



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:02 PM BST

PDB ID : 1ILO
Title : NMR structure of a thioredoxin, MtH895, from the archeon Methanobacterium thermoautotrophicum strain delta H.
Authors : Bhattacharyya, S.; Habibi-Nazhad, B.; Slupsky, C.M.; Sykes, B.D.; Wishart, D.S.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2001-05-08

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

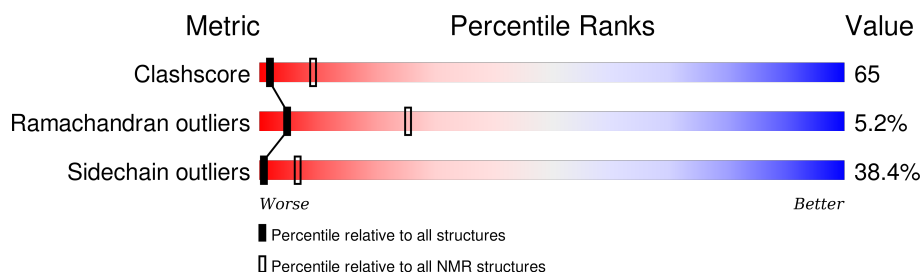
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 65%.

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 ≥ 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	77	<div> <div>25%</div> <div>57%</div> <div>12%</div> <div>• 5%</div> </div>

2 Ensemble composition and analysis

This entry contains 21 models. Model 21 is the overall representative, medoid model (most similar to other models). The authors have identified model 14 as representative, based on the following criterion: *closest to the average*.

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:1-A:73 (73)	0.28	21

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, 3, 4, 5, 6, 7, 8, 9, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21
2	2, 10

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1207 atoms, of which 621 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called conserved hypothetical protein MtH895.

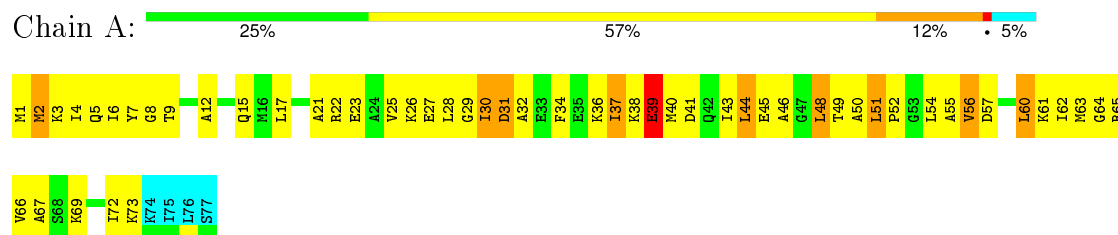
Mol	Chain	Residues	Atoms						Trace
1	A	77	Total	C	H	N	O	S	0
			1207	368	621	97	114	7	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: conserved hypothetical protein MtH895

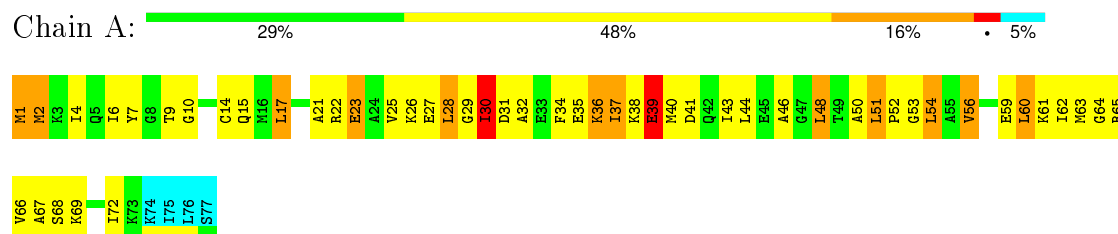


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

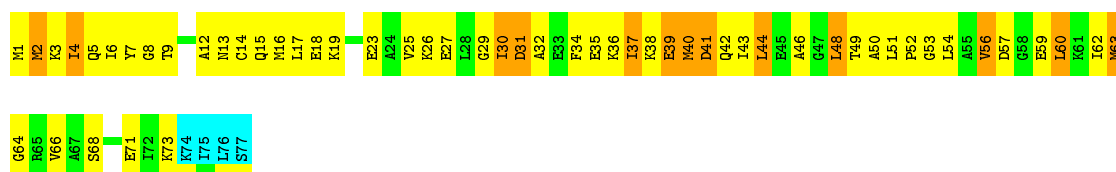
- Molecule 1: conserved hypothetical protein MtH895



4.2.2 Score per residue for model 2

- Molecule 1: conserved hypothetical protein MtH895

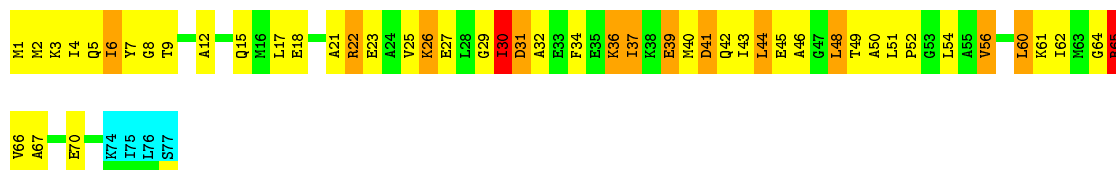




4.2.3 Score per residue for model 3

- Molecule 1: conserved hypothetical protein MtH895

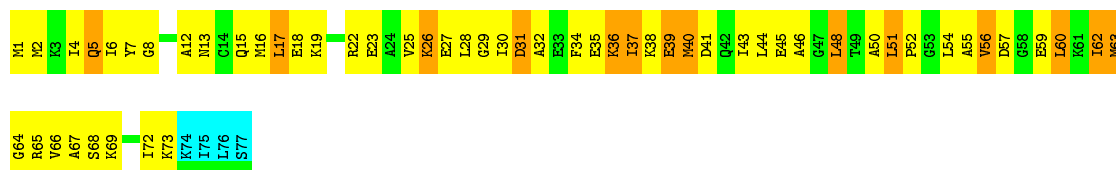
Chain A: 31% 45% 16% 5%



4.2.4 Score per residue for model 4

- Molecule 1: conserved hypothetical protein MtH895

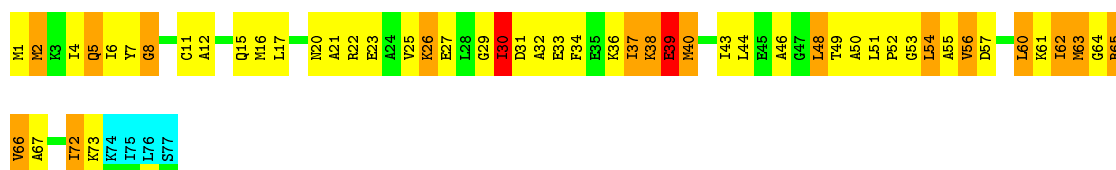
Chain A: 22% 55% 18% 5%



4.2.5 Score per residue for model 5

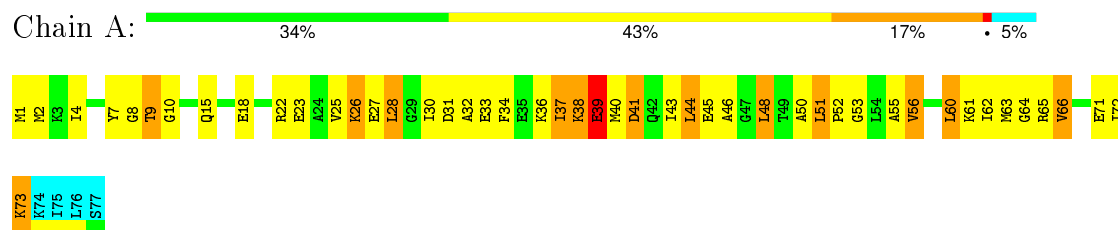
- Molecule 1: conserved hypothetical protein MtH895

Chain A: 26% 45% 21% 5%



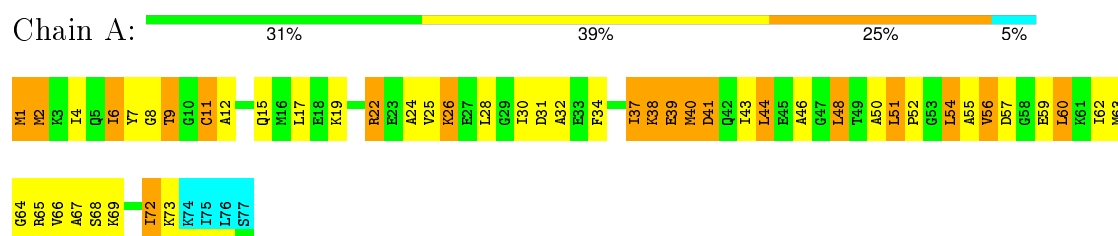
4.2.6 Score per residue for model 6

- Molecule 1: conserved hypothetical protein MtH895



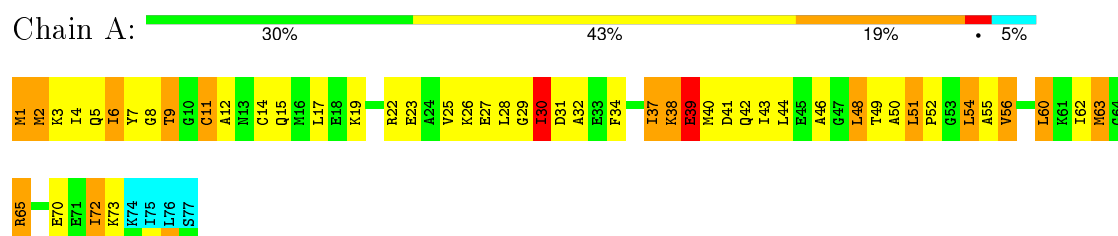
4.2.7 Score per residue for model 7

- Molecule 1: conserved hypothetical protein MtH895



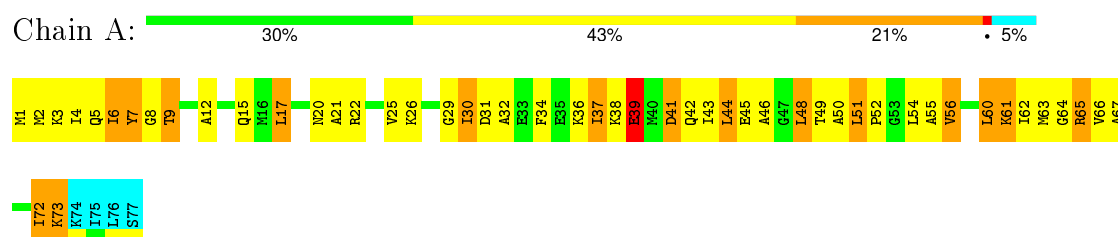
4.2.8 Score per residue for model 8

- Molecule 1: conserved hypothetical protein MtH895



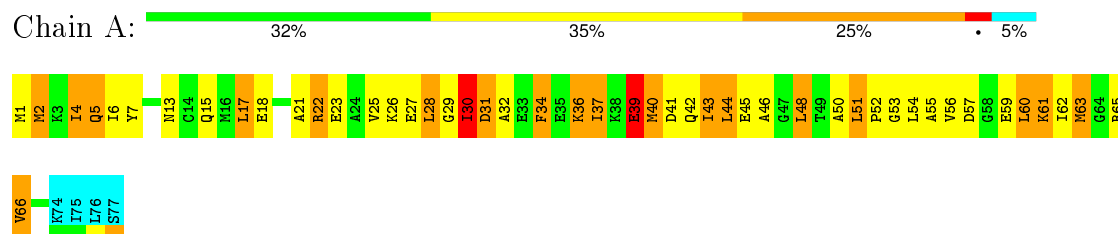
4.2.9 Score per residue for model 9

- Molecule 1: conserved hypothetical protein MtH895



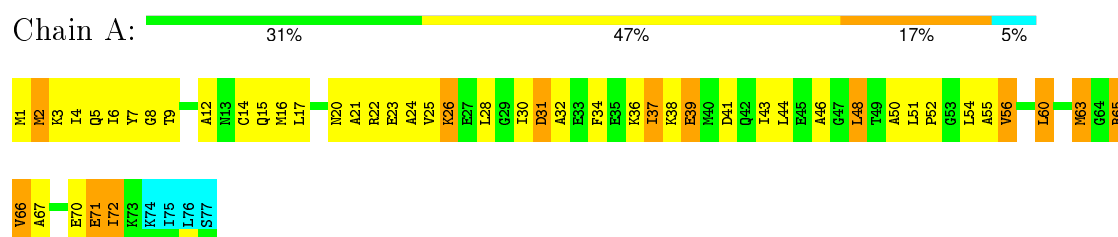
4.2.10 Score per residue for model 10

- Molecule 1: conserved hypothetical protein MtH895



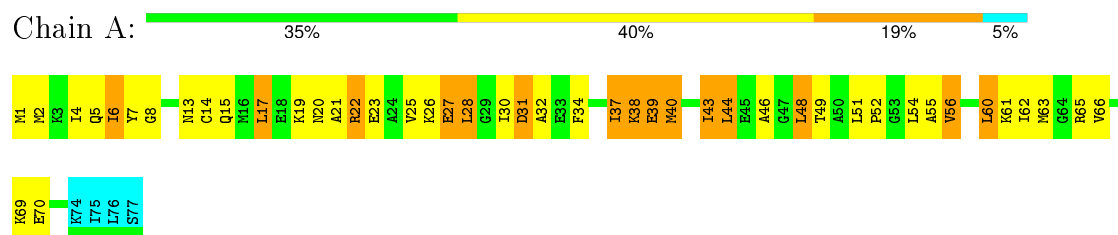
4.2.11 Score per residue for model 11

- Molecule 1: conserved hypothetical protein MtH895



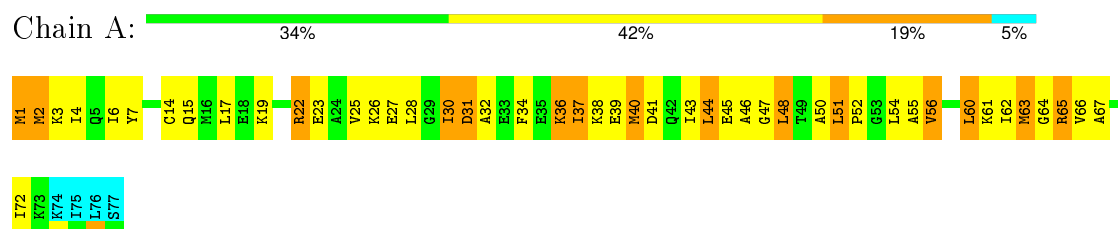
4.2.12 Score per residue for model 12

- Molecule 1: conserved hypothetical protein MtH895



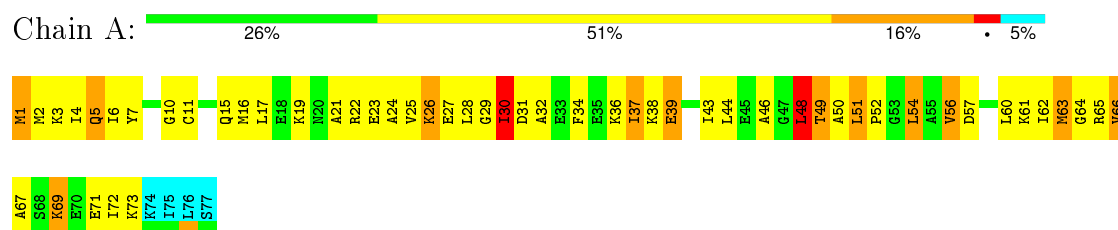
4.2.13 Score per residue for model 13

- Molecule 1: conserved hypothetical protein MtH895



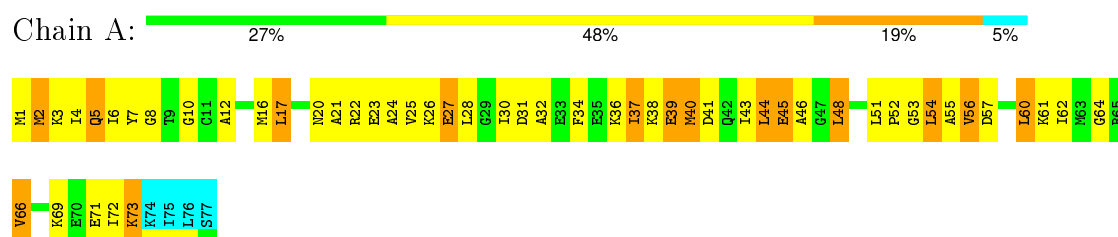
4.2.14 Score per residue for model 14

- Molecule 1: conserved hypothetical protein MtH895



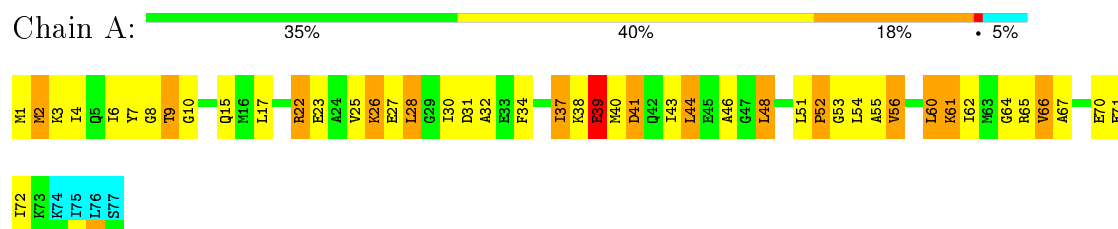
4.2.15 Score per residue for model 15

- Molecule 1: conserved hypothetical protein MtH895



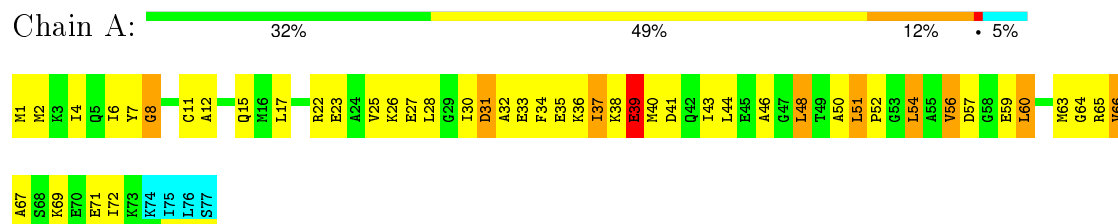
4.2.16 Score per residue for model 16

- Molecule 1: conserved hypothetical protein MtH895



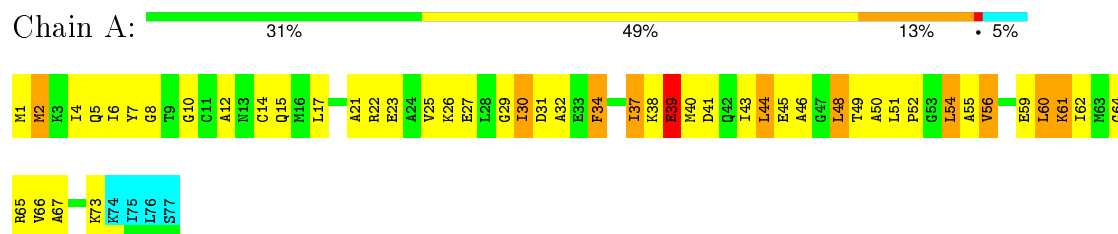
4.2.17 Score per residue for model 17

- Molecule 1: conserved hypothetical protein MtH895



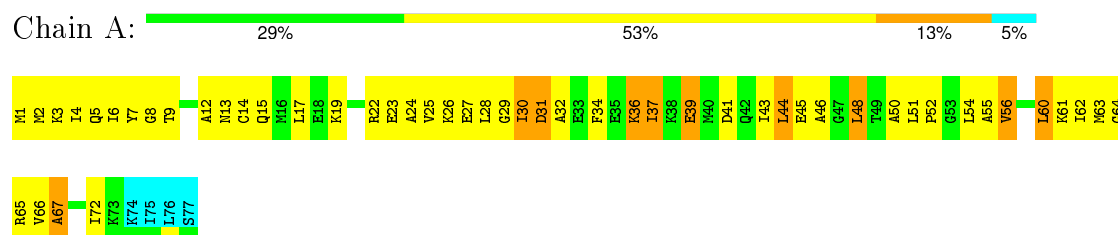
4.2.18 Score per residue for model 18

- Molecule 1: conserved hypothetical protein MtH895



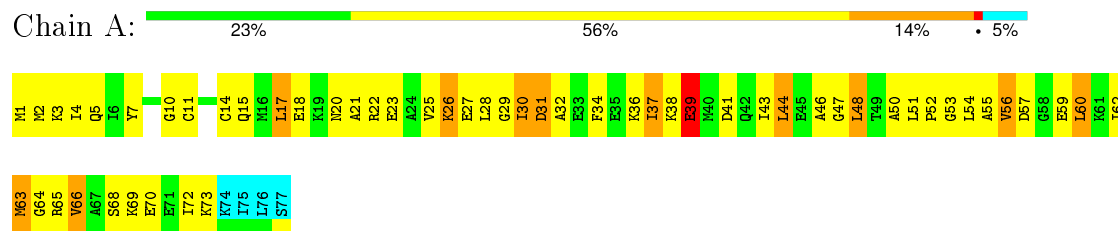
4.2.19 Score per residue for model 19

- Molecule 1: conserved hypothetical protein MtH895



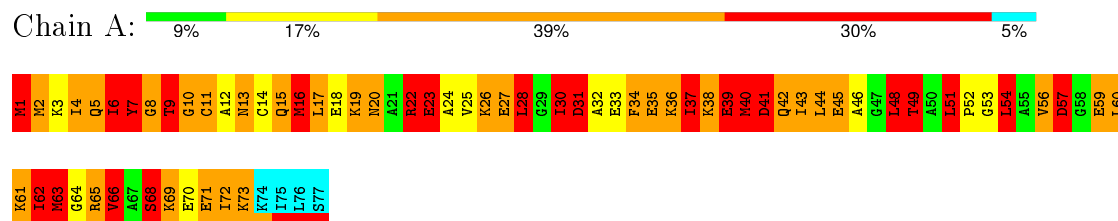
4.2.20 Score per residue for model 20

- Molecule 1: conserved hypothetical protein MtH895



4.2.21 Score per residue for model 21 (medoid)

- Molecule 1: conserved hypothetical protein MtH895



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 21 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
X-PLOR	structure solution	3.851
X-PLOR	refinement	3.851

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

Chemical shift file(s)	BMRB entry 4991
Number of chemical shift lists	1
Total number of shifts	664
Number of shifts mapped to atoms	664
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	65%

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	1.36±4.35	8±37/557 (1.5±6.7%)	1.22±3.43	9±38/742 (1.2±5.1%)
All	All	4.56	177/11697 (1.5%)	3.64	183/15582 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.1±0.6	0.0±0.0
All	All	3	0

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	45	GLU	CD-OE1	-94.08	0.22	1.25	21	1
1	A	39	GLU	CD-OE1	-88.04	0.28	1.25	21	1
1	A	65	ARG	CZ-NH1	-87.68	0.19	1.33	21	1
1	A	22	ARG	CZ-NH1	-86.24	0.20	1.33	21	1
1	A	33	GLU	CD-OE1	-84.25	0.33	1.25	21	1
1	A	71	GLU	CD-OE2	-82.80	0.34	1.25	21	1
1	A	35	GLU	CD-OE2	-82.53	0.34	1.25	21	1
1	A	27	GLU	CD-OE2	-81.12	0.36	1.25	21	1
1	A	59	GLU	CD-OE2	-80.00	0.37	1.25	21	1
1	A	59	GLU	CD-OE1	-79.48	0.38	1.25	21	1
1	A	23	GLU	CD-OE1	-77.03	0.41	1.25	21	1
1	A	70	GLU	CD-OE2	-76.09	0.41	1.25	21	1
1	A	71	GLU	CD-OE1	-75.72	0.42	1.25	21	1
1	A	70	GLU	CD-OE1	-74.22	0.44	1.25	21	1
1	A	18	GLU	CD-OE2	-72.14	0.46	1.25	21	1
1	A	35	GLU	CD-OE1	-70.83	0.47	1.25	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	27	GLU	CD-OE1	-69.67	0.49	1.25	21	1
1	A	23	GLU	CD-OE2	-69.52	0.49	1.25	21	1
1	A	18	GLU	CD-OE1	-69.07	0.49	1.25	21	1
1	A	33	GLU	CD-OE2	-65.97	0.53	1.25	21	1
1	A	45	GLU	CD-OE2	-63.10	0.56	1.25	21	1
1	A	39	GLU	CD-OE2	-62.05	0.57	1.25	21	1
1	A	7	TYR	CE2-CZ	58.13	2.14	1.38	9	2
1	A	65	ARG	NE-CZ	-57.56	0.58	1.33	21	1
1	A	68	SER	CB-OG	-57.18	0.68	1.42	21	1
1	A	7	TYR	CE1-CZ	-52.82	0.69	1.38	21	1
1	A	7	TYR	CG-CD2	-50.82	0.73	1.39	21	1
1	A	7	TYR	CG-CD1	-50.05	0.74	1.39	21	1
1	A	7	TYR	CD2-CE2	49.83	2.14	1.39	9	1
1	A	65	ARG	CZ-NH2	-49.22	0.69	1.33	21	1
1	A	22	ARG	CZ-NH2	-46.06	0.73	1.33	21	1
1	A	45	GLU	CG-CD	-44.93	0.84	1.51	21	1
1	A	34	PHE	CG-CD2	-42.83	0.74	1.38	21	1
1	A	38	LYS	CE-NZ	-42.50	0.42	1.49	21	1
1	A	49	THR	CB-OG1	-41.78	0.59	1.43	21	1
1	A	35	GLU	CG-CD	-41.65	0.89	1.51	21	1
1	A	34	PHE	CG-CD1	-41.60	0.76	1.38	21	1
1	A	65	ARG	CD-NE	-40.48	0.77	1.46	21	1
1	A	42	GLN	CD-OE1	-39.85	0.36	1.24	21	1
1	A	11	CYS	CB-SG	-39.76	1.14	1.82	21	1
1	A	59	GLU	CG-CD	-39.30	0.93	1.51	21	1
1	A	9	THR	C-O	-39.24	0.48	1.23	21	1
1	A	27	GLU	CG-CD	-38.22	0.94	1.51	21	1
1	A	33	GLU	CG-CD	-37.78	0.95	1.51	21	1
1	A	22	ARG	NE-CZ	-37.17	0.84	1.33	21	1
1	A	71	GLU	CG-CD	-36.80	0.96	1.51	21	1
1	A	22	ARG	CD-NE	-36.51	0.84	1.46	21	1
1	A	39	GLU	CG-CD	-36.40	0.97	1.51	21	1
1	A	31	ASP	CG-OD1	-34.39	0.46	1.25	21	1
1	A	34	PHE	CE1-CZ	-33.78	0.73	1.37	21	1
1	A	34	PHE	CE2-CZ	-32.91	0.74	1.37	21	1
1	A	57	ASP	CG-OD1	-32.78	0.49	1.25	21	1
1	A	41	ASP	CG-OD2	-32.50	0.50	1.25	21	1
1	A	2	MET	CG-SD	-32.10	0.97	1.81	21	1
1	A	66	VAL	CB-CG2	-31.86	0.85	1.52	21	1
1	A	61	LYS	CE-NZ	-31.44	0.70	1.49	21	1
1	A	13	ASN	CG-OD1	-30.91	0.56	1.24	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	70	GLU	CG-CD	-30.75	1.05	1.51	21	1
1	A	57	ASP	CG-OD2	-30.37	0.55	1.25	21	1
1	A	31	ASP	CG-OD2	-30.32	0.55	1.25	21	1
1	A	26	LYS	CE-NZ	-30.05	0.73	1.49	21	1
1	A	23	GLU	CB-CG	-29.79	0.95	1.52	21	1
1	A	54	LEU	CG-CD2	-29.69	0.42	1.51	21	1
1	A	9	THR	CB-OG1	-29.66	0.83	1.43	21	1
1	A	38	LYS	CD-CE	-29.60	0.77	1.51	21	1
1	A	66	VAL	CB-CG1	-29.58	0.90	1.52	21	1
1	A	26	LYS	CD-CE	-29.33	0.78	1.51	21	1
1	A	69	LYS	CB-CG	-29.05	0.74	1.52	21	1
1	A	35	GLU	CB-CG	-29.00	0.97	1.52	21	1
1	A	17	LEU	CG-CD2	-28.93	0.44	1.51	21	1
1	A	9	THR	C-N	-28.81	0.81	1.33	21	1
1	A	69	LYS	CE-NZ	-28.11	0.78	1.49	21	1
1	A	70	GLU	CB-CG	-28.05	0.98	1.52	21	1
1	A	40	MET	CB-CG	-28.01	0.61	1.51	21	1
1	A	42	GLN	CG-CD	-27.91	0.86	1.51	21	1
1	A	73	LYS	CE-NZ	-27.84	0.79	1.49	21	1
1	A	5	GLN	CD-OE1	-27.66	0.63	1.24	21	1
1	A	16	MET	CG-SD	-27.52	1.09	1.81	21	1
1	A	23	GLU	CG-CD	-27.41	1.10	1.51	21	1
1	A	36	LYS	CD-CE	-27.11	0.83	1.51	21	1
1	A	42	GLN	CD-NE2	-27.03	0.65	1.32	21	1
1	A	20	ASN	CG-OD1	-26.70	0.65	1.24	21	1
1	A	41	ASP	CG-OD1	-26.55	0.64	1.25	21	1
1	A	19	LYS	CD-CE	-26.46	0.85	1.51	21	1
1	A	69	LYS	CD-CE	-26.35	0.85	1.51	21	1
1	A	73	LYS	CD-CE	-25.88	0.86	1.51	21	1
1	A	18	GLU	CG-CD	-25.76	1.13	1.51	21	1
1	A	30	ILE	CB-CG1	-25.14	0.83	1.54	21	1
1	A	63	MET	CG-SD	-24.98	1.16	1.81	21	1
1	A	49	THR	CB-CG2	-24.83	0.70	1.52	21	1
1	A	13	ASN	CG-ND2	-24.68	0.71	1.32	21	1
1	A	60	LEU	CG-CD1	-24.68	0.60	1.51	21	1
1	A	1	MET	CG-SD	-24.07	1.18	1.81	21	1
1	A	19	LYS	CE-NZ	-23.73	0.89	1.49	21	1
1	A	65	ARG	CG-CD	-23.36	0.93	1.51	21	1
1	A	17	LEU	CG-CD1	-22.72	0.67	1.51	21	1
1	A	28	LEU	CG-CD2	-22.34	0.69	1.51	21	1
1	A	54	LEU	CG-CD1	-22.30	0.69	1.51	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	61	LYS	CD-CE	-21.78	0.96	1.51	21	1
1	A	1	MET	CB-CG	-21.78	0.81	1.51	21	1
1	A	39	GLU	CB-CG	-21.76	1.10	1.52	21	1
1	A	36	LYS	CE-NZ	-21.65	0.94	1.49	21	1
1	A	30	ILE	CB-CG2	-21.55	0.86	1.52	21	1
1	A	3	LYS	CE-NZ	-21.28	0.95	1.49	21	1
1	A	40	MET	CG-SD	-20.63	1.27	1.81	21	1
1	A	62	ILE	CB-CG1	-19.84	0.98	1.54	21	1
1	A	3	LYS	CB-CG	-19.56	0.99	1.52	21	1
1	A	10	GLY	C-O	-19.09	0.93	1.23	21	1
1	A	5	GLN	CG-CD	-19.05	1.07	1.51	21	1
1	A	63	MET	CB-CG	-18.64	0.91	1.51	21	1
1	A	65	ARG	CB-CG	-18.15	1.03	1.52	21	1
1	A	62	ILE	CB-CG2	-18.09	0.96	1.52	21	1
1	A	3	LYS	CD-CE	-17.80	1.06	1.51	21	1
1	A	59	GLU	CB-CG	-17.76	1.18	1.52	21	1
1	A	72	ILE	CB-CG1	-17.76	1.04	1.54	21	1
1	A	16	MET	SD-CE	-17.72	0.78	1.77	21	1
1	A	1	MET	SD-CE	-17.55	0.79	1.77	21	1
1	A	48	LEU	C-O	-17.52	0.90	1.23	21	1
1	A	40	MET	SD-CE	-17.42	0.80	1.77	21	1
1	A	9	THR	CB-CG2	-17.29	0.95	1.52	21	1
1	A	51	LEU	CG-CD1	-17.11	0.88	1.51	21	1
1	A	60	LEU	CG-CD2	-16.73	0.90	1.51	21	1
1	A	28	LEU	CG-CD1	-16.43	0.91	1.51	21	1
1	A	33	GLU	CB-CG	-16.30	1.21	1.52	21	1
1	A	51	LEU	CG-CD2	-15.94	0.92	1.51	21	1
1	A	6	ILE	CB-CG1	-15.85	1.09	1.54	21	1
1	A	72	ILE	CB-CG2	-15.76	1.03	1.52	21	1
1	A	6	ILE	CB-CG2	-14.79	1.07	1.52	21	1
1	A	38	LYS	CG-CD	-14.63	1.02	1.52	21	1
1	A	62	ILE	CG1-CD1	-14.59	0.49	1.50	21	1
1	A	38	LYS	CB-CG	-14.22	1.14	1.52	21	1
1	A	63	MET	SD-CE	-14.20	0.98	1.77	21	1
1	A	61	LYS	CG-CD	-14.12	1.04	1.52	21	1
1	A	37	ILE	CB-CG1	-13.94	1.15	1.54	21	1
1	A	20	ASN	CB-CG	-13.79	1.19	1.51	21	1
1	A	31	ASP	CB-CG	-13.55	1.23	1.51	21	1
1	A	43	ILE	CB-CG1	-13.41	1.16	1.54	21	1
1	A	61	LYS	CB-CG	-12.92	1.17	1.52	21	1
1	A	37	ILE	C-O	-12.84	0.98	1.23	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	15	GLN	CD-OE1	-12.68	0.96	1.24	21	1
1	A	2	MET	SD-CE	-12.49	1.07	1.77	21	1
1	A	36	LYS	CB-CG	-12.26	1.19	1.52	21	1
1	A	72	ILE	CG1-CD1	-11.90	0.68	1.50	21	1
1	A	13	ASN	CB-CG	-11.86	1.23	1.51	21	1
1	A	43	ILE	CB-CG2	-11.81	1.16	1.52	21	1
1	A	73	LYS	CG-CD	-11.74	1.12	1.52	21	1
1	A	60	LEU	CB-CG	-11.69	1.18	1.52	21	1
1	A	10	GLY	C-N	-11.20	1.08	1.34	21	1
1	A	3	LYS	CG-CD	-11.12	1.14	1.52	21	1
1	A	57	ASP	CB-CG	-10.82	1.29	1.51	21	1
1	A	19	LYS	CG-CD	-10.75	1.15	1.52	21	1
1	A	71	GLU	CB-CG	-10.59	1.32	1.52	21	1
1	A	15	GLN	CG-CD	-10.53	1.26	1.51	21	1
1	A	28	LEU	CB-CG	-10.51	1.22	1.52	21	1
1	A	69	LYS	CG-CD	-10.25	1.17	1.52	21	1
1	A	54	LEU	CB-CG	-10.21	1.23	1.52	21	1
1	A	48	LEU	C-N	-9.77	1.11	1.34	21	1
1	A	5	GLN	CB-CG	-9.76	1.26	1.52	21	1
1	A	16	MET	CB-CG	-9.08	1.22	1.51	21	1
1	A	37	ILE	CB-CG2	-9.05	1.24	1.52	21	1
1	A	22	ARG	CG-CD	-9.00	1.29	1.51	21	1
1	A	6	ILE	CG1-CD1	-8.98	0.88	1.50	21	1
1	A	37	ILE	C-N	-8.89	1.13	1.34	21	1
1	A	11	CYS	C-O	-8.33	1.07	1.23	21	1
1	A	20	ASN	CG-ND2	-8.24	1.12	1.32	21	1
1	A	26	LYS	CG-CD	-7.43	1.27	1.52	21	1
1	A	8	GLY	C-O	-7.38	1.11	1.23	21	1
1	A	37	ILE	CG1-CD1	-6.71	1.04	1.50	21	1
1	A	5	GLN	CD-NE2	-6.64	1.16	1.32	21	1
1	A	11	CYS	C-N	-6.62	1.18	1.34	21	1
1	A	1	MET	CA-CB	-6.31	1.40	1.53	21	1
1	A	26	LYS	CB-CG	-6.24	1.35	1.52	21	1
1	A	49	THR	C-O	-5.67	1.12	1.23	21	1
1	A	49	THR	C-N	-5.55	1.21	1.34	21	1
1	A	36	LYS	CG-CD	-5.51	1.33	1.52	21	1
1	A	30	ILE	CG1-CD1	-5.20	1.14	1.50	21	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	65	ARG	NE-CZ-NH1	-115.00	62.80	120.30	21	1
1	A	22	ARG	NE-CZ-NH2	94.72	167.66	120.30	21	1
1	A	65	ARG	NE-CZ-NH2	91.33	165.97	120.30	21	1
1	A	71	GLU	OE1-CD-OE2	-91.33	13.70	123.30	21	1
1	A	7	TYR	CD1-CG-CD2	-85.23	24.15	117.90	21	1
1	A	70	GLU	OE1-CD-OE2	-80.24	27.01	123.30	21	1
1	A	7	TYR	CB-CG-CD2	79.59	168.75	121.00	21	1
1	A	23	GLU	OE1-CD-OE2	-79.48	27.92	123.30	21	1
1	A	59	GLU	OE1-CD-OE2	-77.68	30.09	123.30	21	1
1	A	7	TYR	CB-CG-CD1	76.81	167.09	121.00	21	1
1	A	18	GLU	OE1-CD-OE2	-67.06	42.83	123.30	21	1
1	A	34	PHE	CD1-CG-CD2	-59.66	40.74	118.30	21	1
1	A	7	TYR	CE1-CZ-CE2	-59.19	25.10	119.80	21	2
1	A	7	TYR	CG-CD1-CE1	58.72	168.27	121.30	21	1
1	A	41	ASP	CB-CG-OD1	58.20	170.68	118.30	21	1
1	A	7	TYR	CG-CD2-CE2	57.73	167.49	121.30	21	2
1	A	7	TYR	CZ-CE2-CD2	-57.64	67.92	119.80	9	2
1	A	34	PHE	CB-CG-CD1	55.88	159.91	120.80	21	1
1	A	41	ASP	CB-CG-OD2	55.28	168.06	118.30	21	1
1	A	34	PHE	CB-CG-CD2	55.04	159.33	120.80	21	1
1	A	39	GLU	OE1-CD-OE2	-54.09	58.39	123.30	21	1
1	A	41	ASP	OD1-CG-OD2	-53.70	21.27	123.30	21	1
1	A	27	GLU	OE1-CD-OE2	-53.23	59.42	123.30	21	1
1	A	7	TYR	CD1-CE1-CZ	52.87	167.38	119.80	21	1
1	A	22	ARG	NH1-CZ-NH2	-52.71	61.42	119.40	21	1
1	A	57	ASP	CB-CG-OD2	52.01	165.11	118.30	21	1
1	A	33	GLU	OE1-CD-OE2	-51.83	61.10	123.30	21	1
1	A	31	ASP	CB-CG-OD2	50.84	164.06	118.30	21	1
1	A	57	ASP	CB-CG-OD1	50.04	163.33	118.30	21	1
1	A	35	GLU	OE1-CD-OE2	-49.65	63.72	123.30	21	1
1	A	63	MET	CG-SD-CE	48.32	177.52	100.20	21	1
1	A	57	ASP	OD1-CG-OD2	-48.28	31.56	123.30	21	1
1	A	31	ASP	CB-CG-OD1	46.98	160.58	118.30	21	1
1	A	31	ASP	OD1-CG-OD2	-46.28	35.36	123.30	21	1
1	A	34	PHE	CE1-CZ-CE2	-43.51	41.68	120.00	21	1
1	A	45	GLU	OE1-CD-OE2	-42.73	72.03	123.30	21	1
1	A	9	THR	O-C-N	-42.61	50.77	123.20	21	1
1	A	40	MET	CG-SD-CE	39.61	163.58	100.20	21	1
1	A	2	MET	CG-SD-CE	37.95	160.93	100.20	21	1
1	A	34	PHE	CG-CD1-CE1	35.56	159.92	120.80	21	1
1	A	54	LEU	CB-CG-CD1	35.11	170.69	111.00	21	1
1	A	34	PHE	CG-CD2-CE2	35.09	159.40	120.80	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	17	LEU	CB-CG-CD1	33.57	168.08	111.00	21	1
1	A	34	PHE	CZ-CE2-CD2	32.82	159.48	120.10	21	1
1	A	22	ARG	CD-NE-CZ	32.26	168.76	123.60	21	1
1	A	34	PHE	CD1-CE1-CZ	32.23	158.78	120.10	21	1
1	A	16	MET	CG-SD-CE	31.38	150.40	100.20	21	1
1	A	54	LEU	CB-CG-CD2	31.18	164.00	111.00	21	1
1	A	65	ARG	CD-NE-CZ	30.91	166.87	123.60	21	1
1	A	1	MET	CG-SD-CE	30.81	149.49	100.20	21	1
1	A	54	LEU	CD1-CG-CD2	-30.65	18.55	110.50	21	1
1	A	40	MET	CA-CB-CG	30.20	164.65	113.30	21	1
1	A	17	LEU	CB-CG-CD2	29.70	161.49	111.00	21	1
1	A	71	GLU	CG-CD-OE1	27.75	173.81	118.30	21	1
1	A	17	LEU	CD1-CG-CD2	-27.68	27.47	110.50	21	1
1	A	71	GLU	CG-CD-OE2	27.10	172.49	118.30	21	1
1	A	22	ARG	CG-CD-NE	26.34	167.11	111.80	21	1
1	A	65	ARG	CG-CD-NE	25.79	165.95	111.80	21	1
1	A	26	LYS	CD-CE-NZ	24.92	169.01	111.70	21	1
1	A	23	GLU	CG-CD-OE2	24.54	167.37	118.30	21	1
1	A	70	GLU	CG-CD-OE1	24.26	166.81	118.30	21	1
1	A	61	LYS	CD-CE-NZ	23.99	166.88	111.70	21	1
1	A	70	GLU	CG-CD-OE2	23.94	166.17	118.30	21	1
1	A	59	GLU	CG-CD-OE1	23.41	165.12	118.30	21	1
1	A	59	GLU	CG-CD-OE2	23.24	164.79	118.30	21	1
1	A	23	GLU	CG-CD-OE1	23.21	164.71	118.30	21	1
1	A	69	LYS	CD-CE-NZ	22.50	163.45	111.70	21	1
1	A	49	THR	CA-CB-CG2	22.41	143.77	112.40	21	1
1	A	66	VAL	CG1-CB-CG2	-22.23	75.34	110.90	21	1
1	A	9	THR	CA-C-N	21.83	159.86	116.20	21	1
1	A	45	GLU	CG-CD-OE2	21.72	161.73	118.30	21	1
1	A	39	GLU	CG-CD-OE2	21.55	161.40	118.30	21	1
1	A	63	MET	CA-CB-CG	21.48	149.82	113.30	21	1
1	A	22	ARG	NE-CZ-NH1	21.23	130.92	120.30	21	1
1	A	5	GLN	CB-CG-CD	21.20	166.71	111.60	21	1
1	A	69	LYS	CB-CG-CD	21.17	166.64	111.60	21	1
1	A	38	LYS	CD-CE-NZ	21.02	160.06	111.70	21	1
1	A	18	GLU	CG-CD-OE1	20.54	159.37	118.30	21	1
1	A	13	ASN	OD1-CG-ND2	-20.48	74.80	121.90	21	1
1	A	36	LYS	CD-CE-NZ	20.27	158.31	111.70	21	1
1	A	18	GLU	CG-CD-OE2	19.75	157.79	118.30	21	1
1	A	49	THR	OG1-CB-CG2	-19.55	65.03	110.00	21	1
1	A	33	GLU	CG-CD-OE2	19.52	157.33	118.30	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	19	LYS	CD-CE-NZ	19.46	156.46	111.70	21	1
1	A	40	MET	CB-CG-SD	18.99	169.37	112.40	21	1
1	A	69	LYS	CG-CD-CE	18.68	167.94	111.90	21	1
1	A	9	THR	C-N-CA	18.42	160.98	122.30	21	1
1	A	27	GLU	CG-CD-OE1	18.36	155.01	118.30	21	1
1	A	66	VAL	CA-CB-CG1	17.81	137.61	110.90	21	1
1	A	35	GLU	CG-CD-OE1	17.76	153.82	118.30	21	1
1	A	42	GLN	CB-CG-CD	17.73	157.69	111.60	21	1
1	A	7	TYR	OH-CZ-CE2	17.57	167.53	120.10	21	2
1	A	7	TYR	CE1-CZ-OH	17.51	167.37	120.10	21	1
1	A	69	LYS	CA-CB-CG	17.49	151.87	113.40	21	1
1	A	26	LYS	CG-CD-CE	17.14	163.32	111.90	21	1
1	A	3	LYS	CD-CE-NZ	16.88	150.52	111.70	21	1
1	A	35	GLU	CB-CG-CD	16.50	158.74	114.20	21	1
1	A	2	MET	CB-CG-SD	16.02	160.47	112.40	21	1
1	A	66	VAL	CA-CB-CG2	15.76	134.54	110.90	21	1
1	A	5	GLN	CG-CD-OE1	-15.73	90.13	121.60	21	1
1	A	6	ILE	CB-CG1-CD1	15.57	157.49	113.90	21	1
1	A	61	LYS	CB-CG-CD	15.51	151.92	111.60	21	1
1	A	3	LYS	CG-CD-CE	15.12	157.28	111.90	21	1
1	A	71	GLU	CB-CG-CD	15.04	154.80	114.20	21	1
1	A	72	ILE	CB-CG1-CD1	14.93	155.71	113.90	21	1
1	A	73	LYS	CD-CE-NZ	14.52	145.09	111.70	21	1
1	A	1	MET	CA-CB-CG	14.13	137.32	113.30	21	1
1	A	28	LEU	CB-CG-CD1	14.00	134.80	111.00	21	1
1	A	19	LYS	CG-CD-CE	13.97	153.82	111.90	21	1
1	A	9	THR	CA-C-O	13.94	149.37	120.10	21	1
1	A	49	THR	CA-CB-OG1	13.92	138.24	109.00	21	1
1	A	27	GLU	CG-CD-OE2	13.63	145.57	118.30	21	1
1	A	30	ILE	CG1-CB-CG2	-13.03	82.74	111.40	21	1
1	A	42	GLN	CG-CD-NE2	12.71	147.21	116.70	21	1
1	A	60	LEU	CB-CG-CD2	12.62	132.45	111.00	21	1
1	A	36	LYS	CG-CD-CE	12.59	149.67	111.90	21	1
1	A	42	GLN	OE1-CD-NE2	-12.48	93.19	121.90	21	1
1	A	59	GLU	CB-CG-CD	12.43	147.75	114.20	21	1
1	A	35	GLU	CG-CD-OE2	12.08	142.46	118.30	21	1
1	A	51	LEU	CB-CG-CD2	11.97	131.35	111.00	21	1
1	A	13	ASN	CB-CG-ND2	11.94	145.36	116.70	21	1
1	A	61	LYS	CG-CD-CE	11.77	147.21	111.90	21	1
1	A	9	THR	CA-CB-CG2	11.72	128.81	112.40	21	1
1	A	33	GLU	CG-CD-OE1	11.63	141.57	118.30	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	65	ARG	CB-CG-CD	11.46	141.40	111.60	21	1
1	A	73	LYS	CG-CD-CE	11.40	146.11	111.90	21	1
1	A	39	GLU	CG-CD-OE1	10.96	140.21	118.30	21	1
1	A	1	MET	CB-CG-SD	10.91	145.13	112.40	21	1
1	A	28	LEU	CB-CG-CD2	10.79	129.34	111.00	21	1
1	A	65	ARG	NH1-CZ-NH2	10.76	131.23	119.40	21	1
1	A	5	GLN	CG-CD-NE2	10.74	142.48	116.70	21	1
1	A	30	ILE	CA-CB-CG2	10.62	132.14	110.90	21	1
1	A	45	GLU	CB-CG-CD	10.39	142.26	114.20	21	1
1	A	16	MET	CB-CG-SD	10.32	143.37	112.40	21	1
1	A	33	GLU	CB-CG-CD	10.20	141.74	114.20	21	1
1	A	30	ILE	CA-CB-CG1	10.13	130.24	111.00	21	1
1	A	20	ASN	CB-CG-ND2	9.80	140.21	116.70	21	1
1	A	20	ASN	CB-CG-OD1	-9.38	102.84	121.60	21	1
1	A	51	LEU	CB-CG-CD1	9.21	126.65	111.00	21	1
1	A	38	LYS	CG-CD-CE	9.20	139.51	111.90	21	1
1	A	13	ASN	CB-CG-OD1	9.12	139.85	121.60	21	1
1	A	10	GLY	O-C-N	-8.99	108.32	122.70	21	1
1	A	51	LEU	CD1-CG-CD2	-8.91	83.78	110.50	21	1
1	A	68	SER	CA-CB-OG	8.82	135.02	111.20	21	1
1	A	39	GLU	CB-CG-CD	8.72	137.75	114.20	21	1
1	A	3	LYS	CB-CG-CD	8.72	134.27	111.60	21	1
1	A	28	LEU	CD1-CG-CD2	-8.62	84.64	110.50	21	1
1	A	48	LEU	O-C-N	-8.51	109.08	122.70	21	1
1	A	62	ILE	CG1-CB-CG2	-8.46	92.80	111.40	21	1
1	A	9	THR	OG1-CB-CG2	-8.40	90.69	110.00	21	1
1	A	62	ILE	CB-CG1-CD1	8.14	136.70	113.90	21	1
1	A	37	ILE	O-C-N	-8.11	109.72	122.70	21	1
1	A	23	GLU	CA-CB-CG	8.10	131.21	113.40	21	1
1	A	72	ILE	CG1-CB-CG2	-8.05	93.69	111.40	21	1
1	A	11	CYS	CA-CB-SG	7.99	128.38	114.00	21	1
1	A	35	GLU	CA-CB-CG	7.79	130.54	113.40	21	1
1	A	70	GLU	CB-CG-CD	7.49	134.42	114.20	21	1
1	A	4	ILE	CB-CG1-CD1	7.39	134.60	113.90	21	1
1	A	62	ILE	CA-CB-CG1	7.38	125.02	111.00	21	1
1	A	15	GLN	CG-CD-OE1	-7.11	107.38	121.60	21	1
1	A	23	GLU	CB-CG-CD	7.05	133.23	114.20	21	1
1	A	73	LYS	CB-CG-CD	7.04	129.90	111.60	21	1
1	A	3	LYS	CA-CB-CG	6.93	128.65	113.40	21	1
1	A	65	ARG	CA-CB-CG	6.92	128.62	113.40	21	1
1	A	72	ILE	CA-CB-CG2	6.64	124.18	110.90	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	6	ILE	CG1-CB-CG2	-6.59	96.89	111.40	21	1
1	A	62	ILE	CA-CB-CG2	6.44	123.78	110.90	21	1
1	A	72	ILE	CA-CB-CG1	6.41	123.18	111.00	21	1
1	A	30	ILE	CB-CG1-CD1	6.40	131.83	113.90	21	1
1	A	60	LEU	CA-CB-CG	6.13	129.41	115.30	21	1
1	A	60	LEU	CD1-CG-CD2	-6.13	92.11	110.50	21	1
1	A	9	THR	CA-CB-OG1	5.93	121.45	109.00	21	1
1	A	6	ILE	CA-CB-CG1	5.88	122.16	111.00	21	1
1	A	70	GLU	CA-CB-CG	5.84	126.25	113.40	21	1
1	A	27	GLU	CB-CG-CD	5.74	129.70	114.20	21	1
1	A	37	ILE	CA-CB-CG2	5.55	122.01	110.90	21	1
1	A	48	LEU	CA-C-N	5.47	129.23	117.20	21	1
1	A	43	ILE	CG1-CB-CG2	-5.43	99.45	111.40	21	1
1	A	39	GLU	CA-CB-CG	5.36	125.19	113.40	21	1

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

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	9	THR	CB	1
1	A	30	ILE	CB	1
1	A	49	THR	CB	1

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	554	581	575	73±66
All	All	11634	12201	12195	1540

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 65.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:MET:CG	1:A:16:MET:CE	1.59	1.81	21	1
1:A:30:ILE:CB	1:A:30:ILE:CD1	1.55	1.81	21	1
1:A:65:ARG:CD	1:A:65:ARG:CB	1.54	1.85	21	1
1:A:65:ARG:NE	1:A:65:ARG:CG	1.54	1.69	21	1
1:A:17:LEU:CD2	1:A:17:LEU:CB	1.49	1.90	21	1
1:A:54:LEU:CD1	1:A:54:LEU:CB	1.48	1.91	21	1
1:A:35:GLU:CD	1:A:35:GLU:CB	1.47	1.82	21	1
1:A:19:LYS:NZ	1:A:19:LYS:CD	1.47	1.70	21	1
1:A:69:LYS:CD	1:A:69:LYS:CB	1.47	1.90	21	1
1:A:73:LYS:CG	1:A:73:LYS:CE	1.46	1.90	21	1
1:A:6:ILE:CD1	1:A:6:ILE:CB	1.45	1.94	21	1
1:A:1:MET:CE	1:A:1:MET:CG	1.44	1.91	21	1
1:A:34:PHE:CD1	1:A:34:PHE:CZ	1.43	2.07	21	1
1:A:19:LYS:CG	1:A:19:LYS:CE	1.42	1.95	21	1
1:A:31:ASP:OD1	1:A:31:ASP:CB	1.42	1.67	21	1
1:A:7:TYR:CZ	1:A:7:TYR:CD1	1.42	2.06	21	1
1:A:36:LYS:CD	1:A:36:LYS:NZ	1.41	1.74	21	1
1:A:34:PHE:CG	1:A:34:PHE:CE2	1.40	2.08	21	1
1:A:34:PHE:CD2	1:A:34:PHE:CZ	1.39	2.09	21	1
1:A:7:TYR:CZ	1:A:7:TYR:CD2	1.39	2.07	21	1
1:A:7:TYR:CG	1:A:7:TYR:CE2	1.39	2.09	21	1
1:A:13:ASN:CB	1:A:13:ASN:OD1	1.39	1.70	21	1
1:A:13:ASN:ND2	1:A:13:ASN:CB	1.39	1.86	21	1
1:A:2:MET:CE	1:A:2:MET:CG	1.38	2.02	21	1
1:A:34:PHE:CG	1:A:34:PHE:CE1	1.38	2.10	21	1
1:A:69:LYS:CG	1:A:69:LYS:CE	1.36	2.01	21	1
1:A:26:LYS:CG	1:A:26:LYS:CE	1.36	2.02	21	1
1:A:7:TYR:CD2	1:A:7:TYR:CE2	1.36	2.14	9	1
1:A:7:TYR:CG	1:A:7:TYR:CE1	1.36	2.10	21	1
1:A:7:TYR:CZ	1:A:7:TYR:CE2	1.35	2.14	9	2
1:A:40:MET:CE	1:A:40:MET:CG	1.35	2.05	21	1
1:A:51:LEU:CB	1:A:51:LEU:CD1	1.33	2.05	21	1
1:A:1:MET:CA	1:A:1:MET:CG	1.30	2.07	21	1
1:A:49:THR:CA	1:A:49:THR:CG2	1.30	2.07	21	1
1:A:31:ASP:OD2	1:A:31:ASP:CB	1.30	1.77	21	1
1:A:57:ASP:OD1	1:A:57:ASP:CB	1.30	1.77	21	1
1:A:16:MET:CB	1:A:16:MET:SD	1.30	2.19	21	1
1:A:9:THR:O	1:A:10:GLY:CA	1.28	1.82	21	1
1:A:36:LYS:CG	1:A:36:LYS:CE	1.27	2.09	21	1
1:A:59:GLU:CB	1:A:59:GLU:CD	1.27	2.02	21	1
1:A:1:MET:SD	1:A:1:MET:CG	1.26	1.18	21	1
1:A:51:LEU:CB	1:A:51:LEU:CD2	1.26	2.13	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:LEU:CD1	1:A:17:LEU:CB	1.26	2.14	21	1
1:A:57:ASP:CB	1:A:57:ASP:OD2	1.25	1.82	21	1
1:A:63:MET:SD	1:A:63:MET:CG	1.25	1.16	21	1
1:A:34:PHE:CB	1:A:34:PHE:CD2	1.24	2.20	21	1
1:A:63:MET:CE	1:A:63:MET:CG	1.23	2.14	21	1
1:A:11:CYS:SG	1:A:11:CYS:CB	1.23	1.14	21	1
1:A:30:ILE:CA	1:A:30:ILE:CG1	1.22	2.17	21	1
1:A:9:THR:O	1:A:9:THR:CA	1.22	1.88	21	1
1:A:69:LYS:CG	1:A:69:LYS:CA	1.19	2.19	21	1
1:A:7:TYR:CB	1:A:7:TYR:CD1	1.19	2.24	21	1
1:A:66:VAL:CA	1:A:66:VAL:CG2	1.18	2.19	21	1
1:A:30:ILE:CA	1:A:30:ILE:CG2	1.18	2.20	21	1
1:A:34:PHE:CB	1:A:34:PHE:CD1	1.18	2.22	21	1
1:A:7:TYR:CB	1:A:7:TYR:CD2	1.17	2.23	21	1
1:A:41:ASP:OD2	1:A:41:ASP:CB	1.17	1.93	21	1
1:A:6:ILE:CD1	1:A:6:ILE:CG2	1.15	2.25	21	1
1:A:16:MET:CG	1:A:16:MET:SD	1.15	1.09	21	1
1:A:2:MET:CE	1:A:2:MET:SD	1.14	1.07	21	1
1:A:2:MET:CB	1:A:2:MET:SD	1.13	2.34	21	1
1:A:49:THR:CA	1:A:49:THR:OG1	1.13	1.95	21	1
1:A:11:CYS:SG	1:A:11:CYS:CA	1.13	2.36	21	1
1:A:22:ARG:CG	1:A:22:ARG:NE	1.13	2.12	21	1
1:A:9:THR:C	1:A:10:GLY:CA	1.11	2.17	21	1
1:A:66:VAL:CG2	1:A:66:VAL:HB	1.11	1.68	21	1
1:A:66:VAL:CA	1:A:66:VAL:CG1	1.09	2.26	21	1
1:A:51:LEU:CD1	1:A:51:LEU:HG	1.09	1.66	21	1
1:A:51:LEU:CD2	1:A:51:LEU:HG	1.09	1.66	21	1
1:A:45:GLU:CD	1:A:45:GLU:CB	1.09	2.19	21	1
1:A:63:MET:CA	1:A:63:MET:CG	1.08	2.31	21	1
1:A:42:GLN:CD	1:A:42:GLN:CB	1.08	2.21	21	1
1:A:49:THR:HB	1:A:49:THR:OG1	1.07	1.48	21	1
1:A:17:LEU:HD21	1:A:72:ILE:HD11	1.05	1.27	20	3
1:A:68:SER:CA	1:A:68:SER:OG	1.05	2.04	21	1
1:A:68:SER:HB2	1:A:68:SER:OG	1.05	1.30	21	1
1:A:66:VAL:CG1	1:A:66:VAL:HB	1.04	1.70	21	1
1:A:2:MET:CG	1:A:2:MET:SD	1.03	0.97	21	1
1:A:7:TYR:OH	1:A:7:TYR:CE1	1.03	2.06	21	1
1:A:68:SER:OG	1:A:68:SER:HB3	1.03	1.30	21	1
1:A:7:TYR:OH	1:A:7:TYR:CE2	1.03	2.07	21	2
1:A:41:ASP:OD1	1:A:41:ASP:CB	1.02	2.06	21	1
1:A:9:THR:CA	1:A:10:GLY:N	1.02	2.22	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:GLU:CG	1:A:59:GLU:CD	1.02	0.93	21	1
1:A:43:ILE:HG22	1:A:48:LEU:HD21	1.02	1.30	6	18
1:A:63:MET:CB	1:A:63:MET:HG2	1.02	1.55	21	1
1:A:49:THR:CG2	1:A:49:THR:HB	1.01	1.55	21	1
1:A:11:CYS:HB3	1:A:11:CYS:SG	1.01	1.68	21	1
1:A:37:ILE:N	1:A:37:ILE:HD13	1.01	1.54	21	5
1:A:51:LEU:CG	1:A:51:LEU:HD23	1.01	1.55	21	1
1:A:30:ILE:CG1	1:A:30:ILE:HB	1.01	1.62	21	1
1:A:2:MET:HE2	1:A:2:MET:SD	1.01	1.67	21	1
1:A:59:GLU:HG3	1:A:59:GLU:CD	1.00	1.45	21	1
1:A:49:THR:CG2	1:A:49:THR:OG1	1.00	0.70	21	1
1:A:59:GLU:HG2	1:A:59:GLU:CD	1.00	1.45	21	1
1:A:63:MET:SD	1:A:63:MET:CE	1.00	0.98	21	1
1:A:66:VAL:HG11	1:A:66:VAL:CB	1.00	1.53	21	1
1:A:11:CYS:HB2	1:A:11:CYS:SG	0.99	1.68	21	1
1:A:2:MET:HE1	1:A:2:MET:SD	0.99	1.67	21	1
1:A:66:VAL:HG13	1:A:66:VAL:CB	0.98	1.53	21	1
1:A:49:THR:HG23	1:A:49:THR:OG1	0.98	1.24	21	1
1:A:7:TYR:CD2	1:A:7:TYR:CZ	0.98	2.39	9	1
1:A:25:VAL:HG21	1:A:32:ALA:HB2	0.98	1.30	6	16
1:A:17:LEU:HD11	1:A:72:ILE:HD11	0.98	1.31	1	5
1:A:66:VAL:HG12	1:A:66:VAL:CB	0.98	1.53	21	1
1:A:63:MET:SD	1:A:63:MET:HG2	0.98	1.75	21	1
1:A:51:LEU:HD21	1:A:51:LEU:CG	0.98	1.55	21	1
1:A:51:LEU:CG	1:A:51:LEU:HD12	0.97	1.51	21	1
1:A:68:SER:OG	1:A:68:SER:CB	0.97	0.67	21	1
1:A:2:MET:HE3	1:A:2:MET:SD	0.97	1.67	21	1
1:A:63:MET:CB	1:A:63:MET:HG3	0.97	1.55	21	1
1:A:22:ARG:NE	1:A:22:ARG:CD	0.96	0.84	21	1
1:A:51:LEU:CG	1:A:51:LEU:HD22	0.96	1.55	21	1
1:A:30:ILE:CG2	1:A:30:ILE:HB	0.96	1.62	21	1
1:A:6:ILE:HD12	1:A:6:ILE:CG1	0.96	1.51	21	1
1:A:45:GLU:CD	1:A:45:GLU:HG3	0.96	1.40	21	1
1:A:6:ILE:HD13	1:A:6:ILE:CG1	0.96	1.51	21	1
1:A:42:GLN:CG	1:A:42:GLN:CD	0.96	0.86	21	1
1:A:30:ILE:CB	1:A:30:ILE:HG21	0.95	1.49	21	1
1:A:51:LEU:CG	1:A:51:LEU:HD13	0.95	1.51	21	1
1:A:63:MET:SD	1:A:63:MET:HE2	0.95	1.59	21	1
1:A:6:ILE:HD11	1:A:6:ILE:CG1	0.95	1.51	21	1
1:A:63:MET:SD	1:A:63:MET:HE1	0.95	1.59	21	1
1:A:30:ILE:CB	1:A:30:ILE:HG22	0.95	1.49	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:GLU:HG2	1:A:35:GLU:CD	0.94	1.39	21	1
1:A:37:ILE:H	1:A:37:ILE:HD13	0.94	1.03	21	1
1:A:22:ARG:NE	1:A:22:ARG:HD2	0.94	1.32	21	1
1:A:51:LEU:CG	1:A:51:LEU:HD11	0.94	1.51	21	1
1:A:66:VAL:HG22	1:A:66:VAL:CB	0.94	1.49	21	1
1:A:65:ARG:HG3	1:A:65:ARG:CD	0.94	1.47	21	1
1:A:63:MET:SD	1:A:63:MET:HE3	0.94	1.59	21	1
1:A:45:GLU:CD	1:A:45:GLU:CG	0.93	0.84	21	1
1:A:45:GLU:CD	1:A:45:GLU:HG2	0.93	1.40	21	1
1:A:16:MET:HG3	1:A:16:MET:SD	0.93	1.59	21	1
1:A:22:ARG:NE	1:A:22:ARG:HD3	0.93	1.32	21	1
1:A:66:VAL:HG21	1:A:66:VAL:CB	0.93	1.49	21	1
1:A:66:VAL:HG23	1:A:66:VAL:CB	0.93	1.49	21	1
1:A:16:MET:HG2	1:A:16:MET:SD	0.93	1.59	21	1
1:A:42:GLN:CD	1:A:42:GLN:HG3	0.93	1.37	21	1
1:A:35:GLU:HG3	1:A:35:GLU:CD	0.92	1.39	21	1
1:A:30:ILE:CB	1:A:30:ILE:HG23	0.92	1.49	21	1
1:A:42:GLN:HG2	1:A:42:GLN:CD	0.92	1.37	21	1
1:A:35:GLU:CD	1:A:35:GLU:CG	0.92	0.89	21	1
1:A:51:LEU:CG	1:A:51:LEU:CD2	0.92	0.92	21	1
1:A:63:MET:CB	1:A:63:MET:CG	0.91	0.91	21	1
1:A:4:ILE:HD13	1:A:34:PHE:CZ	0.91	2.01	13	13
1:A:65:ARG:HG2	1:A:65:ARG:CD	0.91	1.47	21	1
1:A:65:ARG:CD	1:A:65:ARG:CG	0.91	0.93	21	1
1:A:63:MET:SD	1:A:63:MET:HG3	0.91	1.75	21	1
1:A:66:VAL:CG1	1:A:66:VAL:CB	0.90	0.90	21	1
1:A:63:MET:CG	1:A:63:MET:HB2	0.90	1.43	21	1
1:A:6:ILE:HG21	1:A:6:ILE:CD1	0.89	1.98	21	1
1:A:49:THR:CB	1:A:49:THR:OG1	0.89	0.59	21	1
1:A:62:ILE:HD13	1:A:66:VAL:HG12	0.88	1.45	15	1
1:A:7:TYR:CE2	1:A:42:GLN:O	0.88	2.26	9	1
1:A:7:TYR:CD2	1:A:48:LEU:HD11	0.88	2.03	12	5
1:A:6:ILE:CG1	1:A:6:ILE:CD1	0.88	0.88	21	1
1:A:51:LEU:CG	1:A:51:LEU:CD1	0.88	0.88	21	1
1:A:37:ILE:HD13	1:A:37:ILE:N	0.88	1.83	10	4
1:A:30:ILE:CB	1:A:30:ILE:HG13	0.87	1.42	21	1
1:A:63:MET:HB3	1:A:63:MET:CG	0.87	1.43	21	1
1:A:30:ILE:CB	1:A:30:ILE:HG12	0.87	1.42	21	1
1:A:73:LYS:HD3	1:A:73:LYS:CE	0.86	1.40	21	1
1:A:2:MET:O	1:A:32:ALA:HB1	0.86	1.70	18	20
1:A:1:MET:SD	1:A:1:MET:CE	0.86	0.79	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:ARG:CG	1:A:65:ARG:HD2	0.86	1.39	21	1
1:A:73:LYS:NZ	1:A:73:LYS:HE3	0.86	1.36	21	1
1:A:4:ILE:HG13	1:A:56:VAL:HG12	0.86	1.48	14	14
1:A:1:MET:HB2	1:A:1:MET:CG	0.85	1.39	21	1
1:A:30:ILE:CG2	1:A:30:ILE:CB	0.85	0.86	21	1
1:A:66:VAL:CG2	1:A:66:VAL:CB	0.85	0.85	21	1
1:A:46:ALA:HB1	1:A:60:LEU:HD21	0.85	1.45	14	3
1:A:4:ILE:HD13	1:A:34:PHE:CE2	0.85	2.06	8	12
1:A:1:MET:HB3	1:A:1:MET:CG	0.85	1.39	21	1
1:A:73:LYS:HD2	1:A:73:LYS:CE	0.85	1.40	21	1
1:A:55:ALA:HB2	1:A:60:LEU:HD23	0.84	1.47	18	2
1:A:65:ARG:CG	1:A:65:ARG:HD3	0.84	1.39	21	1
1:A:73:LYS:CD	1:A:73:LYS:CE	0.84	0.86	21	1
1:A:7:TYR:CD1	1:A:43:ILE:HA	0.84	2.07	16	12
1:A:19:LYS:HD3	1:A:19:LYS:CE	0.84	1.37	21	1
1:A:73:LYS:CD	1:A:73:LYS:HE3	0.84	1.41	21	1
1:A:49:THR:CB	1:A:49:THR:HG23	0.84	1.37	21	1
1:A:16:MET:CE	1:A:16:MET:SD	0.84	0.78	21	1
1:A:40:MET:CE	1:A:40:MET:SD	0.84	0.80	21	1
1:A:36:LYS:HD2	1:A:36:LYS:CE	0.84	1.37	21	1
1:A:9:THR:C	1:A:10:GLY:N	0.84	0.81	21	1
1:A:7:TYR:CD1	1:A:37:ILE:HD12	0.83	2.07	12	5
1:A:49:THR:HG21	1:A:49:THR:CB	0.83	1.37	21	1
1:A:30:ILE:CG1	1:A:30:ILE:CB	0.83	0.83	21	1
1:A:55:ALA:HB2	1:A:60:LEU:CD2	0.83	2.04	10	3
1:A:49:THR:CB	1:A:49:THR:HG22	0.83	1.37	21	1
1:A:6:ILE:HG12	1:A:6:ILE:CD1	0.83	1.38	21	1
1:A:19:LYS:HE2	1:A:19:LYS:CD	0.82	1.36	21	1
1:A:6:ILE:HG13	1:A:6:ILE:CD1	0.82	1.38	21	1
1:A:17:LEU:CG	1:A:17:LEU:HD12	0.82	1.35	21	1
1:A:7:TYR:CD2	1:A:43:ILE:HA	0.82	2.09	7	8
1:A:19:LYS:HD2	1:A:19:LYS:CE	0.82	1.37	21	1
1:A:17:LEU:CG	1:A:17:LEU:HD13	0.82	1.35	21	1
1:A:19:LYS:HE3	1:A:19:LYS:CD	0.82	1.36	21	1
1:A:40:MET:HE2	1:A:40:MET:SD	0.82	1.45	21	1
1:A:36:LYS:HD3	1:A:36:LYS:CE	0.82	1.37	21	1
1:A:4:ILE:HD12	1:A:34:PHE:CE2	0.81	2.10	2	5
1:A:17:LEU:CG	1:A:17:LEU:HD11	0.81	1.35	21	1
1:A:73:LYS:CD	1:A:73:LYS:HE2	0.81	1.41	21	1
1:A:40:MET:HE1	1:A:40:MET:SD	0.81	1.45	21	1
1:A:34:PHE:HZ	1:A:34:PHE:CE2	0.81	1.65	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LYS:CD	1:A:36:LYS:HE2	0.81	1.35	21	1
1:A:54:LEU:HD11	1:A:66:VAL:HG23	0.81	1.50	14	1
1:A:36:LYS:CD	1:A:36:LYS:CE	0.81	0.83	21	1
1:A:36:LYS:CD	1:A:36:LYS:HE3	0.81	1.35	21	1
1:A:50:ALA:HB3	1:A:63:MET:CB	0.81	2.06	5	3
1:A:1:MET:CB	1:A:1:MET:HG2	0.81	1.37	21	1
1:A:19:LYS:CD	1:A:19:LYS:CE	0.81	0.85	21	1
1:A:1:MET:HE2	1:A:1:MET:SD	0.80	1.44	21	1
1:A:50:ALA:HB3	1:A:63:MET:HB2	0.80	1.50	8	3
1:A:1:MET:CB	1:A:1:MET:CG	0.80	0.81	21	1
1:A:5:GLN:O	1:A:54:LEU:HD13	0.80	1.77	12	3
1:A:1:MET:SD	1:A:1:MET:HE1	0.80	1.44	21	1
1:A:41:ASP:CG	1:A:41:ASP:OD1	0.80	0.64	21	1
1:A:25:VAL:HG11	1:A:32:ALA:HB3	0.80	1.54	1	16
1:A:40:MET:HE3	1:A:40:MET:SD	0.80	1.45	21	1
1:A:16:MET:SD	1:A:16:MET:HE1	0.80	1.43	21	1
1:A:65:ARG:CG	1:A:65:ARG:HE	0.80	1.89	21	1
1:A:34:PHE:HZ	1:A:34:PHE:CE1	0.80	1.63	21	1
1:A:16:MET:SD	1:A:16:MET:HE3	0.80	1.43	21	1
1:A:49:THR:HG1	1:A:49:THR:CG2	0.80	1.54	21	1
1:A:2:MET:HG2	1:A:2:MET:SD	0.80	1.44	21	1
1:A:1:MET:HE3	1:A:1:MET:SD	0.80	1.44	21	1
1:A:1:MET:SD	1:A:1:MET:HG3	0.79	1.66	21	1
1:A:69:LYS:HD3	1:A:69:LYS:CE	0.79	1.33	21	1
1:A:16:MET:CE	1:A:16:MET:HG2	0.79	2.05	21	1
1:A:2:MET:HG3	1:A:2:MET:SD	0.79	1.44	21	1
1:A:7:TYR:HA	1:A:37:ILE:CD1	0.79	2.07	18	8
1:A:1:MET:CB	1:A:1:MET:HG3	0.79	1.37	21	1
1:A:73:LYS:NZ	1:A:73:LYS:HE2	0.78	1.36	21	1
1:A:17:LEU:HB2	1:A:66:VAL:HG13	0.78	1.53	21	4
1:A:4:ILE:HD12	1:A:32:ALA:HB1	0.78	1.55	12	4
1:A:69:LYS:CE	1:A:69:LYS:HD2	0.78	1.33	21	1
1:A:16:MET:SD	1:A:16:MET:HE2	0.78	1.44	21	1
1:A:29:GLY:O	1:A:30:ILE:HD13	0.78	1.78	19	1
1:A:17:LEU:HD11	1:A:72:ILE:CD1	0.78	2.07	1	2
1:A:69:LYS:HE2	1:A:69:LYS:CD	0.77	1.34	21	1
1:A:52:PRO:O	1:A:62:ILE:HD12	0.77	1.78	15	2
1:A:4:ILE:HD12	1:A:34:PHE:CZ	0.77	2.13	1	5
1:A:9:THR:O	1:A:10:GLY:N	0.77	0.63	21	1
1:A:55:ALA:HB2	1:A:60:LEU:HD12	0.77	1.56	8	7
1:A:7:TYR:CZ	1:A:46:ALA:HB2	0.77	2.14	13	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:LYS:CG	1:A:69:LYS:HB2	0.77	1.30	21	1
1:A:2:MET:O	1:A:4:ILE:HD12	0.76	1.80	17	9
1:A:26:LYS:CE	1:A:26:LYS:HD3	0.75	1.29	21	1
1:A:13:ASN:HD22	1:A:13:ASN:CG	0.75	1.36	21	1
1:A:46:ALA:HB1	1:A:60:LEU:HD11	0.75	1.59	12	2
1:A:26:LYS:CE	1:A:26:LYS:HD2	0.74	1.29	21	1
1:A:49:THR:HG21	1:A:49:THR:OG1	0.74	0.99	21	1
1:A:69:LYS:CG	1:A:69:LYS:HB3	0.74	1.30	21	1
1:A:6:ILE:N	1:A:37:ILE:HD11	0.74	1.97	10	5
1:A:61:LYS:O	1:A:62:ILE:HD13	0.74	1.81	9	2
1:A:55:ALA:HB2	1:A:60:LEU:HD22	0.74	1.60	7	5
1:A:4:ILE:HG12	1:A:56:VAL:HG12	0.74	1.58	16	4
1:A:69:LYS:HE3	1:A:69:LYS:CD	0.74	1.34	21	1
1:A:63:MET:CE	1:A:63:MET:HB2	0.74	2.13	21	1
1:A:4:ILE:CG1	1:A:56:VAL:HG12	0.73	2.14	5	18
1:A:69:LYS:CE	1:A:69:LYS:CD	0.73	0.85	21	1
1:A:36:LYS:C	1:A:37:ILE:HD13	0.73	2.04	3	8
1:A:13:ASN:HD21	1:A:13:ASN:CG	0.73	1.36	21	1
1:A:17:LEU:O	1:A:17:LEU:HD13	0.72	1.84	8	4
1:A:69:LYS:HG3	1:A:69:LYS:CB	0.72	1.26	21	1
1:A:69:LYS:CG	1:A:69:LYS:CB	0.72	0.74	21	1
1:A:48:LEU:N	1:A:48:LEU:HD22	0.72	1.99	14	5
1:A:69:LYS:NZ	1:A:69:LYS:HE2	0.72	1.30	21	1
1:A:7:TYR:CD1	1:A:37:ILE:HG13	0.72	2.19	16	10
1:A:37:ILE:O	1:A:37:ILE:HD13	0.72	1.84	8	2
1:A:43:ILE:CG2	1:A:48:LEU:HD21	0.72	2.14	2	14
1:A:26:LYS:CD	1:A:26:LYS:HE3	0.71	1.28	21	1
1:A:8:GLY:HA3	1:A:12:ALA:HB3	0.71	1.61	9	13
1:A:17:LEU:HD11	1:A:54:LEU:HG	0.71	1.62	10	1
1:A:22:ARG:HE	1:A:22:ARG:HD3	0.71	1.00	21	1
1:A:7:TYR:CE2	1:A:37:ILE:HG13	0.71	2.21	17	1
1:A:5:GLN:O	1:A:54:LEU:HD22	0.70	1.86	2	5
1:A:69:LYS:CB	1:A:69:LYS:HG2	0.70	1.26	21	1
1:A:48:LEU:HD13	1:A:60:LEU:HD21	0.70	1.62	4	4
1:A:1:MET:CE	1:A:1:MET:HG2	0.70	2.11	21	1
1:A:1:MET:SD	1:A:1:MET:HG2	0.70	1.66	21	1
1:A:34:PHE:CG	1:A:34:PHE:CD1	0.70	0.76	21	1
1:A:42:GLN:HE21	1:A:42:GLN:CD	0.70	1.31	21	1
1:A:5:GLN:C	1:A:6:ILE:HD13	0.70	2.07	8	1
1:A:49:THR:CB	1:A:49:THR:CG2	0.70	0.70	21	1
1:A:4:ILE:HG23	1:A:54:LEU:HD21	0.70	1.63	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LYS:CD	1:A:26:LYS:HE2	0.69	1.27	21	1
1:A:17:LEU:HD23	1:A:67:ALA:O	0.69	1.88	17	6
1:A:7:TYR:CD2	1:A:37:ILE:HG13	0.69	2.22	7	2
1:A:69:LYS:NZ	1:A:69:LYS:HE3	0.69	1.30	21	1
1:A:62:ILE:CD1	1:A:66:VAL:HG12	0.69	2.18	15	2
1:A:6:ILE:HG22	1:A:54:LEU:HD12	0.69	1.63	4	2
1:A:42:GLN:CD	1:A:42:GLN:HE22	0.69	1.31	21	1
1:A:17:LEU:CD1	1:A:67:ALA:HB3	0.69	2.18	7	2
1:A:65:ARG:HG3	1:A:65:ARG:HD2	0.69	1.19	21	1
1:A:17:LEU:HD21	1:A:72:ILE:CD1	0.68	2.15	20	2
1:A:29:GLY:O	1:A:30:ILE:HG23	0.68	1.88	5	11
1:A:48:LEU:H	1:A:48:LEU:HD22	0.68	1.48	14	1
1:A:13:ASN:O	1:A:66:VAL:HG21	0.68	1.87	10	4
1:A:48:LEU:HD12	1:A:60:LEU:HD11	0.68	1.63	7	1
1:A:34:PHE:CG	1:A:34:PHE:CD2	0.68	0.74	21	1
1:A:46:ALA:O	1:A:60:LEU:HD21	0.68	1.89	16	11
1:A:26:LYS:CD	1:A:26:LYS:CE	0.68	0.77	21	1
1:A:55:ALA:CB	1:A:60:LEU:HD12	0.68	2.19	8	2
1:A:26:LYS:HE3	1:A:26:LYS:HD2	0.68	1.01	21	1
1:A:25:VAL:CG2	1:A:32:ALA:HB2	0.67	2.18	3	13
1:A:7:TYR:CE1	1:A:37:ILE:HG13	0.67	2.24	1	8
1:A:54:LEU:HD11	1:A:56:VAL:HG13	0.67	1.67	15	1
1:A:9:THR:O	1:A:9:THR:C	0.67	0.48	21	1
1:A:73:LYS:HZ2	1:A:73:LYS:CE	0.67	1.37	21	1
1:A:17:LEU:CD1	1:A:17:LEU:CG	0.67	0.67	21	1
1:A:22:ARG:HH21	1:A:22:ARG:CZ	0.67	1.38	21	1
1:A:69:LYS:CE	1:A:69:LYS:HZ3	0.67	1.37	21	1
1:A:11:CYS:CB	1:A:11:CYS:HG	0.67	1.91	21	1
1:A:22:ARG:HH22	1:A:22:ARG:CZ	0.67	1.38	21	1
1:A:48:LEU:HD23	1:A:48:LEU:O	0.67	1.90	5	5
1:A:60:LEU:HD13	1:A:60:LEU:N	0.66	2.05	8	4
1:A:73:LYS:HZ3	1:A:73:LYS:CE	0.66	1.37	21	1
1:A:17:LEU:CG	1:A:17:LEU:HD21	0.66	1.19	21	1
1:A:31:ASP:OD2	1:A:31:ASP:CG	0.66	0.55	21	1
1:A:17:LEU:CG	1:A:17:LEU:HD22	0.66	1.19	21	1
1:A:73:LYS:HZ1	1:A:73:LYS:CE	0.66	1.37	21	1
1:A:25:VAL:HA	1:A:28:LEU:HD23	0.66	1.67	16	1
1:A:69:LYS:HD2	1:A:69:LYS:CB	0.66	2.12	21	1
1:A:57:ASP:CG	1:A:57:ASP:OD2	0.66	0.55	21	1
1:A:55:ALA:HB2	1:A:60:LEU:CD1	0.66	2.20	15	7
1:A:17:LEU:CG	1:A:17:LEU:HD23	0.66	1.19	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:LYS:HZ1	1:A:69:LYS:CE	0.66	1.37	21	1
1:A:30:ILE:HD13	1:A:30:ILE:N	0.65	2.05	1	1
1:A:50:ALA:HB3	1:A:63:MET:HG2	0.65	1.66	10	3
1:A:67:ALA:HB1	1:A:71:GLU:HB3	0.65	1.67	11	1
1:A:38:LYS:O	1:A:38:LYS:HG3	0.65	1.92	21	1
1:A:17:LEU:CD2	1:A:72:ILE:HD11	0.65	2.16	20	1
1:A:25:VAL:HG21	1:A:32:ALA:CB	0.65	2.22	10	10
1:A:34:PHE:CZ	1:A:34:PHE:CE2	0.65	0.74	21	1
1:A:13:ASN:ND2	1:A:13:ASN:CG	0.65	0.71	21	1
1:A:69:LYS:CE	1:A:69:LYS:HZ2	0.65	1.37	21	1
1:A:43:ILE:HG22	1:A:48:LEU:CD2	0.65	2.22	16	16
1:A:26:LYS:NZ	1:A:26:LYS:HE3	0.65	1.25	21	1
1:A:34:PHE:CZ	1:A:34:PHE:CE1	0.65	0.73	21	1
1:A:4:ILE:CD1	1:A:32:ALA:HB1	0.65	2.22	3	4
1:A:61:LYS:O	1:A:62:ILE:HD12	0.64	1.92	16	2
1:A:54:LEU:HB3	1:A:62:ILE:HD11	0.64	1.69	15	2
1:A:46:ALA:O	1:A:60:LEU:HD11	0.64	1.92	18	9
1:A:69:LYS:HA	1:A:72:ILE:HD12	0.64	1.69	14	1
1:A:6:ILE:HG23	1:A:14:CYS:HB2	0.64	1.68	13	2
1:A:40:MET:HA	1:A:43:ILE:HG13	0.64	1.70	21	1
1:A:60:LEU:HD12	1:A:63:MET:SD	0.64	2.32	7	1
1:A:4:ILE:HG21	1:A:34:PHE:CD2	0.64	2.27	15	8
1:A:73:LYS:NZ	1:A:73:LYS:CE	0.64	0.79	21	1
1:A:72:ILE:O	1:A:72:ILE:HD13	0.64	1.93	8	3
1:A:7:TYR:HD1	1:A:37:ILE:HD12	0.64	1.52	8	3
1:A:17:LEU:CB	1:A:66:VAL:HG22	0.63	2.23	17	7
1:A:60:LEU:HD22	1:A:60:LEU:H	0.63	1.51	2	3
1:A:28:LEU:O	1:A:28:LEU:HD13	0.63	1.94	12	2
1:A:7:TYR:HD2	1:A:48:LEU:HD11	0.63	1.53	8	3
1:A:69:LYS:NZ	1:A:69:LYS:CE	0.63	0.78	21	1
1:A:54:LEU:CD1	1:A:66:VAL:HG23	0.63	2.22	14	1
1:A:65:ARG:CD	1:A:65:ARG:HB2	0.63	2.13	21	1
1:A:17:LEU:CD1	1:A:17:LEU:HD23	0.63	1.18	21	1
1:A:17:LEU:HD13	1:A:17:LEU:O	0.63	1.94	20	3
1:A:46:ALA:HB1	1:A:60:LEU:HD23	0.63	1.68	10	1
1:A:37:ILE:HD13	1:A:37:ILE:O	0.62	1.93	12	1
1:A:57:ASP:OD1	1:A:57:ASP:CG	0.62	0.49	21	1
1:A:26:LYS:CE	1:A:26:LYS:HZ1	0.62	1.33	21	1
1:A:50:ALA:HB3	1:A:63:MET:HB3	0.62	1.68	5	3
1:A:5:GLN:CB	1:A:37:ILE:HD11	0.62	2.25	4	2
1:A:41:ASP:CG	1:A:41:ASP:OD2	0.62	0.50	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:TYR:CE2	1:A:42:GLN:C	0.62	2.73	9	1
1:A:48:LEU:HD22	1:A:48:LEU:H	0.62	1.53	2	2
1:A:26:LYS:CE	1:A:26:LYS:HZ3	0.62	1.33	21	1
1:A:60:LEU:N	1:A:60:LEU:HD13	0.61	2.10	11	3
1:A:9:THR:O	1:A:9:THR:HB	0.61	1.95	21	1
1:A:7:TYR:CE2	1:A:43:ILE:HA	0.61	2.30	12	3
1:A:26:LYS:CE	1:A:26:LYS:HZ2	0.61	1.33	21	1
1:A:7:TYR:CE2	1:A:37:ILE:HG21	0.61	2.29	9	1
1:A:17:LEU:HD22	1:A:20:ASN:OD1	0.61	1.95	15	2
1:A:46:ALA:HB1	1:A:60:LEU:HD12	0.61	1.71	2	1
1:A:26:LYS:NZ	1:A:26:LYS:HE2	0.61	1.25	21	1
1:A:7:TYR:CG	1:A:7:TYR:CD1	0.61	0.74	21	1
1:A:17:LEU:HD13	1:A:67:ALA:C	0.61	2.15	19	1
1:A:17:LEU:HD22	1:A:54:LEU:HD13	0.61	1.70	3	3
1:A:40:MET:HA	1:A:43:ILE:CG1	0.61	2.26	21	8
1:A:62:ILE:HG21	1:A:66:VAL:HA	0.60	1.73	14	5
1:A:65:ARG:HB2	1:A:65:ARG:HD3	0.60	1.72	21	1
1:A:6:ILE:HD13	1:A:6:ILE:N	0.60	2.12	9	3
1:A:65:ARG:CB	1:A:65:ARG:HD3	0.60	1.85	21	1
1:A:4:ILE:CG2	1:A:54:LEU:HD11	0.60	2.26	2	2
1:A:7:TYR:CD2	1:A:37:ILE:CD1	0.60	2.85	18	4
1:A:7:TYR:CE2	1:A:48:LEU:HD11	0.60	2.31	12	3
1:A:54:LEU:HD11	1:A:66:VAL:CG2	0.60	2.26	14	1
1:A:17:LEU:HD11	1:A:17:LEU:HD23	0.60	0.68	21	1
1:A:17:LEU:CB	1:A:66:VAL:HG21	0.60	2.27	15	1
1:A:7:TYR:CB	1:A:43:ILE:HG23	0.60	2.27	9	4
1:A:42:GLN:NE2	1:A:42:GLN:CD	0.59	0.65	21	1
1:A:37:ILE:C	1:A:37:ILE:HD13	0.59	2.18	5	2
1:A:7:TYR:OH	1:A:46:ALA:HB2	0.59	1.98	13	6
1:A:25:VAL:CG1	1:A:32:ALA:HB3	0.59	2.28	1	4
1:A:73:LYS:HG2	1:A:73:LYS:CE	0.59	2.19	21	1
1:A:39:GLU:O	1:A:43:ILE:HG23	0.59	1.97	10	1
1:A:17:LEU:HD11	1:A:62:ILE:HD12	0.59	1.73	12	1
1:A:7:TYR:CG	1:A:7:TYR:CD2	0.59	0.73	21	1
1:A:17:LEU:HD12	1:A:67:ALA:O	0.59	1.98	3	2
1:A:37:ILE:CD1	1:A:37:ILE:N	0.58	2.39	21	3
1:A:26:LYS:NZ	1:A:26:LYS:CE	0.58	0.73	21	1
1:A:48:LEU:O	1:A:48:LEU:HD23	0.58	1.98	8	5
1:A:7:TYR:CZ	1:A:7:TYR:CE1	0.58	0.69	21	1
1:A:17:LEU:O	1:A:17:LEU:HD22	0.58	1.99	15	1
1:A:48:LEU:HD22	1:A:48:LEU:N	0.58	2.13	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:MET:HA	1:A:43:ILE:HB	0.58	1.75	5	3
1:A:12:ALA:HB1	1:A:52:PRO:HB3	0.57	1.76	8	2
1:A:7:TYR:HB3	1:A:43:ILE:HG23	0.57	1.76	7	7
1:A:37:ILE:N	1:A:37:ILE:CD1	0.57	2.58	3	6
1:A:54:LEU:HD23	1:A:54:LEU:CD1	0.57	1.11	21	1
1:A:22:ARG:NH2	1:A:22:ARG:CZ	0.57	0.73	21	1
1:A:72:ILE:HD13	1:A:72:ILE:O	0.57	1.98	9	2
1:A:54:LEU:HD21	1:A:54:LEU:HD12	0.57	0.62	21	1
1:A:17:LEU:HD23	1:A:67:ALA:C	0.57	2.19	9	3
1:A:50:ALA:HB3	1:A:63:MET:CG	0.57	2.29	10	3
1:A:31:ASP:OD1	1:A:31:ASP:CG	0.57	0.46	21	1
1:A:62:ILE:HD13	1:A:66:VAL:CG1	0.57	2.27	15	1
1:A:40:MET:HA	1:A:43:ILE:HG23	0.56	1.77	13	3
1:A:69:LYS:HD3	1:A:69:LYS:CB	0.56	2.16	21	1
1:A:61:LYS:C	1:A:62:ILE:HD12	0.56	2.20	16	1
1:A:34:PHE:CD1	1:A:34:PHE:N	0.56	2.73	18	5
1:A:21:ALA:O	1:A:25:VAL:HG12	0.56	2.00	14	4
1:A:60:LEU:H	1:A:60:LEU:HD22	0.56	1.59	8	6
1:A:51:LEU:CB	1:A:52:PRO:CD	0.56	2.83	4	6
1:A:17:LEU:HD12	1:A:67:ALA:C	0.56	2.20	7	1
1:A:17:LEU:HD23	1:A:54:LEU:CD2	0.56	2.30	19	1
1:A:17:LEU:HB3	1:A:66:VAL:HG21	0.56	1.78	15	2
1:A:54:LEU:CD2	1:A:54:LEU:HD12	0.56	1.22	21	1
1:A:6:ILE:HG23	1:A:54:LEU:HD21	0.56	1.77	8	1
1:A:46:ALA:C	1:A:60:LEU:HD21	0.56	2.21	18	2
1:A:51:LEU:CB	1:A:52:PRO:HD3	0.56	2.30	13	14
1:A:40:MET:HA	1:A:43:ILE:HD12	0.56	1.77	2	4
1:A:17:LEU:CD2	1:A:54:LEU:HD13	0.56	2.31	3	1
1:A:6:ILE:HG22	1:A:14:CYS:HB2	0.56	1.77	8	3
1:A:6:ILE:HG21	1:A:6:ILE:HD13	0.56	1.62	21	1
1:A:34:PHE:N	1:A:34:PHE:CD1	0.56	2.74	10	1
1:A:46:ALA:HB1	1:A:60:LEU:CD1	0.55	2.31	2	1
1:A:50:ALA:HB3	1:A:64:GLY:N	0.55	2.16	14	2
1:A:1:MET:HB3	1:A:1:MET:HG2	0.55	1.21	21	1
1:A:17:LEU:HB2	1:A:66:VAL:HG22	0.55	1.79	21	5
1:A:24:ALA:O	1:A:28:LEU:HD23	0.55	2.02	15	4
1:A:7:TYR:HA	1:A:37:ILE:HD12	0.55	1.79	20	7
1:A:54:LEU:HD12	1:A:66:VAL:CG2	0.55	2.32	5	1
1:A:22:ARG:HA	1:A:34:PHE:CZ	0.54	2.36	18	2
1:A:25:VAL:HG13	1:A:26:LYS:N	0.54	2.17	6	21
1:A:7:TYR:CD1	1:A:37:ILE:CD1	0.54	2.90	6	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:MET:H3	1:A:31:ASP:C	0.54	2.06	3	1
1:A:68:SER:HG	1:A:68:SER:CB	0.54	1.24	21	1
1:A:17:LEU:CB	1:A:66:VAL:HG13	0.54	2.32	10	1
1:A:54:LEU:O	1:A:54:LEU:HD13	0.54	2.03	11	1
1:A:47:GLY:HA3	1:A:60:LEU:HD21	0.54	1.79	13	2
1:A:2:MET:HB2	1:A:32:ALA:HB2	0.54	1.78	1	2
1:A:6:ILE:HD11	1:A:36:LYS:CG	0.54	2.32	10	1
1:A:2:MET:SD	1:A:30:ILE:HD12	0.54	2.43	2	1
1:A:34:PHE:CZ	1:A:34:PHE:HE2	0.54	1.29	21	1
1:A:34:PHE:CG	1:A:34:PHE:HD2	0.53	1.29	21	1
1:A:53:GLY:O	1:A:54:LEU:HD22	0.53	2.04	20	1
1:A:54:LEU:O	1:A:54:LEU:HD23	0.53	2.04	3	1
1:A:54:LEU:HD13	1:A:54:LEU:C	0.53	2.24	11	4
1:A:34:PHE:CG	1:A:34:PHE:HD1	0.53	1.30	21	1
1:A:4:ILE:HG23	1:A:54:LEU:CD1	0.53	2.33	19	1
1:A:17:LEU:HD13	1:A:17:LEU:C	0.53	2.23	15	1
1:A:54:LEU:CG	1:A:54:LEU:CD1	0.53	0.69	21	1
1:A:34:PHE:HE1	1:A:34:PHE:CZ	0.53	1.28	21	1
1:A:51:LEU:O	1:A:53:GLY:N	0.53	2.42	16	3
1:A:46:ALA:CB	1:A:60:LEU:HD21	0.52	2.28	14	1
1:A:54:LEU:CD2	1:A:54:LEU:HD11	0.52	1.06	21	1
1:A:54:LEU:HD23	1:A:54:LEU:HD11	0.52	0.85	21	1
1:A:54:LEU:HB2	1:A:62:ILE:HD11	0.52	1.82	4	1
1:A:51:LEU:N	1:A:51:LEU:HD23	0.52	2.19	17	1
1:A:7:TYR:CD1	1:A:37:ILE:CG1	0.52	2.93	3	9
1:A:26:LYS:HE2	1:A:26:LYS:HZ3	0.52	1.10	21	1
1:A:48:LEU:C	1:A:48:LEU:HD23	0.52	2.24	3	6
1:A:48:LEU:O	1:A:49:THR:HG23	0.52	2.05	2	1
1:A:17:LEU:HD21	1:A:72:ILE:HB	0.52	1.82	5	1
1:A:6:ILE:HG22	1:A:54:LEU:CD1	0.52	2.34	4	1
1:A:48:LEU:C	1:A:49:THR:HG23	0.51	2.25	2	1
1:A:17:LEU:HD13	1:A:21:ALA:HB2	0.51	1.80	5	1
1:A:21:ALA:HB3	1:A:34:PHE:HE2	0.51	1.65	18	2
1:A:54:LEU:HD22	1:A:62:ILE:HD12	0.51	1.81	7	1
1:A:44:LEU:HD23	1:A:45:GLU:H	0.51	1.65	3	6
1:A:17:LEU:HD23	1:A:54:LEU:HD22	0.51	1.83	19	1
1:A:37:ILE:HD13	1:A:37:ILE:C	0.51	2.26	12	1
1:A:55:ALA:CB	1:A:60:LEU:HD22	0.51	2.34	7	2
1:A:17:LEU:HD13	1:A:67:ALA:HB3	0.51	1.81	14	1
1:A:52:PRO:HD2	1:A:64:GLY:HA2	0.51	1.83	17	8
1:A:50:ALA:CB	1:A:64:GLY:N	0.51	2.74	20	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ILE:HD13	1:A:72:ILE:C	0.51	2.26	11	3
1:A:38:LYS:O	1:A:39:GLU:HG3	0.51	2.07	21	1
1:A:25:VAL:CG1	1:A:26:LYS:N	0.50	2.74	18	21
1:A:17:LEU:CD2	1:A:17:LEU:HD13	0.50	1.11	21	1
1:A:4:ILE:CG2	1:A:34:PHE:CD2	0.50	2.95	19	10
1:A:4:ILE:HG23	1:A:56:VAL:HG13	0.50	1.83	2	4
1:A:46:ALA:HB1	1:A:60:LEU:CD2	0.50	2.36	18	2
1:A:62:ILE:HD11	1:A:67:ALA:HB2	0.50	1.83	18	1
1:A:44:LEU:HD23	1:A:45:GLU:N	0.50	2.21	3	6
1:A:69:LYS:HG3	1:A:69:LYS:CE	0.50	2.23	21	1
1:A:20:ASN:OD1	1:A:21:ALA:N	0.50	2.45	12	6
1:A:29:GLY:C	1:A:30:ILE:HD13	0.50	2.26	1	1
1:A:46:ALA:CB	1:A:60:LEU:HD11	0.50	2.36	12	1
1:A:1:MET:HG3	1:A:1:MET:CA	0.50	2.01	21	1
1:A:48:LEU:O	1:A:49:THR:CB	0.49	2.59	14	2
1:A:32:ALA:HB3	1:A:34:PHE:HE1	0.49	1.68	10	2
1:A:48:LEU:HD23	1:A:48:LEU:C	0.49	2.26	5	3
1:A:43:ILE:CG1	1:A:44:LEU:N	0.49	2.76	12	3
1:A:7:TYR:CD2	1:A:37:ILE:CG1	0.49	2.95	7	2
1:A:7:TYR:CD2	1:A:37:ILE:HD12	0.49	2.43	18	3
1:A:17:LEU:CD2	1:A:54:LEU:HD22	0.49	2.38	13	1
1:A:23:GLU:O	1:A:27:GLU:CB	0.49	2.60	10	18
1:A:30:ILE:CB	1:A:30:ILE:HD12	0.49	2.18	21	1
1:A:60:LEU:HD22	1:A:60:LEU:N	0.49	2.21	2	1
1:A:17:LEU:HD13	1:A:17:LEU:HD22	0.49	0.59	21	1
1:A:1:MET:HE3	1:A:1:MET:CG	0.49	2.19	21	1
1:A:7:TYR:HE2	1:A:46:ALA:CB	0.49	2.21	8	3
1:A:6:ILE:HD11	1:A:34:PHE:HB3	0.49	1.84	11	1
1:A:26:LYS:HE3	1:A:26:LYS:HZ1	0.49	1.10	21	1
1:A:43:ILE:HG23	1:A:48:LEU:HD21	0.49	1.84	5	1
1:A:5:GLN:CA	1:A:37:ILE:HD11	0.48	2.38	14	1
1:A:48:LEU:HB2	1:A:63:MET:HG2	0.48	1.85	19	6
1:A:17:LEU:HD13	1:A:67:ALA:O	0.48	2.08	13	2
1:A:48:LEU:N	1:A:48:LEU:CD2	0.48	2.73	14	1
1:A:32:ALA:HB3	1:A:34:PHE:CE1	0.48	2.43	14	3
1:A:4:ILE:HG23	1:A:54:LEU:HD11	0.48	1.85	1	3
1:A:17:LEU:HD23	1:A:18:GLU:N	0.48	2.22	10	1
1:A:7:TYR:CG	1:A:7:TYR:HD1	0.48	1.24	21	1
1:A:7:TYR:HD2	1:A:7:TYR:CG	0.48	1.24	21	1
1:A:39:GLU:O	1:A:43:ILE:HG13	0.48	2.08	17	9
1:A:1:MET:N	1:A:31:ASP:O	0.48	2.46	21	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ILE:HD13	1:A:66:VAL:HA	0.48	1.86	19	3
1:A:25:VAL:HG22	1:A:30:ILE:O	0.48	2.09	14	2
1:A:5:GLN:HB3	1:A:7:TYR:CE1	0.48	2.44	5	1
1:A:22:ARG:HA	1:A:34:PHE:CE1	0.48	2.44	5	13
1:A:17:LEU:HD11	1:A:62:ILE:CD1	0.48	2.37	12	1
1:A:6:ILE:HG22	1:A:14:CYS:SG	0.48	2.49	18	3
1:A:22:ARG:CG	1:A:34:PHE:CD1	0.48	2.96	6	4
1:A:49:THR:HG1	1:A:49:THR:CB	0.48	1.18	21	1
1:A:7:TYR:CE2	1:A:46:ALA:HB2	0.47	2.44	6	3
1:A:7:TYR:CZ	1:A:7:TYR:HE2	0.47	1.23	21	1
1:A:6:ILE:HD11	1:A:36:LYS:HG3	0.47	1.85	10	1
1:A:53:GLY:HA2	1:A:62:ILE:O	0.47	2.09	10	4
1:A:54:LEU:HD12	1:A:62:ILE:CB	0.47	2.38	14	1
1:A:50:ALA:HB1	1:A:64:GLY:N	0.47	2.25	20	4
1:A:46:ALA:HB3	1:A:48:LEU:HD13	0.47	1.86	6	3
1:A:66:VAL:CG1	1:A:66:VAL:C	0.47	2.82	21	1
1:A:54:LEU:HD23	1:A:54:LEU:C	0.47	2.30	3	1
1:A:48:LEU:CD1	1:A:60:LEU:HD21	0.47	2.39	19	1
1:A:40:MET:HA	1:A:43:ILE:CG2	0.47	2.40	13	1
1:A:6:ILE:HG22	1:A:54:LEU:HD22	0.47	1.87	14	1
1:A:17:LEU:HD22	1:A:66:VAL:HB	0.47	1.86	13	1
1:A:48:LEU:C	1:A:48:LEU:CD2	0.47	2.83	3	5
1:A:4:ILE:HG12	1:A:56:VAL:CG1	0.46	2.40	15	3
1:A:17:LEU:C	1:A:17:LEU:HD13	0.46	2.30	18	2
1:A:7:TYR:CZ	1:A:7:TYR:HE1	0.46	1.22	21	1
1:A:54:LEU:N	1:A:62:ILE:O	0.46	2.48	8	1
1:A:54:LEU:HD12	1:A:62:ILE:CG1	0.46	2.40	14	1
1:A:4:ILE:CD1	1:A:34:PHE:CE2	0.46	2.99	15	1
1:A:48:LEU:CD2	1:A:48:LEU:C	0.46	2.83	15	5
1:A:28:LEU:HD21	1:A:73:LYS:HG2	0.46	1.86	15	1
1:A:4:ILE:CG2	1:A:54:LEU:HD21	0.46	2.40	11	1
1:A:1:MET:N	1:A:1:MET:CG	0.46	2.72	21	1
1:A:17:LEU:HB3	1:A:66:VAL:HG22	0.46	1.87	10	2
1:A:6:ILE:HD11	1:A:36:LYS:HB2	0.46	1.87	5	1
1:A:38:LYS:O	1:A:39:GLU:CB	0.46	2.63	12	11
1:A:16:MET:CB	1:A:66:VAL:HG11	0.46	2.40	2	1
1:A:59:GLU:O	1:A:59:GLU:CG	0.46	2.64	1	1
1:A:17:LEU:HD22	1:A:20:ASN:HD21	0.46	1.69	20	2
1:A:40:MET:HA	1:A:43:ILE:HG12	0.46	1.87	10	2
1:A:17:LEU:HD13	1:A:66:VAL:HG22	0.46	1.87	11	1
1:A:50:ALA:CB	1:A:63:MET:HB2	0.46	2.41	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:MET:CA	1:A:31:ASP:O	0.46	2.64	10	19
1:A:7:TYR:CE1	1:A:37:ILE:HD12	0.46	2.46	16	2
1:A:6:ILE:HD13	1:A:18:GLU:HG3	0.46	1.87	3	1
1:A:6:ILE:HG23	1:A:54:LEU:CD2	0.46	2.41	8	1
1:A:62:ILE:HG21	1:A:66:VAL:HG12	0.46	1.86	3	1
1:A:1:MET:CB	1:A:31:ASP:O	0.45	2.64	1	1
1:A:24:ALA:O	1:A:28:LEU:HB2	0.45	2.10	21	1
1:A:30:ILE:N	1:A:30:ILE:HD13	0.45	2.26	20	1
1:A:72:ILE:HG23	1:A:73:LYS:N	0.45	2.26	15	4
1:A:17:LEU:HB2	1:A:66:VAL:CG1	0.45	2.36	21	1
1:A:46:ALA:HB3	1:A:48:LEU:CD1	0.45	2.41	9	1
1:A:6:ILE:C	1:A:37:ILE:HD11	0.45	2.31	15	2
1:A:46:ALA:O	1:A:60:LEU:CD2	0.45	2.64	21	1
1:A:36:LYS:HD2	1:A:36:LYS:HE3	0.45	1.31	21	1
1:A:6:ILE:HG23	1:A:54:LEU:HD11	0.45	1.88	12	1
1:A:40:MET:HA	1:A:43:ILE:CD1	0.45	2.41	21	1
1:A:7:TYR:HE2	1:A:46:ALA:HB2	0.45	1.72	8	1
1:A:4:ILE:O	1:A:34:PHE:HA	0.45	2.11	7	1
1:A:54:LEU:HD13	1:A:54:LEU:O	0.45	2.12	9	1
1:A:48:LEU:CB	1:A:63:MET:CG	0.45	2.94	14	3
1:A:73:LYS:CG	1:A:73:LYS:HE2	0.45	2.00	21	1
1:A:8:GLY:CA	1:A:12:ALA:HB3	0.45	2.42	17	2
1:A:40:MET:CA	1:A:43:ILE:HD12	0.44	2.42	2	1
1:A:7:TYR:CE2	1:A:37:ILE:HD12	0.44	2.46	7	1
1:A:54:LEU:CG	1:A:54:LEU:HD12	0.44	1.36	21	1
1:A:65:ARG:CD	1:A:65:ARG:HB3	0.44	2.18	21	1
1:A:8:GLY:O	1:A:10:GLY:N	0.44	2.50	6	2
1:A:43:ILE:O	1:A:48:LEU:HD22	0.44	2.12	13	1
1:A:41:ASP:O	1:A:44:LEU:HD23	0.44	2.13	13	11
1:A:73:LYS:HD2	1:A:73:LYS:HE3	0.44	1.31	21	1
1:A:12:ALA:HB1	1:A:52:PRO:CB	0.44	2.43	4	2
1:A:17:LEU:CD1	1:A:72:ILE:HD11	0.44	2.22	1	1
1:A:46:ALA:CB	1:A:60:LEU:HD12	0.44	2.43	2	1
1:A:60:LEU:H	1:A:60:LEU:HD13	0.44	1.70	11	1
1:A:6:ILE:HD13	1:A:18:GLU:CD	0.44	2.33	4	1
1:A:7:TYR:N	1:A:7:TYR:CD1	0.44	2.84	8	2
1:A:7:TYR:CD1	1:A:37:ILE:HB	0.44	2.47	4	1
1:A:6:ILE:CD1	1:A:6:ILE:N	0.44	2.81	8	2
1:A:48:LEU:CD2	1:A:48:LEU:O	0.43	2.66	9	4
1:A:50:ALA:CB	1:A:63:MET:CB	0.43	2.90	5	1
1:A:28:LEU:HD13	1:A:28:LEU:O	0.43	2.12	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:MET:N	1:A:32:ALA:HA	0.43	2.28	17	5
1:A:26:LYS:HG2	1:A:31:ASP:HA	0.43	1.89	21	1
1:A:34:PHE:N	1:A:34:PHE:HD1	0.43	2.09	18	2
1:A:48:LEU:HB2	1:A:63:MET:CG	0.43	2.43	9	5
1:A:17:LEU:CD2	1:A:62:ILE:HD11	0.43	2.43	2	1
1:A:6:ILE:HD13	1:A:6:ILE:H	0.43	1.74	7	1
1:A:7:TYR:CE1	1:A:37:ILE:HG21	0.43	2.48	8	1
1:A:6:ILE:CG2	1:A:14:CYS:CB	0.43	2.96	1	1
1:A:4:ILE:CG1	1:A:56:VAL:CG1	0.43	2.95	20	4
1:A:7:TYR:CE1	1:A:37:ILE:CG2	0.43	3.02	8	2
1:A:2:MET:CE	1:A:30:ILE:HG21	0.43	2.43	13	1
1:A:13:ASN:CG	1:A:13:ASN:OD1	0.43	0.55	21	1
1:A:17:LEU:O	1:A:20:ASN:OD1	0.43	2.37	20	1
1:A:37:ILE:HG12	1:A:38:LYS:N	0.43	2.28	20	2
1:A:1:MET:HA	1:A:31:ASP:O	0.43	2.14	10	4
1:A:7:TYR:HA	1:A:37:ILE:HD11	0.43	1.87	18	1
1:A:22:ARG:HG3	1:A:34:PHE:CD1	0.43	2.49	9	6
1:A:23:GLU:HG3	1:A:24:ALA:N	0.43	2.28	14	1
1:A:48:LEU:CB	1:A:63:MET:HG2	0.43	2.44	7	1
1:A:17:LEU:CD1	1:A:17:LEU:HD22	0.43	1.03	21	1
1:A:4:ILE:HB	1:A:34:PHE:CD2	0.43	2.49	14	4
1:A:2:MET:CE	1:A:30:ILE:HD12	0.43	2.44	3	1
1:A:72:ILE:C	1:A:72:ILE:HD13	0.43	2.33	8	1
1:A:7:TYR:HA	1:A:37:ILE:CG1	0.43	2.44	7	3
1:A:54:LEU:HD21	1:A:56:VAL:HG13	0.43	1.89	3	1
1:A:14:CYS:HA	1:A:66:VAL:HG21	0.42	1.90	20	1
1:A:17:LEU:CD2	1:A:17:LEU:HD11	0.42	0.96	21	1
1:A:30:ILE:CD1	1:A:30:ILE:N	0.42	2.76	1	1
1:A:2:MET:HE3	1:A:30:ILE:HD12	0.42	1.89	3	1
1:A:48:LEU:HD12	1:A:53:GLY:HA3	0.42	1.91	6	1
1:A:48:LEU:O	1:A:48:LEU:CD2	0.42	2.67	8	3
1:A:5:GLN:C	1:A:37:ILE:HD11	0.42	2.34	10	1
1:A:17:LEU:HD21	1:A:17:LEU:HD12	0.42	0.43	21	1
1:A:17:LEU:CB	1:A:66:VAL:CG2	0.42	2.96	17	3
1:A:8:GLY:HA3	1:A:12:ALA:CB	0.42	2.44	21	1
1:A:8:GLY:C	1:A:9:THR:HG1	0.42	2.17	16	1
1:A:43:ILE:O	1:A:48:LEU:HD21	0.42	2.13	17	1
1:A:5:GLN:HB2	1:A:37:ILE:HD11	0.42	1.92	14	1
1:A:72:ILE:CG2	1:A:73:LYS:N	0.42	2.83	5	1
1:A:7:TYR:HD1	1:A:43:ILE:HG22	0.42	1.75	10	1
1:A:5:GLN:O	1:A:54:LEU:HA	0.42	2.15	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:CB	1:A:63:MET:CB	0.42	2.98	2	1
1:A:17:LEU:CD2	1:A:17:LEU:CA	0.42	2.88	21	1
1:A:46:ALA:C	1:A:60:LEU:HD11	0.42	2.35	20	1
1:A:17:LEU:HG	1:A:67:ALA:HB3	0.42	1.91	1	1
1:A:54:LEU:C	1:A:54:LEU:HD12	0.42	2.35	15	1
1:A:4:ILE:HG13	1:A:56:VAL:CG1	0.41	2.44	19	1
1:A:17:LEU:HD21	1:A:72:ILE:HG12	0.41	1.91	1	1
1:A:43:ILE:O	1:A:48:LEU:CD2	0.41	2.67	13	1
1:A:62:ILE:HG21	1:A:66:VAL:CA	0.41	2.45	9	1
1:A:52:PRO:O	1:A:62:ILE:CG2	0.41	2.68	18	1
1:A:5:GLN:CB	1:A:37:ILE:CD1	0.41	2.99	14	2
1:A:25:VAL:HG11	1:A:32:ALA:CB	0.41	2.37	1	2
1:A:54:LEU:CD1	1:A:66:VAL:CG2	0.41	2.98	5	1
1:A:62:ILE:HD13	1:A:67:ALA:H	0.41	1.75	13	1
1:A:48:LEU:HD13	1:A:60:LEU:CD1	0.41	2.45	12	1
1:A:7:TYR:CD1	1:A:7:TYR:N	0.41	2.86	12	1
1:A:22:ARG:HG2	1:A:34:PHE:CD1	0.41	2.50	19	1
1:A:51:LEU:HD12	1:A:52:PRO:HD3	0.41	1.92	7	1
1:A:5:GLN:O	1:A:54:LEU:CD2	0.41	2.68	11	1
1:A:60:LEU:N	1:A:60:LEU:CD1	0.41	2.77	8	1
1:A:38:LYS:O	1:A:38:LYS:CG	0.41	2.62	21	1
1:A:2:MET:CG	1:A:25:VAL:CG2	0.41	2.99	19	1
1:A:62:ILE:HD12	1:A:62:ILE:N	0.41	2.31	14	1
1:A:4:ILE:HG22	1:A:54:LEU:HD21	0.41	1.93	2	1
1:A:6:ILE:HG22	1:A:54:LEU:HD23	0.41	1.93	10	1
1:A:48:LEU:O	1:A:63:MET:HG3	0.41	2.16	2	1
1:A:68:SER:HG	1:A:68:SER:HB3	0.41	1.36	21	1
1:A:4:ILE:HG21	1:A:34:PHE:CE2	0.40	2.51	4	1
1:A:6:ILE:H	1:A:37:ILE:HD11	0.40	1.70	2	1
1:A:17:LEU:HD21	1:A:72:ILE:CG1	0.40	2.46	1	1
1:A:17:LEU:CD2	1:A:17:LEU:CG	0.40	0.44	21	1
1:A:41:ASP:O	1:A:44:LEU:CD2	0.40	2.70	10	1
1:A:52:PRO:HG2	1:A:65:ARG:N	0.40	2.31	3	1
1:A:17:LEU:HD23	1:A:62:ILE:HD11	0.40	1.94	2	1
1:A:7:TYR:O	1:A:51:LEU:O	0.40	2.39	11	1
1:A:22:ARG:HG2	1:A:34:PHE:CE1	0.40	2.51	11	1
1:A:40:MET:O	1:A:43:ILE:HG12	0.40	2.17	13	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	72/77 (94%)	58±2 (80±2%)	11±1 (15±2%)	4±1 (5±1%)	5	25
All	All	1512/1617 (94%)	1209 (80%)	225 (15%)	78 (5%)	5	25

All 13 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	39	GLU	21
1	A	30	ILE	16
1	A	65	ARG	15
1	A	9	THR	8
1	A	10	GLY	5
1	A	66	VAL	3
1	A	8	GLY	3
1	A	11	CYS	2
1	A	67	ALA	1
1	A	48	LEU	1
1	A	51	LEU	1
1	A	52	PRO	1
1	A	49	THR	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	58/62 (94%)	36±4 (62±6%)	22±4 (38±6%)	1	6
All	All	1218/1302 (94%)	750 (62%)	468 (38%)	1	6

All 55 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	56	VAL	21
1	A	44	LEU	21
1	A	37	ILE	21
1	A	48	LEU	21
1	A	15	GLN	20
1	A	60	LEU	19
1	A	41	ASP	14
1	A	61	LYS	14
1	A	36	LYS	12
1	A	38	LYS	12
1	A	40	MET	11
1	A	3	LYS	11
1	A	31	ASP	11
1	A	63	MET	11
1	A	2	MET	11
1	A	39	GLU	11
1	A	30	ILE	10
1	A	57	ASP	10
1	A	51	LEU	10
1	A	54	LEU	9
1	A	26	LYS	9
1	A	28	LEU	9
1	A	73	LYS	9
1	A	65	ARG	9
1	A	66	VAL	8
1	A	22	ARG	8
1	A	5	GLN	8
1	A	69	LYS	8
1	A	19	LYS	8
1	A	59	GLU	7
1	A	17	LEU	7
1	A	49	THR	7
1	A	9	THR	7
1	A	6	ILE	7
1	A	68	SER	6
1	A	72	ILE	6
1	A	16	MET	6
1	A	70	GLU	6
1	A	11	CYS	6
1	A	1	MET	6
1	A	71	GLU	5
1	A	35	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	42	GLN	4
1	A	62	ILE	4
1	A	45	GLU	4
1	A	33	GLU	3
1	A	23	GLU	3
1	A	18	GLU	3
1	A	34	PHE	2
1	A	4	ILE	2
1	A	27	GLU	2
1	A	43	ILE	2
1	A	13	ASN	1
1	A	7	TYR	1
1	A	20	ASN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 65% for the well-defined parts and 65% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4991

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	664
Number of shifts mapped to atoms	664
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	75	-0.34 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	69	-0.07 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	73	0.29 ± 0.56	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 65%, i.e. 572 atoms were assigned a chemical shift out of a possible 878. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	282/363 (78%)	142/145 (98%)	71/146 (49%)	69/72 (96%)
Sidechain	281/498 (56%)	211/290 (73%)	65/189 (34%)	5/19 (26%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	9/17 (53%)	9/9 (100%)	0/8 (0%)	0/0 (—%)
Overall	572/878 (65%)	362/444 (82%)	136/343 (40%)	74/91 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 65%, i.e. 607 atoms were assigned a chemical shift out of a possible 932. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	298/383 (78%)	150/153 (98%)	75/154 (49%)	73/76 (96%)
Sidechain	300/532 (56%)	226/310 (73%)	69/202 (34%)	5/20 (25%)
Aromatic	9/17 (53%)	9/9 (100%)	0/8 (0%)	0/0 (—%)
Overall	607/932 (65%)	385/472 (82%)	144/364 (40%)	78/96 (81%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	50	ALA	CB	44.68	28.03 – 9.93	14.2
1	A	22	ARG	HD2	0.64	4.27 – 1.97	-10.8

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:

