120:PHE:CE2	1:A:121:VAL:CG2	0.55	2.90	8	2
1:A:131:ASN:C	1:A:131:ASN:OD1	0.55	2.45	11	2
1:A:124:ILE:CG2	1:A:125:GLN:N	0.55	2.69	7	17
1:A:96:CYS:SG	1:A:98:LEU:HD11	0.55	2.42	15	7
1:A:122:SER:O	1:A:125:GLN:CD	0.55	2.45	4	5
1:A:67:LEU:CB	1:A:71:ASP:OD2	0.55	2.54	3	1
1:A:98:LEU:C	1:A:99:GLN:OE1	0.55	2.46	17	1
1:A:60:ASP:CG	1:A:60:ASP:O	0.55	2.44	15	1
1:A:31:CYS:SG	1:A:98:LEU:HD13	0.55	2.42	20	5
1:A:77:SER:C	1:A:79:THR:N	0.55	2.61	16	12
1:A:107:ARG:HH11	1:A:107:ARG:CG	0.55	2.15	16	4
1:A:38:ILE:HD12	1:A:38:ILE:C	0.55	2.21	12	2
1:A:13:SER:CB	1:A:116:TYR:CE2	0.55	2.90	16	1
1:A:126:HIS:CD2	1:A:127:ASP:OD1	0.55	2.60	5	1
1:A:11:PHE:CD1	1:A:19:LEU:HD13	0.55	2.36	4	2
1:A:55:MET:CG	1:A:56:GLU:N	0.54	2.70	19	2
1:A:12:GLU:OE2	1:A:12:GLU:O	0.54	2.25	2	1
1:A:54:SER:CB	1:A:94:THR:OG1	0.54	2.55	13	7
1:A:104:LYS:CD	1:A:104:LYS:N	0.54	2.70	20	1
1:A:44:LEU:CD2	1:A:75:SER:H	0.54	2.16	19	1
1:A:98:LEU:CD1	1:A:98:LEU:N	0.54	2.61	7	3
1:A:128:LEU:HD12	1:A:129:THR:N	0.54	2.17	18	1
1:A:40:GLN:CD	1:A:89:ASN:OD1	0.54	2.46	19	1
1:A:40:GLN:H	1:A:89:ASN:CG	0.54	2.06	18	4
1:A:125:GLN:CD	1:A:126:HIS:N	0.54	2.61	7	4
1:A:128:LEU:CD1	1:A:128:LEU:C	0.54	2.75	3	1
1:A:113:TYR:CD1	1:A:116:TYR:CE2	0.54	2.96	6	1
1:A:81:GLU:CG	1:A:82:GLN:N	0.54	2.70	17	2
1:A:107:ARG:NH1	1:A:110:LEU:HD23	0.54	2.17	6	1
1:A:59:LYS:CB	1:A:64:LEU:HD13	0.54	2.31	8	16
1:A:20:ARG:NE	1:A:20:ARG:O	0.54	2.40	4	1
1:A:125:GLN:OE1	1:A:126:HIS:N	0.54	2.41	1	1
1:A:59:LYS:NZ	1:A:87:ASN:O	0.54	2.30	16	2
1:A:125:GLN:C	1:A:125:GLN:OE1	0.54	2.46	16	1
1:A:30:PHE:N	1:A:30:PHE:CD1	0.54	2.76	3	1
1:A:25:ILE:HG23	1:A:25:ILE:O	0.54	2.03	17	9
1:A:76:ASP:H	1:A:131:ASN:CG	0.54	2.06	3	1
1:A:38:ILE:CG1	1:A:90:VAL:HG23	0.53	2.33	12	7
1:A:108:GLU:O	1:A:111:ARG:N	0.53	2.42	6	3
1:A:39:ARG:H	1:A:39:ARG:HD3	0.53	1.64	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:PHE:CD1	1:A:30:PHE:N	0.53	2.77	14	3
1:A:118:GLN:N	1:A:118:GLN:CD	0.53	2.58	6	1
1:A:46:ALA:HB1	1:A:101:ILE:O	0.53	2.03	11	9
1:A:107:ARG:NH1	1:A:110:LEU:CD2	0.53	2.71	6	1
1:A:102:SER:O	1:A:105:GLY:N	0.53	2.41	13	8
1:A:58:LEU:C	1:A:58:LEU:CD1	0.53	2.74	20	1
1:A:50:VAL:HG22	1:A:96:CYS:SG	0.53	2.44	5	5
1:A:121:VAL:HG23	1:A:122:SER:N	0.53	2.17	12	8
1:A:71:ASP:C	1:A:71:ASP:OD1	0.53	2.46	10	11
1:A:14:ALA:HB1	1:A:18:CYS:CB	0.53	2.33	11	4
1:A:48:TYR:HB2	1:A:73:ILE:CG2	0.53	2.34	13	11
1:A:38:ILE:HG22	1:A:90:VAL:HB	0.53	1.79	16	2
1:A:11:PHE:CD2	1:A:19:LEU:HD22	0.53	2.39	17	10
1:A:40:GLN:CB	1:A:89:ASN:OD1	0.53	2.57	3	5
1:A:10:LEU:HD13	1:A:120:PHE:CZ	0.53	2.39	6	2
1:A:101:ILE:HD11	1:A:106:LEU:HB2	0.53	1.81	13	8
1:A:110:LEU:HD21	1:A:120:PHE:HB2	0.53	1.81	6	1
1:A:101:ILE:C	1:A:101:ILE:CD1	0.52	2.78	16	6
1:A:78:LEU:HD13	1:A:124:ILE:CD1	0.52	2.35	13	2
1:A:131:ASN:OD1	1:A:131:ASN:C	0.52	2.47	10	1
1:A:76:ASP:H	1:A:131:ASN:HD21	0.52	1.47	3	1
1:A:15:SER:O	1:A:18:CYS:N	0.52	2.42	17	15
1:A:36:PHE:CD1	1:A:36:PHE:N	0.52	2.77	6	3
1:A:30:PHE:CD1	1:A:30:PHE:C	0.52	2.83	15	4
1:A:107:ARG:NH1	1:A:118:GLN:NE2	0.52	2.57	2	1
1:A:21:SER:O	1:A:109:VAL:CG1	0.52	2.57	13	19
1:A:40:GLN:CB	1:A:87:ASN:O	0.52	2.56	16	12
1:A:81:GLU:O	1:A:82:GLN:CD	0.52	2.47	7	2
1:A:77:SER:C	1:A:79:THR:H	0.52	2.07	16	7
1:A:89:ASN:ND2	1:A:90:VAL:N	0.52	2.57	4	1
1:A:125:GLN:CD	1:A:125:GLN:C	0.52	2.68	8	4
1:A:109:VAL:HG23	1:A:110:LEU:H	0.52	1.65	14	10
1:A:74:GLY:O	1:A:128:LEU:HD21	0.52	2.04	3	1
1:A:20:ARG:CD	1:A:24:LEU:HD23	0.52	2.34	19	2
1:A:120:PHE:C	1:A:120:PHE:CD1	0.52	2.82	17	2
1:A:72:LEU:H	1:A:129:THR:CB	0.52	2.16	20	2
1:A:110:LEU:O	1:A:113:TYR:O	0.52	2.27	8	12
1:A:82:GLN:NE2	1:A:83:VAL:HG22	0.52	2.19	14	4
1:A:40:GLN:CD	1:A:87:ASN:O	0.52	2.47	1	1
1:A:73:ILE:C	1:A:73:ILE:CD1	0.52	2.68	7	2
1:A:101:ILE:HD11	1:A:106:LEU:CB	0.52	2.35	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:ILE:HD12	1:A:74:GLY:H	0.51	1.61	19	1
1:A:77:SER:O	1:A:77:SER:OG	0.51	2.27	10	2
1:A:99:GLN:N	1:A:99:GLN:OE1	0.51	2.42	17	1
1:A:50:VAL:HG21	1:A:55:MET:SD	0.51	2.45	3	2
1:A:126:HIS:ND1	1:A:126:HIS:C	0.51	2.62	16	1
1:A:82:GLN:CD	1:A:83:VAL:H	0.51	2.09	2	6
1:A:18:CYS:SG	1:A:113:TYR:CD2	0.51	2.94	20	2
1:A:120:PHE:CG	1:A:121:VAL:N	0.51	2.78	8	10
1:A:31:CYS:SG	1:A:37:LEU:CD2	0.51	2.99	13	5
1:A:60:ASP:OD2	1:A:64:LEU:CD1	0.51	2.59	3	1
1:A:40:GLN:HE21	1:A:87:ASN:CG	0.51	2.09	1	1
1:A:124:ILE:CG2	1:A:125:GLN:HE21	0.51	2.19	12	1
1:A:71:ASP:OD1	1:A:71:ASP:O	0.51	2.29	16	1
1:A:89:ASN:CG	1:A:90:VAL:N	0.51	2.64	6	2
1:A:85:LYS:HB3	1:A:85:LYS:HZ2	0.51	1.66	6	1
1:A:40:GLN:NE2	1:A:89:ASN:HD21	0.51	2.04	19	1
1:A:56:GLU:C	1:A:56:GLU:CD	0.51	2.69	16	7
1:A:80:LYS:CG	1:A:80:LYS:O	0.51	2.59	16	1
1:A:10:LEU:CD1	1:A:11:PHE:CG	0.51	2.94	20	5
1:A:107:ARG:NH1	1:A:107:ARG:CG	0.51	2.73	18	4
1:A:84:ILE:N	1:A:84:ILE:HD12	0.51	2.20	12	1
1:A:72:LEU:HD23	1:A:128:LEU:HA	0.51	1.81	9	2
1:A:127:ASP:OD1	1:A:127:ASP:N	0.51	2.44	16	4
1:A:126:HIS:CG	1:A:126:HIS:O	0.50	2.65	12	5
1:A:73:ILE:HD13	1:A:130:TYR:CZ	0.50	2.41	6	2
1:A:85:LYS:NZ	1:A:85:LYS:CB	0.50	2.75	6	1
1:A:84:ILE:HG21	1:A:132:LEU:O	0.50	2.06	17	1
1:A:107:ARG:CG	1:A:107:ARG:NH1	0.50	2.71	16	1
1:A:77:SER:O	1:A:80:LYS:N	0.50	2.43	5	2
1:A:94:THR:HG22	1:A:95:TYR:CE1	0.50	2.42	18	3
1:A:134:GLU:CD	1:A:134:GLU:O	0.50	2.50	3	1
1:A:83:VAL:HG22	1:A:83:VAL:O	0.50	2.07	9	1
1:A:68:GLY:N	1:A:71:ASP:OD2	0.50	2.43	3	1
1:A:101:ILE:CD1	1:A:101:ILE:C	0.50	2.70	3	4
1:A:20:ARG:CA	1:A:20:ARG:HE	0.50	2.19	4	1
1:A:128:LEU:HD13	1:A:128:LEU:C	0.50	2.26	3	1
1:A:44:LEU:HD22	1:A:132:LEU:HD12	0.50	1.82	6	1
1:A:40:GLN:OE1	1:A:40:GLN:O	0.50	2.30	12	1
1:A:35:GLU:OE1	1:A:37:LEU:CD2	0.50	2.59	16	1
1:A:40:GLN:NE2	1:A:59:LYS:HZ3	0.50	2.05	3	1
1:A:15:SER:CB	1:A:113:TYR:OH	0.50	2.60	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:LYS:O	1:A:123:GLU:N	0.49	2.45	4	4
1:A:127:ASP:C	1:A:127:ASP:OD1	0.49	2.48	14	1
1:A:112:LEU:N	1:A:112:LEU:HD22	0.49	2.21	16	1
1:A:134:GLU:H	1:A:134:GLU:CD	0.49	2.08	16	1
1:A:85:LYS:H	1:A:85:LYS:HZ3	0.49	1.48	17	1
1:A:124:ILE:CG2	1:A:125:GLN:NE2	0.49	2.75	2	1
1:A:133:ARG:NH2	1:A:134:GLU:O	0.49	2.46	9	1
1:A:31:CYS:SG	1:A:98:LEU:HD12	0.49	2.47	16	2
1:A:125:GLN:C	1:A:125:GLN:CD	0.49	2.69	14	2
1:A:39:ARG:N	1:A:39:ARG:HD3	0.49	2.22	20	5
1:A:107:ARG:CZ	1:A:118:GLN:HE22	0.49	2.21	14	4
1:A:76:ASP:CB	1:A:128:LEU:HD21	0.49	2.36	8	1
1:A:11:PHE:CD1	1:A:19:LEU:HD22	0.49	2.42	4	1
1:A:39:ARG:CD	1:A:42:ASP:CG	0.49	2.81	15	4
1:A:126:HIS:ND1	1:A:127:ASP:OD1	0.49	2.46	2	1
1:A:44:LEU:HD22	1:A:132:LEU:HD23	0.49	1.82	16	2
1:A:44:LEU:O	1:A:84:ILE:O	0.49	2.30	16	2
1:A:39:ARG:H	1:A:42:ASP:CG	0.49	2.10	1	2
1:A:132:LEU:CG	1:A:132:LEU:O	0.49	2.60	8	1
1:A:44:LEU:CB	1:A:84:ILE:O	0.49	2.61	1	1
1:A:57:VAL:O	1:A:57:VAL:CG2	0.49	2.60	20	2
1:A:38:ILE:HG12	1:A:90:VAL:HG23	0.49	1.85	12	7
1:A:22:LEU:CD1	1:A:109:VAL:HG21	0.49	2.33	6	13
1:A:97:ASP:C	1:A:97:ASP:OD1	0.49	2.50	12	1
1:A:130:TYR:C	1:A:130:TYR:CD1	0.48	2.85	13	1
1:A:13:SER:CB	1:A:116:TYR:CE1	0.48	2.96	2	2
1:A:73:ILE:CD1	1:A:132:LEU:HD23	0.48	2.38	17	2
1:A:72:LEU:HD22	1:A:73:ILE:N	0.48	2.23	6	1
1:A:78:LEU:CD2	1:A:124:ILE:HD12	0.48	2.36	20	11
1:A:62:THR:HG22	1:A:63:VAL:N	0.48	2.23	16	16
1:A:20:ARG:NE	1:A:20:ARG:C	0.48	2.66	4	1
1:A:57:VAL:HG22	1:A:65:ALA:CB	0.48	2.38	1	2
1:A:13:SER:OG	1:A:116:TYR:CE2	0.48	2.65	16	1
1:A:59:LYS:O	1:A:64:LEU:CD1	0.48	2.62	5	1
1:A:39:ARG:HD3	1:A:39:ARG:N	0.48	2.22	6	5
1:A:46:ALA:O	1:A:48:TYR:CE1	0.48	2.66	7	1
1:A:48:TYR:H	1:A:73:ILE:HG13	0.48	1.69	3	1
1:A:50:VAL:CG2	1:A:55:MET:SD	0.48	3.02	3	1
1:A:103:LEU:HD13	1:A:103:LEU:O	0.48	2.09	14	1
1:A:78:LEU:HB3	1:A:121:VAL:HG12	0.48	1.85	6	2
1:A:85:LYS:NZ	1:A:135:GLY:H	0.48	2.07	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:TYR:O	1:A:72:LEU:CD2	0.48	2.61	6	1
1:A:10:LEU:HD12	1:A:11:PHE:N	0.47	2.24	10	6
1:A:134:GLU:C	1:A:134:GLU:OE1	0.47	2.52	9	1
1:A:55:MET:C	1:A:56:GLU:CG	0.47	2.81	9	2
1:A:76:ASP:OD1	1:A:76:ASP:C	0.47	2.50	9	2
1:A:40:GLN:O	1:A:40:GLN:NE2	0.47	2.47	6	1
1:A:85:LYS:HZ2	1:A:85:LYS:CB	0.47	2.22	6	1
1:A:21:SER:OG	1:A:109:VAL:HB	0.47	2.08	1	6
1:A:57:VAL:CG2	1:A:64:LEU:CB	0.47	2.92	8	1
1:A:72:LEU:HD22	1:A:73:ILE:H	0.47	1.68	6	1
1:A:118:GLN:CD	1:A:118:GLN:N	0.47	2.65	17	1
1:A:15:SER:O	1:A:16:ARG:C	0.47	2.53	16	20
1:A:33:PRO:HG3	1:A:95:TYR:CD2	0.47	2.44	2	14
1:A:20:ARG:HG3	1:A:21:SER:N	0.47	2.23	4	3
1:A:21:SER:C	1:A:109:VAL:CG1	0.47	2.83	13	15
1:A:38:ILE:CD1	1:A:88:ALA:O	0.47	2.62	12	2
1:A:39:ARG:NH1	1:A:89:ASN:HD21	0.47	2.06	14	1
1:A:13:SER:HB3	1:A:116:TYR:CZ	0.47	2.44	16	1
1:A:44:LEU:O	1:A:84:ILE:HD12	0.47	2.09	15	1
1:A:50:VAL:CG2	1:A:98:LEU:HD22	0.47	2.40	2	1
1:A:126:HIS:O	1:A:126:HIS:CG	0.47	2.68	4	3
1:A:100:TYR:CD1	1:A:100:TYR:O	0.47	2.67	8	2
1:A:13:SER:HB2	1:A:116:TYR:CZ	0.47	2.44	16	1
1:A:77:SER:H	1:A:125:GLN:HE21	0.47	1.52	5	1
1:A:80:LYS:O	1:A:80:LYS:CG	0.47	2.62	5	1
1:A:132:LEU:O	1:A:132:LEU:HD13	0.47	2.10	2	2
1:A:60:ASP:O	1:A:61:ASN:CB	0.47	2.63	20	1
1:A:55:MET:O	1:A:67:LEU:CD1	0.47	2.63	18	16
1:A:79:THR:OG1	1:A:121:VAL:CG1	0.47	2.52	8	1
1:A:22:LEU:HD21	1:A:106:LEU:HD12	0.47	1.85	2	1
1:A:38:ILE:HD13	1:A:86:THR:HB	0.47	1.86	12	1
1:A:13:SER:OG	1:A:116:TYR:CE1	0.47	2.56	4	2
1:A:128:LEU:C	1:A:128:LEU:HD12	0.47	2.30	18	1
1:A:106:LEU:HD22	1:A:120:PHE:CE1	0.47	2.45	1	4
1:A:80:LYS:NZ	1:A:80:LYS:O	0.47	2.31	17	1
1:A:103:LEU:O	1:A:103:LEU:HD13	0.47	2.10	1	1
1:A:109:VAL:HG23	1:A:110:LEU:N	0.46	2.24	16	8
1:A:13:SER:O	1:A:116:TYR:CD1	0.46	2.68	9	2
1:A:65:ALA:HB2	1:A:130:TYR:CZ	0.46	2.44	4	4
1:A:97:ASP:OD1	1:A:97:ASP:C	0.46	2.53	15	1
1:A:48:TYR:CD1	1:A:73:ILE:CG1	0.46	2.97	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:SER:CA	1:A:131:ASN:ND2	0.46	2.79	8	1
1:A:13:SER:O	1:A:13:SER:OG	0.46	2.31	15	1
1:A:110:LEU:HD23	1:A:117:ALA:HA	0.46	1.88	19	5
1:A:98:LEU:N	1:A:98:LEU:CD1	0.46	2.78	3	2
1:A:56:GLU:CD	1:A:56:GLU:C	0.46	2.73	10	4
1:A:106:LEU:HD21	1:A:120:PHE:CE1	0.46	2.45	14	2
1:A:38:ILE:HG12	1:A:86:THR:HG21	0.46	1.86	4	4
1:A:20:ARG:CA	1:A:20:ARG:NE	0.46	2.79	4	1
1:A:100:TYR:CD1	1:A:100:TYR:C	0.46	2.88	8	7
1:A:58:LEU:CD2	1:A:63:VAL:HG13	0.46	2.40	1	2
1:A:52:SER:C	1:A:96:CYS:HG	0.46	2.09	12	1
1:A:59:LYS:HZ1	1:A:87:ASN:C	0.46	2.13	18	1
1:A:40:GLN:CB	1:A:89:ASN:ND2	0.46	2.79	15	2
1:A:60:ASP:N	1:A:60:ASP:OD1	0.46	2.47	10	1
1:A:57:VAL:O	1:A:64:LEU:N	0.46	2.47	8	5
1:A:106:LEU:HD21	1:A:120:PHE:CD1	0.46	2.46	13	3
1:A:80:LYS:NZ	1:A:80:LYS:CB	0.46	2.77	14	1
1:A:72:LEU:HD21	1:A:124:ILE:HD11	0.46	1.87	17	1
1:A:76:ASP:O	1:A:77:SER:OG	0.46	2.28	15	3
1:A:23:SER:HA	1:A:26:ILE:CG1	0.46	2.41	19	20
1:A:15:SER:C	1:A:17:GLY:H	0.46	2.13	13	11
1:A:38:ILE:HD13	1:A:86:THR:CB	0.46	2.41	12	1
1:A:48:TYR:CD1	1:A:73:ILE:HG23	0.46	2.46	5	4
1:A:30:PHE:O	1:A:30:PHE:CD1	0.46	2.69	18	1
1:A:101:ILE:HG12	1:A:102:SER:N	0.46	2.26	10	11
1:A:50:VAL:HG12	1:A:70:GLY:H	0.46	1.71	3	9
1:A:86:THR:HA	1:A:132:LEU:HD11	0.46	1.87	13	1
1:A:96:CYS:HG	1:A:98:LEU:HD11	0.46	1.71	14	2
1:A:16:ARG:CG	1:A:16:ARG:HH11	0.46	2.24	18	1
1:A:106:LEU:HD23	1:A:107:ARG:N	0.46	2.26	11	2
1:A:76:ASP:H	1:A:131:ASN:HD22	0.46	1.54	11	1
1:A:110:LEU:HD21	1:A:120:PHE:CG	0.46	2.45	6	1
1:A:29:SER:HB3	1:A:100:TYR:CZ	0.46	2.46	7	1
1:A:67:LEU:H	1:A:67:LEU:HD12	0.46	1.70	11	4
1:A:54:SER:OG	1:A:94:THR:CB	0.46	2.64	11	1
1:A:122:SER:CA	1:A:125:GLN:NE2	0.45	2.79	9	1
1:A:125:GLN:O	1:A:125:GLN:CD	0.45	2.55	14	1
1:A:20:ARG:HE	1:A:20:ARG:C	0.45	2.14	4	1
1:A:76:ASP:N	1:A:131:ASN:HD22	0.45	2.09	8	1
1:A:40:GLN:N	1:A:89:ASN:ND2	0.45	2.63	15	1
1:A:32:ALA:HB1	1:A:33:PRO:HD2	0.45	1.87	19	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:SER:CA	1:A:125:GLN:HE22	0.45	2.24	9	1
1:A:82:GLN:HE22	1:A:83:VAL:HG22	0.45	1.72	2	2
1:A:20:ARG:CD	1:A:21:SER:N	0.45	2.79	2	2
1:A:64:LEU:HD22	1:A:88:ALA:HB2	0.45	1.88	14	1
1:A:132:LEU:HD12	1:A:132:LEU:C	0.45	2.32	8	1
1:A:60:ASP:C	1:A:61:ASN:CG	0.45	2.75	1	1
1:A:85:LYS:HB3	1:A:85:LYS:NZ	0.45	2.27	6	1
1:A:85:LYS:NZ	1:A:134:GLU:OE1	0.45	2.50	2	1
1:A:57:VAL:HA	1:A:89:ASN:O	0.45	2.12	9	12
1:A:11:PHE:O	1:A:14:ALA:N	0.45	2.49	13	5
1:A:110:LEU:HD23	1:A:120:PHE:HB3	0.45	1.88	10	1
1:A:134:GLU:O	1:A:134:GLU:OE2	0.45	2.34	3	1
1:A:46:ALA:CB	1:A:101:ILE:O	0.45	2.65	4	2
1:A:108:GLU:CD	1:A:108:GLU:C	0.45	2.75	20	1
1:A:47:ILE:CD1	1:A:124:ILE:HD11	0.45	2.41	15	2
1:A:57:VAL:CG2	1:A:57:VAL:O	0.45	2.64	13	1
1:A:85:LYS:NZ	1:A:85:LYS:O	0.45	2.50	4	1
1:A:128:LEU:HD13	1:A:129:THR:N	0.45	2.26	3	1
1:A:71:ASP:HB2	1:A:129:THR:HG21	0.45	1.89	18	2
1:A:61:ASN:N	1:A:61:ASN:ND2	0.45	2.65	19	1
1:A:81:GLU:O	1:A:82:GLN:NE2	0.45	2.50	18	1
1:A:40:GLN:CB	1:A:89:ASN:HD21	0.45	2.25	18	2
1:A:54:SER:O	1:A:96:CYS:SG	0.45	2.75	8	1
1:A:20:ARG:HD2	1:A:21:SER:N	0.44	2.27	2	7
1:A:39:ARG:HH11	1:A:89:ASN:HD22	0.44	1.51	16	1
1:A:100:TYR:C	1:A:100:TYR:CD1	0.44	2.89	10	4
1:A:63:VAL:HG23	1:A:66:ILE:HD11	0.44	1.88	6	3
1:A:120:PHE:CD2	1:A:121:VAL:HG23	0.44	2.47	8	2
1:A:69:LYS:NZ	1:A:69:LYS:HB3	0.44	2.26	17	1
1:A:59:LYS:NZ	1:A:88:ALA:HA	0.44	2.27	18	5
1:A:56:GLU:HB3	1:A:65:ALA:O	0.44	2.12	9	1
1:A:69:LYS:HD3	1:A:69:LYS:H	0.44	1.72	16	1
1:A:25:ILE:C	1:A:27:LYS:HZ3	0.44	2.16	3	1
1:A:67:LEU:HD12	1:A:67:LEU:H	0.44	1.72	9	2
1:A:118:GLN:NE2	1:A:118:GLN:CA	0.44	2.81	13	1
1:A:81:GLU:O	1:A:82:GLN:C	0.44	2.55	5	1
1:A:78:LEU:CD2	1:A:103:LEU:HD21	0.44	2.42	1	1
1:A:61:ASN:ND2	1:A:61:ASN:N	0.44	2.65	1	1
1:A:56:GLU:CB	1:A:65:ALA:O	0.44	2.66	4	3
1:A:20:ARG:HD3	1:A:24:LEU:HD23	0.44	1.88	19	1
1:A:110:LEU:HD21	1:A:120:PHE:CD2	0.44	2.48	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:GLU:O	1:A:125:GLN:OE1	0.44	2.36	18	3
1:A:112:LEU:N	1:A:112:LEU:CD2	0.44	2.80	16	1
1:A:13:SER:HB2	1:A:116:TYR:CE2	0.44	2.48	16	1
1:A:57:VAL:O	1:A:63:VAL:HG12	0.44	2.11	13	1
1:A:87:ASN:ND2	1:A:135:GLY:O	0.44	2.45	17	1
1:A:39:ARG:HD2	1:A:89:ASN:ND2	0.44	2.25	1	1
1:A:39:ARG:HD3	1:A:89:ASN:ND2	0.44	2.25	1	1
1:A:72:LEU:H	1:A:129:THR:HB	0.44	1.73	7	6
1:A:78:LEU:CD2	1:A:120:PHE:CE1	0.44	3.01	19	2
1:A:47:ILE:HD11	1:A:72:LEU:HD11	0.44	1.90	12	1
1:A:55:MET:SD	1:A:67:LEU:CD1	0.44	3.06	5	1
1:A:82:GLN:O	1:A:82:GLN:NE2	0.43	2.51	17	1
1:A:11:PHE:H	1:A:11:PHE:HD1	0.43	1.44	20	1
1:A:25:ILE:HG21	1:A:105:GLY:C	0.43	2.33	19	2
1:A:42:ASP:O	1:A:85:LYS:CA	0.43	2.66	19	2
1:A:70:GLY:O	1:A:71:ASP:O	0.43	2.36	10	1
1:A:33:PRO:HG2	1:A:95:TYR:CE2	0.43	2.48	6	1
1:A:37:LEU:CD1	1:A:37:LEU:C	0.43	2.79	7	1
1:A:48:TYR:CD1	1:A:73:ILE:HG12	0.43	2.48	7	1
1:A:13:SER:HB2	1:A:116:TYR:CE1	0.43	2.48	2	1
1:A:131:ASN:ND2	1:A:133:ARG:CG	0.43	2.81	1	1
1:A:44:LEU:HD11	1:A:46:ALA:O	0.43	2.12	9	3
1:A:11:PHE:HD2	1:A:19:LEU:HD22	0.43	1.72	3	4
1:A:73:ILE:HD13	1:A:130:TYR:CE2	0.43	2.48	6	1
1:A:100:TYR:C	1:A:101:ILE:HG22	0.43	2.33	11	6
1:A:44:LEU:O	1:A:82:GLN:NE2	0.43	2.51	12	1
1:A:69:LYS:CD	1:A:69:LYS:N	0.43	2.78	16	1
1:A:118:GLN:CA	1:A:118:GLN:NE2	0.43	2.81	6	1
1:A:64:LEU:CD1	1:A:64:LEU:N	0.43	2.81	20	1
1:A:35:GLU:OE1	1:A:36:PHE:N	0.43	2.52	19	1
1:A:78:LEU:HB2	1:A:121:VAL:HG13	0.43	1.90	13	2
1:A:73:ILE:CD1	1:A:74:GLY:N	0.43	2.66	7	2
1:A:122:SER:HA	1:A:125:GLN:NE2	0.43	2.28	9	1
1:A:79:THR:HG23	1:A:121:VAL:HG21	0.43	1.91	14	1
1:A:66:ILE:N	1:A:66:ILE:HD12	0.43	2.29	8	1
1:A:10:LEU:HB2	1:A:120:PHE:CZ	0.43	2.49	6	1
1:A:125:GLN:CD	1:A:125:GLN:N	0.43	2.66	13	1
1:A:78:LEU:HB3	1:A:121:VAL:HG22	0.43	1.90	13	1
1:A:57:VAL:CG2	1:A:64:LEU:HB2	0.43	2.44	15	2
1:A:124:ILE:HG22	1:A:125:GLN:NE2	0.43	2.28	2	1
1:A:56:GLU:OE2	1:A:93:LEU:HD22	0.43	2.13	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:CYS:HG	1:A:113:TYR:HD2	0.43	1.56	6	1
1:A:56:GLU:OE1	1:A:63:VAL:HG12	0.43	2.14	11	3
1:A:11:PHE:C	1:A:13:SER:N	0.43	2.72	4	1
1:A:75:SER:CA	1:A:131:ASN:HD22	0.43	2.27	8	1
1:A:106:LEU:C	1:A:106:LEU:HD23	0.43	2.34	11	1
1:A:134:GLU:OE1	1:A:134:GLU:C	0.42	2.58	10	1
1:A:50:VAL:HG12	1:A:70:GLY:N	0.42	2.29	16	5
1:A:72:LEU:HG	1:A:73:ILE:N	0.42	2.28	16	4
1:A:85:LYS:HZ2	1:A:85:LYS:HB3	0.42	1.75	9	1
1:A:123:GLU:CA	1:A:123:GLU:OE1	0.42	2.64	18	1
1:A:84:ILE:HD12	1:A:84:ILE:N	0.42	2.29	3	1
1:A:38:ILE:CG2	1:A:86:THR:HG21	0.42	2.44	6	1
1:A:87:ASN:CB	1:A:135:GLY:CA	0.42	2.97	12	1
1:A:55:MET:C	1:A:55:MET:SD	0.42	2.98	7	1
1:A:127:ASP:N	1:A:127:ASP:OD1	0.42	2.52	2	1
1:A:133:ARG:O	1:A:134:GLU:C	0.42	2.58	12	1
1:A:113:TYR:CD1	1:A:116:TYR:CD2	0.42	3.08	6	1
1:A:67:LEU:HB2	1:A:71:ASP:CB	0.42	2.45	9	9
1:A:104:LYS:N	1:A:104:LYS:HD3	0.42	2.29	12	1
1:A:16:ARG:NH1	1:A:16:ARG:CG	0.42	2.79	18	1
1:A:86:THR:HG23	1:A:132:LEU:CD1	0.42	2.42	18	1
1:A:38:ILE:CG2	1:A:90:VAL:HB	0.42	2.45	16	1
1:A:61:ASN:O	1:A:61:ASN:OD1	0.42	2.38	16	1
1:A:97:ASP:OD1	1:A:98:LEU:N	0.42	2.53	12	1
1:A:124:ILE:O	1:A:127:ASP:OD1	0.42	2.38	11	2
1:A:106:LEU:O	1:A:110:LEU:HB2	0.42	2.15	5	1
1:A:48:TYR:CE2	1:A:73:ILE:HG21	0.42	2.50	15	1
1:A:110:LEU:HD23	1:A:120:PHE:CD2	0.42	2.50	9	2
1:A:49:PHE:CE2	1:A:72:LEU:HD22	0.42	2.50	15	1
1:A:77:SER:OG	1:A:77:SER:O	0.42	2.27	6	1
1:A:118:GLN:NE2	1:A:118:GLN:HA	0.41	2.30	6	2
1:A:80:LYS:CD	1:A:80:LYS:O	0.41	2.68	16	1
1:A:99:GLN:C	1:A:99:GLN:HE21	0.41	2.16	3	1
1:A:98:LEU:CD2	1:A:98:LEU:N	0.41	2.75	2	1
1:A:125:GLN:N	1:A:125:GLN:OE1	0.41	2.53	1	1
1:A:78:LEU:CD1	1:A:78:LEU:N	0.41	2.83	5	1
1:A:125:GLN:HA	1:A:128:LEU:HD23	0.41	1.92	8	1
1:A:82:GLN:O	1:A:84:ILE:CD1	0.41	2.68	3	1
1:A:78:LEU:HG	1:A:103:LEU:HD21	0.41	1.92	6	1
1:A:132:LEU:CD1	1:A:132:LEU:C	0.41	2.85	2	1
1:A:132:LEU:HD22	1:A:133:ARG:N	0.41	2.31	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:CYS:SG	1:A:113:TYR:CG	0.41	3.11	18	1
1:A:39:ARG:HD2	1:A:89:ASN:HD21	0.41	1.75	1	1
1:A:110:LEU:O	1:A:117:ALA:HB2	0.41	2.15	16	4
1:A:79:THR:O	1:A:79:THR:HG22	0.41	2.16	8	1
1:A:87:ASN:HD22	1:A:87:ASN:C	0.41	2.18	11	1
1:A:121:VAL:O	1:A:124:ILE:N	0.41	2.49	6	1
1:A:38:ILE:CG1	1:A:90:VAL:CG2	0.41	2.99	12	4
1:A:76:ASP:CG	1:A:77:SER:N	0.41	2.74	12	1
1:A:132:LEU:HD12	1:A:133:ARG:N	0.41	2.31	16	1
1:A:44:LEU:CD1	1:A:48:TYR:CE1	0.41	3.04	10	1
1:A:85:LYS:C	1:A:85:LYS:HZ3	0.41	2.19	4	1
1:A:49:PHE:CB	1:A:99:GLN:OE1	0.41	2.69	8	1
1:A:38:ILE:HG22	1:A:90:VAL:CB	0.41	2.44	15	1
1:A:32:ALA:HB1	1:A:33:PRO:CD	0.41	2.45	15	3
1:A:58:LEU:CD1	1:A:59:LYS:N	0.41	2.82	14	1
1:A:123:GLU:CA	1:A:125:GLN:OE1	0.41	2.68	7	1
1:A:47:ILE:HD12	1:A:124:ILE:HD11	0.41	1.91	20	1
1:A:58:LEU:HD13	1:A:59:LYS:H	0.41	1.75	14	1
1:A:98:LEU:HD12	1:A:98:LEU:H	0.41	1.76	3	1
1:A:10:LEU:HB2	1:A:120:PHE:CE2	0.41	2.51	13	1
1:A:59:LYS:HD3	1:A:60:ASP:N	0.41	2.31	13	1
1:A:71:ASP:OD1	1:A:72:LEU:N	0.41	2.54	11	2
1:A:99:GLN:N	1:A:99:GLN:CD	0.41	2.73	17	1
1:A:10:LEU:HG	1:A:10:LEU:H	0.41	1.51	9	1
1:A:125:GLN:CD	1:A:126:HIS:H	0.41	2.19	13	1
1:A:89:ASN:ND2	1:A:89:ASN:N	0.41	2.68	18	1
1:A:81:GLU:O	1:A:81:GLU:OE1	0.41	2.39	10	1
1:A:113:TYR:CD1	1:A:113:TYR:N	0.41	2.88	8	1
1:A:117:ALA:C	1:A:119:LYS:N	0.41	2.72	6	1
1:A:51:CYS:SG	1:A:52:SER:N	0.41	2.94	15	1
1:A:47:ILE:CG1	1:A:72:LEU:HD11	0.41	2.46	15	1
1:A:37:LEU:HG	1:A:38:ILE:N	0.41	2.30	7	1
1:A:47:ILE:HG13	1:A:48:TYR:N	0.41	2.30	7	1
1:A:127:ASP:O	1:A:128:LEU:C	0.41	2.59	12	1
1:A:11:PHE:HD1	1:A:11:PHE:H	0.41	1.57	13	1
1:A:25:ILE:HG23	1:A:101:ILE:CD1	0.41	2.45	14	1
1:A:22:LEU:CD1	1:A:109:VAL:CG2	0.41	2.97	14	1
1:A:75:SER:HB3	1:A:131:ASN:ND2	0.41	2.28	8	1
1:A:75:SER:HA	1:A:131:ASN:ND2	0.41	2.31	8	1
1:A:107:ARG:HG2	1:A:107:ARG:NH1	0.40	2.30	16	1
1:A:106:LEU:CD2	1:A:120:PHE:CE2	0.40	3.04	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:VAL:HG22	1:A:98:LEU:HD22	0.40	1.90	2	1
1:A:82:GLN:NE2	1:A:83:VAL:H	0.40	2.13	2	1
1:A:63:VAL:HG12	1:A:66:ILE:HD12	0.40	1.92	16	1
1:A:40:GLN:HE21	1:A:59:LYS:NZ	0.40	2.12	20	1
1:A:55:MET:CE	1:A:98:LEU:HD21	0.40	2.47	12	1
1:A:134:GLU:OE1	1:A:134:GLU:O	0.40	2.40	9	1
1:A:38:ILE:HG13	1:A:90:VAL:N	0.40	2.32	14	1
1:A:60:ASP:OD2	1:A:64:LEU:HD11	0.40	2.16	3	1
1:A:69:LYS:CB	1:A:69:LYS:HZ2	0.40	2.30	17	1
1:A:57:VAL:O	1:A:63:VAL:HA	0.40	2.16	20	1
1:A:76:ASP:O	1:A:77:SER:CB	0.40	2.69	12	1
1:A:110:LEU:CD2	1:A:120:PHE:CG	0.40	3.05	9	1
1:A:27:LYS:HB3	1:A:100:TYR:CE1	0.40	2.52	14	1
1:A:131:ASN:C	1:A:131:ASN:ND2	0.40	2.74	14	1
1:A:47:ILE:O	1:A:100:TYR:HB2	0.40	2.16	6	1
1:A:40:GLN:NE2	1:A:87:ASN:ND2	0.40	2.69	1	1
1:A:48:TYR:CD2	1:A:100:TYR:HB3	0.40	2.52	16	1
1:A:118:GLN:HA	1:A:118:GLN:NE2	0.40	2.31	4	1
1:A:47:ILE:HG13	1:A:72:LEU:HD11	0.40	1.93	15	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	125/143 (87%)	116±2 (93±1%)	6±2 (5±1%)	3±1 (3±1%)	9	44
All	All	2500/2860 (87%)	2314 (93%)	117 (5%)	69 (3%)	9	44

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	40	GLN	20
1	A	81	GLU	17
1	A	76	ASP	7

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Mol	Chain	Res	Type	Models (Total)
1	A	71	ASP	7
1	A	78	LEU	6
1	A	16	ARG	5
1	A	128	LEU	4
1	A	82	GLN	3

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	109/126 (87%)	63±3 (58±2%)	46±3 (42±2%)	0 4
All	All	2180/2520 (87%)	1263 (58%)	917 (42%)	0 4

All 96 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	24	LEU	20
1	A	38	ILE	20
1	A	49	PHE	20
1	A	85	LYS	20
1	A	67	LEU	20
1	A	25	ILE	20
1	A	120	PHE	20
1	A	124	ILE	20
1	A	18	CYS	20
1	A	95	TYR	20
1	A	10	LEU	20
1	A	101	ILE	19
1	A	63	VAL	19
1	A	100	TYR	19
1	A	26	ILE	19
1	A	56	GLU	18
1	A	23	SER	17
1	A	75	SER	17
1	A	54	SER	17
1	A	52	SER	16

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Mol	Chain	Res	Type	Models (Total)
1	A	11	PHE	16
1	A	64	LEU	16
1	A	48	TYR	15
1	A	107	ARG	15
1	A	98	LEU	14
1	A	55	MET	14
1	A	39	ARG	14
1	A	103	LEU	14
1	A	20	ARG	14
1	A	35	GLU	13
1	A	22	LEU	12
1	A	73	ILE	12
1	A	50	VAL	11
1	A	44	LEU	11
1	A	58	LEU	11
1	A	42	ASP	11
1	A	57	VAL	10
1	A	15	SER	10
1	A	59	LYS	10
1	A	131	ASN	10
1	A	79	THR	10
1	A	71	ASP	10
1	A	127	ASP	10
1	A	61	ASN	10
1	A	93	LEU	9
1	A	125	GLN	9
1	A	47	ILE	9
1	A	82	GLN	9
1	A	28	THR	9
1	A	134	GLU	9
1	A	13	SER	8
1	A	69	LYS	8
1	A	89	ASN	8
1	A	112	LEU	8
1	A	36	PHE	8
1	A	80	LYS	7
1	A	132	LEU	7
1	A	106	LEU	7
1	A	122	SER	6
1	A	60	ASP	6
1	A	97	ASP	6
1	A	30	PHE	6

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Mol	Chain	Res	Type	Models (Total)
1	A	40	GLN	5
1	A	78	LEU	5
1	A	99	GLN	5
1	A	130	TYR	5
1	A	123	GLU	5
1	A	126	HIS	5
1	A	113	TYR	5
1	A	128	LEU	5
1	A	84	ILE	4
1	A	119	LYS	4
1	A	77	SER	4
1	A	27	LYS	4
1	A	81	GLU	4
1	A	51	CYS	4
1	A	87	ASN	3
1	A	16	ARG	3
1	A	86	THR	3
1	A	115	GLU	3
1	A	45	GLN	3
1	A	76	ASP	3
1	A	133	ARG	2
1	A	104	LYS	2
1	A	12	GLU	2
1	A	94	THR	2
1	A	29	SER	2
1	A	37	LEU	2
1	A	66	ILE	2
1	A	110	LEU	2
1	A	116	TYR	1
1	A	108	GLU	1
1	A	121	VAL	1
1	A	96	CYS	1
1	A	83	VAL	1
1	A	111	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [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

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: 2mhf_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1524
Number of shifts mapped to atoms	1524
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	133	-0.27 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	123	-0.06 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	129	0.10 ± 0.09	None needed (< 0.5 ppm)
^{15}N	130	0.43 ± 0.20	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 1277 atoms were assigned a chemical shift out of a possible 1548. 18 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	623/626 (100%)	250/250 (100%)	249/252 (99%)	124/124 (100%)
Sidechain	625/821 (76%)	361/478 (76%)	258/307 (84%)	6/36 (17%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	29/101 (29%)	18/53 (34%)	11/46 (24%)	0/2 (0%)
Overall	1277/1548 (82%)	629/781 (81%)	518/605 (86%)	130/162 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1340 atoms were assigned a chemical shift out of a possible 1672. 20 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	649/669 (97%)	260/267 (97%)	261/270 (97%)	128/132 (97%)
Sidechain	662/902 (73%)	383/526 (73%)	272/337 (81%)	7/39 (18%)
Aromatic	29/101 (29%)	18/53 (34%)	11/46 (24%)	0/2 (0%)
Overall	1340/1672 (80%)	661/846 (78%)	544/653 (83%)	135/173 (78%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:

