



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 12:16 AM UTC

PDB ID : 1ILO / pdb_00001ilo
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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

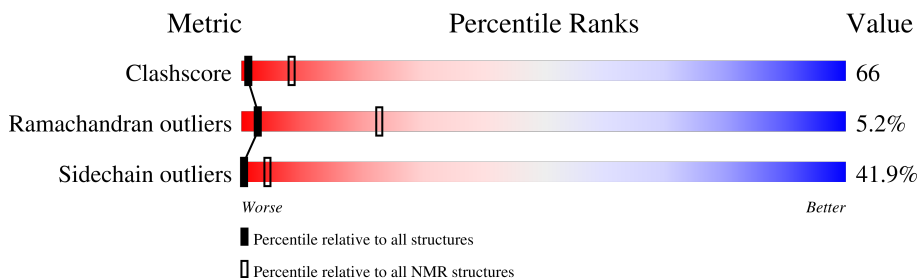
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	

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)	0.48	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

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.

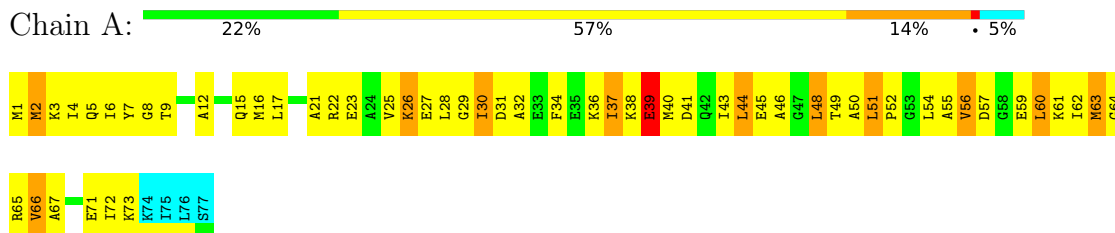
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	77	1207	368	621	97	114	7	0

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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 MthH895

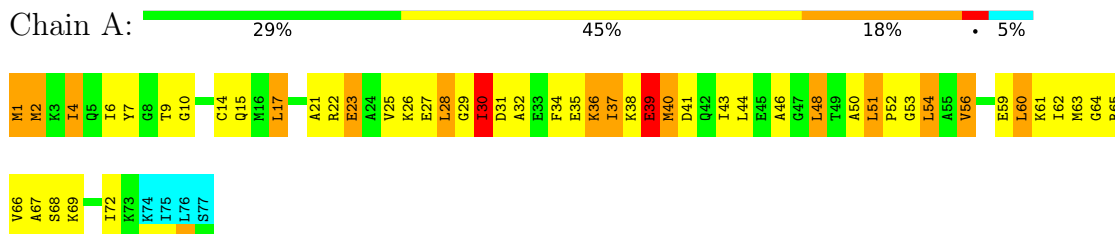


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

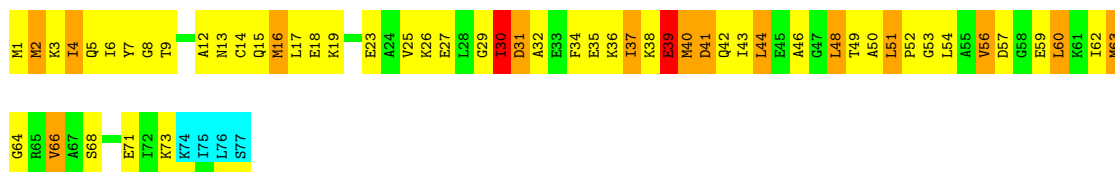
- Molecule 1: conserved hypothetical protein MthH895



4.2.2 Score per residue for model 2

- Molecule 1: conserved hypothetical protein MthH895

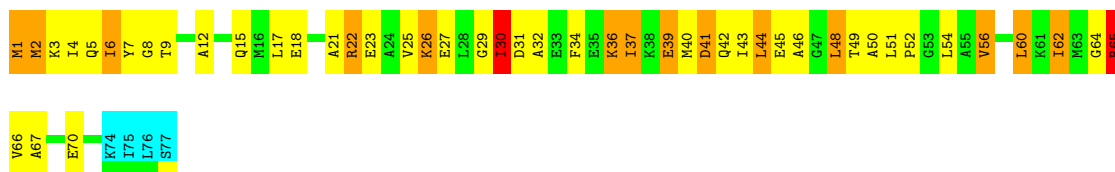




4.2.3 Score per residue for model 3

- Molecule 1: conserved hypothetical protein MtH895

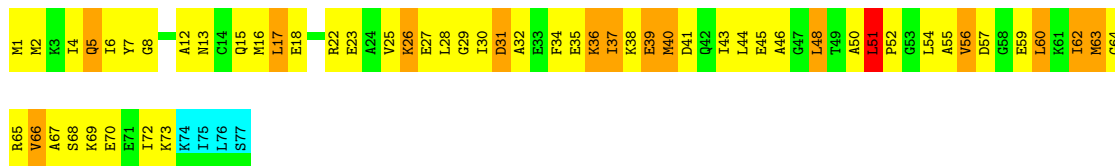
Chain A: 32% 42% 18% 5%



4.2.4 Score per residue for model 4

- Molecule 1: conserved hypothetical protein MtH895

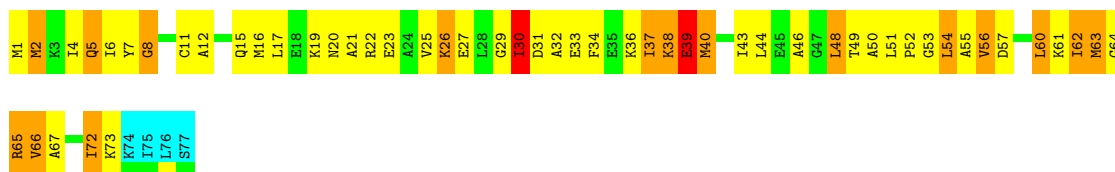
Chain A: 22% 53% 18% 5%



4.2.5 Score per residue for model 5

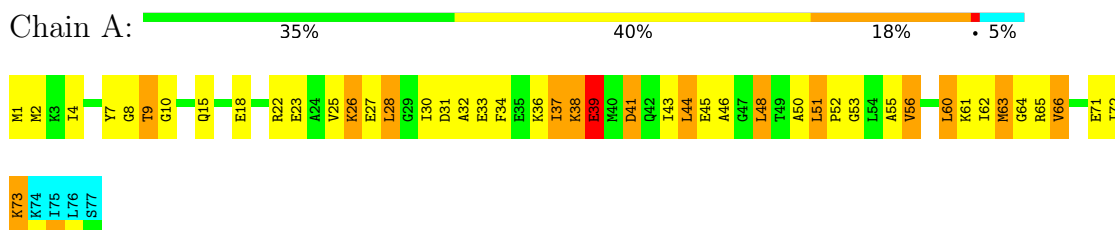
- Molecule 1: conserved hypothetical protein MtH895

Chain A: 25% 47% 21% 5%



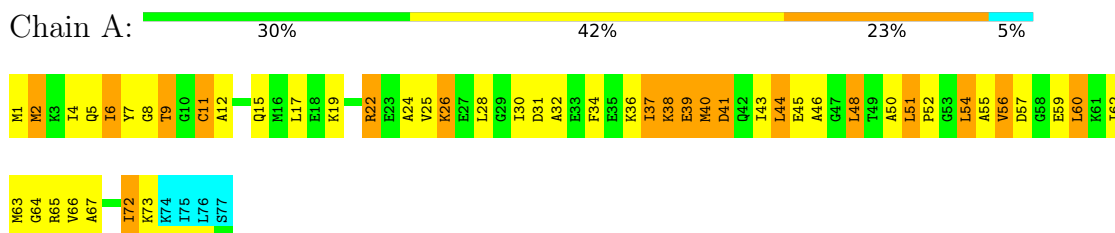
4.2.6 Score per residue for model 6

- Molecule 1: conserved hypothetical protein MtH895



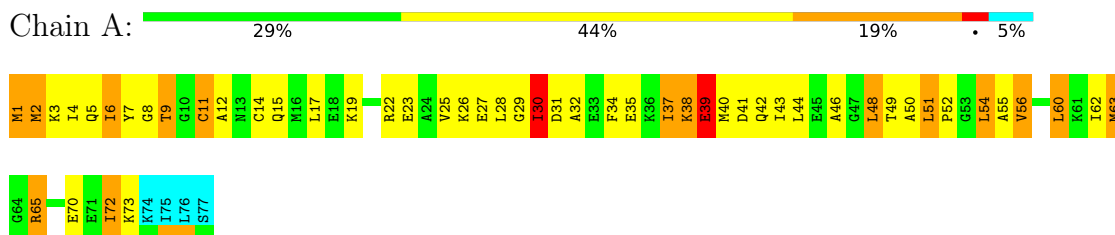
4.2.7 Score per residue for model 7

- Molecule 1: conserved hypothetical protein MtH895



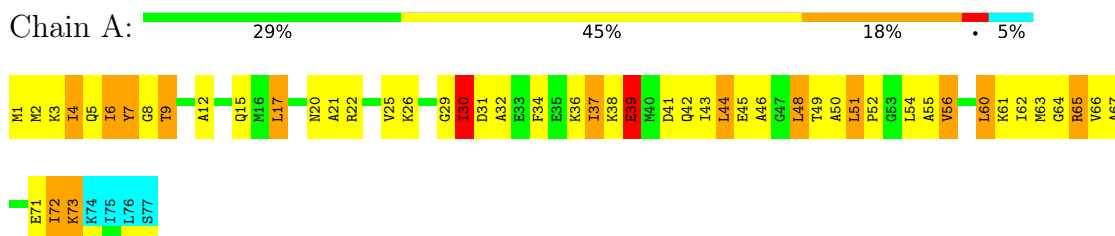
4.2.8 Score per residue for model 8

- Molecule 1: conserved hypothetical protein MtH895



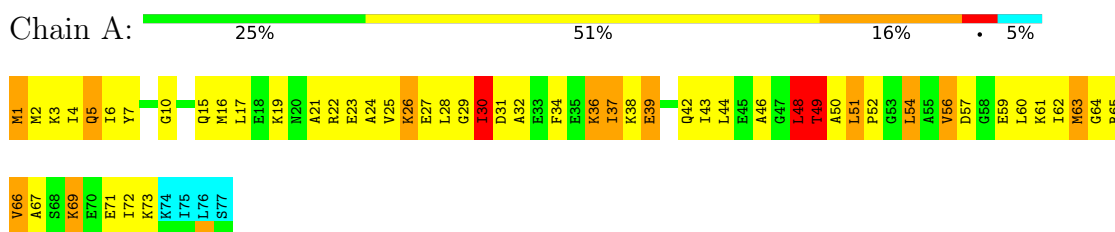
4.2.9 Score per residue for model 9

- Molecule 1: conserved hypothetical protein MtH895



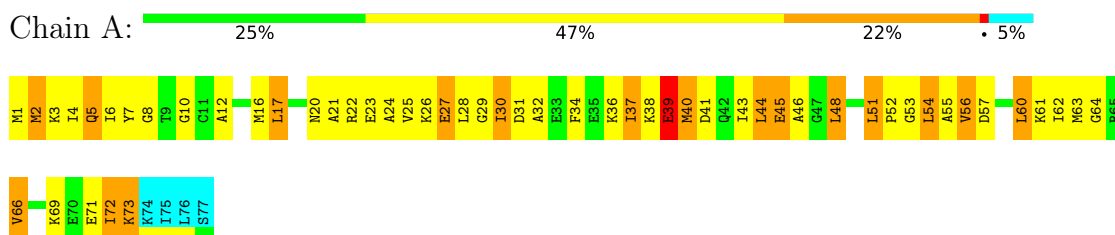
4.2.14 Score per residue for model 14

- Molecule 1: conserved hypothetical protein MtH895



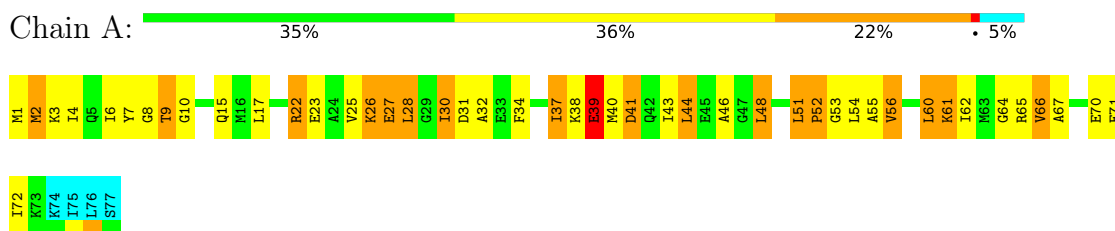
4.2.15 Score per residue for model 15

- Molecule 1: conserved hypothetical protein MtH895



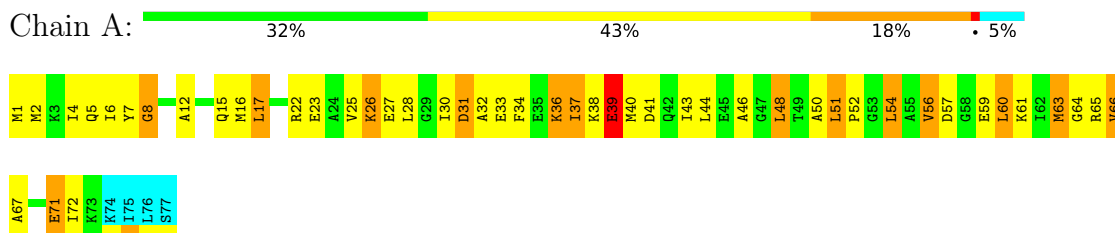
4.2.16 Score per residue for model 16

- Molecule 1: conserved hypothetical protein MtH895



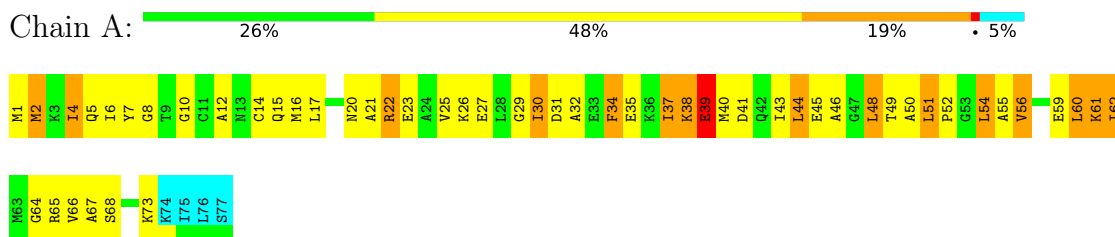
4.2.17 Score per residue for model 17

- Molecule 1: conserved hypothetical protein MtH895



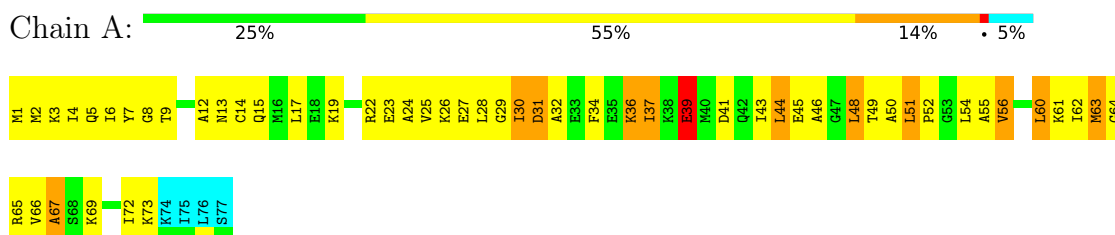
4.2.18 Score per residue for model 18

- Molecule 1: conserved hypothetical protein MtH895



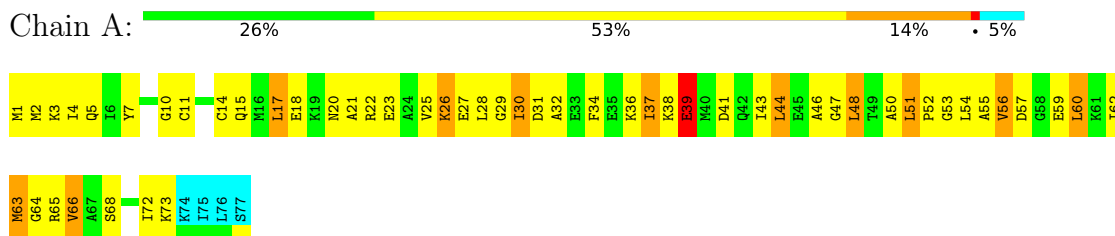
4.2.19 Score per residue for model 19

- Molecule 1: conserved hypothetical protein MtH895



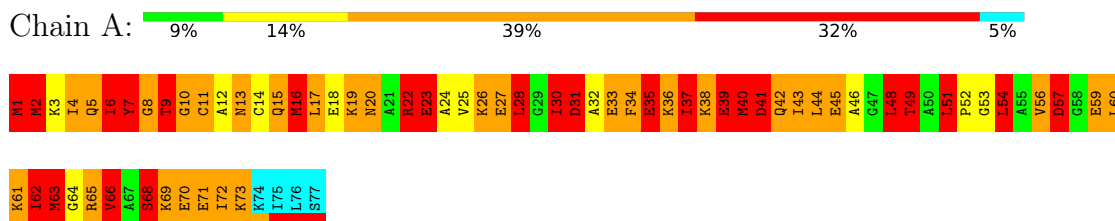
4.2.20 Score per residue for model 20

- 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

No chemical shift data was provided.

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	1.17±3.44	9±39/557 (1.6± 7.0%)	1.19±2.28	9±40/742 (1.2± 5.4%)
All	All	3.63	186/11697 (1.6%)	2.58	193/15582 (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	65	ARG	CZ-NH1	-81.20	0.19	1.32	21	1
1	A	22	ARG	CZ-NH1	-79.86	0.20	1.32	21	1
1	A	65	ARG	NE-CZ	-68.03	0.58	1.33	21	1
1	A	45	GLU	CD-OE1	-54.31	0.22	1.25	21	1
1	A	49	THR	CB-OG1	-52.54	0.59	1.43	21	1
1	A	39	GLU	CD-OE1	-50.81	0.28	1.25	21	1
1	A	65	ARG	CZ-NH2	-49.53	0.69	1.33	21	1
1	A	65	ARG	CD-NE	-49.01	0.77	1.46	21	1
1	A	9	THR	C-O	-48.65	0.48	1.23	21	1
1	A	33	GLU	CD-OE1	-48.62	0.33	1.25	21	1
1	A	71	GLU	CD-OE2	-47.78	0.34	1.25	21	1
1	A	35	GLU	CD-OE2	-47.62	0.34	1.25	21	1
1	A	27	GLU	CD-OE2	-46.81	0.36	1.25	21	1
1	A	22	ARG	CZ-NH2	-46.37	0.73	1.33	21	1
1	A	59	GLU	CD-OE2	-46.16	0.37	1.25	21	1
1	A	42	GLN	CD-OE1	-45.93	0.36	1.23	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	59	GLU	CD-OE1	-45.86	0.38	1.25	21	1
1	A	23	GLU	CD-OE1	-44.44	0.41	1.25	21	1
1	A	22	ARG	CD-NE	-44.19	0.84	1.46	21	1
1	A	22	ARG	NE-CZ	-43.93	0.84	1.33	21	1
1	A	70	GLU	CD-OE2	-43.89	0.41	1.25	21	1
1	A	71	GLU	CD-OE1	-43.68	0.42	1.25	21	1
1	A	70	GLU	CD-OE1	-42.81	0.44	1.25	21	1
1	A	31	ASP	CG-OD1	-41.63	0.46	1.25	21	1
1	A	18	GLU	CD-OE2	-41.61	0.46	1.25	21	1
1	A	35	GLU	CD-OE1	-40.85	0.47	1.25	21	1
1	A	16	MET	SD-CE	-40.38	0.78	1.79	21	1
1	A	27	GLU	CD-OE1	-40.17	0.49	1.25	21	1
1	A	23	GLU	CD-OE2	-40.09	0.49	1.25	21	1
1	A	1	MET	SD-CE	-39.98	0.79	1.79	21	1
1	A	18	GLU	CD-OE1	-39.83	0.49	1.25	21	1
1	A	40	MET	SD-CE	-39.70	0.80	1.79	21	1
1	A	57	ASP	CG-OD1	-39.69	0.49	1.25	21	1
1	A	41	ASP	CG-OD2	-39.35	0.50	1.25	21	1
1	A	33	GLU	CD-OE2	-38.03	0.53	1.25	21	1
1	A	9	THR	CB-OG1	-37.38	0.83	1.43	21	1
1	A	68	SER	CB-OG	-37.12	0.68	1.42	21	1
1	A	57	ASP	CG-OD2	-36.76	0.55	1.25	21	1
1	A	31	ASP	CG-OD2	-36.70	0.55	1.25	21	1
1	A	45	GLU	CD-OE2	-36.37	0.56	1.25	21	1
1	A	9	THR	C-N	-35.83	0.81	1.33	21	1
1	A	39	GLU	CD-OE2	-35.77	0.57	1.25	21	1
1	A	13	ASN	CG-OD1	-35.58	0.56	1.23	21	1
1	A	38	LYS	CE-NZ	-35.52	0.42	1.49	21	1
1	A	30	ILE	CB-CG1	-34.90	0.83	1.53	21	1
1	A	54	LEU	CG-CD2	-33.50	0.42	1.52	21	1
1	A	2	MET	CG-SD	-33.22	0.97	1.80	21	1
1	A	17	LEU	CG-CD2	-32.65	0.44	1.52	21	1
1	A	63	MET	SD-CE	-32.49	0.98	1.79	21	1
1	A	42	GLN	CD-NE2	-32.37	0.65	1.33	21	1
1	A	41	ASP	CG-OD1	-32.14	0.64	1.25	21	1
1	A	5	GLN	CD-OE1	-31.81	0.63	1.23	21	1
1	A	7	TYR	CE2-CZ	31.61	2.14	1.38	9	2
1	A	7	TYR	CG-CD2	-31.55	0.73	1.39	21	1
1	A	7	TYR	CG-CD1	-31.08	0.74	1.39	21	1
1	A	20	ASN	CG-OD1	-30.70	0.65	1.23	21	1
1	A	34	PHE	CG-CD2	-30.64	0.74	1.38	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	40	MET	CB-CG	-30.25	0.61	1.52	21	1
1	A	34	PHE	CG-CD1	-29.76	0.76	1.38	21	1
1	A	13	ASN	CG-ND2	-29.58	0.71	1.33	21	1
1	A	2	MET	SD-CE	-28.65	1.07	1.79	21	1
1	A	7	TYR	CE1-CZ	-28.49	0.69	1.38	21	1
1	A	16	MET	CG-SD	-28.47	1.09	1.80	21	1
1	A	60	LEU	CG-CD1	-27.89	0.60	1.52	21	1
1	A	62	ILE	CB-CG1	-27.48	0.98	1.53	21	1
1	A	45	GLU	CG-CD	-27.00	0.84	1.52	21	1
1	A	61	LYS	CE-NZ	-26.30	0.70	1.49	21	1
1	A	62	ILE	CG1-CD1	-26.15	0.49	1.51	21	1
1	A	69	LYS	CB-CG	-26.11	0.74	1.52	21	1
1	A	42	GLN	CG-CD	-26.07	0.86	1.52	21	1
1	A	63	MET	CG-SD	-25.82	1.16	1.80	21	1
1	A	17	LEU	CG-CD1	-25.69	0.67	1.52	21	1
1	A	28	LEU	CG-CD2	-25.26	0.69	1.52	21	1
1	A	54	LEU	CG-CD1	-25.22	0.69	1.52	21	1
1	A	7	TYR	CD2-CE2	25.15	2.14	1.38	9	1
1	A	26	LYS	CE-NZ	-25.14	0.73	1.49	21	1
1	A	38	LYS	CD-CE	-25.07	0.77	1.52	21	1
1	A	35	GLU	CG-CD	-25.03	0.89	1.52	21	1
1	A	49	THR	CB-CG2	-24.89	0.70	1.52	21	1
1	A	48	LEU	C-O	-24.87	0.90	1.23	21	1
1	A	1	MET	CG-SD	-24.87	1.18	1.80	21	1
1	A	26	LYS	CD-CE	-24.84	0.78	1.52	21	1
1	A	37	ILE	C-O	-24.60	0.98	1.24	21	1
1	A	72	ILE	CB-CG1	-24.57	1.04	1.53	21	1
1	A	59	GLU	CG-CD	-23.62	0.93	1.52	21	1
1	A	1	MET	CB-CG	-23.59	0.81	1.52	21	1
1	A	69	LYS	CE-NZ	-23.53	0.78	1.49	21	1
1	A	73	LYS	CE-NZ	-23.30	0.79	1.49	21	1
1	A	36	LYS	CD-CE	-22.99	0.83	1.52	21	1
1	A	27	GLU	CG-CD	-22.97	0.94	1.52	21	1
1	A	10	GLY	C-O	-22.83	0.93	1.23	21	1
1	A	33	GLU	CG-CD	-22.71	0.95	1.52	21	1
1	A	19	LYS	CD-CE	-22.45	0.85	1.52	21	1
1	A	69	LYS	CD-CE	-22.36	0.85	1.52	21	1
1	A	71	GLU	CG-CD	-22.12	0.96	1.52	21	1
1	A	73	LYS	CD-CE	-21.97	0.86	1.52	21	1
1	A	6	ILE	CB-CG1	-21.89	1.09	1.53	21	1
1	A	39	GLU	CG-CD	-21.88	0.97	1.52	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	34	PHE	CE1-CZ	-21.83	0.73	1.38	21	1
1	A	72	ILE	CG1-CD1	-21.40	0.68	1.51	21	1
1	A	40	MET	CG-SD	-21.30	1.27	1.80	21	1
1	A	34	PHE	CE2-CZ	-21.28	0.74	1.38	21	1
1	A	63	MET	CB-CG	-20.25	0.91	1.52	21	1
1	A	66	VAL	CB-CG2	-20.19	0.85	1.52	21	1
1	A	11	CYS	CB-SG	-20.18	1.14	1.81	21	1
1	A	30	ILE	CB-CG2	-20.15	0.86	1.52	21	1
1	A	19	LYS	CE-NZ	-19.88	0.89	1.49	21	1
1	A	65	ARG	CG-CD	-19.63	0.93	1.52	21	1
1	A	51	LEU	CG-CD1	-19.40	0.88	1.52	21	1
1	A	37	ILE	CB-CG1	-19.22	1.15	1.53	21	1
1	A	60	LEU	CG-CD2	-18.97	0.90	1.52	21	1
1	A	23	GLU	CB-CG	-18.97	0.95	1.52	21	1
1	A	66	VAL	CB-CG1	-18.73	0.90	1.52	21	1
1	A	28	LEU	CG-CD1	-18.63	0.91	1.52	21	1
1	A	61	LYS	CD-CE	-18.55	0.96	1.52	21	1
1	A	70	GLU	CG-CD	-18.49	1.05	1.52	21	1
1	A	43	ILE	CB-CG1	-18.47	1.16	1.53	21	1
1	A	35	GLU	CB-CG	-18.47	0.97	1.52	21	1
1	A	36	LYS	CE-NZ	-18.14	0.94	1.49	21	1
1	A	51	LEU	CG-CD2	-18.09	0.92	1.52	21	1
1	A	5	GLN	CG-CD	-17.92	1.07	1.52	21	1
1	A	70	GLU	CB-CG	-17.87	0.98	1.52	21	1
1	A	3	LYS	CE-NZ	-17.83	0.95	1.49	21	1
1	A	3	LYS	CB-CG	-17.57	0.99	1.52	21	1
1	A	60	LEU	CB-CG	-17.40	1.18	1.53	21	1
1	A	9	THR	CB-CG2	-17.35	0.95	1.52	21	1
1	A	62	ILE	CB-CG2	-16.91	0.96	1.52	21	1
1	A	38	LYS	CG-CD	-16.58	1.02	1.52	21	1
1	A	23	GLU	CG-CD	-16.48	1.10	1.52	21	1
1	A	10	GLY	C-N	-16.41	1.08	1.33	21	1
1	A	65	ARG	CB-CG	-16.30	1.03	1.52	21	1
1	A	6	ILE	CG1-CD1	-16.22	0.88	1.51	21	1
1	A	61	LYS	CG-CD	-16.00	1.04	1.52	21	1
1	A	37	ILE	C-N	-15.96	1.13	1.33	21	1
1	A	28	LEU	CB-CG	-15.69	1.22	1.53	21	1
1	A	18	GLU	CG-CD	-15.50	1.13	1.52	21	1
1	A	54	LEU	CB-CG	-15.25	1.23	1.53	21	1
1	A	3	LYS	CD-CE	-15.24	1.06	1.52	21	1
1	A	72	ILE	CB-CG2	-14.72	1.03	1.52	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	48	LEU	C-N	-14.68	1.11	1.33	21	1
1	A	15	GLN	CD-OE1	-14.47	0.96	1.23	21	1
1	A	39	GLU	CB-CG	-13.88	1.10	1.52	21	1
1	A	6	ILE	CB-CG2	-13.80	1.07	1.52	21	1
1	A	73	LYS	CG-CD	-13.31	1.12	1.52	21	1
1	A	20	ASN	CB-CG	-13.09	1.19	1.52	21	1
1	A	38	LYS	CB-CG	-12.76	1.14	1.52	21	1
1	A	3	LYS	CG-CD	-12.60	1.14	1.52	21	1
1	A	11	CYS	C-O	-12.54	1.07	1.24	21	1
1	A	37	ILE	CG1-CD1	-12.20	1.04	1.51	21	1
1	A	19	LYS	CG-CD	-12.19	1.15	1.52	21	1
1	A	69	LYS	CG-CD	-11.62	1.17	1.52	21	1
1	A	61	LYS	CB-CG	-11.60	1.17	1.52	21	1
1	A	31	ASP	CB-CG	-11.50	1.23	1.52	21	1
1	A	59	GLU	CB-CG	-11.35	1.18	1.52	21	1
1	A	13	ASN	CB-CG	-11.31	1.23	1.52	21	1
1	A	43	ILE	CB-CG2	-11.01	1.16	1.52	21	1
1	A	36	LYS	CB-CG	-11.00	1.19	1.52	21	1
1	A	33	GLU	CB-CG	-10.43	1.21	1.52	21	1
1	A	11	CYS	C-N	-10.33	1.18	1.33	21	1
1	A	15	GLN	CG-CD	-10.09	1.26	1.52	21	1
1	A	16	MET	CB-CG	-10.05	1.22	1.52	21	1
1	A	20	ASN	CG-ND2	-9.99	1.12	1.33	21	1
1	A	30	ILE	CG1-CD1	-9.54	1.14	1.51	21	1
1	A	8	GLY	C-N	-9.36	1.22	1.33	21	1
1	A	57	ASP	CB-CG	-9.21	1.29	1.52	21	1
1	A	9	THR	CA-C	-9.15	1.45	1.53	21	1
1	A	8	GLY	C-O	-8.95	1.11	1.23	21	1
1	A	4	ILE	CG1-CD1	-8.82	1.17	1.51	21	1
1	A	5	GLN	CB-CG	-8.75	1.26	1.52	21	1
1	A	49	THR	C-O	-8.75	1.12	1.24	21	1
1	A	26	LYS	CG-CD	-8.42	1.27	1.52	21	1
1	A	37	ILE	CB-CG2	-8.41	1.24	1.52	21	1
1	A	5	GLN	CD-NE2	-8.10	1.16	1.33	21	1
1	A	22	ARG	CG-CD	-7.67	1.29	1.52	21	1
1	A	49	THR	C-N	-7.03	1.21	1.33	21	1
1	A	71	GLU	CB-CG	-6.81	1.32	1.52	21	1
1	A	1	MET	CA-CB	-6.69	1.40	1.53	21	1
1	A	51	LEU	CB-CG	-6.40	1.40	1.53	21	1
1	A	61	LYS	CA-CB	-6.37	1.44	1.54	21	1
1	A	36	LYS	CG-CD	-6.25	1.33	1.52	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	9	THR	CA-CB	-5.86	1.45	1.53	21	1
1	A	48	LEU	CA-C	-5.86	1.45	1.53	21	1
1	A	26	LYS	CB-CG	-5.58	1.35	1.52	21	1
1	A	49	THR	CA-CB	-5.35	1.46	1.54	21	1
1	A	1	MET	N-CA	-5.06	1.36	1.46	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	7	TYR	CD1-CG-CD2	-62.63	24.15	118.10	21	1
1	A	9	THR	O-C-N	-59.48	50.77	123.33	21	1
1	A	65	ARG	NE-CZ-NH1	-58.70	62.80	121.50	21	1
1	A	22	ARG	NE-CZ-NH2	53.84	167.66	119.20	21	1
1	A	65	ARG	NE-CZ-NH2	51.96	165.97	119.20	21	1
1	A	34	PHE	CD1-CG-CD2	-51.91	40.74	118.60	21	1
1	A	13	ASN	OD1-CG-ND2	-47.80	74.80	122.60	21	1
1	A	7	TYR	CE1-CZ-CE2	-47.60	25.10	120.30	21	2
1	A	71	GLU	OE1-CD-OE2	-45.50	13.70	122.90	21	1
1	A	22	ARG	NH1-CZ-NH2	-44.52	61.42	119.30	21	1
1	A	34	PHE	CE1-CZ-CE2	-43.51	41.68	120.00	21	1
1	A	41	ASP	OD1-CG-OD2	-42.35	21.27	122.90	21	1
1	A	54	LEU	CD1-CG-CD2	-41.93	18.55	110.80	21	1
1	A	70	GLU	OE1-CD-OE2	-39.95	27.01	122.90	21	1
1	A	23	GLU	OE1-CD-OE2	-39.58	27.92	122.90	21	1
1	A	59	GLU	OE1-CD-OE2	-38.67	30.09	122.90	21	1
1	A	57	ASP	OD1-CG-OD2	-38.06	31.56	122.90	21	1
1	A	17	LEU	CD1-CG-CD2	-37.88	27.47	110.80	21	1
1	A	31	ASP	OD1-CG-OD2	-36.47	35.36	122.90	21	1
1	A	63	MET	CG-SD-CE	34.83	177.52	100.90	21	1
1	A	18	GLU	OE1-CD-OE2	-33.36	42.83	122.90	21	1
1	A	7	TYR	CB-CG-CD2	31.97	168.75	120.80	21	1
1	A	5	GLN	CB-CG-CD	31.83	166.71	112.60	21	1
1	A	22	ARG	CD-NE-CZ	31.69	168.76	124.40	21	1
1	A	7	TYR	CG-CD1-CE1	31.38	168.27	121.20	21	1
1	A	7	TYR	CG-CD2-CE2	30.86	167.49	121.20	21	2
1	A	7	TYR	CB-CG-CD1	30.86	167.09	120.80	21	1
1	A	65	ARG	CD-NE-CZ	30.34	166.87	124.40	21	1
1	A	42	GLN	OE1-CD-NE2	-29.41	93.19	122.60	21	1
1	A	7	TYR	CZ-CE2-CD2	-28.71	67.92	119.60	9	2
1	A	40	MET	CG-SD-CE	28.49	163.58	100.90	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	2	MET	CG-SD-CE	27.29	160.93	100.90	21	1
1	A	35	GLU	CB-CG-CD	27.14	158.74	112.60	21	1
1	A	39	GLU	OE1-CD-OE2	-26.88	58.39	122.90	21	1
1	A	7	TYR	CD1-CE1-CZ	26.54	167.38	119.60	21	1
1	A	42	GLN	CB-CG-CD	26.53	157.69	112.60	21	1
1	A	27	GLU	OE1-CD-OE2	-26.45	59.42	122.90	21	1
1	A	33	GLU	OE1-CD-OE2	-25.75	61.10	122.90	21	1
1	A	40	MET	CA-CB-CG	25.27	164.65	114.10	21	1
1	A	22	ARG	CG-CD-NE	25.05	167.11	112.00	21	1
1	A	71	GLU	CB-CG-CD	24.82	154.80	112.60	21	1
1	A	35	GLU	OE1-CD-OE2	-24.66	63.72	122.90	21	1
1	A	69	LYS	CG-CD-CE	24.62	167.94	111.30	21	1
1	A	65	ARG	CG-CD-NE	24.52	165.95	112.00	21	1
1	A	71	GLU	CG-CD-OE1	24.09	173.81	118.40	21	1
1	A	69	LYS	CB-CG-CD	24.06	166.64	111.30	21	1
1	A	71	GLU	CG-CD-OE2	23.52	172.49	118.40	21	1
1	A	34	PHE	CG-CD1-CE1	23.07	159.92	120.70	21	1
1	A	34	PHE	CB-CG-CD1	23.07	159.91	120.70	21	1
1	A	34	PHE	CG-CD2-CE2	22.77	159.40	120.70	21	1
1	A	41	ASP	CB-CG-OD1	22.73	170.68	118.40	21	1
1	A	34	PHE	CB-CG-CD2	22.72	159.33	120.70	21	1
1	A	26	LYS	CG-CD-CE	22.62	163.32	111.30	21	1
1	A	16	MET	CG-SD-CE	22.50	150.40	100.90	21	1
1	A	49	THR	OG1-CB-CG2	-22.14	65.03	109.30	21	1
1	A	1	MET	CG-SD-CE	22.09	149.49	100.90	21	1
1	A	34	PHE	CZ-CE2-CD2	21.93	159.48	120.00	21	1
1	A	41	ASP	CB-CG-OD2	21.59	168.06	118.40	21	1
1	A	34	PHE	CD1-CE1-CZ	21.55	158.78	120.00	21	1
1	A	23	GLU	CG-CD-OE2	21.29	167.37	118.40	21	1
1	A	45	GLU	OE1-CD-OE2	-21.20	72.03	122.90	21	1
1	A	70	GLU	CG-CD-OE1	21.05	166.81	118.40	21	1
1	A	6	ILE	CB-CG1-CD1	20.80	157.49	113.80	21	1
1	A	70	GLU	CG-CD-OE2	20.77	166.17	118.40	21	1
1	A	59	GLU	CB-CG-CD	20.68	147.75	112.60	21	1
1	A	42	GLN	CG-CD-NE2	20.54	147.21	116.40	21	1
1	A	9	THR	CA-C-O	20.40	149.37	122.44	21	1
1	A	59	GLU	CG-CD-OE1	20.32	165.12	118.40	21	1
1	A	57	ASP	CB-CG-OD2	20.31	165.11	118.40	21	1
1	A	9	THR	CA-C-N	20.19	160.98	121.41	21	1
1	A	9	THR	C-N-CA	20.19	160.98	121.41	21	1
1	A	59	GLU	CG-CD-OE2	20.17	164.79	118.40	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	23	GLU	CG-CD-OE1	20.14	164.71	118.40	21	1
1	A	54	LEU	CB-CG-CD1	20.00	170.69	110.70	21	1
1	A	3	LYS	CG-CD-CE	19.99	157.28	111.30	21	1
1	A	72	ILE	CB-CG1-CD1	19.96	155.71	113.80	21	1
1	A	31	ASP	CB-CG-OD2	19.85	164.06	118.40	21	1
1	A	49	THR	CA-CB-CG2	19.57	143.77	110.50	21	1
1	A	57	ASP	CB-CG-OD1	19.54	163.33	118.40	21	1
1	A	13	ASN	CB-CG-ND2	19.30	145.36	116.40	21	1
1	A	17	LEU	CB-CG-CD1	19.12	168.08	110.70	21	1
1	A	49	THR	CA-CB-OG1	19.09	138.24	109.60	21	1
1	A	40	MET	CB-CG-SD	18.89	169.37	112.70	21	1
1	A	69	LYS	CA-CB-CG	18.89	151.87	114.10	21	1
1	A	45	GLU	CG-CD-OE2	18.84	161.73	118.40	21	1
1	A	39	GLU	CG-CD-OE2	18.70	161.40	118.40	21	1
1	A	19	LYS	CG-CD-CE	18.49	153.82	111.30	21	1
1	A	31	ASP	CB-CG-OD1	18.34	160.58	118.40	21	1
1	A	63	MET	CA-CB-CG	17.86	149.82	114.10	21	1
1	A	26	LYS	CD-CE-NZ	17.85	169.01	111.90	21	1
1	A	18	GLU	CG-CD-OE1	17.81	159.37	118.40	21	1
1	A	54	LEU	CB-CG-CD2	17.77	164.00	110.70	21	1
1	A	61	LYS	CB-CG-CD	17.66	151.92	111.30	21	1
1	A	45	GLU	CB-CG-CD	17.45	142.26	112.60	21	1
1	A	5	GLN	CG-CD-NE2	17.38	142.48	116.40	21	1
1	A	61	LYS	CD-CE-NZ	17.18	166.88	111.90	21	1
1	A	33	GLU	CB-CG-CD	17.14	141.74	112.60	21	1
1	A	18	GLU	CG-CD-OE2	17.13	157.79	118.40	21	1
1	A	17	LEU	CB-CG-CD2	16.93	161.49	110.70	21	1
1	A	33	GLU	CG-CD-OE2	16.93	157.33	118.40	21	1
1	A	36	LYS	CG-CD-CE	16.68	149.67	111.30	21	1
1	A	66	VAL	CG1-CB-CG2	-16.12	75.34	110.80	21	1
1	A	69	LYS	CD-CE-NZ	16.11	163.45	111.90	21	1
1	A	66	VAL	CA-CB-CG1	16.01	137.61	110.40	21	1
1	A	2	MET	CB-CG-SD	15.92	160.47	112.70	21	1
1	A	27	GLU	CG-CD-OE1	15.92	155.01	118.40	21	1
1	A	7	TYR	OH-CZ-CE2	15.88	167.53	119.90	21	2
1	A	20	ASN	CB-CG-ND2	15.87	140.21	116.40	21	1
1	A	7	TYR	CE1-CZ-OH	15.82	167.37	119.90	21	1
1	A	61	LYS	CG-CD-CE	15.61	147.21	111.30	21	1
1	A	35	GLU	CG-CD-OE1	15.40	153.82	118.40	21	1
1	A	5	GLN	CG-CD-OE1	-15.34	90.13	120.80	21	1
1	A	73	LYS	CG-CD-CE	15.14	146.11	111.30	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	38	LYS	CD-CE-NZ	15.05	160.06	111.90	21	1
1	A	39	GLU	CB-CG-CD	14.79	137.75	112.60	21	1
1	A	36	LYS	CD-CE-NZ	14.51	158.31	111.90	21	1
1	A	66	VAL	CA-CB-CG2	14.20	134.54	110.40	21	1
1	A	19	LYS	CD-CE-NZ	13.92	156.46	111.90	21	1
1	A	65	ARG	CB-CG-CD	13.09	141.40	111.30	21	1
1	A	70	GLU	CB-CG-CD	12.83	134.42	112.60	21	1
1	A	30	ILE	CA-CB-CG2	12.73	132.14	110.50	21	1
1	A	37	ILE	O-C-N	-12.46	109.72	123.18	21	1
1	A	51	LEU	CD1-CG-CD2	-12.28	83.78	110.80	21	1
1	A	38	LYS	CG-CD-CE	12.26	139.51	111.30	21	1
1	A	23	GLU	CB-CG-CD	12.14	133.23	112.60	21	1
1	A	3	LYS	CD-CE-NZ	12.07	150.52	111.90	21	1
1	A	48	LEU	O-C-N	-12.03	109.08	122.79	21	1
1	A	68	SER	CA-CB-OG	11.96	135.02	111.10	21	1
1	A	28	LEU	CD1-CG-CD2	-11.89	84.64	110.80	21	1
1	A	27	GLU	CG-CD-OE2	11.81	145.57	118.40	21	1
1	A	30	ILE	CA-CB-CG1	11.67	130.24	110.40	21	1
1	A	1	MET	CA-CB-CG	11.61	137.32	114.10	21	1
1	A	10	GLY	O-C-N	-11.06	108.32	122.70	21	1
1	A	62	ILE	CB-CG1-CD1	10.90	136.70	113.80	21	1
1	A	1	MET	CB-CG-SD	10.81	145.13	112.70	21	1
1	A	9	THR	CA-CB-CG2	10.77	128.81	110.50	21	1
1	A	35	GLU	CG-CD-OE2	10.46	142.46	118.40	21	1
1	A	73	LYS	CD-CE-NZ	10.37	145.09	111.90	21	1
1	A	16	MET	CB-CG-SD	10.22	143.37	112.70	21	1
1	A	33	GLU	CG-CD-OE1	10.07	141.57	118.40	21	1
1	A	27	GLU	CB-CG-CD	10.06	129.70	112.60	21	1
1	A	3	LYS	CB-CG-CD	9.99	134.27	111.30	21	1
1	A	4	ILE	CB-CG1-CD1	9.91	134.60	113.80	21	1
1	A	20	ASN	CA-CB-CG	9.70	122.30	112.60	21	1
1	A	13	ASN	CB-CG-OD1	9.52	139.85	120.80	21	1
1	A	39	GLU	CG-CD-OE1	9.48	140.21	118.40	21	1
1	A	22	ARG	NE-CZ-NH1	9.42	130.92	121.50	21	1
1	A	30	ILE	CG1-CB-CG2	-9.32	82.74	110.70	21	1
1	A	9	THR	OG1-CB-CG2	-9.31	90.69	109.30	21	1
1	A	65	ARG	NH1-CZ-NH2	9.18	131.23	119.30	21	1
1	A	20	ASN	CB-CG-OD1	-8.98	102.84	120.80	21	1
1	A	62	ILE	CA-CB-CG1	8.60	125.02	110.40	21	1
1	A	30	ILE	CB-CG1-CD1	8.59	131.83	113.80	21	1
1	A	23	GLU	CA-CB-CG	8.56	131.21	114.10	21	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	60	LEU	CD1-CG-CD2	-8.49	92.11	110.80	21	1
1	A	35	GLU	CA-CB-CG	8.22	130.54	114.10	21	1
1	A	73	LYS	CB-CG-CD	8.09	129.90	111.30	21	1
1	A	72	ILE	CA-CB-CG2	8.05	124.18	110.50	21	1
1	A	28	LEU	CB-CG-CD1	8.03	134.80	110.70	21	1
1	A	9	THR	CA-CB-OG1	7.90	121.45	109.60	21	1
1	A	62	ILE	CA-CB-CG2	7.81	123.78	110.50	21	1
1	A	72	ILE	CA-CB-CG1	7.52	123.18	110.40	21	1
1	A	3	LYS	CA-CB-CG	7.28	128.65	114.10	21	1
1	A	65	ARG	CA-CB-CG	7.26	128.62	114.10	21	1
1	A	60	LEU	CB-CG-CD2	7.25	132.45	110.70	21	1
1	A	48	LEU	CA-C-N	7.14	133.46	122.24	21	1
1	A	48	LEU	C-N-CA	7.14	133.46	122.24	21	1
1	A	6	ILE	CA-CB-CG1	6.92	122.16	110.40	21	1
1	A	51	LEU	CB-CG-CD2	6.88	131.35	110.70	21	1
1	A	15	GLN	CG-CD-NE2	6.85	126.67	116.40	21	1
1	A	37	ILE	CA-CB-CG2	6.77	122.01	110.50	21	1
1	A	15	GLN	CG-CD-OE1	-6.71	107.38	120.80	21	1
1	A	28	LEU	CB-CG-CD2	6.21	129.34	110.70	21	1
1	A	11	CYS	CA-CB-SG	6.08	128.38	114.40	21	1
1	A	70	GLU	CA-CB-CG	6.07	126.25	114.10	21	1
1	A	62	ILE	CG1-CB-CG2	-5.97	92.80	110.70	21	1
1	A	6	ILE	CA-CB-CG2	5.95	120.61	110.50	21	1
1	A	72	ILE	CG1-CB-CG2	-5.67	93.69	110.70	21	1
1	A	20	ASN	OD1-CG-ND2	-5.65	116.95	122.60	21	1
1	A	18	GLU	CB-CG-CD	5.58	122.08	112.60	21	1
1	A	39	GLU	CA-CB-CG	5.55	125.19	114.10	21	1
1	A	13	ASN	CA-CB-CG	5.50	118.10	112.60	21	1
1	A	10	GLY	CA-C-N	5.40	131.16	121.66	21	1
1	A	10	GLY	C-N-CA	5.40	131.16	121.66	21	1
1	A	38	LYS	CB-CG-CD	5.37	123.66	111.30	21	1
1	A	51	LEU	CB-CG-CD1	5.32	126.65	110.70	21	1
1	A	19	LYS	CB-CG-CD	5.31	123.52	111.30	21	1
1	A	43	ILE	CA-CB-CG1	5.26	119.34	110.40	21	1
1	A	11	CYS	O-C-N	-5.25	115.27	122.46	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

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Mol	Chain	Res	Type	Atoms	Models (Total)
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	577	75±65
All	All	11634	12201	12197	1568

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 66.

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:CG	1:A:65:ARG:NE	1.54	1.69	21	1
1:A:35:GLU:CD	1:A:35:GLU:CB	1.52	1.82	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:19:LYS:CD	1:A:19:LYS:NZ	1.47	1.70	21	1
1:A:69:LYS:CB	1:A:69:LYS:CD	1.47	1.90	21	1
1:A:73:LYS:CE	1:A:73:LYS:CG	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:CZ	1:A:34:PHE:CD1	1.43	2.07	21	1
1:A:19:LYS:CE	1:A:19:LYS:CG	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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ASN:OD1	1:A:13:ASN:CB	1.39	1.70	21	1
1:A:34:PHE:CZ	1:A:34:PHE:CD2	1.39	2.09	21	1
1:A:13:ASN:CB	1:A:13:ASN:ND2	1.39	1.86	21	1
1:A:2:MET:CG	1:A:2:MET:CE	1.38	2.02	21	1
1:A:34:PHE:CG	1:A:34:PHE:CE1	1.38	2.10	21	1
1:A:7:TYR:CD2	1:A:7:TYR:CE2	1.36	2.14	9	1
1:A:26:LYS:CE	1:A:26:LYS:CG	1.36	2.02	21	1
1:A:69:LYS:CE	1:A:69:LYS:CG	1.36	2.01	21	1
1:A:7:TYR:CG	1:A:7:TYR:CE1	1.36	2.10	21	1
1:A:7:TYR:CE2	1:A:7:TYR:CZ	1.35	2.14	9	1
1:A:40:MET:CE	1:A:40:MET:CG	1.35	2.05	21	1
1:A:51:LEU:CD1	1:A:51:LEU:CB	1.33	2.05	21	1
1:A:59:GLU:CD	1:A:59:GLU:CB	1.31	2.02	21	1
1:A:1:MET:CG	1:A:1:MET:CA	1.30	2.07	21	1
1:A:49:THR:CG2	1:A:49:THR:CA	1.30	2.07	21	1
1:A:31:ASP:CB	1:A:31:ASP:OD2	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:SD	1:A:16:MET:CB	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:CE	1:A:36:LYS:CG	1.27	2.09	21	1
1:A:1:MET:CG	1:A:1:MET:SD	1.26	1.18	21	1
1:A:51:LEU:CB	1:A:51:LEU:CD2	1.26	2.13	21	1
1:A:17:LEU:CB	1:A:17:LEU:CD1	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:CG	1:A:63:MET:SD	1.25	1.16	21	1
1:A:34:PHE:CD2	1:A:34:PHE:CB	1.24	2.20	21	1
1:A:11:CYS:CB	1:A:11:CYS:SG	1.23	1.14	21	1
1:A:63:MET:CG	1:A:63:MET:CE	1.23	2.14	21	1
1:A:9:THR:O	1:A:9:THR:CA	1.22	1.88	21	1
1:A:30:ILE:CG1	1:A:30:ILE:CA	1.22	2.17	21	1
1:A:69:LYS:CG	1:A:69:LYS:CA	1.19	2.19	21	1
1:A:7:TYR:CD1	1:A:7:TYR:CB	1.19	2.24	21	1
1:A:66:VAL:CG2	1:A:66:VAL:CA	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:CD1	1:A:34:PHE:CB	1.18	2.22	21	1
1:A:7:TYR:CD2	1:A:7:TYR:CB	1.17	2.23	21	1
1:A:9:THR:C	1:A:10:GLY:CA	1.17	2.17	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:MET:SD	1:A:2:MET:CB	1.13	2.34	21	1
1:A:45:GLU:CD	1:A:45:GLU:CB	1.13	2.19	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:NE	1:A:22:ARG:CG	1.13	2.12	21	1
1:A:42:GLN:CD	1:A:42:GLN:CB	1.12	2.21	21	1
1:A:66:VAL:CG2	1:A:66:VAL:HB	1.11	1.68	21	1
1:A:51:LEU:CD1	1:A:51:LEU:HG	1.09	1.66	21	1
1:A:66:VAL:CA	1:A:66:VAL:CG1	1.09	2.26	21	1
1:A:51:LEU:CD2	1:A:51:LEU:HG	1.09	1.66	21	1
1:A:63:MET:CG	1:A:63:MET:CA	1.08	2.31	21	1
1:A:49:THR:OG1	1:A:49:THR:HB	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:OG	1:A:68:SER:CA	1.05	2.04	21	1
1:A:68:SER:OG	1:A:68:SER:HB2	1.05	1.30	21	1
1:A:66:VAL:HB	1:A:66:VAL:CG1	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:CE1	1:A:7:TYR:OH	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:CE2	1:A:7:TYR:OH	1.03	2.07	21	2
1:A:41:ASP:CB	1:A:41:ASP:OD1	1.02	2.06	21	1
1:A:9:THR:CA	1:A:10:GLY:N	1.02	2.22	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:11:CYS:SG	1:A:11:CYS:HB3	1.01	1.68	21	1
1:A:49:THR:CG2	1:A:49:THR:HB	1.01	1.55	21	1
1:A:37:ILE:HD13	1:A:37:ILE:N	1.01	1.54	21	9
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:49:THR:CG2	1:A:49:THR:OG1	1.00	0.70	21	1
1:A:63:MET:SD	1:A:63:MET:CE	1.00	0.98	21	1
1:A:66:VAL:CB	1:A:66:VAL:HG11	1.00	1.53	21	1
1:A:11:CYS:SG	1:A:11:CYS:HB2	0.99	1.68	21	1
1:A:2:MET:SD	1:A:2:MET:HE3	0.99	1.67	21	1
1:A:7:TYR:CD2	1:A:7:TYR:CZ	0.98	2.39	9	1
1:A:49:THR:OG1	1:A:49:THR:HG23	0.98	1.24	21	1
1:A:66:VAL:CB	1:A:66:VAL:HG13	0.98	1.53	21	1
1:A:17:LEU:HD11	1:A:72:ILE:HD11	0.98	1.31	1	5
1:A:25:VAL:HG21	1:A:32:ALA:HB2	0.98	1.30	6	16
1:A:2:MET:SD	1:A:2:MET:HE1	0.98	1.67	21	1
1:A:2:MET:SD	1:A:2:MET:HE2	0.98	1.67	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:MET:SD	1:A:63:MET:HG2	0.98	1.75	21	1
1:A:66:VAL:CB	1:A:66:VAL:HG12	0.98	1.53	21	1
1:A:51:LEU:CG	1:A:51:LEU:HD21	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: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:6:ILE:CG1	1:A:6:ILE:HD12	0.96	1.51	21	1
1:A:30:ILE:CG2	1:A:30:ILE:HB	0.96	1.62	21	1
1:A:59:GLU:CD	1:A:59:GLU:HG3	0.96	1.45	21	1
1:A:6:ILE:CG1	1:A:6:ILE:HD13	0.96	1.51	21	1
1:A:59:GLU:CD	1:A:59:GLU:HG2	0.96	1.45	21	1
1:A:59:GLU:CD	1:A:59:GLU:CG	0.95	0.93	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:6:ILE:CG1	1:A:6:ILE:HD11	0.95	1.51	21	1
1:A:30:ILE:CB	1:A:30:ILE:HG22	0.95	1.49	21	1
1:A:37:ILE:HD13	1:A:37:ILE:H	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:CB	1:A:66:VAL:HG22	0.94	1.49	21	1
1:A:65:ARG:CD	1:A:65:ARG:HG3	0.94	1.47	21	1
1:A:63:MET:SD	1:A:63:MET:HE2	0.94	1.59	21	1
1:A:63:MET:SD	1:A:63:MET:HE3	0.94	1.59	21	1
1:A:16:MET:SD	1:A:16:MET:HG3	0.93	1.59	21	1
1:A:22:ARG:NE	1:A:22:ARG:HD3	0.93	1.32	21	1
1:A:63:MET:SD	1:A:63:MET:HE1	0.93	1.59	21	1
1:A:66:VAL:CB	1:A:66:VAL:HG21	0.93	1.49	21	1
1:A:66:VAL:CB	1:A:66:VAL:HG23	0.93	1.49	21	1
1:A:16:MET:SD	1:A:16:MET:HG2	0.93	1.59	21	1
1:A:30:ILE:CB	1:A:30:ILE:HG23	0.92	1.49	21	1
1:A:45:GLU:CD	1:A:45:GLU:HG3	0.92	1.40	21	1
1:A:51:LEU:CD2	1:A:51:LEU:CG	0.92	0.92	21	1
1:A:63:MET:CG	1:A:63:MET:CB	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:CD	1:A:65:ARG:HG2	0.91	1.47	21	1
1:A:9:THR:C	1:A:10:GLY:N	0.91	0.81	21	1
1:A:63:MET:SD	1:A:63:MET:HG3	0.91	1.75	21	1
1:A:65:ARG:CD	1:A:65:ARG:CG	0.91	0.93	21	1
1:A:63:MET:CG	1:A:63:MET:HB2	0.90	1.43	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:VAL:CG1	1:A:66:VAL:CB	0.90	0.90	21	1
1:A:6:ILE:CD1	1:A:6:ILE:HG21	0.89	1.98	21	1
1:A:45:GLU:CD	1:A:45:GLU:HG2	0.89	1.40	21	1
1:A:49:THR:OG1	1:A:49:THR:CB	0.89	0.59	21	1
1:A:45:GLU:CD	1:A:45:GLU:CG	0.89	0.84	21	1
1:A:42:GLN:CD	1:A:42:GLN:CG	0.89	0.86	21	1
1:A:35:GLU:CD	1:A:35:GLU:HG2	0.89	1.39	21	1
1:A:7:TYR:CE2	1:A:42:GLN:O	0.88	2.26	9	1
1:A:62:ILE:HD13	1:A:66:VAL:HG12	0.88	1.45	15	1
1:A:35:GLU:CD	1:A:35:GLU:HG3	0.88	1.39	21	1
1:A:42:GLN:CD	1:A:42:GLN:HG3	0.88	1.37	21	1
1:A:7:TYR:CD2	1:A:48:LEU:HD11	0.88	2.03	12	5
1:A:42:GLN:CD	1:A:42:GLN:HG2	0.88	1.37	21	1
1:A:6:ILE:CD1	1:A:6:ILE:CG1	0.88	0.88	21	1
1:A:51:LEU:CD1	1:A:51:LEU:CG	0.88	0.88	21	1
1:A:30:ILE:CB	1:A:30:ILE:HG13	0.87	1.42	21	1
1:A:63:MET:CG	1:A:63:MET:HB3	0.87	1.43	21	1
1:A:30:ILE:CB	1:A:30:ILE:HG12	0.87	1.42	21	1
1:A:41:ASP:OD1	1:A:41:ASP:CG	0.86	0.64	21	1
1:A:73:LYS:CE	1:A:73:LYS:HD3	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:CE	1:A:1:MET:SD	0.86	0.79	21	1
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:CG	1:A:1:MET:HB2	0.85	1.39	21	1
1:A:30:ILE:CB	1:A:30:ILE:CG2	0.85	0.86	21	1
1:A:66:VAL:CG2	1:A:66:VAL:CB	0.85	0.85	21	1
1:A:4:ILE:HD13	1:A:34:PHE:CE2	0.85	2.06	8	12
1:A:46:ALA:HB1	1:A:60:LEU:HD21	0.85	1.45	14	3
1:A:1:MET:CG	1:A:1:MET:HB3	0.85	1.39	21	1
1:A:35:GLU:CD	1:A:35:GLU:CG	0.85	0.89	21	1
1:A:73:LYS:CE	1:A:73:LYS:HD2	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:CE	1:A:73:LYS:CD	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:CE	1:A:19:LYS:HD3	0.84	1.37	21	1
1:A:49:THR:HG23	1:A:49:THR:CB	0.84	1.37	21	1
1:A:73:LYS:HE3	1:A:73:LYS:CD	0.84	1.41	21	1
1:A:16:MET:CE	1:A:16:MET:SD	0.84	0.78	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LYS:CE	1:A:36:LYS:HD2	0.84	1.37	21	1
1:A:40:MET:CE	1:A:40:MET:SD	0.84	0.80	21	1
1:A:7:TYR:CD1	1:A:37:ILE:HD12	0.83	2.07	12	5
1:A:49:THR:CB	1:A:49:THR:HG21	0.83	1.37	21	1
1:A:30:ILE:CB	1:A:30:ILE:CG1	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:CD1	1:A:6:ILE:HG12	0.83	1.38	21	1
1:A:19:LYS:CD	1:A:19:LYS:HE2	0.82	1.36	21	1
1:A:6:ILE:CD1	1:A:6:ILE:HG13	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:CE	1:A:19:LYS:HD2	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:CD	1:A:19:LYS:HE3	0.82	1.36	21	1
1:A:36:LYS:CE	1:A:36:LYS:HD3	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:40:MET:SD	1:A:40:MET:HE3	0.81	1.45	21	1
1:A:73:LYS:CD	1:A:73:LYS:HE2	0.81	1.41	21	1
1:A:34:PHE:CE2	1:A:34:PHE:HZ	0.81	1.65	21	1
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:40:MET:SD	1:A:40:MET:HE2	0.81	1.45	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:40:MET:SD	1:A:40:MET:HE1	0.81	1.45	21	1
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:50:ALA:HB3	1:A:63:MET:HB2	0.80	1.50	8	3
1:A:16:MET:SD	1:A:16:MET:HE1	0.80	1.43	21	1
1:A:1:MET:CG	1:A:1:MET:CB	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:HE2	0.80	1.44	21	1
1:A:25:VAL:HG11	1:A:32:ALA:HB3	0.80	1.54	1	16
1:A:34:PHE:CE1	1:A:34:PHE:HZ	0.80	1.63	21	1
1:A:65:ARG:CG	1:A:65:ARG:HE	0.80	1.89	21	1
1:A:49:THR:CG2	1:A:49:THR:HG1	0.80	1.54	21	1
1:A:1:MET:SD	1:A:1:MET:HE1	0.80	1.44	21	1
1:A:2:MET:SD	1:A:2:MET:HG2	0.80	1.44	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:MET:SD	1:A:16:MET:HE2	0.80	1.43	21	1
1:A:1:MET:SD	1:A:1:MET:HG3	0.79	1.66	21	1
1:A:2:MET:HE3	1:A:30:ILE:HD12	0.79	1.52	3	1
1:A:69:LYS:CE	1:A:69:LYS:HD3	0.79	1.33	21	1
1:A:1:MET:SD	1:A:1:MET:HE3	0.79	1.44	21	1
1:A:16:MET:CE	1:A:16:MET:HG2	0.79	2.05	21	1
1:A:2:MET:SD	1:A:2:MET:HG3	0.79	1.44	21	1
1:A:7:TYR:HA	1:A:37:ILE:CD1	0.79	2.07	18	8
1:A:16:MET:SD	1:A:16:MET:HE3	0.79	1.43	21	1
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:11:CYS:CB	1:A:11:CYS:HG	0.78	1.91	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: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:36:LYS:C	1:A:37:ILE:HD13	0.77	2.03	1	9
1:A:69:LYS:CD	1:A:69:LYS:HE2	0.77	1.34	21	1
1:A:4:ILE:HD12	1:A:34:PHE:CZ	0.77	2.13	1	5
1:A:52:PRO:O	1:A:62:ILE:HD12	0.77	1.78	15	2
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
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: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:OG1	1:A:49:THR:HG21	0.74	0.99	21	1
1:A:5:GLN:C	1:A:6:ILE:HD13	0.74	2.07	8	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:63:MET:CE	1:A:63:MET:HB2	0.74	2.13	21	1
1:A:69:LYS:CD	1:A:69:LYS:HE3	0.74	1.34	21	1
1:A:4:ILE:CG1	1:A:56:VAL:HG12	0.73	2.14	5	18
1:A:69:LYS:CD	1:A:69:LYS:CE	0.73	0.85	21	1
1:A:17:LEU:HD13	1:A:17:LEU:O	0.72	1.84	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:LYS:CB	1:A:69:LYS:HG3	0.72	1.26	21	1
1:A:9:THR:O	1:A:9:THR:C	0.72	0.48	21	1
1:A:69:LYS:CB	1:A:69:LYS:CG	0.72	0.74	21	1
1:A:48:LEU:HD22	1:A:48:LEU:N	0.72	1.99	14	7
1:A:57:ASP:OD2	1:A:57:ASP:CG	0.72	0.55	21	1
1:A:69:LYS:HE2	1:A:69:LYS:NZ	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:HD13	1:A:37:ILE:O	0.72	1.84	8	3
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:HD3	1:A:22:ARG:HE	0.71	1.00	21	1
1:A:31:ASP:OD2	1:A:31:ASP:CG	0.71	0.55	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:CD1	1:A:34:PHE:CG	0.70	0.76	21	1
1:A:49:THR:CG2	1:A:49:THR:CB	0.70	0.70	21	1
1:A:4:ILE:HG23	1:A:54:LEU:HD21	0.70	1.63	4	3
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:13:ASN:CG	1:A:13:ASN:HD22	0.69	1.36	21	1
1:A:41:ASP:OD2	1:A:41:ASP:CG	0.69	0.50	21	1
1:A:69:LYS:HE3	1:A:69:LYS:NZ	0.69	1.30	21	1
1:A:6:ILE:HG22	1:A:54:LEU:HD12	0.69	1.63	4	2
1:A:62:ILE:CD1	1:A:66:VAL:HG12	0.69	2.18	15	2
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:HD22	1:A:48:LEU:H	0.68	1.48	14	1
1:A:13:ASN:CG	1:A:13:ASN:HD21	0.68	1.36	21	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LYS:CE	1:A:26:LYS:CD	0.68	0.77	21	1
1:A:55:ALA:CB	1:A:60:LEU:HD12	0.68	2.19	8	2
1:A:49:THR:HG22	1:A:63:MET:HE3	0.68	1.65	19	1
1:A:26:LYS:HD2	1:A:26:LYS:HE3	0.68	1.01	21	1
1:A:7:TYR:CE1	1:A:37:ILE:HG13	0.67	2.24	1	8
1:A:25:VAL:CG2	1:A:32:ALA:HB2	0.67	2.18	3	13
1:A:54:LEU:HD11	1:A:56:VAL:HG13	0.67	1.67	15	1
1:A:57:ASP:OD1	1:A:57:ASP:CG	0.67	0.49	21	1
1:A:73:LYS:CE	1:A:73:LYS:HZ2	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:CZ	1:A:22:ARG:HH21	0.67	1.38	21	1
1:A:69:LYS:CE	1:A:69:LYS:HZ3	0.67	1.37	21	1
1:A:22:ARG:CZ	1:A:22:ARG:HH22	0.67	1.38	21	1
1:A:48:LEU:HD23	1:A:48:LEU:O	0.67	1.90	5	10
1:A:7:TYR:CE2	1:A:42:GLN:C	0.67	2.73	9	1
1:A:60:LEU:HD13	1:A:60:LEU:N	0.66	2.05	8	5
1:A:73:LYS:CE	1:A:73:LYS:HZ3	0.66	1.37	21	1
1:A:17:LEU:CG	1:A:17:LEU:HD21	0.66	1.19	21	1
1:A:25:VAL:HA	1:A:28:LEU:HD23	0.66	1.67	16	1
1:A:17:LEU:CG	1:A:17:LEU:HD22	0.66	1.19	21	1
1:A:73:LYS:CE	1:A:73:LYS:HZ1	0.66	1.37	21	1
1:A:17:LEU:HD13	1:A:67:ALA:C	0.66	2.15	19	1
1:A:69:LYS:CB	1:A:69:LYS:HD2	0.66	2.12	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
1:A:42:GLN:CD	1:A:42:GLN:HE21	0.66	1.31	21	1
1:A:69:LYS:CE	1:A:69:LYS:HZ1	0.66	1.37	21	1
1:A:30:ILE:N	1:A:30:ILE:HD13	0.65	2.05	1	2
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:17:LEU:CD2	1:A:72:ILE:HD11	0.65	2.16	20	1
1:A:38:LYS:O	1:A:38:LYS:HG3	0.65	1.92	21	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: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:HE3	1:A:26:LYS:NZ	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:54:LEU:HB3	1:A:62:ILE:HD11	0.64	1.69	15	2
1:A:61:LYS:O	1:A:62:ILE:HD12	0.64	1.92	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:ILE:HG23	1:A:14:CYS:HB2	0.64	1.68	13	2
1:A:37:ILE:C	1:A:37:ILE:HD13	0.64	2.18	5	6
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: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:42:GLN:CD	1:A:42:GLN:HE22	0.64	1.31	21	1
1:A:4:ILE:HG21	1:A:34:PHE:CD2	0.64	2.27	15	8
1:A:73:LYS:CE	1:A:73:LYS:NZ	0.64	0.79	21	1
1:A:72:ILE:O	1:A:72:ILE:HD13	0.64	1.93	8	4
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:H	1:A:60:LEU:HD22	0.63	1.51	2	9
1:A:28:LEU:O	1:A:28:LEU:HD13	0.63	1.94	12	3
1:A:7:TYR:HD2	1:A:48:LEU:HD11	0.63	1.53	8	3
1:A:69:LYS:CE	1:A:69:LYS:NZ	0.63	0.78	21	1
1:A:54:LEU:CD1	1:A:66:VAL:HG23	0.63	2.22	14	1
1:A:46:ALA:HB1	1:A:60:LEU:HD23	0.63	1.68	10	1
1:A:17:LEU:CD1	1:A:17:LEU:HD23	0.63	1.18	21	1
1:A:65:ARG:CD	1:A:65:ARG:HB2	0.63	2.13	21	1
1:A:2:MET:HE1	1:A:30:ILE:HG21	0.62	1.69	13	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:48:LEU:H	1:A:48:LEU:HD22	0.62	1.53	2	2
1:A:26:LYS:CE	1:A:26:LYS:HZ3	0.62	1.33	21	1
1:A:17:LEU:HD23	1:A:67:ALA:C	0.62	2.19	9	3
1:A:31:ASP:OD1	1:A:31:ASP:CG	0.62	0.46	21	1
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:7:TYR:CE2	1:A:37:ILE:HG21	0.61	2.29	9	1
1:A:26:LYS:CE	1:A:26:LYS:HZ2	0.61	1.33	21	1
1:A:61:LYS:C	1:A:62:ILE:HD12	0.61	2.20	16	1
1:A:46:ALA:HB1	1:A:60:LEU:HD12	0.61	1.71	2	1
1:A:17:LEU:HD22	1:A:20:ASN:OD1	0.61	1.95	15	2
1:A:7:TYR:CD1	1:A:7:TYR:CG	0.61	0.74	21	1
1:A:26:LYS:HE2	1:A:26:LYS:NZ	0.61	1.25	21	1
1:A:40:MET:HA	1:A:43:ILE:CG1	0.61	2.26	21	8
1:A:17:LEU:HD22	1:A:54:LEU:HD13	0.61	1.70	3	3
1:A:17:LEU:HD12	1:A:67:ALA:C	0.61	2.20	7	1
1:A:62:ILE:HG21	1:A:66:VAL:HA	0.60	1.73	14	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ALA:C	1:A:60:LEU:HD21	0.60	2.21	18	2
1:A:65:ARG:HD3	1:A:65:ARG:HB2	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:13:ASN:ND2	1:A:13:ASN:CG	0.60	0.71	21	1
1:A:7:TYR:CE2	1:A:48:LEU:HD11	0.60	2.31	12	3
1:A:7:TYR:CD2	1:A:37:ILE:CD1	0.60	2.85	18	4
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:7:TYR:CZ	1:A:7:TYR:CE2	0.59	0.71	21	1
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:CE	1:A:73:LYS:HG2	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:CD2	1:A:7:TYR:CG	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:N	1:A:37:ILE:CD1	0.58	2.39	21	9
1:A:26:LYS:CE	1:A:26:LYS:NZ	0.58	0.73	21	1
1:A:7:TYR:CZ	1:A:7:TYR:CE1	0.58	0.69	21	1
1:A:54:LEU:C	1:A:54:LEU:HD13	0.58	2.24	11	4
1:A:17:LEU:HD22	1:A:17:LEU:O	0.58	1.99	15	1
1:A:37:ILE:HD13	1:A:37:ILE:C	0.58	2.24	8	2
1:A:40:MET:HA	1:A:43:ILE:HB	0.58	1.75	5	3
1:A:17:LEU:C	1:A:17:LEU:HD13	0.58	2.23	15	1
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:22:ARG:CZ	1:A:22:ARG:NH2	0.57	0.73	21	1
1:A:54:LEU:CD1	1:A:54:LEU:HD23	0.57	1.11	21	1
1:A:2:MET:HE3	1:A:30:ILE:CD1	0.57	2.29	3	1
1:A:54:LEU:HD21	1:A:54:LEU:HD12	0.57	0.62	21	1
1:A:50:ALA:HB3	1:A:63:MET:CG	0.57	2.29	10	3
1:A:62:ILE:HD13	1:A:66:VAL:CG1	0.57	2.27	15	1
1:A:48:LEU:C	1:A:48:LEU:HD23	0.56	2.24	3	7
1:A:40:MET:HA	1:A:43:ILE:HG23	0.56	1.77	13	3
1:A:69:LYS:CB	1:A:69:LYS:HD3	0.56	2.16	21	1
1:A:1:MET:H3	1:A:31:ASP:C	0.56	2.09	3	1
1:A:34:PHE:CD1	1:A:34:PHE:N	0.56	2.73	18	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ALA:O	1:A:25:VAL:HG12	0.56	2.00	14	4
1:A:51:LEU:CB	1:A:52:PRO:CD	0.56	2.83	4	6
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:6:ILE:HG23	1:A:54:LEU:HD21	0.56	1.77	8	1
1:A:54:LEU:HD12	1:A:54:LEU:CD2	0.56	1.22	21	1
1:A:48:LEU:C	1:A:49:THR:HG23	0.56	2.25	2	1
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:HD13	1:A:6:ILE:HG21	0.56	1.62	21	1
1:A:46:ALA:HB1	1:A:60:LEU:CD1	0.55	2.31	2	1
1:A:72:ILE:HD13	1:A:72:ILE:C	0.55	2.26	11	4
1:A:50:ALA:HB3	1:A:64:GLY:N	0.55	2.16	14	2
1:A:72:ILE:C	1:A:72:ILE:HD13	0.55	2.26	7	1
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:42:GLN:CD	1:A:42:GLN:NE2	0.55	0.65	21	1
1:A:29:GLY:C	1:A:30:ILE:HD13	0.55	2.26	1	1
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:24:ALA:O	1:A:28:LEU:HD23	0.55	2.02	15	4
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
1:A:22:ARG:HA	1:A:34:PHE:CZ	0.54	2.36	18	2
1:A:48:LEU:HD23	1:A:48:LEU:C	0.54	2.26	5	5
1:A:68:SER:CB	1:A:68:SER:HG	0.54	1.24	21	1
1:A:17:LEU:CB	1:A:66:VAL:HG13	0.54	2.32	10	1
1:A:2:MET:HB2	1:A:32:ALA:HB2	0.54	1.78	1	2
1:A:54:LEU:HD13	1:A:54:LEU:O	0.54	2.03	11	2
1:A:6:ILE:HD11	1:A:36:LYS:CG	0.54	2.32	10	1
1:A:47:GLY:HA3	1:A:60:LEU:HD21	0.54	1.79	13	2
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:53:GLY:O	1:A:54:LEU:HD22	0.53	2.04	20	1
1:A:34:PHE:CG	1:A:34:PHE:HD2	0.53	1.29	21	1
1:A:54:LEU:O	1:A:54:LEU:HD23	0.53	2.04	3	1
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:34:PHE:CZ	1:A:34:PHE:HE1	0.53	1.28	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:LEU:CD1	1:A:54:LEU:CG	0.53	0.69	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:66:VAL:CG1	1:A:66:VAL:C	0.52	2.82	21	1
1:A:54:LEU:HB2	1:A:62:ILE:HD11	0.52	1.82	4	1
1:A:51:LEU:HD23	1:A:51:LEU:N	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:O	1:A:49:THR:HG23	0.52	2.05	2	1
1:A:6:ILE:HG22	1:A:54:LEU:CD1	0.52	2.34	4	1
1:A:17:LEU:HD21	1:A:72:ILE:HB	0.52	1.82	5	1
1:A:54:LEU:HD23	1:A:54:LEU:C	0.52	2.30	3	1
1:A:17:LEU:HD13	1:A:21:ALA:HB2	0.51	1.80	5	1
1:A:54:LEU:HD22	1:A:62:ILE:HD12	0.51	1.81	7	1
1:A:21:ALA:HB3	1:A:34:PHE:HE2	0.51	1.65	18	2
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:48:LEU:C	1:A:48:LEU:CD2	0.51	2.83	3	4
1:A:17:LEU:HD13	1:A:17:LEU:C	0.51	2.30	18	2
1:A:48:LEU:CD2	1:A:48:LEU:C	0.51	2.83	15	11
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
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:HG23	1:A:56:VAL:HG13	0.50	1.83	2	4
1:A:4:ILE:CG2	1:A:34:PHE:CD2	0.50	2.95	19	10
1:A:44:LEU:HD23	1:A:45:GLU:N	0.50	2.21	3	6
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:69:LYS:CE	1:A:69:LYS:HG3	0.50	2.23	21	1
1:A:20:ASN:OD1	1:A:21:ALA:N	0.50	2.45	12	6
1:A:46:ALA:CB	1:A:60:LEU:HD11	0.50	2.36	12	1
1:A:6:ILE:C	1:A:37:ILE:HD11	0.50	2.31	15	3
1:A:1:MET:CA	1:A:1:MET:HG3	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:43:ILE:HG23	1:A:48:LEU:HD21	0.49	1.84	5	1
1:A:26:LYS:HE3	1:A:26:LYS:HZ1	0.49	1.10	21	1
1:A:48:LEU:HB2	1:A:63:MET:HG2	0.48	1.85	19	6
1:A:5:GLN:CA	1:A:37:ILE:HD11	0.48	2.38	14	1
1:A:17:LEU:HD13	1:A:67:ALA:O	0.48	2.08	13	2
1:A:4:ILE:HG23	1:A:54:LEU:HD11	0.48	1.85	1	3
1:A:32:ALA:HB3	1:A:34:PHE:CE1	0.48	2.43	14	3
1:A:17:LEU:HD23	1:A:18:GLU:N	0.48	2.22	10	1
1:A:48:LEU:N	1:A:48:LEU:CD2	0.48	2.73	14	1
1:A:7:TYR:CG	1:A:7:TYR:HD1	0.48	1.24	21	1
1:A:7:TYR:CG	1:A:7:TYR:HD2	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
1:A:2:MET:N	1:A:2:MET:HE2	0.48	2.23	3	1
1:A:6:ILE:HD13	1:A:18:GLU:CD	0.48	2.33	4	1
1:A:62:ILE:HD13	1:A:66:VAL:HA	0.48	1.86	19	3
1:A:5:GLN:HB3	1:A:7:TYR:CE1	0.48	2.44	5	1
1:A:25:VAL:HG22	1:A:30:ILE:O	0.48	2.09	14	2
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:13:ASN:OD1	1:A:13:ASN:CG	0.48	0.55	21	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:CB	1:A:49:THR:HG1	0.48	1.18	21	1
1:A:7:TYR:CE2	1:A:46:ALA:HB2	0.47	2.44	6	3
1:A:6:ILE:HD11	1:A:36:LYS:HG3	0.47	1.85	10	1
1:A:7:TYR:CZ	1:A:7:TYR:HE2	0.47	1.23	21	1
1:A:53:GLY:HA2	1:A:62:ILE:O	0.47	2.09	10	4
1:A:48:LEU:O	1:A:49:THR:OG1	0.47	2.33	2	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:LEU:HD12	1:A:62:ILE:CB	0.47	2.38	14	1
1:A:5:GLN:C	1:A:37:ILE:HD11	0.47	2.34	10	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:17:LEU:HD22	1:A:66:VAL:HB	0.47	1.86	13	1
1:A:6:ILE:HG22	1:A:54:LEU:HD22	0.47	1.87	14	1
1:A:4:ILE:HG12	1:A:56:VAL:CG1	0.46	2.40	15	3
1:A:46:ALA:C	1:A:60:LEU:HD11	0.46	2.35	20	2
1:A:72:ILE:HD13	1:A:72:ILE:O	0.46	2.10	7	1
1:A:54:LEU:N	1:A:62:ILE:O	0.46	2.48	8	1
1:A:54:LEU:C	1:A:54:LEU:HD12	0.46	2.35	15	1
1:A:7:TYR:CZ	1:A:7:TYR:HE1	0.46	1.22	21	1
1:A:17:LEU:HB3	1:A:66:VAL:HG22	0.46	1.87	10	2
1:A:4:ILE:CG2	1:A:54:LEU:HD21	0.46	2.40	11	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:28:LEU:HD21	1:A:73:LYS:HG2	0.46	1.86	15	1
1:A:1:MET:CG	1:A:1:MET:N	0.46	2.72	21	1
1:A:6:ILE:HD11	1:A:36:LYS:HB2	0.46	1.87	5	1
1:A:59:GLU:O	1:A:59:GLU:CG	0.46	2.64	1	1
1:A:16:MET:CB	1:A:66:VAL:HG11	0.46	2.40	2	1
1:A:38:LYS:O	1:A:39:GLU:CB	0.46	2.63	12	11
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
1:A:1:MET:CA	1:A:31:ASP:O	0.46	2.64	10	19
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:7:TYR:CE1	1:A:37:ILE:HD12	0.46	2.46	16	2
1:A:62:ILE:HG21	1:A:66:VAL:HG12	0.46	1.86	3	1
1:A:8:GLY:C	1:A:9:THR:HG1	0.45	2.18	16	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:60:LEU:N	1:A:60:LEU:HD13	0.45	2.26	2	2
1:A:72:ILE:HG23	1:A:73:LYS:N	0.45	2.26	15	4
1:A:46:ALA:HB3	1:A:48:LEU:CD1	0.45	2.41	9	1
1:A:17:LEU:HB2	1:A:66:VAL:CG1	0.45	2.36	21	1
1:A:36:LYS:HD2	1:A:36:LYS:HE3	0.45	1.31	21	1
1:A:46:ALA:O	1:A:60:LEU:CD2	0.45	2.64	21	1
1:A:7:TYR:HE2	1:A:46:ALA:HB2	0.45	1.72	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:4:ILE:O	1:A:34:PHE:HA	0.45	2.11	7	1
1:A:8:GLY:CA	1:A:12:ALA:HB3	0.45	2.42	17	2
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: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:HD12	1:A:54:LEU:CG	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:HE3	1:A:73:LYS:HD2	0.44	1.31	21	1
1:A:17:LEU:CD1	1:A:72:ILE:HD11	0.44	2.22	1	1
1:A:12:ALA:HB1	1:A:52:PRO:CB	0.44	2.43	4	2
1:A:46:ALA:CB	1:A:60:LEU:HD12	0.44	2.43	2	1
1:A:60:LEU:HD13	1:A:60:LEU:H	0.44	1.70	11	1
1:A:7:TYR:CD1	1:A:37:ILE:HB	0.44	2.47	4	1
1:A:7:TYR:CD1	1:A:7:TYR:N	0.44	2.84	8	3
1:A:6:ILE:N	1:A:6:ILE:CD1	0.44	2.81	8	2
1:A:50:ALA:CB	1:A:63:MET:CB	0.43	2.90	5	1
1:A:48:LEU:O	1:A:48:LEU:CD2	0.43	2.66	9	4
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:6:ILE:CG2	1:A:14:CYS:CB	0.43	2.96	1	1
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:34:PHE:N	1:A:34:PHE:HD1	0.43	2.09	18	2
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:1:MET:HA	1:A:31:ASP:O	0.43	2.14	10	4
1:A:37:ILE:HG12	1:A:38:LYS:N	0.43	2.28	20	2
1:A:17:LEU:O	1:A:20:ASN:OD1	0.43	2.37	20	1
1:A:22:ARG:HG3	1:A:34:PHE:CD1	0.43	2.49	9	6
1:A:7:TYR:HA	1:A:37:ILE:HD11	0.43	1.87	18	1
1:A:48:LEU:CB	1:A:63:MET:HG2	0.43	2.44	7	1
1:A:23:GLU:HG3	1:A:24:ALA:N	0.43	2.28	14	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: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:69:LYS:CG	1:A:69:LYS:C	0.43	2.89	21	1
1:A:54:LEU:HD21	1:A:56:VAL:HG13	0.43	1.89	3	1
1:A:7:TYR:HA	1:A:37:ILE:CG1	0.43	2.44	7	3
1:A:17:LEU:HD23	1:A:17:LEU:C	0.43	2.38	10	1
1:A:48:LEU:CD2	1:A:48:LEU:O	0.42	2.67	4	3
1:A:37:ILE:CD1	1:A:37:ILE:C	0.42	2.83	5	2
1:A:14:CYS:HA	1:A:66:VAL:HG21	0.42	1.90	20	1
1:A:30:ILE:N	1:A:30:ILE:CD1	0.42	2.76	1	1
1:A:17:LEU:CD2	1:A:17:LEU:HD11	0.42	0.96	21	1
1:A:48:LEU:HD12	1:A:53:GLY:HA3	0.42	1.91	6	1
1:A:17:LEU:HD12	1:A:17:LEU:HD21	0.42	0.43	21	1
1:A:17:LEU:CB	1:A:66:VAL:CG2	0.42	2.96	17	3
1:A:43:ILE:O	1:A:48:LEU:HD21	0.42	2.13	17	1
1:A:8:GLY:HA3	1:A:12:ALA:CB	0.42	2.44	21	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:17:LEU:HG	1:A:67:ALA:HB3	0.42	1.91	1	1
1:A:48:LEU:CB	1:A:63:MET:CB	0.42	2.98	2	1
1:A:5:GLN:O	1:A:54:LEU:HA	0.42	2.15	15	1
1:A:17:LEU:CD2	1:A:17:LEU:CA	0.42	2.88	21	1
1:A:29:GLY:C	1:A:30:ILE:CG1	0.42	2.93	15	2
1:A:48:LEU:N	1:A:48:LEU:HD22	0.41	2.30	9	2
1:A:17:LEU:HD21	1:A:72:ILE:HG12	0.41	1.91	1	1
1:A:62:ILE:HG21	1:A:66:VAL:CA	0.41	2.45	9	1
1:A:43:ILE:O	1:A:48:LEU:CD2	0.41	2.67	13	1
1:A:4:ILE:HG13	1:A:56:VAL:CG1	0.41	2.44	19	1
1:A:52:PRO:O	1:A:62:ILE:CG2	0.41	2.68	18	1
1:A:25:VAL:HG11	1:A:32:ALA:CB	0.41	2.37	1	2
1:A:5:GLN:CB	1:A:37:ILE:CD1	0.41	2.97	4	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: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:60:LEU:N	1:A:60:LEU:CD1	0.41	2.77	8	1
1:A:5:GLN:O	1:A:54:LEU:CD2	0.41	2.68	11	1
1:A:2:MET:CG	1:A:25:VAL:CG2	0.41	2.99	19	1
1:A:38:LYS:O	1:A:38:LYS:CG	0.41	2.62	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:62:ILE:HD12	1:A:62:ILE:N	0.41	2.31	14	1
1:A:48:LEU:O	1:A:63:MET:HG3	0.41	2.16	2	1
1:A:17:LEU:O	1:A:17:LEU:HD13	0.41	2.16	4	1
1:A:68:SER:HB3	1:A:68:SER:HG	0.41	1.36	21	1
1:A:4:ILE:HG21	1:A:34:PHE:CE2	0.40	2.51	4	1
1:A:72:ILE:C	1:A:72:ILE:CD1	0.40	2.94	11	1
1:A:17:LEU:HD21	1:A:72:ILE:CG1	0.40	2.46	1	1
1:A:6:ILE:H	1:A:37:ILE:HD11	0.40	1.70	2	1
1:A:41:ASP:O	1:A:44:LEU:CD2	0.40	2.70	10	1
1:A:17:LEU:CD2	1:A:17:LEU:CG	0.40	0.44	21	1
1:A:17:LEU:HD23	1:A:62:ILE:HD11	0.40	1.94	2	1
1:A:52:PRO:HG2	1:A:65:ARG:N	0.40	2.31	3	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:54:LEU:C	1:A:54:LEU:CD1	0.40	2.94	10	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%)	3	23
All	All	1512/1617 (94%)	1209 (80%)	225 (15%)	78 (5%)	3	23

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

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Mol	Chain	Res	Type	Models (Total)
1	A	10	GLY	5
1	A	8	GLY	3
1	A	66	VAL	3
1	A	11	CYS	2
1	A	51	LEU	1
1	A	48	LEU	1
1	A	49	THR	1
1	A	52	PRO	1
1	A	67	ALA	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%)	34±4 (58±6%)	24±4 (42±6%)	0 4
All	All	1218/1302 (94%)	708 (58%)	510 (42%)	0 4

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	37	ILE	21
1	A	44	LEU	21
1	A	48	LEU	21
1	A	56	VAL	21
1	A	15	GLN	20
1	A	60	LEU	19
1	A	51	LEU	17
1	A	63	MET	15
1	A	36	LYS	14
1	A	39	GLU	14
1	A	2	MET	13
1	A	30	ILE	13
1	A	38	LYS	13
1	A	41	ASP	13
1	A	61	LYS	13
1	A	40	MET	11

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Mol	Chain	Res	Type	Models (Total)
1	A	3	LYS	11
1	A	5	GLN	11
1	A	57	ASP	10
1	A	66	VAL	10
1	A	73	LYS	10
1	A	26	LYS	10
1	A	28	LEU	9
1	A	54	LEU	9
1	A	17	LEU	8
1	A	16	MET	8
1	A	19	LYS	8
1	A	59	GLU	8
1	A	22	ARG	8
1	A	49	THR	8
1	A	65	ARG	8
1	A	9	THR	7
1	A	31	ASP	7
1	A	71	GLU	7
1	A	6	ILE	7
1	A	70	GLU	7
1	A	72	ILE	7
1	A	1	MET	6
1	A	35	GLU	6
1	A	68	SER	6
1	A	69	LYS	6
1	A	62	ILE	6
1	A	45	GLU	6
1	A	4	ILE	5
1	A	42	GLN	5
1	A	33	GLU	5
1	A	11	CYS	4
1	A	23	GLU	3
1	A	18	GLU	3
1	A	27	GLU	3
1	A	34	PHE	2
1	A	43	ILE	2
1	A	13	ASN	2
1	A	20	ASN	2
1	A	7	TYR	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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	21-A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
21	A	11:CYS	C	12:ALA	N	1.18
21	A	37:ILE	C	38:LYS	N	1.13
21	A	48:LEU	C	49:THR	N	1.11
21	A	10:GLY	C	11:CYS	N	1.08
21	A	9:THR	C	10:GLY	N	0.81

7 Chemical shift validation

No chemical shift data were provided