



Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 10:58 PM UTC

PDB ID : 1NCV / pdb_00001ncv
Title : DETERMINATION CC-CHEMOKINE MCP-3, NMR, 7 STRUCTURES
Authors : Meunier, S.; Bernassau, J.M.; Guillemot, J.C.; Ferrara, P.; Darbon, H.
Deposited on : 1997-02-05

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

<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

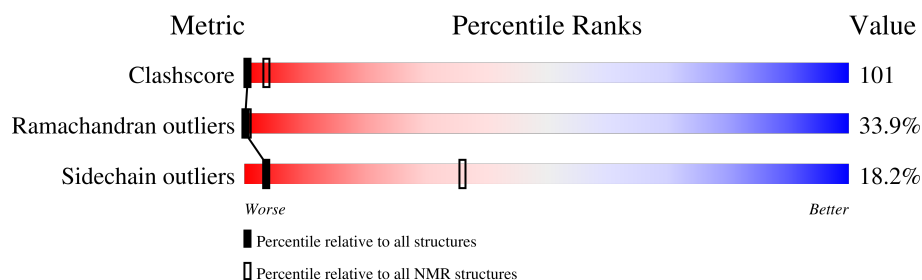
1 Overall quality at a glance

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	76	46% 39% 14%
1	B	76	49% 30% 21%

2 Ensemble composition and analysis

This entry contains 7 models. Model 4 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:11-A:75, B:11-B:70 (125)	3.49	4

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

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

The models can be grouped into 1 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 6, 7
Single-model clusters	3; 5

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2545 atoms, of which 1292 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MONOCYTE CHEMOATTRACTANT PROTEIN 3.

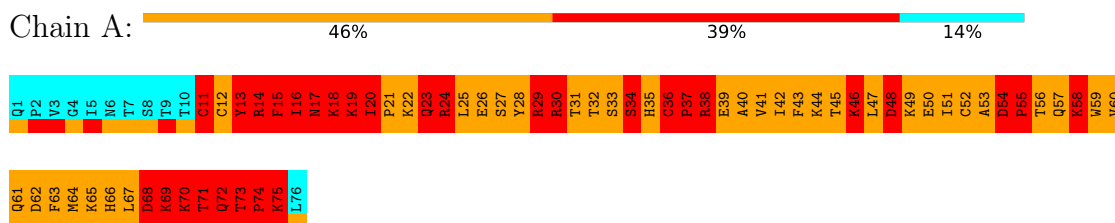
Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1273	395	647	114	112	5	
1	B	76	Total	C	H	N	O	S	0
			1272	395	645	114	113	5	

4 Residue-property plots [i](#)

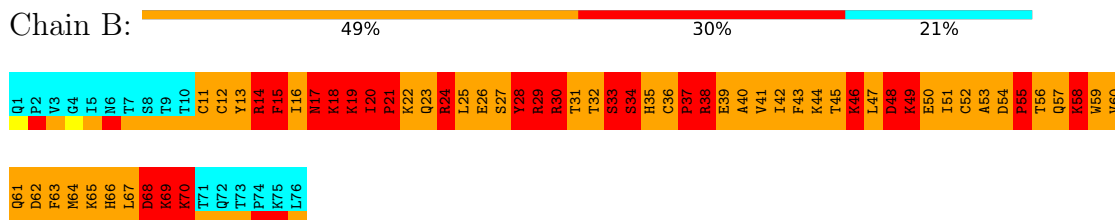
4.1 Average score per residue in the NMR ensemble

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: MONOCYTE CHEMOATTRACTANT PROTEIN 3



• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

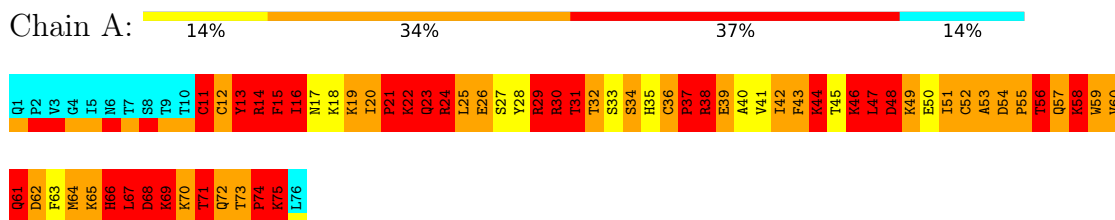


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

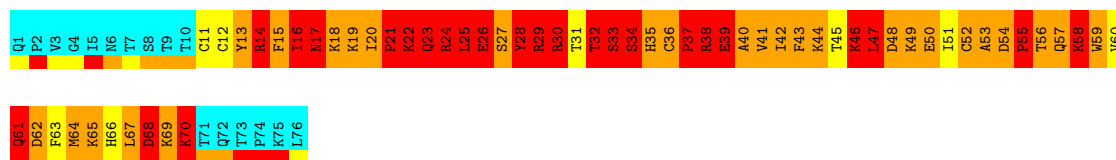
4.2.1 Score per residue for model 1

• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3



- Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

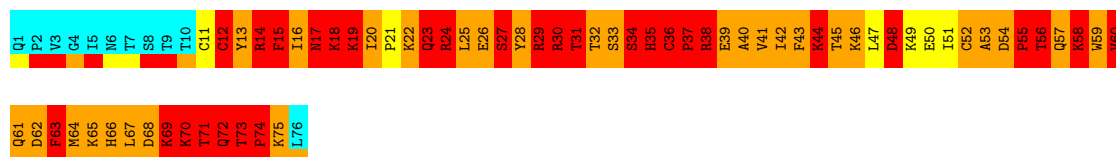
Chain B: 11% 36% 33% 21%



4.2.2 Score per residue for model 2

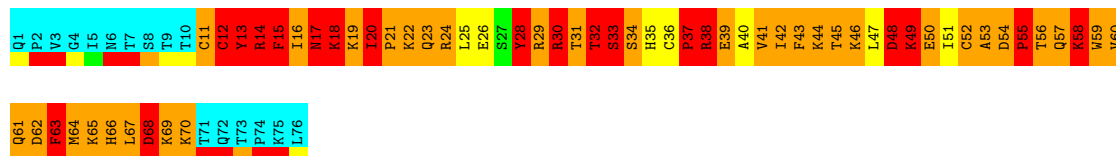
- Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain A: 8% 38% 39% 14%



- Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

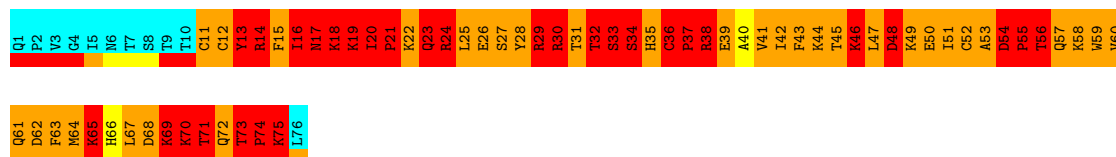
Chain B: 9% 43% 25% 21%



4.2.3 Score per residue for model 3

- Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain A: 43% 39% 14%



- Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain B: 8% 33% 38% 21%

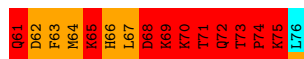




4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain A: . . 33% 47% 14%



- Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain B: 5% 42% 32% 21%



4.2.5 Score per residue for model 5

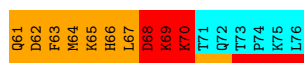
- Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain A: 9% 37% 39% 14%



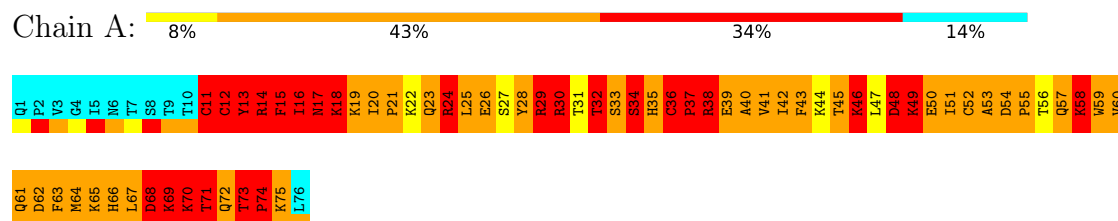
- Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain B: . 43% 33% 21%

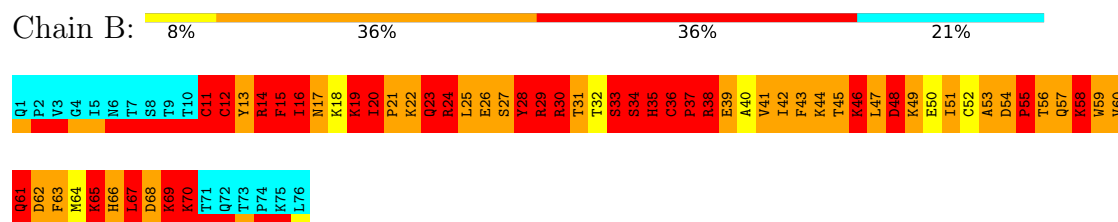


4.2.6 Score per residue for model 6

- Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

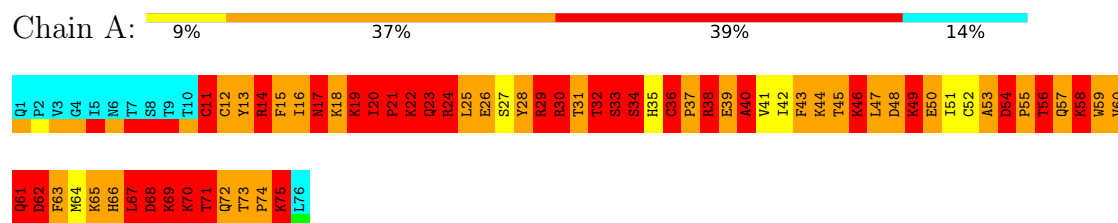


- Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

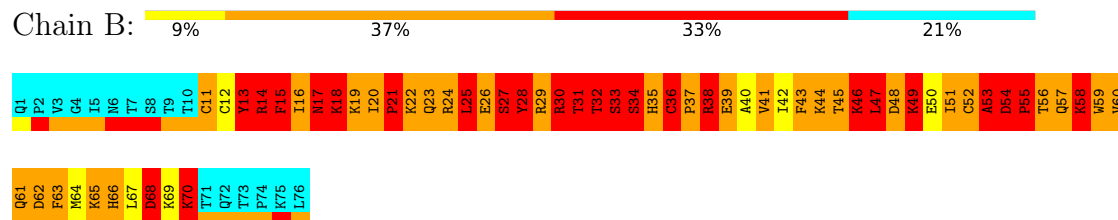


4.2.7 Score per residue for model 7

- Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3



- Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY SIMULATED ANNEALING*.

Of the 50 calculated structures, 7 were deposited, based on the following criterion: *NOE VIOLATION*.

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

Software name	Classification	Version
X-PLOR	refinement	
DIANA	structure solution	
XPLOR	structure solution	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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	2.90±0.05	50±3/561 (9.0± 0.5%)	5.48±0.53	208±12/752 (27.6± 1.6%)
1	B	2.94±0.14	47±5/521 (9.0± 1.0%)	5.47±0.43	192±15/697 (27.5± 2.1%)
All	All	2.92	682/7574 (9.0%)	5.50	2797/10143 (27.6%)

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	1.0±0.5	5.1±0.3
1	B	1.6±0.9	4.7±0.5
All	All	18	69

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	15	PHE	CB-CG	17.78	1.91	1.50	7	1
1	B	28	TYR	CB-CG	17.19	1.89	1.51	7	1
1	A	40	ALA	N-CA	11.34	1.60	1.46	4	3
1	B	28	TYR	CE1-CZ	11.25	1.65	1.38	7	1
1	B	14	ARG	CZ-NH2	-11.10	1.19	1.33	2	7
1	A	29	ARG	CZ-NH2	-10.49	1.19	1.33	6	7
1	B	27	SER	N-CA	9.89	1.58	1.46	3	5
1	A	14	ARG	CA-CB	9.88	1.70	1.53	3	2
1	A	38	ARG	CZ-NH2	-9.81	1.20	1.33	3	7
1	B	38	ARG	CZ-NH2	-9.77	1.20	1.33	6	7
1	A	14	ARG	CZ-NH2	-9.74	1.20	1.33	2	7
1	B	28	TYR	CZ-OH	9.72	1.58	1.38	7	1
1	B	29	ARG	CZ-NH2	-9.63	1.21	1.33	6	7
1	B	30	ARG	CZ-NH2	-9.61	1.21	1.33	1	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	30	ARG	NE-CZ	-9.51	1.22	1.33	4	6
1	A	15	PHE	CD1-CE1	9.43	1.67	1.38	7	1
1	B	28	TYR	CG-CD1	9.40	1.59	1.39	7	1
1	A	30	ARG	CZ-NH2	-9.36	1.21	1.33	6	7
1	A	30	ARG	CZ-NH1	-9.30	1.19	1.32	4	6
1	B	38	ARG	NE-CZ	-9.27	1.22	1.33	3	7
1	A	15	PHE	CG-CD2	9.11	1.57	1.38	7	1
1	A	24	ARG	NE-CZ	-9.10	1.23	1.33	7	7
1	B	25	LEU	N-CA	9.08	1.57	1.46	7	1
1	A	24	ARG	CZ-NH2	-9.06	1.21	1.33	2	7
1	B	24	ARG	CZ-NH2	-9.02	1.21	1.33	3	6
1	B	14	ARG	NE-CZ	-8.94	1.23	1.33	2	7
1	B	24	ARG	N-CA	8.86	1.55	1.46	6	5
1	B	66	HIS	CG-ND1	-8.85	1.28	1.38	5	7
1	B	29	ARG	CZ-NH1	-8.77	1.20	1.32	6	7
1	B	22	LYS	CA-C	8.72	1.58	1.52	7	1
1	B	54	ASP	CA-C	8.72	1.63	1.52	1	6
1	B	30	ARG	CZ-NH1	-8.71	1.20	1.32	4	7
1	A	38	ARG	CZ-NH1	-8.70	1.20	1.32	4	7
1	B	57	GLN	CA-C	8.65	1.64	1.52	3	2
1	A	45	THR	CA-CB	-8.65	1.40	1.53	7	1
1	A	29	ARG	CZ-NH1	-8.62	1.20	1.32	1	6
1	B	28	TYR	CD2-CE2	8.61	1.64	1.38	7	1
1	B	14	ARG	CZ-NH1	-8.61	1.20	1.32	4	7
1	A	26	GLU	N-CA	8.58	1.54	1.46	2	2
1	A	66	HIS	CG-ND1	-8.53	1.28	1.38	7	7
1	A	35	HIS	CG-ND1	-8.51	1.28	1.38	4	7
1	B	35	HIS	CG-ND1	-8.50	1.28	1.38	5	7
1	B	30	ARG	NE-CZ	-8.44	1.23	1.33	5	7
1	B	70	LYS	CA-C	8.43	1.64	1.52	5	3
1	A	12	CYS	N-CA	8.37	1.56	1.46	6	4
1	B	38	ARG	CZ-NH1	-8.36	1.21	1.32	5	7
1	A	14	ARG	NE-CZ	-8.36	1.23	1.33	6	7
1	A	14	ARG	CZ-NH1	-8.35	1.21	1.32	2	7
1	B	24	ARG	CZ-NH1	-8.34	1.21	1.32	5	7
1	A	38	ARG	NE-CZ	-8.33	1.23	1.33	3	7
1	B	53	ALA	CA-C	8.31	1.63	1.52	6	5
1	B	24	ARG	NE-CZ	-8.29	1.24	1.33	2	6
1	A	34	SER	N-CA	8.25	1.56	1.46	3	5
1	A	38	ARG	N-CA	8.22	1.56	1.46	6	2
1	B	29	ARG	NE-CZ	-8.20	1.24	1.33	6	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	54	ASP	CA-CB	8.11	1.64	1.54	1	1
1	B	67	LEU	CA-C	-8.11	1.46	1.52	5	1
1	A	29	ARG	NE-CZ	-8.07	1.24	1.33	2	6
1	A	54	ASP	CA-C	8.03	1.62	1.52	4	5
1	A	71	THR	N-CA	7.96	1.56	1.46	5	6
1	B	57	GLN	N-CA	7.93	1.57	1.46	3	1
1	A	73	THR	N-CA	7.93	1.57	1.46	4	4
1	A	15	PHE	CE2-CZ	7.88	1.62	1.38	7	1
1	A	33	SER	N-CA	7.88	1.55	1.46	5	6
1	B	56	THR	N-CA	7.84	1.54	1.46	1	5
1	A	24	ARG	CZ-NH1	-7.81	1.21	1.32	6	7
1	B	12	CYS	N-CA	7.80	1.56	1.46	3	4
1	A	39	GLU	N-CA	7.76	1.54	1.45	6	2
1	A	74	PRO	CA-C	7.74	1.63	1.52	3	1
1	B	51	ILE	N-CA	7.71	1.54	1.46	5	4
1	A	20	ILE	CA-C	7.71	1.60	1.52	7	4
1	B	66	HIS	CA-C	-7.63	1.42	1.52	5	1
1	A	35	HIS	CA-C	7.61	1.60	1.52	1	3
1	B	45	THR	N-CA	7.61	1.56	1.45	5	3
1	A	45	THR	N-CA	7.60	1.55	1.45	2	5
1	B	23	GLN	CA-C	7.59	1.62	1.53	3	4
1	A	36	CYS	N-CA	7.57	1.56	1.46	6	6
1	B	15	PHE	CA-C	7.54	1.62	1.52	5	1
1	B	54	ASP	N-CA	7.52	1.56	1.46	3	4
1	A	55	PRO	CA-C	7.47	1.63	1.52	2	1
1	A	26	GLU	CA-C	7.44	1.62	1.53	2	1
1	A	33	SER	CA-CB	7.42	1.63	1.53	5	1
1	B	53	ALA	N-CA	7.37	1.55	1.46	7	2
1	B	24	ARG	CA-C	7.33	1.62	1.52	3	4
1	B	69	LYS	CA-CB	-7.33	1.41	1.53	5	1
1	A	33	SER	CA-C	7.26	1.62	1.52	5	1
1	B	60	VAL	CA-CB	-7.25	1.45	1.54	6	1
1	B	59	TRP	NE1-CE2	-7.21	1.29	1.37	5	6
1	B	49	LYS	N-CA	7.17	1.54	1.45	7	5
1	B	34	SER	N-CA	7.15	1.55	1.46	3	4
1	A	38	ARG	CA-C	7.14	1.62	1.52	6	1
1	B	44	LYS	CA-CB	-7.11	1.42	1.53	6	1
1	A	50	GLU	CA-CB	-7.11	1.40	1.53	5	1
1	A	11	CYS	N-CA	7.10	1.55	1.46	7	3
1	B	36	CYS	CA-C	7.02	1.61	1.52	6	1
1	A	12	CYS	CA-C	6.98	1.59	1.52	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	17	ASN	CA-CB	6.97	1.65	1.53	6	1
1	A	54	ASP	N-CA	6.90	1.55	1.46	4	2
1	A	72	GLN	CA-C	6.86	1.61	1.52	2	3
1	A	64	MET	CA-C	6.79	1.61	1.52	2	1
1	B	33	SER	N-CA	6.76	1.54	1.46	4	5
1	A	59	TRP	NE1-CE2	-6.75	1.30	1.37	2	6
1	B	52	CYS	N-CA	6.73	1.54	1.46	5	5
1	A	75	LYS	CA-C	6.71	1.61	1.52	3	3
1	A	11	CYS	CA-C	6.65	1.61	1.52	1	2
1	A	17	ASN	CA-C	6.63	1.61	1.52	5	3
1	B	14	ARG	CA-C	6.60	1.61	1.52	2	2
1	A	51	ILE	N-CA	6.60	1.54	1.46	6	4
1	B	46	LYS	N-CA	6.59	1.54	1.46	5	1
1	A	24	ARG	N-CA	6.58	1.54	1.46	2	4
1	B	20	ILE	CA-C	6.56	1.59	1.52	3	3
1	B	11	CYS	N-CA	6.55	1.54	1.46	5	3
1	A	30	ARG	CA-CB	-6.53	1.44	1.53	5	3
1	A	47	LEU	N-CA	6.51	1.54	1.46	1	1
1	B	32	THR	N-CA	6.50	1.54	1.46	4	2
1	A	70	LYS	CA-C	6.50	1.61	1.52	5	4
1	A	27	SER	N-CA	6.48	1.54	1.46	5	3
1	A	36	CYS	CA-CB	6.48	1.63	1.53	1	3
1	B	26	GLU	CA-C	6.46	1.58	1.52	7	3
1	A	31	THR	N-CA	6.46	1.54	1.46	3	2
1	A	46	LYS	N-CA	6.43	1.53	1.46	2	4
1	B	16	ILE	N-CA	6.43	1.54	1.46	5	2
1	A	74	PRO	N-CA	6.40	1.55	1.47	3	2
1	B	66	HIS	CD2-NE2	-6.38	1.30	1.37	7	7
1	B	11	CYS	CA-C	6.37	1.61	1.52	5	6
1	B	18	LYS	N-CA	6.35	1.54	1.45	7	2
1	B	29	ARG	CA-CB	6.33	1.62	1.53	7	1
1	B	55	PRO	N-CA	6.33	1.55	1.47	6	1
1	B	70	LYS	N-CA	6.31	1.54	1.46	3	2
1	A	52	CYS	CA-CB	6.31	1.63	1.53	6	1
1	A	56	THR	N-CA	6.31	1.54	1.46	3	4
1	A	35	HIS	CD2-NE2	-6.29	1.30	1.37	2	7
1	B	19	LYS	CA-C	6.27	1.60	1.52	4	1
1	B	12	CYS	CA-CB	6.26	1.64	1.53	3	3
1	B	56	THR	CA-C	6.25	1.61	1.52	3	1
1	B	66	HIS	CA-CB	-6.25	1.43	1.53	5	1
1	A	72	GLN	N-CA	6.17	1.54	1.46	5	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	16	ILE	CA-CB	6.14	1.62	1.54	7	3
1	B	35	HIS	CD2-NE2	-6.12	1.31	1.37	6	7
1	A	44	LYS	CA-CB	-6.12	1.44	1.53	3	1
1	B	57	GLN	CA-CB	6.11	1.62	1.53	3	1
1	B	40	ALA	N-CA	6.11	1.53	1.45	1	2
1	A	18	LYS	CA-C	6.11	1.60	1.52	2	1
1	B	55	PRO	CA-C	6.10	1.61	1.52	6	1
1	B	35	HIS	CA-C	6.08	1.58	1.52	2	2
1	A	36	CYS	CA-C	6.05	1.60	1.52	2	3
1	A	24	ARG	CD-NE	6.04	1.54	1.46	6	1
1	A	75	LYS	N-CA	6.03	1.53	1.46	3	4
1	B	19	LYS	C-N	-6.03	1.26	1.33	1	2
1	B	38	ARG	CA-C	6.03	1.60	1.52	7	3
1	A	57	GLN	CA-CB	-6.00	1.43	1.53	4	1
1	B	17	ASN	N-CA	6.00	1.53	1.46	2	2
1	A	60	VAL	CA-CB	-5.99	1.46	1.54	1	3
1	A	57	GLN	N-CA	5.99	1.53	1.46	4	1
1	B	24	ARG	CA-CB	5.98	1.63	1.53	3	2
1	B	14	ARG	N-CA	5.97	1.53	1.46	2	3
1	A	30	ARG	CD-NE	5.94	1.54	1.46	5	1
1	B	27	SER	CA-CB	5.94	1.62	1.53	6	1
1	B	15	PHE	N-CA	5.93	1.53	1.46	6	4
1	B	39	GLU	CA-C	5.93	1.60	1.52	5	1
1	B	35	HIS	N-CA	5.92	1.53	1.46	1	2
1	A	66	HIS	CD2-NE2	-5.91	1.31	1.37	3	7
1	B	31	THR	N-CA	5.91	1.53	1.45	4	2
1	B	36	CYS	N-CA	5.90	1.53	1.45	3	2
1	B	20	ILE	N-CA	5.85	1.53	1.46	2	1
1	A	52	CYS	N-CA	5.83	1.55	1.46	4	2
1	A	11	CYS	CA-CB	5.82	1.63	1.53	6	2
1	A	34	SER	CA-CB	-5.81	1.43	1.53	7	1
1	A	17	ASN	N-CA	5.80	1.53	1.46	3	1
1	A	59	TRP	CG-CD2	-5.80	1.33	1.43	5	1
1	A	15	PHE	N-CA	5.80	1.53	1.46	1	2
1	A	53	ALA	CA-C	5.80	1.59	1.52	1	2
1	A	31	THR	C-N	-5.79	1.25	1.33	5	1
1	A	24	ARG	CA-CB	5.79	1.63	1.53	3	1
1	A	20	ILE	N-CA	5.78	1.53	1.46	7	3
1	A	26	GLU	CA-CB	-5.76	1.44	1.53	1	1
1	A	37	PRO	N-CA	5.76	1.54	1.47	5	1
1	A	35	HIS	N-CA	5.75	1.54	1.46	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	24	ARG	CD-NE	5.75	1.54	1.46	1	3
1	A	69	LYS	CA-C	5.75	1.60	1.52	2	1
1	A	70	LYS	N-CA	5.74	1.53	1.46	5	2
1	A	58	LYS	C-N	-5.74	1.26	1.34	2	1
1	B	53	ALA	CA-CB	5.73	1.61	1.53	1	1
1	A	14	ARG	CA-C	5.70	1.60	1.52	4	1
1	B	17	ASN	CA-C	5.70	1.60	1.52	7	3
1	B	25	LEU	CA-CB	5.68	1.64	1.53	3	1
1	A	49	LYS	N-CA	5.66	1.53	1.45	7	2
1	A	50	GLU	CA-C	5.65	1.59	1.52	6	2
1	A	65	LYS	CA-CB	5.65	1.61	1.53	4	1
1	A	14	ARG	N-CA	5.64	1.53	1.46	2	2
1	B	39	GLU	N-CA	5.62	1.53	1.46	5	2
1	A	22	LYS	CA-C	5.60	1.57	1.52	2	2
1	A	55	PRO	N-CA	5.60	1.54	1.47	2	1
1	A	71	THR	CA-C	5.59	1.60	1.52	5	1
1	B	42	ILE	CA-C	5.59	1.59	1.52	6	1
1	B	57	GLN	C-N	-5.54	1.25	1.33	6	1
1	A	23	GLN	N-CA	5.53	1.53	1.46	4	3
1	B	70	LYS	CG-CD	5.52	1.69	1.52	7	1
1	B	13	TYR	N-CA	5.52	1.53	1.46	2	1
1	B	21	PRO	CA-C	5.49	1.58	1.53	3	1
1	B	47	LEU	N-CA	5.47	1.53	1.46	1	1
1	B	18	LYS	CA-C	5.47	1.59	1.52	7	1
1	B	23	GLN	N-CA	5.45	1.53	1.46	7	2
1	B	16	ILE	CA-C	5.44	1.59	1.52	2	2
1	B	46	LYS	CA-C	5.39	1.59	1.52	1	3
1	A	13	TYR	N-CA	5.38	1.53	1.46	4	3
1	A	18	LYS	N-CA	5.37	1.52	1.46	3	1
1	A	29	ARG	CD-NE	5.36	1.53	1.46	5	2
1	A	39	GLU	CA-C	5.36	1.59	1.52	4	1
1	A	30	ARG	C-N	-5.35	1.26	1.33	5	1
1	A	75	LYS	CA-CB	5.35	1.62	1.53	6	1
1	A	57	GLN	C-N	-5.32	1.26	1.33	3	1
1	A	16	ILE	CA-C	5.28	1.59	1.52	5	1
1	A	32	THR	N-CA	5.27	1.52	1.46	1	3
1	A	25	LEU	N-CA	5.26	1.52	1.46	1	1
1	B	56	THR	CA-CB	5.26	1.62	1.53	3	1
1	A	38	ARG	CD-NE	5.26	1.53	1.46	4	2
1	B	29	ARG	CD-NE	5.26	1.53	1.46	4	1
1	A	37	PRO	CA-C	5.25	1.59	1.52	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	20	ILE	CA-CB	5.25	1.60	1.54	3	1
1	A	49	LYS	CA-C	5.23	1.58	1.52	6	2
1	B	41	VAL	N-CA	5.22	1.51	1.46	6	1
1	A	19	LYS	N-CA	5.22	1.52	1.46	4	1
1	A	73	THR	CA-C	5.22	1.58	1.53	1	1
1	B	38	ARG	CD-NE	5.21	1.53	1.46	2	2
1	A	28	TYR	C-N	-5.21	1.27	1.33	5	1
1	A	65	LYS	CA-C	5.19	1.59	1.53	2	1
1	A	42	ILE	C-N	-5.17	1.26	1.33	4	1
1	A	39	GLU	CA-CB	-5.13	1.46	1.52	3	1
1	B	20	ILE	CA-CB	5.13	1.60	1.54	2	1
1	B	14	ARG	CD-NE	5.11	1.53	1.46	1	1
1	A	15	PHE	CA-CB	5.11	1.61	1.53	7	1
1	B	13	TYR	CA-CB	5.09	1.62	1.53	7	1
1	B	30	ARG	CA-CB	5.07	1.62	1.53	6	1
1	B	62	ASP	CA-CB	5.04	1.61	1.53	7	1
1	A	16	ILE	N-CA	5.04	1.52	1.46	5	1
1	A	34	SER	CA-C	5.02	1.59	1.52	2	1
1	B	61	GLN	N-CA	5.02	1.52	1.46	7	1
1	B	45	THR	CA-C	5.01	1.58	1.52	3	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	B	28	TYR	CG-CD2-CE2	-61.56	28.86	121.20	7	1
1	B	57	GLN	OE1-CD-NE2	-58.97	63.63	122.60	3	5
1	A	15	PHE	CG-CD1-CE1	-54.22	28.53	120.70	7	1
1	A	15	PHE	CD1-CE1-CZ	-48.92	31.95	120.00	7	1
1	B	24	ARG	NE-CZ-NH2	-47.79	76.19	119.20	1	3
1	B	28	TYR	CZ-CE2-CD2	-47.44	34.20	119.60	7	1
1	A	29	ARG	NE-CZ-NH1	-43.92	77.58	121.50	5	4
1	A	30	ARG	NH1-CZ-NH2	-43.16	63.19	119.30	5	5
1	A	30	ARG	NE-CZ-NH1	-42.44	79.06	121.50	5	5
1	A	61	GLN	OE1-CD-NE2	39.42	162.02	122.60	6	3
1	B	61	GLN	OE1-CD-NE2	38.01	160.61	122.60	4	4
1	A	29	ARG	NH1-CZ-NH2	-37.92	70.01	119.30	5	3
1	B	61	GLN	CG-CD-NE2	-36.95	60.98	116.40	4	3
1	B	62	ASP	CA-CB-CG	34.75	147.35	112.60	7	7
1	B	28	TYR	CD1-CG-CD2	-33.30	68.16	118.10	7	1
1	B	24	ARG	NH1-CZ-NH2	-32.74	76.74	119.30	1	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	15	PHE	CD1-CG-CD2	-32.49	69.87	118.60	7	1
1	A	29	ARG	NE-CZ-NH2	31.51	147.56	119.20	5	4
1	B	24	ARG	NE-CZ-NH1	31.43	152.93	121.50	1	6
1	A	15	PHE	CE1-CZ-CE2	-29.32	67.23	120.00	7	1
1	B	28	TYR	CE1-CZ-CE2	-28.12	64.07	120.30	7	1
1	A	62	ASP	CA-CB-CG	28.05	140.65	112.60	3	6
1	B	57	GLN	N-CA-C	27.93	148.84	109.18	3	6
1	B	28	TYR	CG-CD1-CE1	-27.72	79.62	121.20	7	1
1	A	75	LYS	N-CA-C	26.73	148.17	109.69	2	5
1	B	57	GLN	CG-CD-NE2	26.42	156.04	116.40	3	4
1	B	53	ALA	N-CA-C	26.02	146.31	114.04	3	7
1	A	30	ARG	NE-CZ-NH2	25.60	142.24	119.20	5	3
1	A	16	ILE	N-CA-C	25.43	138.45	113.53	2	3
1	B	68	ASP	CA-CB-CG	25.39	137.99	112.60	2	3
1	B	45	THR	N-CA-C	25.34	147.93	109.41	3	6
1	B	43	PHE	CA-CB-CG	24.71	138.51	113.80	6	7
1	A	41	VAL	N-CA-C	24.65	148.65	107.24	2	6
1	A	15	PHE	CG-CD2-CE2	-24.12	79.69	120.70	7	1
1	A	61	GLN	CG-CD-NE2	-23.76	80.76	116.40	6	2
1	B	48	ASP	OD1-CG-OD2	-23.32	66.94	122.90	4	2
1	A	35	HIS	N-CA-C	23.16	143.04	109.69	6	3
1	A	74	PRO	N-CA-CB	-22.53	79.60	103.25	3	4
1	A	43	PHE	CA-CB-CG	22.33	136.13	113.80	3	7
1	A	33	SER	N-CA-C	22.25	139.74	112.59	5	2
1	A	50	GLU	N-CA-C	22.03	151.01	107.62	7	3
1	A	53	ALA	N-CA-C	21.94	136.76	110.44	3	5
1	A	57	GLN	OE1-CD-NE2	-21.84	100.77	122.60	4	4
1	A	53	ALA	N-CA-CB	-21.36	78.61	110.87	4	7
1	B	11	CYS	N-CA-C	21.34	136.29	108.34	3	4
1	B	23	GLN	N-CA-C	21.17	138.39	108.54	2	6
1	B	28	TYR	CB-CG-CD2	21.09	152.43	120.80	7	3
1	B	60	VAL	N-CA-C	-20.99	91.93	111.45	5	5
1	B	57	GLN	CA-C-O	20.88	145.71	121.49	3	7
1	A	15	PHE	CZ-CE2-CD2	-20.70	82.74	120.00	7	1
1	A	17	ASN	CA-CB-CG	20.28	132.88	112.60	1	5
1	A	45	THR	N-CA-C	20.14	140.63	109.81	4	4
1	A	40	ALA	N-CA-C	20.13	142.86	109.24	6	3
1	A	61	GLN	CG-CD-OE1	-19.77	81.27	120.80	6	2
1	A	33	SER	O-C-N	-19.65	98.09	122.26	5	1
1	B	26	GLU	N-CA-C	19.63	139.02	112.13	1	5
1	B	28	TYR	CD1-CE1-CZ	-19.17	85.09	119.60	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	54	ASP	CA-CB-CG	19.12	131.72	112.60	1	4
1	B	12	CYS	N-CA-C	18.96	151.18	110.80	4	3
1	A	17	ASN	N-CA-C	18.90	151.06	110.80	1	5
1	A	38	ARG	NE-CZ-NH2	18.76	136.08	119.20	1	5
1	A	55	PRO	N-CA-CB	-18.70	83.62	103.25	2	4
1	A	33	SER	CA-C-N	18.65	155.26	121.70	5	5
1	A	33	SER	C-N-CA	18.65	155.26	121.70	5	5
1	B	69	LYS	N-CA-C	18.28	134.58	109.54	2	3
1	A	61	GLN	CB-CG-CD	18.27	143.66	112.60	6	6
1	B	35	HIS	N-CA-C	18.03	136.05	113.88	3	6
1	A	39	GLU	N-CA-C	17.92	137.92	110.14	1	4
1	B	22	LYS	N-CA-C	17.83	136.02	113.55	5	3
1	A	26	GLU	CA-C-N	17.75	155.43	121.54	2	1
1	A	26	GLU	C-N-CA	17.75	155.43	121.54	2	1
1	A	66	HIS	CA-CB-CG	-17.67	96.13	113.80	6	4
1	B	57	GLN	N-CA-CB	-17.64	83.13	110.65	1	5
1	A	29	ARG	N-CA-C	17.57	135.91	108.67	6	2
1	A	17	ASN	OD1-CG-ND2	-17.51	105.09	122.60	6	7
1	A	15	PHE	CA-CB-CG	17.50	131.30	113.80	5	4
1	B	25	LEU	N-CA-CB	-17.42	80.88	110.50	3	5
1	A	31	THR	OG1-CB-CG2	-17.35	74.60	109.30	5	6
1	A	54	ASP	N-CA-C	17.34	148.13	109.81	4	4
1	A	52	CYS	N-CA-CB	-17.29	83.59	110.56	6	3
1	A	31	THR	N-CA-C	17.12	147.26	110.80	1	7
1	B	24	ARG	O-C-N	-17.07	105.06	121.79	6	4
1	A	37	PRO	N-CA-C	16.77	147.01	112.47	3	4
1	B	29	ARG	NE-CZ-NH1	-16.73	104.77	121.50	7	5
1	A	24	ARG	NE-CZ-NH1	-16.59	104.91	121.50	1	5
1	B	23	GLN	OE1-CD-NE2	-16.59	106.01	122.60	1	6
1	A	36	CYS	CA-CB-SG	16.50	152.35	114.40	6	4
1	B	38	ARG	NE-CZ-NH1	-16.44	105.06	121.50	5	6
1	A	45	THR	OG1-CB-CG2	-16.44	76.42	109.30	4	6
1	B	32	THR	OG1-CB-CG2	-16.38	76.55	109.30	1	7
1	A	21	PRO	N-CA-CB	-16.37	86.06	103.25	7	2
1	B	31	THR	CA-CB-CG2	-16.18	82.99	110.50	3	3
1	B	70	LYS	N-CA-C	15.99	144.87	110.80	6	6
1	A	23	GLN	OE1-CD-NE2	-15.96	106.64	122.60	7	7
1	A	28	TYR	CA-CB-CG	15.88	142.49	113.90	2	4
1	B	33	SER	N-CA-C	15.88	144.62	110.80	3	5
1	B	48	ASP	CB-CG-OD2	-15.84	81.97	118.40	4	4
1	B	53	ALA	N-CA-CB	-15.83	87.38	110.81	3	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	14	ARG	N-CA-C	15.72	131.01	110.88	6	4
1	B	30	ARG	NE-CZ-NH1	-15.69	105.81	121.50	5	3
1	A	72	GLN	N-CA-C	15.63	144.09	110.80	5	6
1	A	57	GLN	CA-C-O	15.63	140.33	121.11	5	6
1	A	15	PHE	CB-CG-CD1	15.61	147.23	120.70	7	3
1	A	23	GLN	CA-C-N	15.46	151.07	121.54	7	5
1	A	23	GLN	C-N-CA	15.46	151.07	121.54	7	5
1	A	50	GLU	CB-CG-CD	15.42	138.81	112.60	3	5
1	B	44	LYS	N-CA-CB	-15.29	86.38	110.85	5	7
1	A	48	ASP	N-CA-C	15.23	130.38	110.88	7	7
1	A	32	THR	N-CA-C	15.23	143.25	110.80	4	3
1	B	61	GLN	N-CA-CB	-15.22	87.26	109.94	2	2
1	B	15	PHE	N-CA-C	15.07	131.65	109.95	2	7
1	B	39	GLU	N-CA-C	14.98	132.73	109.81	2	3
1	B	39	GLU	CB-CG-CD	14.89	137.91	112.60	5	3
1	B	41	VAL	N-CA-C	14.88	132.91	108.81	2	5
1	A	66	HIS	N-CA-C	-14.75	93.31	112.93	2	3
1	A	38	ARG	NE-CZ-NH1	-14.62	106.89	121.50	3	3
1	B	17	ASN	OD1-CG-ND2	-14.55	108.05	122.60	6	6
1	A	30	ARG	CA-C-O	14.55	136.32	120.32	5	1
1	B	40	ALA	N-CA-C	14.54	130.63	109.69	6	5
1	A	15	PHE	N-CA-C	14.51	141.70	110.80	3	5
1	B	53	ALA	CA-C-O	-14.44	101.01	119.06	3	4
1	A	13	TYR	N-CA-C	-14.43	95.25	113.43	7	5
1	B	11	CYS	CA-C-N	14.39	149.02	121.54	3	4
1	B	11	CYS	C-N-CA	14.39	149.02	121.54	3	4
1	B	30	ARG	NE-CZ-NH2	14.28	132.05	119.20	4	2
1	A	62	ASP	N-CA-CB	-14.25	89.35	110.01	1	4
1	B	57	GLN	CG-CD-OE1	-14.19	92.42	120.80	3	1
1	B	49	LYS	N-CA-CB	-14.15	88.69	111.62	2	2
1	A	72	GLN	CB-CG-CD	14.10	136.58	112.60	5	1
1	B	17	ASN	N-CA-C	14.02	140.66	110.80	6	7
1	B	55	PRO	N-CD-CG	-13.91	82.33	103.20	4	6
1	A	48	ASP	N-CA-CB	-13.91	90.92	111.51	7	7
1	B	31	THR	OG1-CB-CG2	-13.90	81.50	109.30	3	6
1	B	47	LEU	N-CA-CB	-13.86	94.42	110.35	6	1
1	B	31	THR	N-CA-C	13.85	131.88	109.72	5	5
1	B	14	ARG	N-CA-CB	-13.82	91.05	111.51	6	7
1	A	30	ARG	CA-CB-CG	13.72	141.54	114.10	7	1
1	A	30	ARG	CA-C-N	13.71	146.37	121.70	4	3
1	A	30	ARG	C-N-CA	13.71	146.37	121.70	4	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	31	THR	CA-C-N	13.69	147.69	121.54	3	5
1	A	31	THR	C-N-CA	13.69	147.69	121.54	3	5
1	A	52	CYS	CB-CA-C	13.57	132.19	109.80	6	1
1	A	55	PRO	CA-C-N	13.53	147.38	121.54	2	2
1	A	55	PRO	C-N-CA	13.53	147.38	121.54	2	2
1	A	72	GLN	OE1-CD-NE2	-13.50	109.10	122.60	5	6
1	B	54	ASP	N-CA-CB	-13.49	86.36	110.37	5	6
1	B	22	LYS	N-CA-CB	-13.46	90.88	110.40	5	6
1	A	24	ARG	NH1-CZ-NH2	13.46	136.80	119.30	1	6
1	A	35	HIS	N-CA-CB	-13.37	90.68	110.87	6	5
1	A	27	SER	N-CA-CB	-13.36	87.91	110.49	2	1
1	A	52	CYS	CA-CB-SG	13.32	145.03	114.40	1	5
1	B	50	GLU	N-CA-C	13.29	136.20	107.49	7	4
1	B	63	PHE	CA-CB-CG	-13.29	100.51	113.80	6	4
1	A	37	PRO	N-CA-CB	-13.27	89.31	103.25	2	5
1	A	39	GLU	CB-CG-CD	13.27	135.15	112.60	2	4
1	B	48	ASP	CB-CG-OD1	13.27	148.91	118.40	4	1
1	B	21	PRO	N-CA-CB	-13.20	89.39	103.25	1	4
1	B	30	ARG	CD-NE-CZ	13.20	142.88	124.40	1	6
1	B	55	PRO	N-CA-CB	-13.20	89.39	103.25	7	3
1	B	45	THR	CA-CB-OG1	13.18	129.38	109.60	5	5
1	B	18	LYS	N-CA-C	13.15	135.18	107.70	1	5
1	A	26	GLU	N-CA-C	-13.14	95.91	112.72	5	2
1	B	67	LEU	N-CA-CB	-13.08	90.82	109.91	1	3
1	A	27	SER	CA-C-O	-13.07	101.81	120.51	2	1
1	A	15	PHE	CB-CG-CD2	13.04	142.88	120.70	7	1
1	B	30	ARG	NH1-CZ-NH2	13.04	136.25	119.30	5	2
1	B	66	HIS	CA-CB-CG	-13.03	100.77	113.80	6	5
1	A	25	LEU	N-CA-C	13.03	128.45	109.69	5	3
1	A	14	ARG	NE-CZ-NH1	-12.98	108.52	121.50	5	4
1	A	47	LEU	N-CA-C	-12.95	94.42	110.61	3	3
1	B	25	LEU	CB-CA-C	12.91	134.63	110.10	3	3
1	B	28	TYR	CA-C-O	12.88	134.48	120.32	5	1
1	A	62	ASP	N-CA-C	-12.87	97.24	111.14	2	4
1	B	28	TYR	CA-CB-CG	12.86	137.04	113.90	2	4
1	B	30	ARG	CB-CG-CD	12.83	140.81	111.30	5	7
1	A	16	ILE	CA-C-O	-12.82	105.77	118.98	2	3
1	A	16	ILE	CA-C-N	12.81	146.02	121.54	5	1
1	A	16	ILE	C-N-CA	12.81	146.02	121.54	5	1
1	B	52	CYS	CA-C-O	-12.81	106.72	121.58	7	1
1	A	73	THR	OG1-CB-CG2	-12.79	83.72	109.30	2	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	ASP	CA-CB-CG	12.73	125.33	112.60	7	3
1	A	46	LYS	CA-C-N	12.71	140.63	121.83	5	5
1	A	46	LYS	C-N-CA	12.71	140.63	121.83	5	5
1	B	14	ARG	NE-CZ-NH2	-12.70	107.77	119.20	5	1
1	A	26	GLU	CA-C-O	12.69	132.70	119.51	2	3
1	A	69	LYS	N-CA-C	12.67	129.51	113.55	5	2
1	B	65	LYS	N-CA-CB	-12.66	93.09	110.56	6	5
1	B	49	LYS	CA-CB-CG	12.65	139.41	114.10	2	1
1	A	62	ASP	CB-CA-C	12.62	130.69	110.88	1	5
1	A	37	PRO	CA-C-N	12.58	145.56	121.54	5	3
1	A	37	PRO	C-N-CA	12.58	145.56	121.54	5	3
1	A	20	ILE	CA-CB-CG1	12.57	131.76	110.40	3	1
1	A	48	ASP	CA-CB-CG	-12.54	100.06	112.60	1	4
1	B	56	THR	OG1-CB-CG2	-12.50	84.30	109.30	3	6
1	A	32	THR	OG1-CB-CG2	-12.45	84.39	109.30	7	5
1	A	60	VAL	N-CA-C	-12.45	99.88	111.45	4	7
1	B	62	ASP	N-CA-C	-12.44	96.23	111.40	2	6
1	B	15	PHE	O-C-N	-12.42	106.07	122.59	5	2
1	A	18	LYS	N-CA-CB	-12.41	89.51	110.49	6	5
1	B	28	TYR	CB-CG-CD1	12.41	139.42	120.80	7	2
1	B	62	ASP	N-CA-CB	-12.41	91.79	109.91	1	3
1	A	40	ALA	N-CA-CB	-12.34	89.63	110.49	7	3
1	B	68	ASP	N-CA-CB	-12.34	89.64	110.49	5	7
1	A	38	ARG	CA-CB-CG	12.33	138.76	114.10	5	2
1	B	32	THR	N-CA-C	12.28	136.96	110.80	2	5
1	A	58	LYS	N-CA-CB	-12.26	89.77	110.49	5	4
1	A	14	ARG	NH1-CZ-NH2	12.25	135.23	119.30	5	4
1	B	19	LYS	N-CA-C	-12.17	90.62	109.85	4	5
1	B	62	ASP	CB-CA-C	12.17	129.70	110.96	1	3
1	A	71	THR	N-CA-C	12.17	136.72	110.80	2	4
1	B	29	ARG	NE-CZ-NH2	-12.15	108.26	119.20	5	4
1	A	41	VAL	CB-CA-C	-12.15	96.27	110.73	2	4
1	A	75	LYS	CA-C-N	12.15	143.57	121.70	2	4
1	A	75	LYS	C-N-CA	12.15	143.57	121.70	2	4
1	B	56	THR	O-C-N	-12.13	106.45	122.59	3	2
1	B	55	PRO	N-CA-C	12.11	137.42	112.47	6	5
1	A	36	CYS	O-C-N	-12.09	107.42	121.32	6	1
1	A	73	THR	N-CA-C	12.08	136.50	109.81	5	5
1	B	49	LYS	N-CA-C	12.06	127.11	109.14	2	3
1	B	34	SER	N-CA-C	12.04	136.44	110.80	1	4
1	A	65	LYS	CA-C-N	12.03	143.25	122.79	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	65	LYS	C-N-CA	12.03	143.25	122.79	2	2
1	A	56	THR	OG1-CB-CG2	-12.01	85.28	109.30	5	7
1	A	18	LYS	N-CA-C	11.98	125.43	108.54	7	7
1	A	71	THR	OG1-CB-CG2	-11.96	85.38	109.30	7	7
1	B	23	GLN	CB-CG-CD	11.95	132.91	112.60	2	3
1	A	14	ARG	CA-C-N	11.93	144.33	121.54	5	4
1	A	14	ARG	C-N-CA	11.93	144.33	121.54	5	4
1	B	28	TYR	CA-C-N	11.87	141.16	123.12	6	3
1	B	28	TYR	C-N-CA	11.87	141.16	123.12	6	3
1	A	38	ARG	N-CA-C	11.84	128.35	113.43	7	4
1	B	50	GLU	CA-C-N	11.83	143.27	121.97	3	1
1	B	50	GLU	C-N-CA	11.83	143.27	121.97	3	1
1	B	44	LYS	CB-CA-C	11.80	130.96	109.37	5	5
1	A	33	SER	CA-C-O	-11.80	106.03	119.95	5	4
1	B	26	GLU	CA-C-N	11.80	144.07	121.54	3	3
1	B	26	GLU	C-N-CA	11.80	144.07	121.54	3	3
1	B	54	ASP	O-C-N	-11.79	111.33	121.35	1	4
1	B	58	LYS	N-CA-CB	-11.78	90.59	110.49	5	5
1	A	48	ASP	CA-C-O	11.74	137.31	120.51	2	6
1	A	68	ASP	CA-CB-CG	-11.74	100.86	112.60	2	2
1	B	52	CYS	CA-CB-SG	11.73	141.39	114.40	6	4
1	B	65	LYS	CG-CD-CE	11.69	138.20	111.30	3	2
1	B	66	HIS	N-CA-CB	-11.68	93.20	110.49	4	4
1	A	75	LYS	N-CA-CB	-11.67	92.45	110.77	6	4
1	A	28	TYR	N-CA-C	-11.66	91.40	109.95	5	6
1	B	62	ASP	CB-CG-OD1	11.64	145.18	118.40	7	2
1	B	28	TYR	OH-CZ-CE2	11.63	154.79	119.90	7	1
1	A	21	PRO	N-CD-CG	-11.58	85.82	103.20	3	5
1	A	68	ASP	N-CA-CB	-11.58	90.92	110.49	2	5
1	B	24	ARG	CA-C-O	-11.58	109.06	121.45	7	3
1	B	61	GLN	CB-CG-CD	11.56	132.25	112.60	1	3
1	B	30	ARG	N-CA-C	-11.54	90.43	109.24	7	3
1	A	31	THR	CA-CB-OG1	-11.49	92.37	109.60	2	3
1	A	70	LYS	N-CA-C	11.48	135.25	110.80	6	6
1	B	47	LEU	N-CA-C	-11.46	96.20	110.65	6	4
1	B	13	TYR	N-CA-C	11.46	125.09	110.65	5	7
1	B	48	ASP	N-CA-C	11.45	135.19	110.80	5	5
1	A	50	GLU	N-CA-CB	-11.40	91.52	110.68	5	5
1	A	74	PRO	N-CA-C	11.40	135.95	112.47	6	4
1	B	61	GLN	CA-C-O	11.38	134.33	121.02	3	7
1	A	31	THR	CA-C-O	11.37	132.82	120.77	5	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	70	LYS	CA-C-N	11.35	143.22	121.54	2	3
1	A	70	LYS	C-N-CA	11.35	143.22	121.54	2	3
1	A	61	GLN	CA-C-O	11.33	133.53	121.07	6	6
1	B	39	GLU	N-CA-CB	-11.32	91.37	110.49	6	2
1	A	23	GLN	N-CA-C	11.31	134.89	110.80	3	5
1	B	38	ARG	CA-C-N	11.25	143.02	121.54	3	3
1	B	38	ARG	C-N-CA	11.25	143.02	121.54	3	3
1	A	29	ARG	CA-CB-CG	11.24	136.58	114.10	5	2
1	B	70	LYS	CA-C-O	-11.23	104.45	120.51	7	2
1	B	60	VAL	CA-CB-CG1	11.21	129.46	110.40	6	3
1	A	64	MET	O-C-N	11.18	134.97	122.11	5	1
1	B	57	GLN	CB-CG-CD	11.17	131.59	112.60	2	4
1	A	30	ARG	CB-CG-CD	11.15	136.95	111.30	4	3
1	A	62	ASP	CB-CG-OD1	11.11	143.96	118.40	6	3
1	B	17	ASN	CA-CB-CG	11.11	123.70	112.60	6	1
1	B	64	MET	CA-C-O	11.09	133.27	121.07	3	2
1	A	74	PRO	N-CD-CG	-11.09	86.57	103.20	5	4
1	A	36	CYS	N-CA-C	11.06	128.40	109.82	4	3
1	B	48	ASP	N-CA-CB	-11.05	91.81	110.49	1	6
1	B	30	ARG	CA-C-O	11.05	132.81	120.43	5	3
1	A	72	GLN	N-CA-CB	-11.02	91.87	110.49	5	5
1	B	50	GLU	N-CA-CB	-11.01	91.07	111.00	5	7
1	A	72	GLN	CA-C-N	11.00	148.64	121.80	3	4
1	A	72	GLN	C-N-CA	11.00	148.64	121.80	3	4
1	A	29	ARG	CD-NE-CZ	10.97	139.75	124.40	4	3
1	A	57	GLN	N-CA-CB	-10.96	91.98	110.49	4	5
1	B	45	THR	N-CA-CB	-10.96	94.01	111.43	3	2
1	B	65	LYS	CA-C-O	10.96	133.06	119.59	6	4
1	B	66	HIS	N-CA-C	-10.93	99.78	113.55	6	2
1	B	49	LYS	CA-C-N	10.92	140.05	123.23	2	3
1	B	49	LYS	C-N-CA	10.92	140.05	123.23	2	3
1	A	15	PHE	CA-C-N	10.92	141.62	121.97	4	2
1	A	15	PHE	C-N-CA	10.92	141.62	121.97	4	2
1	A	54	ASP	N-CA-CB	-10.92	90.93	110.37	5	6
1	A	39	GLU	N-CA-CB	-10.88	94.09	110.85	1	5
1	A	74	PRO	CB-CA-C	10.88	129.51	111.56	3	2
1	B	19	LYS	CG-CD-CE	10.88	136.31	111.30	6	3
1	A	53	ALA	CB-CA-C	10.85	127.61	112.09	5	3
1	A	70	LYS	N-CA-CB	-10.85	92.16	110.49	3	6
1	A	12	CYS	CA-C-O	10.84	139.22	122.20	7	1
1	B	44	LYS	CG-CD-CE	10.84	136.24	111.30	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	19	LYS	N-CA-CB	-10.83	92.19	110.49	1	5
1	A	25	LEU	N-CA-CB	-10.82	94.23	111.43	4	7
1	B	66	HIS	CA-C-N	-10.81	106.35	122.56	5	1
1	B	66	HIS	C-N-CA	-10.81	106.35	122.56	5	1
1	B	66	HIS	CB-CG-CD2	-10.79	117.17	131.20	5	1
1	B	37	PRO	N-CA-CB	-10.75	91.96	103.25	3	6
1	B	62	ASP	OD1-CG-OD2	-10.75	97.09	122.90	4	1
1	B	18	LYS	N-CA-CB	-10.74	93.37	110.87	1	2
1	B	47	LEU	CA-C-N	10.73	142.03	121.54	4	6
1	B	47	LEU	C-N-CA	10.73	142.03	121.54	4	6
1	A	23	GLN	N-CA-CB	-10.69	96.37	110.59	6	5
1	A	30	ARG	N-CA-C	10.67	124.34	109.18	6	4
1	A	31	THR	O-C-N	-10.67	111.10	122.84	5	3
1	B	21	PRO	CA-C-N	10.67	140.87	123.37	3	1
1	B	21	PRO	C-N-CA	10.67	140.87	123.37	3	1
1	B	35	HIS	N-CA-CB	-10.67	96.40	110.59	3	5
1	A	55	PRO	N-CD-CG	-10.65	87.23	103.20	4	3
1	B	14	ARG	NE-CZ-NH1	-10.65	110.85	121.50	1	3
1	A	57	GLN	O-C-N	-10.60	110.12	122.84	5	4
1	A	65	LYS	N-CA-CB	-10.59	92.61	110.41	7	3
1	A	22	LYS	N-CA-C	10.58	126.62	112.13	2	4
1	B	61	GLN	CG-CD-OE1	-10.58	99.64	120.80	4	5
1	B	23	GLN	N-CA-CB	-10.57	91.57	110.60	5	5
1	B	17	ASN	CA-C-O	10.57	135.62	120.51	6	1
1	B	41	VAL	CA-CB-CG2	10.56	128.35	110.40	1	2
1	A	72	GLN	CG-CD-NE2	10.56	132.24	116.40	5	3
1	B	61	GLN	CB-CA-C	10.55	127.69	110.81	2	2
1	B	20	ILE	CA-CB-CG1	10.54	128.31	110.40	2	1
1	B	38	ARG	NH1-CZ-NH2	10.52	132.97	119.30	4	6
1	B	67	LEU	CA-C-N	10.51	141.62	121.54	5	2
1	B	67	LEU	C-N-CA	10.51	141.62	121.54	5	2
1	A	73	THR	CA-CB-CG2	10.51	128.36	110.50	4	2
1	B	16	ILE	N-CA-C	10.50	121.76	106.85	5	5
1	B	67	LEU	CB-CA-C	10.49	127.11	110.96	1	3
1	B	24	ARG	N-CA-CB	-10.47	92.32	111.37	2	2
1	A	57	GLN	CG-CD-NE2	10.45	132.07	116.40	4	3
1	A	11	CYS	CA-CB-SG	10.43	138.39	114.40	6	2
1	A	29	ARG	CA-C-N	10.43	141.46	121.54	4	1
1	A	29	ARG	C-N-CA	10.43	141.46	121.54	4	1
1	A	38	ARG	CA-C-O	-10.37	105.68	120.51	6	1
1	A	17	ASN	N-CA-CB	-10.34	93.01	110.49	1	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	29	ARG	NH1-CZ-NH2	10.34	132.74	119.30	7	4
1	B	56	THR	CB-CA-C	-10.34	91.95	110.35	1	2
1	A	11	CYS	CA-C-O	-10.32	105.75	120.51	6	2
1	A	41	VAL	CA-C-O	10.31	131.22	120.39	4	2
1	A	19	LYS	N-CA-C	10.31	132.76	110.80	2	2
1	A	50	GLU	CA-CB-CG	10.29	134.69	114.10	5	2
1	B	24	ARG	CD-NE-CZ	10.29	138.81	124.40	2	2
1	B	19	LYS	N-CA-CB	-10.28	93.12	110.49	5	5
1	A	22	LYS	N-CA-CB	-10.27	93.13	110.49	3	5
1	A	44	LYS	N-CA-CB	-10.27	94.56	111.20	5	4
1	B	38	ARG	N-CA-CB	-10.27	93.14	110.49	3	1
1	B	63	PHE	CA-C-O	-10.25	109.80	121.07	5	3
1	B	54	ASP	N-CA-C	10.22	132.40	109.81	7	6
1	A	12	CYS	CA-CB-SG	10.22	137.90	114.40	4	2
1	A	16	ILE	N-CA-CB	-10.17	94.44	111.23	1	4
1	A	71	THR	CA-C-N	10.17	140.97	121.54	2	3
1	A	71	THR	C-N-CA	10.17	140.97	121.54	2	3
1	A	14	ARG	N-CA-C	10.16	132.45	110.80	2	3
1	A	26	GLU	CG-CD-OE1	10.15	141.76	118.40	3	2
1	B	59	TRP	CA-C-N	10.14	136.66	121.65	5	2
1	B	59	TRP	C-N-CA	10.14	136.66	121.65	5	2
1	A	69	LYS	N-CA-CB	-10.13	93.38	110.49	1	4
1	B	29	ARG	N-CA-C	10.11	125.92	107.73	6	2
1	A	17	ASN	CA-C-O	10.09	134.94	120.51	2	3
1	A	74	PRO	CA-C-N	10.07	140.78	121.54	3	4
1	A	74	PRO	C-N-CA	10.07	140.78	121.54	3	4
1	A	14	ARG	NE-CZ-NH2	-10.06	110.15	119.20	6	3
1	A	34	SER	CA-C-N	10.06	140.75	121.54	2	3
1	A	34	SER	C-N-CA	10.06	140.75	121.54	2	3
1	A	14	ARG	CG-CD-NE	-10.05	89.89	112.00	3	2
1	B	28	TYR	N-CA-C	-9.99	92.24	108.52	5	4
1	B	45	THR	CA-CB-CG2	9.97	127.46	110.50	3	3
1	B	33	SER	CA-C-O	9.95	134.74	120.51	5	4
1	A	36	CYS	CA-C-N	9.93	132.26	119.84	3	4
1	A	36	CYS	C-N-CA	9.93	132.26	119.84	3	4
1	B	32	THR	CA-CB-OG1	9.91	124.47	109.60	5	2
1	A	63	PHE	CA-C-O	-9.91	110.39	120.80	5	2
1	A	75	LYS	CB-CA-C	9.90	125.97	110.14	6	2
1	B	14	ARG	NH1-CZ-NH2	9.89	132.16	119.30	5	4
1	B	52	CYS	N-CA-C	9.89	125.49	107.99	5	4
1	A	73	THR	CA-CB-OG1	9.89	124.43	109.60	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	34	SER	CA-C-N	9.88	140.41	121.54	1	4
1	B	34	SER	C-N-CA	9.88	140.41	121.54	1	4
1	B	24	ARG	CA-C-N	9.88	139.48	121.70	6	4
1	B	24	ARG	C-N-CA	9.88	139.48	121.70	6	4
1	B	61	GLN	N-CA-C	9.84	122.91	111.11	2	2
1	A	34	SER	N-CA-CB	9.81	127.18	110.50	5	1
1	B	46	LYS	N-CA-CB	-9.81	95.80	110.61	2	4
1	A	51	ILE	CA-C-O	-9.80	108.38	121.32	1	5
1	B	46	LYS	CA-C-N	9.80	136.16	123.03	2	5
1	B	46	LYS	C-N-CA	9.80	136.16	123.03	2	5
1	B	14	ARG	CD-NE-CZ	9.80	138.12	124.40	7	3
1	B	11	CYS	N-CA-CB	-9.79	93.25	110.87	3	4
1	B	48	ASP	CA-C-O	9.77	134.49	120.51	4	6
1	A	64	MET	N-CA-CB	-9.76	94.00	110.49	2	1
1	A	16	ILE	CB-CA-C	9.75	127.29	111.29	6	2
1	A	38	ARG	NH1-CZ-NH2	-9.71	106.68	119.30	1	2
1	A	45	THR	CA-C-O	-9.70	109.37	121.78	2	4
1	B	56	THR	CA-C-N	9.68	136.68	122.16	4	2
1	B	56	THR	C-N-CA	9.68	136.68	122.16	4	2
1	A	55	PRO	CB-CA-C	9.68	127.53	111.56	2	2
1	B	65	LYS	CB-CG-CD	9.68	133.56	111.30	7	1
1	A	53	ALA	CA-C-N	9.67	145.40	121.80	4	2
1	A	53	ALA	C-N-CA	9.67	145.40	121.80	4	2
1	B	64	MET	N-CA-CB	-9.64	95.16	109.82	3	2
1	A	52	CYS	N-CA-C	9.63	126.86	107.41	4	3
1	A	68	ASP	CB-CA-C	9.61	129.54	110.42	2	3
1	A	24	ARG	NE-CZ-NH2	-9.60	110.56	119.20	7	4
1	A	11	CYS	N-CA-CB	-9.60	94.27	110.49	1	3
1	B	56	THR	CA-C-O	9.60	134.23	120.51	5	4
1	A	60	VAL	CA-CB-CG1	9.58	126.68	110.40	2	1
1	A	63	PHE	CA-CB-CG	-9.57	104.22	113.80	2	4
1	A	46	LYS	CB-CG-CD	9.56	133.29	111.30	5	2
1	B	43	PHE	N-CA-C	-9.56	93.81	109.40	5	3
1	A	27	SER	N-CA-C	9.56	131.16	110.80	2	1
1	B	66	HIS	CB-CG-ND1	9.54	137.02	122.70	5	2
1	B	36	CYS	CA-CB-SG	9.54	136.34	114.40	5	5
1	B	68	ASP	CA-C-N	9.48	139.65	121.54	5	2
1	B	68	ASP	C-N-CA	9.48	139.65	121.54	5	2
1	B	22	LYS	CB-CA-C	9.46	126.40	111.73	2	4
1	A	64	MET	CA-C-O	-9.42	110.37	120.92	5	3
1	A	73	THR	N-CA-CB	-9.42	93.60	110.37	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	65	LYS	N-CA-C	9.40	123.85	112.38	3	3
1	B	28	TYR	CB-CA-C	9.40	125.61	110.19	5	1
1	B	11	CYS	CA-CB-SG	9.40	136.01	114.40	6	1
1	A	75	LYS	CG-CD-CE	9.39	132.89	111.30	4	1
1	A	57	GLN	N-CA-C	9.38	121.70	110.44	3	4
1	A	51	ILE	CA-C-N	9.37	135.34	122.79	1	2
1	A	51	ILE	C-N-CA	9.37	135.34	122.79	1	2
1	B	70	LYS	CB-CG-CD	9.36	132.82	111.30	5	3
1	A	19	LYS	CG-CD-CE	9.35	132.81	111.30	7	4
1	B	26	GLU	N-CA-CB	-9.34	95.87	110.44	3	2
1	A	62	ASP	OD1-CG-OD2	-9.34	100.48	122.90	5	5
1	B	16	ILE	N-CA-CB	-9.34	95.82	111.23	4	7
1	B	41	VAL	CB-CA-C	-9.33	96.72	110.62	1	2
1	B	68	ASP	CB-CA-C	9.33	128.99	110.42	5	5
1	A	31	THR	N-CA-CB	-9.33	95.64	111.50	4	1
1	A	56	THR	N-CA-C	9.32	130.66	110.80	2	3
1	B	17	ASN	CA-C-N	9.31	139.32	121.54	3	4
1	B	17	ASN	C-N-CA	9.31	139.32	121.54	3	4
1	A	33	SER	CA-CB-OG	-9.31	92.48	111.10	1	4
1	B	21	PRO	CA-N-CD	-9.31	98.97	112.00	4	1
1	B	35	HIS	CA-CB-CG	-9.25	104.55	113.80	4	3
1	A	67	LEU	N-CA-CB	-9.24	96.49	110.26	4	6
1	B	48	ASP	CA-CB-CG	-9.24	103.36	112.60	2	3
1	B	26	GLU	CG-CD-OE1	9.21	139.59	118.40	3	1
1	A	50	GLU	CA-C-O	9.21	131.20	120.70	7	1
1	B	15	PHE	CA-CB-CG	-9.19	104.61	113.80	6	3
1	B	58	LYS	N-CA-C	-9.19	100.22	111.33	2	1
1	A	46	LYS	CA-CB-CG	9.18	132.47	114.10	5	2
1	A	26	GLU	CB-CG-CD	9.17	128.19	112.60	7	3
1	A	72	GLN	CA-CB-CG	9.16	132.42	114.10	2	2
1	B	17	ASN	CB-CG-ND2	9.16	130.14	116.40	6	5
1	B	13	TYR	N-CA-CB	-9.16	95.01	110.49	4	5
1	B	65	LYS	N-CA-C	9.14	130.28	110.80	5	2
1	A	14	ARG	CA-CB-CG	9.12	132.34	114.10	3	1
1	A	59	TRP	CB-CG-CD2	-9.11	114.05	126.80	6	4
1	A	71	THR	O-C-N	-9.10	110.49	122.59	5	4
1	B	26	GLU	CB-CA-C	9.07	127.97	109.55	3	1
1	B	49	LYS	CB-CA-C	-9.06	92.79	109.37	5	2
1	A	46	LYS	CG-CD-CE	9.04	132.09	111.30	5	2
1	A	18	LYS	CG-CD-CE	9.03	132.07	111.30	7	2
1	A	38	ARG	CG-CD-NE	-9.00	92.20	112.00	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	48	ASP	O-C-N	-9.00	109.68	121.83	7	1
1	B	21	PRO	N-CD-CG	-8.99	89.72	103.20	3	3
1	A	32	THR	CA-C-N	8.98	138.69	121.54	6	6
1	A	32	THR	C-N-CA	8.98	138.69	121.54	6	6
1	B	26	GLU	CB-CG-CD	8.96	127.84	112.60	3	3
1	B	20	ILE	N-CA-C	8.95	128.22	108.88	6	3
1	A	41	VAL	N-CA-CB	8.95	123.17	111.90	1	1
1	B	19	LYS	CB-CG-CD	8.94	131.87	111.30	4	4
1	B	16	ILE	O-C-N	-8.92	114.39	122.69	7	4
1	B	59	TRP	O-C-N	8.92	132.36	122.20	7	1
1	A	49	LYS	CA-C-N	8.89	135.53	122.99	5	1
1	A	49	LYS	C-N-CA	8.89	135.53	122.99	5	1
1	A	65	LYS	CA-C-O	8.89	130.35	119.78	4	4
1	B	25	LEU	N-CA-C	-8.87	86.15	111.00	3	3
1	B	24	ARG	N-CA-C	8.87	129.69	110.80	5	5
1	B	29	ARG	CA-C-O	-8.86	110.59	121.58	6	1
1	B	45	THR	CA-C-N	8.84	138.42	121.54	4	6
1	B	45	THR	C-N-CA	8.84	138.42	121.54	4	6
1	B	21	PRO	CB-CA-C	8.84	126.14	111.56	4	3
1	B	36	CYS	CA-C-N	8.83	130.88	119.84	6	3
1	B	36	CYS	C-N-CA	8.83	130.88	119.84	6	3
1	B	36	CYS	N-CA-CB	-8.82	94.67	110.37	5	2
1	A	40	ALA	CB-CA-C	8.81	127.95	110.42	7	1
1	B	62	ASP	CB-CG-OD2	8.81	138.66	118.40	4	3
1	B	45	THR	OG1-CB-CG2	-8.81	91.69	109.30	4	4
1	A	26	GLU	N-CA-CB	-8.79	94.53	110.27	4	4
1	A	12	CYS	N-CA-CB	-8.79	96.76	111.17	5	1
1	B	51	ILE	N-CA-C	8.78	122.58	108.97	4	3
1	A	28	TYR	CA-C-N	8.76	135.04	121.99	6	4
1	A	28	TYR	C-N-CA	8.76	135.04	121.99	6	4
1	B	35	HIS	CB-CG-ND1	8.76	135.83	122.70	6	1
1	A	68	ASP	CA-C-N	8.75	138.25	121.54	1	2
1	A	68	ASP	C-N-CA	8.75	138.25	121.54	1	2
1	A	21	PRO	CA-C-N	8.74	138.23	121.54	7	1
1	A	21	PRO	C-N-CA	8.74	138.23	121.54	7	1
1	B	70	LYS	N-CA-CB	-8.73	95.73	110.49	4	4
1	B	38	ARG	CG-CD-NE	-8.73	92.80	112.00	5	4
1	B	28	TYR	N-CA-CB	-8.73	96.85	110.55	5	2
1	B	40	ALA	N-CA-CB	-8.72	97.70	110.87	6	5
1	A	55	PRO	N-CA-C	-8.70	94.54	112.47	7	6
1	B	38	ARG	NE-CZ-NH2	8.70	127.03	119.20	5	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	55	PRO	CA-C-O	8.69	136.41	120.60	2	1
1	A	34	SER	CB-CA-C	-8.68	93.61	110.10	5	1
1	B	41	VAL	O-C-N	8.66	132.87	123.00	3	1
1	A	43	PHE	N-CA-C	-8.66	97.28	110.70	7	2
1	A	47	LEU	CA-C-N	8.62	139.42	123.13	7	5
1	A	47	LEU	C-N-CA	8.62	139.42	123.13	7	5
1	A	69	LYS	CA-C-N	8.61	136.75	123.23	1	2
1	A	69	LYS	C-N-CA	8.61	136.75	123.23	1	2
1	B	24	ARG	CB-CA-C	8.61	127.37	109.38	2	2
1	B	66	HIS	CB-CA-C	8.59	126.35	110.11	3	4
1	B	27	SER	N-CA-CB	-8.58	95.99	110.49	3	1
1	B	18	LYS	CA-C-O	8.57	131.65	121.11	4	2
1	B	23	GLN	CG-CD-OE1	8.54	137.89	120.80	1	1
1	B	44	LYS	N-CA-C	8.54	123.39	110.14	6	2
1	A	40	ALA	CA-C-O	-8.55	110.83	120.66	6	3
1	B	20	ILE	CA-C-N	8.54	130.51	119.84	4	3
1	B	20	ILE	C-N-CA	8.54	130.51	119.84	4	3
1	A	68	ASP	OD1-CG-OD2	-8.54	102.41	122.90	7	1
1	B	53	ALA	O-C-N	8.53	132.49	122.25	3	2
1	B	44	LYS	CA-C-O	8.51	129.34	120.40	1	2
1	A	31	THR	CA-CB-CG2	8.51	124.96	110.50	5	3
1	A	69	LYS	CA-C-O	8.50	132.66	120.51	1	3
1	B	31	THR	CA-C-O	-8.49	111.51	121.11	5	2
1	B	30	ARG	CA-C-N	8.49	137.75	121.54	7	3
1	B	30	ARG	C-N-CA	8.49	137.75	121.54	7	3
1	B	59	TRP	CG-CD1-NE1	-8.49	99.17	110.20	7	6
1	A	51	ILE	N-CA-C	8.48	121.78	108.89	2	3
1	A	37	PRO	N-CD-CG	-8.47	90.49	103.20	1	5
1	A	14	ARG	CD-NE-CZ	8.47	136.26	124.40	2	3
1	A	37	PRO	CB-CA-C	8.45	125.51	111.56	2	2
1	B	52	CYS	N-CA-CB	-8.45	96.49	110.68	6	3
1	A	50	GLU	CB-CA-C	8.45	123.38	110.62	2	2
1	A	30	ARG	CD-NE-CZ	8.44	136.22	124.40	2	2
1	B	36	CYS	N-CA-C	8.42	128.42	109.81	7	3
1	B	17	ASN	N-CA-CB	-8.41	96.28	110.49	4	5
1	B	61	GLN	CA-CB-CG	-8.41	97.28	114.10	3	3
1	B	70	LYS	CA-CB-CG	8.41	130.91	114.10	7	3
1	A	20	ILE	N-CA-C	8.40	127.03	108.88	5	7
1	A	21	PRO	N-CA-C	8.40	129.77	112.47	7	3
1	A	16	ILE	CA-CB-CG1	8.38	124.65	110.40	3	1
1	A	32	THR	CA-CB-OG1	-8.38	97.03	109.60	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	64	MET	CB-CA-C	8.36	127.06	110.42	2	1
1	A	58	LYS	CG-CD-CE	8.35	130.49	111.30	1	3
1	A	15	PHE	O-C-N	8.33	133.67	122.59	6	2
1	B	64	MET	O-C-N	-8.32	113.18	122.08	3	4
1	B	26	GLU	CA-CB-CG	8.32	130.73	114.10	5	4
1	A	41	VAL	CA-CB-CG2	-8.31	96.27	110.40	4	3
1	B	70	LYS	O-C-N	-8.28	111.57	122.59	5	3
1	A	40	ALA	CA-C-N	8.28	136.87	121.97	7	1
1	A	40	ALA	C-N-CA	8.28	136.87	121.97	7	1
1	A	75	LYS	CA-C-O	-8.27	111.48	120.24	6	3
1	B	50	GLU	CB-CA-C	8.26	125.22	111.51	4	3
1	B	23	GLN	CA-C-N	8.24	137.28	121.54	3	1
1	B	23	GLN	C-N-CA	8.24	137.28	121.54	3	1
1	B	14	ARG	CG-CD-NE	-8.23	93.89	112.00	6	4
1	A	44	LYS	CA-CB-CG	8.23	130.56	114.10	5	2
1	A	59	TRP	O-C-N	8.23	131.58	122.20	2	1
1	B	31	THR	CA-C-N	8.19	137.18	121.54	3	1
1	B	31	THR	C-N-CA	8.19	137.18	121.54	3	1
1	B	56	THR	N-CA-C	8.19	128.24	110.80	5	2
1	A	38	ARG	CA-C-N	-8.19	109.06	122.65	7	2
1	A	38	ARG	C-N-CA	-8.19	109.06	122.65	7	2
1	A	23	GLN	O-C-N	8.17	133.46	122.59	7	1
1	A	38	ARG	O-C-N	-8.16	111.86	122.72	3	2
1	A	28	TYR	CB-CG-CD1	8.16	133.04	120.80	5	1
1	B	32	THR	CB-CA-C	-8.13	98.49	111.18	5	2
1	B	54	ASP	CB-CA-C	8.11	126.15	110.17	5	3
1	A	11	CYS	O-C-N	-8.11	111.81	122.59	7	3
1	A	18	LYS	CA-C-N	8.10	137.01	121.54	4	2
1	A	18	LYS	C-N-CA	8.10	137.01	121.54	4	2
1	B	33	SER	CA-C-N	8.10	137.00	121.54	1	4
1	B	33	SER	C-N-CA	8.10	137.00	121.54	1	4
1	B	13	TYR	CA-C-O	8.09	132.08	120.51	4	3
1	A	65	LYS	CB-CA-C	8.09	126.05	109.95	7	1
1	A	71	THR	CA-C-O	8.09	132.08	120.51	5	1
1	B	41	VAL	CG1-CB-CG2	-8.08	93.03	110.80	7	3
1	B	37	PRO	CA-C-N	8.08	136.97	121.54	5	3
1	B	37	PRO	C-N-CA	8.08	136.97	121.54	5	3
1	B	56	THR	CA-CB-CG2	8.06	124.21	110.50	3	1
1	A	45	THR	CA-CB-OG1	-8.06	97.50	109.60	6	2
1	A	21	PRO	CB-CA-C	8.04	124.83	111.56	1	2
1	B	15	PHE	N-CA-CB	-8.04	96.90	110.49	7	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	12	CYS	CA-C-N	8.04	136.90	121.54	4	2
1	B	12	CYS	C-N-CA	8.04	136.90	121.54	4	2
1	A	67	LEU	CB-CA-C	8.03	122.81	109.56	1	3
1	B	19	LYS	CA-C-N	8.03	136.98	122.13	4	3
1	B	19	LYS	C-N-CA	8.03	136.98	122.13	4	3
1	B	51	ILE	CA-C-O	-8.00	111.32	121.48	4	3
1	B	66	HIS	O-C-N	7.99	134.03	122.28	5	2
1	A	17	ASN	CB-CG-ND2	7.99	128.38	116.40	6	3
1	B	47	LEU	CB-CA-C	7.96	122.65	111.74	6	1
1	B	45	THR	CB-CA-C	-7.96	96.94	110.16	4	1
1	A	48	ASP	CA-C-N	7.95	136.73	121.54	1	2
1	A	48	ASP	C-N-CA	7.95	136.73	121.54	1	2
1	B	53	ALA	CA-C-N	7.93	141.14	121.80	4	2
1	B	53	ALA	C-N-CA	7.93	141.14	121.80	4	2
1	A	46	LYS	N-CA-CB	-7.92	97.10	110.49	6	3
1	A	46	LYS	N-CA-C	7.92	121.52	112.57	3	2
1	B	64	MET	CB-CA-C	7.92	123.51	110.92	3	1
1	A	35	HIS	CA-C-N	7.91	141.10	121.80	6	3
1	A	35	HIS	C-N-CA	7.91	141.10	121.80	6	3
1	A	58	LYS	CB-CA-C	7.90	126.14	110.42	6	3
1	A	54	ASP	CB-CA-C	7.89	125.71	110.17	5	2
1	B	46	LYS	CG-CD-CE	7.87	129.40	111.30	1	2
1	A	29	ARG	CA-C-O	-7.86	111.72	120.60	6	2
1	A	46	LYS	CA-C-O	7.84	130.26	120.15	3	4
1	A	32	THR	CB-CA-C	-7.82	94.85	110.42	4	2
1	B	58	LYS	CB-CA-C	7.82	125.98	110.42	5	3
1	A	24	ARG	N-CA-C	-7.81	94.17	110.80	5	3
1	B	12	CYS	N-CA-CB	-7.80	97.30	110.49	2	3
1	B	33	SER	CA-CB-OG	-7.80	95.50	111.10	7	2
1	B	12	CYS	CB-CA-C	-7.79	94.91	110.42	3	1
1	A	49	LYS	N-CA-C	-7.79	97.26	109.72	6	2
1	A	30	ARG	N-CA-CB	-7.78	98.40	110.46	2	2
1	B	32	THR	CA-C-O	7.77	131.62	120.51	3	2
1	A	18	LYS	CB-CG-CD	7.77	129.17	111.30	5	2
1	B	64	MET	N-CA-C	-7.77	101.54	111.02	2	2
1	A	56	THR	CA-C-N	7.76	136.36	121.54	2	2
1	A	56	THR	C-N-CA	7.76	136.36	121.54	2	2
1	B	58	LYS	CB-CG-CD	-7.75	93.47	111.30	5	2
1	A	25	LEU	CB-CA-C	7.75	125.64	110.30	4	2
1	A	61	GLN	CA-CB-CG	-7.74	98.61	114.10	3	3
1	A	29	ARG	CB-CG-CD	7.73	129.09	111.30	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	34	SER	CA-CB-OG	-7.73	95.65	111.10	5	2
1	A	62	ASP	CA-C-O	-7.72	112.74	120.70	2	4
1	B	54	ASP	CA-C-O	-7.70	109.61	120.16	4	2
1	A	66	HIS	N-CA-CB	7.69	121.55	110.40	4	3
1	A	24	ARG	CA-C-O	7.68	131.49	120.51	4	2
1	A	70	LYS	O-C-N	-7.68	112.38	122.59	5	3
1	B	44	LYS	CA-CB-CG	7.68	129.45	114.10	5	1
1	A	44	LYS	CG-CD-CE	7.66	128.91	111.30	1	2
1	B	39	GLU	CA-C-N	7.65	137.93	123.09	5	2
1	B	39	GLU	C-N-CA	7.65	137.93	123.09	5	2
1	B	57	GLN	CA-CB-CG	-7.65	98.81	114.10	7	3
1	B	38	ARG	CD-NE-CZ	7.64	135.10	124.40	2	1
1	B	41	VAL	CA-CB-CG1	7.64	123.39	110.40	5	2
1	A	24	ARG	CG-CD-NE	-7.64	95.20	112.00	2	2
1	B	57	GLN	O-C-N	-7.63	113.49	122.87	7	4
1	A	41	VAL	CA-CB-CG1	7.63	123.36	110.40	5	2
1	A	32	THR	CA-C-O	7.62	131.41	120.51	6	3
1	B	22	LYS	CA-C-N	7.61	136.07	121.54	6	2
1	B	22	LYS	C-N-CA	7.61	136.07	121.54	6	2
1	A	13	TYR	CA-C-N	7.60	134.52	122.21	1	3
1	A	13	TYR	C-N-CA	7.60	134.52	122.21	1	3
1	A	18	LYS	CB-CA-C	7.59	125.53	110.42	6	3
1	A	50	GLU	CG-CD-OE1	7.59	135.86	118.40	4	2
1	A	56	THR	N-CA-CB	7.59	123.31	110.49	1	1
1	A	34	SER	CA-CB-OG	-7.58	95.94	111.10	7	5
1	B	53	ALA	CB-CA-C	7.56	127.53	110.67	6	2
1	A	23	GLN	CA-C-O	7.53	127.75	119.24	6	2
1	B	63	PHE	CA-C-N	-7.53	110.33	120.79	5	1
1	B	63	PHE	C-N-CA	-7.53	110.33	120.79	5	1
1	B	35	HIS	CB-CG-CD2	-7.51	121.43	131.20	6	1
1	B	39	GLU	CA-CB-CG	-7.51	99.08	114.10	1	2
1	B	18	LYS	CB-CG-CD	7.50	128.54	111.30	2	1
1	B	46	LYS	CB-CG-CD	7.49	128.53	111.30	7	1
1	B	29	ARG	CG-CD-NE	-7.49	95.52	112.00	4	1
1	A	19	LYS	CA-CB-CG	7.49	129.08	114.10	4	3
1	A	59	TRP	CG-CD1-NE1	-7.47	100.48	110.20	6	7
1	B	54	ASP	CA-C-N	7.47	129.18	119.84	5	2
1	B	54	ASP	C-N-CA	7.47	129.18	119.84	5	2
1	B	49	LYS	CG-CD-CE	7.46	128.46	111.30	7	1
1	B	12	CYS	CA-CB-SG	7.44	131.52	114.40	3	3
1	A	75	LYS	O-C-N	-7.44	112.69	122.59	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	58	LYS	CG-CD-CE	7.43	128.40	111.30	1	3
1	A	44	LYS	O-C-N	7.42	131.97	123.06	7	2
1	B	42	ILE	CA-C-N	7.42	133.24	123.00	3	3
1	B	42	ILE	C-N-CA	7.42	133.24	123.00	3	3
1	A	45	THR	CB-CA-C	-7.42	96.14	109.71	1	3
1	B	20	ILE	N-CA-CB	-7.41	100.84	111.21	4	3
1	A	19	LYS	CB-CG-CD	7.40	128.33	111.30	1	3
1	A	58	LYS	CA-C-O	7.39	131.08	120.51	2	2
1	B	31	THR	CB-CA-C	-7.39	95.70	110.42	3	1
1	A	31	THR	CB-CA-C	-7.39	95.72	110.42	1	1
1	B	33	SER	CB-CA-C	-7.37	95.75	110.42	3	1
1	A	75	LYS	CB-CG-CD	-7.37	94.35	111.30	7	3
1	A	39	GLU	CG-CD-OE1	7.37	135.34	118.40	2	2
1	B	39	GLU	CB-CA-C	7.36	125.07	110.42	6	2
1	A	66	HIS	CA-C-O	7.35	128.20	119.60	5	2
1	B	55	PRO	O-C-N	-7.35	112.72	122.64	7	2
1	A	70	LYS	CA-C-O	-7.34	112.57	121.89	4	2
1	A	41	VAL	O-C-N	-7.34	115.91	123.03	2	1
1	B	57	GLN	CB-CA-C	7.34	120.86	111.40	2	3
1	B	42	ILE	O-C-N	-7.32	115.26	123.10	6	2
1	A	56	THR	CA-CB-OG1	7.32	120.58	109.60	7	5
1	A	20	ILE	N-CA-CB	-7.31	100.97	111.21	7	5
1	A	27	SER	CB-CA-C	7.31	124.97	110.42	2	3
1	B	50	GLU	CA-C-O	7.31	134.80	120.69	2	2
1	A	56	THR	CA-C-O	7.30	130.95	120.51	6	1
1	B	65	LYS	CB-CA-C	7.29	123.42	110.81	6	1
1	A	62	ASP	CB-CG-OD2	7.27	135.12	118.40	1	2
1	B	23	GLN	CG-CD-NE2	7.27	127.30	116.40	2	3
1	A	71	THR	N-CA-CB	-7.25	98.23	110.49	2	2
1	B	66	HIS	CG-CD2-NE2	7.25	114.45	107.20	7	1
1	A	57	GLN	CA-CB-CG	-7.23	99.65	114.10	2	3
1	B	19	LYS	CB-CA-C	7.23	123.68	109.66	4	1
1	A	15	PHE	CB-CA-C	-7.21	96.06	110.42	1	2
1	A	57	GLN	CG-CD-OE1	7.19	135.18	120.80	5	1
1	B	24	ARG	CA-CB-CG	7.19	128.47	114.10	7	1
1	A	56	THR	CB-CA-C	-7.18	96.13	110.42	1	2
1	A	60	VAL	CA-CB-CG2	-7.18	98.19	110.40	4	1
1	B	46	LYS	CB-CA-C	7.17	122.29	110.17	2	3
1	A	70	LYS	CB-CA-C	7.17	122.86	110.45	4	3
1	B	31	THR	O-C-N	7.16	132.50	123.19	5	2
1	B	32	THR	CA-C-N	7.16	135.21	121.54	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	32	THR	C-N-CA	7.16	135.21	121.54	3	3
1	A	11	CYS	N-CA-C	7.15	126.02	110.80	3	2
1	A	75	LYS	CA-CB-CG	7.14	128.38	114.10	1	4
1	A	53	ALA	CA-C-O	-7.13	112.97	121.60	4	1
1	A	71	THR	CA-CB-OG1	7.13	120.30	109.60	4	1
1	A	61	GLN	O-C-N	7.13	132.07	122.59	7	1
1	B	70	LYS	CA-C-N	7.10	135.09	121.54	4	3
1	B	70	LYS	C-N-CA	7.10	135.09	121.54	4	3
1	A	23	GLN	CG-CD-OE1	7.09	134.98	120.80	6	2
1	B	18	LYS	CA-CB-CG	7.09	128.28	114.10	3	2
1	B	28	TYR	CE1-CZ-OH	7.08	141.14	119.90	7	1
1	A	56	THR	O-C-N	-7.06	113.20	122.59	7	2
1	B	68	ASP	N-CA-C	-7.05	95.78	110.80	5	1
1	B	34	SER	N-CA-CB	-7.04	98.58	110.49	4	2
1	B	37	PRO	N-CD-CG	-7.04	92.64	103.20	2	2
1	B	29	ARG	CB-CA-C	7.04	120.90	110.62	4	2
1	A	12	CYS	CA-C-N	7.04	134.98	121.54	3	3
1	A	12	CYS	C-N-CA	7.04	134.98	121.54	3	3
1	A	18	LYS	CA-C-O	7.02	126.57	119.97	3	3
1	A	72	GLN	CA-C-O	7.01	130.54	120.51	5	3
1	A	44	LYS	N-CA-C	-7.00	93.82	107.62	4	1
1	A	26	GLU	OE1-CD-OE2	-7.00	106.09	122.90	2	2
1	B	18	LYS	CA-C-N	7.00	134.57	122.81	4	3
1	B	18	LYS	C-N-CA	7.00	134.57	122.81	4	3
1	A	18	LYS	CA-CB-CG	6.99	128.08	114.10	5	2
1	A	38	ARG	CD-NE-CZ	6.99	134.18	124.40	2	2
1	A	58	LYS	CA-CB-CG	6.98	128.06	114.10	2	1
1	A	28	TYR	O-C-N	6.98	131.36	123.27	6	2
1	B	49	LYS	CA-C-O	-6.98	112.85	121.78	7	1
1	B	19	LYS	CA-C-O	6.97	130.33	121.55	1	1
1	B	29	ARG	CA-CB-CG	6.97	128.03	114.10	4	2
1	A	26	GLU	CB-CA-C	6.96	121.68	111.65	6	2
1	A	26	GLU	CA-CB-CG	-6.96	100.18	114.10	5	1
1	B	66	HIS	CE1-NE2-CD2	-6.95	102.05	109.00	7	3
1	A	27	SER	CA-CB-OG	-6.94	97.22	111.10	5	3
1	B	37	PRO	CB-CA-C	6.94	123.01	111.56	1	4
1	A	42	ILE	CA-C-N	6.93	133.19	123.07	4	2
1	A	42	ILE	C-N-CA	6.93	133.19	123.07	4	2
1	A	64	MET	CA-CB-CG	6.92	127.95	114.10	4	2
1	B	32	THR	O-C-N	-6.92	115.33	122.18	4	2
1	B	29	ARG	CD-NE-CZ	6.90	134.06	124.40	3	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	51	ILE	O-C-N	-6.90	115.14	123.00	5	1
1	A	53	ALA	O-C-N	6.88	132.57	122.81	4	1
1	A	36	CYS	N-CA-CB	-6.86	98.15	110.37	5	3
1	B	23	GLN	CA-C-O	-6.86	113.07	121.58	3	2
1	A	52	CYS	O-C-N	-6.86	115.28	123.03	6	2
1	A	64	MET	CA-C-N	6.85	129.46	120.28	5	1
1	A	64	MET	C-N-CA	6.85	129.46	120.28	5	1
1	A	66	HIS	CB-CG-CD2	-6.84	122.31	131.20	1	1
1	A	35	HIS	CB-CG-ND1	6.83	132.95	122.70	5	2
1	A	28	TYR	CB-CG-CD2	-6.83	110.56	120.80	5	1
1	B	29	ARG	N-CA-CB	-6.81	100.02	110.65	2	3
1	A	19	LYS	O-C-N	6.81	131.65	122.59	2	2
1	B	66	HIS	CA-C-O	6.80	127.31	119.35	4	3
1	A	54	ASP	CA-C-N	6.80	128.34	119.84	3	1
1	A	54	ASP	C-N-CA	6.80	128.34	119.84	3	1
1	A	14	ARG	CA-C-O	6.79	133.33	121.38	7	1
1	A	14	ARG	N-CA-CB	-6.78	99.90	111.69	1	2
1	A	29	ARG	N-CA-CB	-6.77	99.11	109.94	6	2
1	A	39	GLU	CA-C-N	6.76	134.44	121.54	4	1
1	A	39	GLU	C-N-CA	6.76	134.44	121.54	4	1
1	B	19	LYS	CA-CB-CG	6.76	127.61	114.10	4	3
1	B	56	THR	N-CA-CB	-6.75	99.08	110.49	3	2
1	A	44	LYS	CB-CA-C	6.73	122.72	109.66	5	3
1	B	62	ASP	CA-C-O	-6.72	113.97	120.90	3	2
1	B	42	ILE	N-CA-CB	6.72	121.33	111.52	2	2
1	A	74	PRO	CA-CB-CG	-6.71	91.74	104.50	4	1
1	A	59	TRP	CB-CG-CD1	6.71	136.96	126.90	5	1
1	A	22	LYS	CG-CD-CE	6.70	126.71	111.30	1	3
1	A	47	LEU	CA-C-O	6.68	130.07	120.51	7	1
1	B	48	ASP	CB-CA-C	6.67	123.69	110.42	1	1
1	A	69	LYS	CB-CA-C	6.66	123.67	110.42	1	2
1	A	43	PHE	N-CA-CB	-6.65	100.14	110.65	4	2
1	A	55	PRO	CA-CB-CG	-6.65	91.87	104.50	3	1
1	B	64	MET	CA-C-N	6.65	131.23	120.60	1	1
1	B	64	MET	C-N-CA	6.65	131.23	120.60	1	1
1	B	38	ARG	CA-C-O	6.65	130.01	120.51	7	1
1	B	11	CYS	O-C-N	-6.64	113.20	122.10	1	1
1	B	38	ARG	N-CA-C	6.63	124.92	110.80	3	2
1	A	24	ARG	CD-NE-CZ	6.62	133.67	124.40	7	1
1	B	65	LYS	CA-C-N	6.60	134.11	122.42	7	1
1	B	65	LYS	C-N-CA	6.60	134.11	122.42	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	37	PRO	CA-C-O	6.60	132.61	120.60	6	1
1	A	29	ARG	CG-CD-NE	-6.57	97.55	112.00	5	2
1	B	35	HIS	CE1-NE2-CD2	-6.56	102.44	109.00	5	4
1	A	17	ASN	CB-CA-C	6.56	123.48	110.42	2	1
1	A	24	ARG	CB-CG-CD	6.55	126.37	111.30	6	1
1	A	42	ILE	O-C-N	-6.55	116.16	123.03	6	2
1	A	66	HIS	CB-CA-C	-6.55	99.19	109.34	4	1
1	A	15	PHE	N-CA-CB	-6.54	99.43	110.49	3	2
1	B	14	ARG	CA-C-O	-6.54	111.16	120.51	5	1
1	A	39	GLU	OE1-CD-OE2	-6.54	107.21	122.90	2	2
1	A	65	LYS	CG-CD-CE	6.52	126.29	111.30	4	1
1	A	51	ILE	CA-CB-CG2	-6.51	99.44	110.50	7	2
1	A	47	LEU	N-CA-CB	-6.46	96.16	111.74	6	1
1	B	52	CYS	CB-CA-C	6.46	121.71	109.37	2	1
1	B	22	LYS	CA-CB-CG	6.46	127.02	114.10	1	1
1	A	42	ILE	CA-CB-CG1	-6.44	99.45	110.40	2	2
1	B	44	LYS	O-C-N	-6.43	115.06	123.16	5	1
1	B	46	LYS	O-C-N	-6.42	114.05	122.59	5	3
1	A	27	SER	CA-C-N	-6.42	112.54	122.87	2	1
1	A	27	SER	C-N-CA	-6.42	112.54	122.87	2	1
1	A	23	GLN	CG-CD-NE2	6.42	126.03	116.40	5	1
1	A	57	GLN	CB-CA-C	6.41	121.10	109.37	7	1
1	B	69	LYS	O-C-N	6.41	131.12	122.59	5	1
1	A	68	ASP	O-C-N	6.41	131.11	122.59	1	2
1	A	54	ASP	OD1-CG-OD2	-6.41	107.52	122.90	3	1
1	B	46	LYS	CA-C-O	6.40	126.94	119.32	2	1
1	B	48	ASP	O-C-N	-6.40	114.08	122.59	7	1
1	B	16	ILE	CA-C-O	6.39	128.77	120.78	6	1
1	A	49	LYS	CB-CA-C	-6.38	96.76	109.33	3	1
1	B	26	GLU	O-C-N	-6.38	114.24	122.09	7	1
1	A	19	LYS	CB-CA-C	6.38	123.11	110.42	1	1
1	B	38	ARG	O-C-N	-6.37	114.12	122.59	2	3
1	A	11	CYS	CB-CA-C	6.37	123.09	110.42	1	2
1	B	69	LYS	CD-CE-NZ	-6.36	91.54	111.90	3	1
1	A	14	ARG	CB-CG-CD	6.36	125.92	111.30	3	1
1	A	39	GLU	CA-C-O	6.34	129.23	121.56	1	3
1	A	66	HIS	CB-CG-ND1	6.34	132.21	122.70	1	1
1	B	68	ASP	CA-C-O	6.33	129.56	120.51	7	2
1	B	51	ILE	CB-CA-C	-6.32	100.92	111.29	3	1
1	A	38	ARG	CB-CG-CD	6.32	125.84	111.30	4	1
1	B	69	LYS	CA-C-O	-6.31	112.30	120.00	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	42	ILE	N-CA-C	-6.31	99.34	108.36	1	1
1	B	31	THR	N-CA-CB	6.29	121.12	110.49	3	1
1	A	48	ASP	OD1-CG-OD2	6.29	137.99	122.90	7	1
1	B	67	LEU	N-CA-C	-6.29	104.12	110.97	1	1
1	A	13	TYR	N-CA-CB	-6.29	100.24	110.11	2	1
1	A	70	LYS	CG-CD-CE	6.29	125.76	111.30	6	3
1	A	33	SER	N-CA-CB	-6.29	100.86	110.92	5	1
1	A	35	HIS	CA-CB-CG	-6.26	107.54	113.80	2	2
1	A	67	LEU	CA-C-O	-6.26	111.84	119.61	3	4
1	B	60	VAL	CA-C-N	6.26	129.00	120.54	2	1
1	B	60	VAL	C-N-CA	6.26	129.00	120.54	2	1
1	A	59	TRP	CA-C-N	6.26	128.57	120.56	6	3
1	A	59	TRP	C-N-CA	6.26	128.57	120.56	6	3
1	A	30	ARG	CB-CA-C	6.26	121.28	110.45	2	2
1	A	45	THR	CA-C-N	6.26	133.49	121.54	4	2
1	A	45	THR	C-N-CA	6.26	133.49	121.54	4	2
1	A	39	GLU	CB-CA-C	-6.25	99.48	109.80	6	1
1	A	72	GLN	O-C-N	6.24	130.73	122.56	3	3
1	B	69	LYS	CA-C-N	6.24	133.45	121.54	2	1
1	B	69	LYS	C-N-CA	6.24	133.45	121.54	2	1
1	A	50	GLU	OE1-CD-OE2	-6.22	107.97	122.90	3	1
1	A	15	PHE	CA-C-O	6.20	129.38	120.51	2	1
1	A	28	TYR	CA-C-O	6.20	128.17	121.16	5	1
1	A	17	ASN	O-C-N	-6.20	114.35	122.59	2	1
1	B	47	LEU	O-C-N	6.20	130.83	122.59	5	1
1	B	50	GLU	CA-CB-CG	6.19	126.48	114.10	6	2
1	B	46	LYS	N-CA-C	-6.19	105.01	113.30	2	1
1	A	51	ILE	CA-CB-CG1	6.18	120.91	110.40	1	2
1	B	43	PHE	CB-CG-CD2	-6.18	110.19	120.70	7	1
1	A	74	PRO	O-C-N	-6.17	114.31	122.64	5	2
1	A	14	ARG	O-C-N	6.16	130.36	122.10	5	2
1	A	16	ILE	O-C-N	-6.16	114.86	122.57	1	1
1	B	35	HIS	CG-CD2-NE2	6.16	113.36	107.20	5	2
1	B	60	VAL	CA-C-O	6.14	127.80	121.41	2	1
1	B	59	TRP	CD2-CE2-CZ2	-6.14	116.26	122.40	6	1
1	A	58	LYS	CB-CG-CD	-6.14	97.18	111.30	4	3
1	A	52	CYS	CA-C-O	6.13	128.26	121.39	7	2
1	A	23	GLN	CB-CG-CD	6.13	123.02	112.60	7	4
1	B	35	HIS	CA-C-O	-6.13	112.31	119.24	3	2
1	B	12	CYS	O-C-N	-6.13	114.44	122.59	6	2
1	B	23	GLN	O-C-N	-6.12	114.44	122.59	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	38	ARG	N-CA-CB	-6.12	100.15	110.49	1	1
1	A	60	VAL	CB-CA-C	-6.11	103.91	111.92	2	2
1	A	69	LYS	O-C-N	6.11	130.72	122.59	6	2
1	A	29	ARG	O-C-N	-6.11	115.29	123.23	1	1
1	A	18	LYS	O-C-N	-6.11	114.47	122.59	2	1
1	B	19	LYS	CD-CE-NZ	-6.09	92.40	111.90	4	1
1	B	67	LEU	CA-C-O	6.09	127.40	121.00	1	2
1	A	61	GLN	N-CA-C	6.08	117.78	111.03	5	1
1	B	44	LYS	CB-CG-CD	-6.08	97.31	111.30	6	2
1	A	54	ASP	CB-CG-OD1	6.08	132.38	118.40	3	1
1	A	68	ASP	CA-C-O	6.06	129.17	120.51	5	2
1	B	69	LYS	CG-CD-CE	6.05	125.22	111.30	1	1
1	A	63	PHE	N-CA-CB	-6.05	101.17	110.07	5	1
1	A	13	TYR	CB-CG-CD1	-6.05	111.72	120.80	7	1
1	B	38	ARG	CB-CA-C	6.05	122.46	110.42	5	1
1	B	59	TRP	NE1-CE2-CZ2	6.04	139.16	130.10	2	1
1	B	27	SER	N-CA-C	6.03	119.37	109.72	1	1
1	A	71	THR	CB-CA-C	-6.03	98.42	110.42	1	1
1	B	39	GLU	CA-C-O	6.03	129.12	120.51	6	2
1	B	32	THR	N-CA-CB	6.02	120.27	111.54	5	1
1	A	73	THR	CA-C-N	6.01	127.35	119.84	1	3
1	A	73	THR	C-N-CA	6.01	127.35	119.84	1	3
1	B	28	TYR	O-C-N	6.00	130.95	123.15	6	1
1	B	37	PRO	N-CA-C	6.00	124.82	112.47	3	3
1	B	27	SER	CB-CA-C	-5.99	98.49	110.42	7	2
1	A	35	HIS	CE1-NE2-CD2	-5.99	103.01	109.00	5	3
1	B	57	GLN	CA-C-N	5.98	132.96	121.54	6	4
1	B	57	GLN	C-N-CA	5.98	132.96	121.54	6	4
1	B	23	GLN	CB-CA-C	5.98	120.55	111.70	5	1
1	A	70	LYS	CA-CB-CG	5.97	126.03	114.10	2	2
1	B	55	PRO	CA-C-N	5.96	131.43	123.20	6	1
1	B	55	PRO	C-N-CA	5.96	131.43	123.20	6	1
1	B	70	LYS	CB-CA-C	-5.95	98.58	110.42	3	1
1	B	27	SER	CA-CB-OG	5.95	123.00	111.10	6	1
1	B	18	LYS	CG-CD-CE	5.94	124.97	111.30	5	2
1	B	60	VAL	CB-CA-C	-5.94	104.10	111.94	7	2
1	A	34	SER	O-C-N	-5.93	114.70	122.59	7	2
1	B	29	ARG	CA-C-N	5.90	132.07	122.81	2	1
1	B	29	ARG	C-N-CA	5.90	132.07	122.81	2	1
1	A	22	LYS	CA-CB-CG	5.89	125.89	114.10	4	1
1	A	34	SER	N-CA-C	-5.89	98.25	110.80	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	55	PRO	O-C-N	-5.88	114.70	122.64	3	1
1	B	49	LYS	O-C-N	5.88	130.37	122.96	2	1
1	A	12	CYS	CB-CA-C	5.87	120.58	111.13	5	1
1	B	42	ILE	CB-CA-C	-5.87	101.76	110.33	2	1
1	A	32	THR	CA-CB-CG2	-5.86	100.53	110.50	5	1
1	B	68	ASP	O-C-N	5.86	130.38	122.59	7	2
1	A	21	PRO	CA-N-CD	-5.86	103.80	112.00	7	1
1	B	13	TYR	CA-C-N	5.86	132.73	121.54	1	1
1	B	13	TYR	C-N-CA	5.86	132.73	121.54	1	1
1	A	44	LYS	CB-CG-CD	5.85	124.76	111.30	2	3
1	A	66	HIS	CE1-NE2-CD2	-5.84	103.16	109.00	7	3
1	A	49	LYS	CA-CB-CG	5.83	125.76	114.10	6	1
1	B	37	PRO	CA-CB-CG	-5.82	93.45	104.50	3	1
1	A	49	LYS	CA-C-O	-5.81	114.55	121.11	3	2
1	A	59	TRP	CB-CA-C	5.80	120.06	110.90	5	1
1	A	40	ALA	O-C-N	-5.79	114.89	122.59	5	1
1	B	70	LYS	CD-CE-NZ	-5.79	93.36	111.90	6	1
1	A	71	THR	CA-CB-CG2	5.79	120.34	110.50	5	2
1	B	14	ARG	CA-C-N	5.79	133.97	123.27	2	1
1	B	14	ARG	C-N-CA	5.79	133.97	123.27	2	1
1	A	17	ASN	CA-C-N	5.78	132.57	121.54	5	2
1	A	17	ASN	C-N-CA	5.78	132.57	121.54	5	2
1	B	59	TRP	CH2-CZ2-CE2	5.77	125.01	117.50	6	1
1	B	16	ILE	CA-C-N	5.77	132.56	121.54	1	1
1	B	16	ILE	C-N-CA	5.77	132.56	121.54	1	1
1	A	37	PRO	CA-CB-CG	-5.76	93.56	104.50	4	1
1	B	65	LYS	O-C-N	-5.74	115.02	122.37	6	1
1	B	55	PRO	CA-N-CD	-5.71	104.00	112.00	3	2
1	A	69	LYS	CB-CG-CD	-5.68	98.23	111.30	7	1
1	B	21	PRO	CA-C-O	5.68	130.94	120.60	2	1
1	A	48	ASP	CB-CG-OD2	-5.67	105.35	118.40	7	1
1	B	50	GLU	O-C-N	-5.67	113.86	122.93	2	1
1	B	61	GLN	O-C-N	5.67	128.15	122.08	6	1
1	A	50	GLU	O-C-N	-5.66	116.56	123.30	5	2
1	B	46	LYS	CD-CE-NZ	-5.66	93.79	111.90	1	1
1	B	30	ARG	CA-CB-CG	-5.66	102.78	114.10	5	1
1	B	11	CYS	CA-C-O	-5.66	114.64	121.32	3	2
1	A	13	TYR	CA-C-O	5.65	128.59	120.51	5	1
1	A	22	LYS	CA-C-N	5.63	132.30	121.54	2	2
1	A	22	LYS	C-N-CA	5.63	132.30	121.54	2	2
1	A	13	TYR	CA-CB-CG	-5.63	103.77	113.90	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	69	LYS	CG-CD-CE	5.63	124.25	111.30	1	3
1	A	20	ILE	CA-C-O	-5.63	112.41	119.95	3	1
1	A	49	LYS	CB-CG-CD	-5.63	98.36	111.30	1	1
1	A	70	LYS	CD-CE-NZ	-5.61	93.97	111.90	3	2
1	A	47	LEU	CD1-CG-CD2	-5.60	98.47	110.80	1	1
1	B	66	HIS	ND1-CG-CD2	-5.60	100.50	106.10	7	1
1	B	48	ASP	CA-C-N	5.59	132.22	121.54	3	1
1	B	48	ASP	C-N-CA	5.59	132.22	121.54	3	1
1	A	73	THR	O-C-N	-5.57	114.92	121.32	3	2
1	B	67	LEU	O-C-N	5.56	129.15	121.92	5	1
1	B	49	LYS	CB-CG-CD	5.56	124.08	111.30	7	2
1	A	58	LYS	N-CA-C	5.55	122.63	110.80	5	1
1	B	56	THR	CA-CB-OG1	5.54	117.91	109.60	1	1
1	A	25	LEU	CD1-CG-CD2	-5.54	98.62	110.80	6	3
1	B	59	TRP	CG-CD2-CE3	5.53	139.43	133.90	5	1
1	A	47	LEU	O-C-N	-5.52	115.10	122.28	6	1
1	B	52	CYS	CA-C-N	5.51	132.07	121.54	7	1
1	B	52	CYS	C-N-CA	5.51	132.07	121.54	7	1
1	B	21	PRO	CA-CB-CG	-5.50	94.04	104.50	5	1
1	B	51	ILE	CA-CB-CG2	5.49	119.83	110.50	3	1
1	B	25	LEU	O-C-N	-5.49	114.22	123.00	5	1
1	B	32	THR	CA-CB-CG2	5.48	119.82	110.50	2	1
1	A	48	ASP	CB-CA-C	5.48	120.87	111.45	7	2
1	B	63	PHE	O-C-N	5.47	127.94	122.08	5	1
1	B	46	LYS	CA-CB-CG	5.47	125.04	114.10	7	1
1	A	39	GLU	CA-CB-CG	-5.47	103.16	114.10	5	2
1	A	65	LYS	CA-CB-CG	5.47	125.03	114.10	4	1
1	B	63	PHE	N-CA-C	5.46	117.68	111.02	5	1
1	A	22	LYS	CD-CE-NZ	-5.46	94.43	111.90	3	1
1	A	23	GLN	CB-CA-C	5.46	117.87	109.03	6	1
1	B	59	TRP	CB-CG-CD2	-5.46	119.16	126.80	6	2
1	A	65	LYS	O-C-N	-5.45	115.65	122.35	4	1
1	A	49	LYS	CD-CE-NZ	-5.44	94.50	111.90	3	1
1	A	54	ASP	O-C-N	-5.43	115.08	121.32	4	2
1	A	51	ILE	N-CA-CB	-5.43	104.62	111.46	4	1
1	A	35	HIS	CB-CG-CD2	-5.43	124.14	131.20	7	2
1	B	14	ARG	CB-CA-C	5.42	120.78	111.45	6	1
1	B	24	ARG	CB-CG-CD	5.41	123.75	111.30	1	1
1	B	13	TYR	CA-CB-CG	5.40	123.63	113.90	2	1
1	B	41	VAL	CA-C-N	5.40	130.50	122.99	3	1
1	B	41	VAL	C-N-CA	5.40	130.50	122.99	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	59	TRP	CD1-NE1-CE2	5.40	118.62	108.90	5	3
1	B	26	GLU	OE1-CD-OE2	-5.39	109.96	122.90	3	1
1	A	72	GLN	CB-CA-C	5.39	118.69	109.80	6	1
1	A	27	SER	O-C-N	-5.38	117.45	123.48	1	1
1	A	57	GLN	CB-CG-CD	-5.38	103.46	112.60	4	1
1	A	25	LEU	O-C-N	-5.38	115.17	122.81	5	1
1	A	66	HIS	O-C-N	5.38	130.00	122.36	7	1
1	A	20	ILE	O-C-N	-5.37	114.98	121.10	6	2
1	B	14	ARG	CA-CB-CG	5.36	124.82	114.10	1	1
1	A	35	HIS	CG-CD2-NE2	5.36	112.56	107.20	5	2
1	A	49	LYS	O-C-N	5.35	129.70	122.59	1	1
1	A	44	LYS	CD-CE-NZ	-5.34	94.81	111.90	4	1
1	B	40	ALA	CA-C-N	5.33	131.11	122.68	6	1
1	B	40	ALA	C-N-CA	5.33	131.11	122.68	6	1
1	A	32	THR	N-CA-CB	5.33	119.49	110.49	3	1
1	B	50	GLU	CB-CG-CD	5.32	121.64	112.60	6	2
1	A	49	LYS	N-CA-CB	5.32	120.18	111.08	3	1
1	B	55	PRO	CB-CA-C	5.32	120.34	111.56	7	1
1	A	36	CYS	CA-C-O	-5.31	112.88	120.16	3	1
1	B	18	LYS	O-C-N	-5.30	114.93	122.99	1	1
1	B	65	LYS	CA-CB-CG	5.29	124.68	114.10	3	1
1	B	15	PHE	CA-C-O	5.28	127.91	121.68	3	1
1	B	51	ILE	CA-CB-CG1	5.28	119.37	110.40	4	1
1	A	67	LEU	CA-C-N	5.26	131.58	121.54	5	1
1	A	67	LEU	C-N-CA	5.26	131.58	121.54	5	1
1	A	42	ILE	CA-C-O	5.25	128.25	121.32	6	2
1	B	65	LYS	CD-CE-NZ	-5.24	95.12	111.90	7	1
1	B	42	ILE	N-CA-C	-5.24	100.58	108.12	2	1
1	A	14	ARG	CB-CA-C	5.24	121.59	110.07	1	1
1	A	59	TRP	CA-CB-CG	-5.23	103.66	113.60	2	1
1	B	11	CYS	CB-CA-C	5.23	120.51	109.79	2	2
1	B	20	ILE	CA-C-O	-5.23	112.95	119.95	7	1
1	A	19	LYS	CA-C-N	5.22	131.79	122.13	2	2
1	A	19	LYS	C-N-CA	5.22	131.79	122.13	2	2
1	A	59	TRP	CD2-CE2-CZ2	-5.22	117.18	122.40	1	1
1	B	27	SER	CA-C-N	-5.20	113.71	123.03	4	1
1	B	27	SER	C-N-CA	-5.20	113.71	123.03	4	1
1	B	25	LEU	CD1-CG-CD2	-5.20	99.36	110.80	1	1
1	B	27	SER	O-C-N	-5.20	115.68	122.59	3	1
1	A	43	PHE	CB-CG-CD2	-5.19	111.88	120.70	2	1
1	B	23	GLN	CA-CB-CG	-5.17	103.75	114.10	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	73	THR	CA-C-O	-5.17	115.02	119.72	1	1
1	B	35	HIS	CB-CA-C	5.17	118.20	110.08	2	1
1	B	22	LYS	CA-C-O	5.17	127.90	120.51	4	1
1	A	59	TRP	CD1-NE1-CE2	5.17	118.20	108.90	7	1
1	B	39	GLU	CG-CD-OE1	-5.16	106.54	118.40	4	1
1	B	69	LYS	CA-CB-CG	-5.15	103.79	114.10	4	1
1	A	39	GLU	O-C-N	-5.15	117.21	123.03	6	1
1	B	30	ARG	O-C-N	-5.15	117.45	123.27	7	2
1	A	73	THR	CB-CA-C	5.14	120.31	110.17	3	2
1	B	51	ILE	N-CA-CB	-5.13	103.86	112.47	7	1
1	B	22	LYS	CG-CD-CE	5.12	123.06	111.30	1	1
1	B	69	LYS	CB-CG-CD	-5.09	99.60	111.30	3	1
1	A	63	PHE	CB-CG-CD2	-5.09	112.05	120.70	6	1
1	A	38	ARG	CB-CA-C	-5.09	101.10	109.65	7	1
1	B	38	ARG	CB-CG-CD	-5.08	99.61	111.30	3	1
1	B	21	PRO	O-C-N	-5.08	116.95	123.04	5	2
1	B	13	TYR	CB-CA-C	5.07	120.51	110.42	4	1
1	B	30	ARG	N-CA-CB	-5.07	102.61	110.46	4	1
1	A	59	TRP	NE1-CE2-CZ2	5.06	137.69	130.10	3	1
1	A	42	ILE	CB-CG1-CD1	5.06	124.42	113.80	2	1
1	B	25	LEU	CA-C-O	5.06	129.40	120.80	5	1
1	A	57	GLN	CA-C-N	5.05	131.20	121.54	4	1
1	A	57	GLN	C-N-CA	5.05	131.20	121.54	4	1
1	B	49	LYS	CD-CE-NZ	-5.05	95.73	111.90	6	1
1	A	66	HIS	CG-CD2-NE2	5.05	112.25	107.20	7	1
1	A	21	PRO	CA-C-O	5.05	129.78	120.60	5	1
1	B	15	PHE	CA-C-N	5.03	131.03	121.97	2	1
1	B	15	PHE	C-N-CA	5.03	131.03	121.97	2	1
1	B	33	SER	N-CA-CB	5.01	118.95	110.49	4	1
1	A	75	LYS	CD-CE-NZ	-5.01	95.88	111.90	6	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	B	45	THR	CB	4
1	A	31	THR	CB	3
1	B	20	ILE	CB	2
1	B	56	THR	CB	2
1	A	73	THR	CB	2
1	B	31	THR	CB	2
1	B	32	THR	CB	1

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Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	32	THR	CB	1
1	A	16	ILE	CB	1

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	14	ARG	Sidechain	7
1	A	24	ARG	Sidechain	7
1	A	30	ARG	Sidechain	7
1	A	38	ARG	Sidechain	7
1	B	29	ARG	Sidechain	7
1	B	30	ARG	Sidechain	7
1	B	38	ARG	Sidechain	7
1	A	29	ARG	Sidechain	6
1	B	14	ARG	Sidechain	6
1	B	24	ARG	Sidechain	6
1	A	54	ASP	Peptide	2

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	548	564	564	135±36
1	B	509	522	522	123±22
All	All	7399	7602	7600	1521

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 101.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:28:TYR:CG	1:B:28:TYR:CB	1.52	1.89	7	1
1:A:15:PHE:CG	1:A:15:PHE:CB	1.50	1.91	7	1
1:A:15:PHE:CB	1:A:15:PHE:CZ	1.11	2.32	7	1
1:A:17:ASN:HA	1:A:59:TRP:CD1	1.11	1.80	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:28:TYR:CB	1:B:28:TYR:CE2	1.06	2.36	7	1
1:B:28:TYR:CB	1:B:28:TYR:CZ	1.05	2.35	7	1
1:B:62:ASP:HB3	1:B:66:HIS:ND1	1.04	1.67	7	1
1:A:15:PHE:CB	1:A:15:PHE:CE1	1.03	2.40	7	1
1:B:26:GLU:HG2	1:B:44:LYS:C	1.01	1.80	5	1
1:A:58:LYS:HD2	1:A:58:LYS:C	0.98	1.82	4	3
1:A:29:ARG:HH22	1:A:50:GLU:HG2	0.95	1.20	4	1
1:A:30:ARG:HD3	1:A:41:VAL:C	0.92	1.89	4	1
1:B:26:GLU:HG2	1:B:45:THR:N	0.90	1.79	5	1
1:A:58:LYS:HD2	1:A:58:LYS:H	0.88	1.25	1	1
1:A:30:ARG:HH21	1:A:31:THR:HG22	0.87	1.29	5	1
1:A:30:ARG:NH1	1:A:52:CYS:SG	0.87	2.48	4	1
1:A:73:THR:OG1	1:B:57:GLN:HA	0.87	1.69	3	1
1:B:53:ALA:HB1	1:B:60:VAL:HG21	0.86	1.44	2	1
1:A:34:SER:N	1:B:27:SER:HB3	0.86	1.85	3	1
1:B:25:LEU:HD22	1:B:63:PHE:CE1	0.85	2.06	5	1
1:A:39:GLU:HG2	1:B:70:LYS:HB2	0.85	1.47	3	1
1:A:71:THR:HA	1:B:39:GLU:HB2	0.84	1.49	3	1
1:A:75:LYS:HB3	1:B:18:LYS:N	0.82	1.89	3	1
1:A:61:GLN:HG3	1:A:65:LYS:NZ	0.82	1.89	7	1
1:B:53:ALA:CB	1:B:60:VAL:HG21	0.82	2.04	2	1
1:A:64:MET:SD	1:B:69:LYS:HD3	0.81	2.14	2	1
1:B:60:VAL:O	1:B:64:MET:HG3	0.81	1.76	2	1
1:B:69:LYS:O	1:B:69:LYS:HD3	0.81	1.73	4	1
1:A:30:ARG:NH2	1:A:31:THR:C	0.80	2.39	5	1
1:A:38:ARG:HG3	1:A:52:CYS:SG	0.80	2.16	4	1
1:A:70:LYS:HD2	1:B:39:GLU:HG3	0.79	1.54	5	1
1:A:16:ILE:C	1:A:17:ASN:HD22	0.79	1.84	6	1
1:B:30:ARG:HA	1:B:41:VAL:HG22	0.79	1.52	6	1
1:A:29:ARG:HH22	1:A:50:GLU:CG	0.78	1.91	4	1
1:B:30:ARG:HG2	1:B:41:VAL:CG2	0.78	2.08	5	5
1:B:41:VAL:CG1	1:B:42:ILE:N	0.76	2.48	6	3
1:A:42:ILE:HA	1:A:51:ILE:O	0.75	1.82	1	3
1:B:23:GLN:N	1:B:25:LEU:HD13	0.74	1.97	3	1
1:A:29:ARG:NH2	1:A:50:GLU:HG2	0.74	1.98	4	1
1:B:69:LYS:HD3	1:B:69:LYS:C	0.74	2.06	4	1
1:A:24:ARG:HH12	1:B:35:HIS:CG	0.74	2.00	1	1
1:A:31:THR:C	1:B:68:ASP:HA	0.74	2.08	7	1
1:A:32:THR:HA	1:B:27:SER:HB2	0.74	1.56	1	1
1:A:34:SER:CA	1:B:27:SER:HB3	0.74	2.12	3	1
1:A:18:LYS:HB3	1:A:18:LYS:HZ2	0.74	1.42	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:28:TYR:CD2	1:B:30:ARG:HD2	0.74	2.18	5	1
1:B:30:ARG:HG2	1:B:41:VAL:HG22	0.74	1.59	2	3
1:B:38:ARG:HG3	1:B:39:GLU:HG2	0.74	1.58	7	1
1:A:58:LYS:HD2	1:A:58:LYS:N	0.73	1.98	1	1
1:A:11:CYS:HB3	1:A:38:ARG:HA	0.73	1.61	1	1
1:A:36:CYS:SG	1:A:37:PRO:CD	0.73	2.77	2	3
1:A:33:SER:O	1:B:70:LYS:HA	0.73	1.84	5	1
1:A:30:ARG:NH2	1:A:39:GLU:C	0.73	2.47	4	1
1:A:30:ARG:NH2	1:A:31:THR:HG22	0.73	1.97	5	1
1:A:53:ALA:HB1	1:A:60:VAL:HG21	0.72	1.60	4	2
1:A:30:ARG:HG3	1:A:40:ALA:O	0.72	1.83	4	1
1:B:25:LEU:HD22	1:B:63:PHE:CD1	0.72	2.19	5	1
1:A:36:CYS:SG	1:A:38:ARG:HB2	0.71	2.26	7	1
1:B:14:ARG:NH1	1:B:14:ARG:HB3	0.71	2.01	1	1
1:B:30:ARG:HD2	1:B:64:MET:HE1	0.71	1.62	1	1
1:B:57:GLN:CD	1:B:57:GLN:N	0.71	2.49	3	1
1:A:44:LYS:HD2	1:A:48:ASP:HA	0.71	1.62	7	1
1:A:30:ARG:HA	1:B:27:SER:HB2	0.71	1.62	4	1
1:A:58:LYS:C	1:A:58:LYS:CD	0.70	2.62	4	2
1:B:15:PHE:CD1	1:B:59:TRP:CH2	0.70	2.79	5	1
1:A:15:PHE:O	1:A:17:ASN:N	0.70	2.24	6	1
1:B:18:LYS:HA	1:B:59:TRP:CD1	0.70	2.22	2	1
1:A:34:SER:N	1:B:27:SER:CB	0.70	2.54	3	1
1:B:30:ARG:HD2	1:B:64:MET:SD	0.69	2.27	2	1
1:B:58:LYS:HD3	1:B:58:LYS:C	0.69	2.11	2	1
1:B:65:LYS:HD2	1:B:65:LYS:O	0.69	1.87	6	2
1:A:54:ASP:H	1:A:57:GLN:CD	0.69	1.95	4	2
1:A:44:LYS:HD3	1:A:44:LYS:C	0.69	2.11	4	1
1:B:26:GLU:HG3	1:B:44:LYS:HE2	0.69	1.64	5	1
1:B:26:GLU:HG3	1:B:44:LYS:HG3	0.69	1.64	5	1
1:B:43:PHE:CE2	1:B:63:PHE:CD2	0.69	2.81	4	5
1:A:33:SER:HA	1:B:26:GLU:HB3	0.69	1.63	4	1
1:B:30:ARG:CD	1:B:64:MET:SD	0.69	2.81	2	1
1:A:74:PRO:HG2	1:B:60:VAL:HG21	0.68	1.65	3	1
1:A:72:GLN:HA	1:B:55:PRO:HG3	0.68	1.65	5	1
1:B:46:LYS:O	1:B:46:LYS:HE2	0.68	1.88	7	1
1:B:12:CYS:SG	1:B:40:ALA:CB	0.68	2.82	3	1
1:B:49:LYS:CE	1:B:49:LYS:H	0.68	2.01	3	1
1:B:26:GLU:HG3	1:B:44:LYS:CE	0.68	2.18	5	1
1:A:57:GLN:C	1:A:61:GLN:NE2	0.68	2.51	7	7
1:A:28:TYR:CD1	1:A:30:ARG:HD3	0.68	2.24	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:64:MET:O	1:B:68:ASP:HB2	0.68	1.89	5	3
1:B:36:CYS:SG	1:B:37:PRO:CD	0.68	2.82	7	1
1:B:36:CYS:SG	1:B:37:PRO:HG2	0.68	2.29	7	1
1:A:53:ALA:CB	1:A:60:VAL:HG21	0.67	2.19	4	1
1:A:17:ASN:HA	1:A:59:TRP:NE1	0.67	2.04	3	1
1:B:28:TYR:OH	1:B:67:LEU:HB3	0.67	1.89	2	1
1:A:75:LYS:HD2	1:B:17:ASN:O	0.67	1.90	4	1
1:A:30:ARG:HE	1:A:41:VAL:HB	0.67	1.48	5	1
1:B:19:LYS:O	1:B:19:LYS:NZ	0.67	2.25	6	1
1:A:61:GLN:HG3	1:A:65:LYS:HZ2	0.67	1.46	7	1
1:A:54:ASP:O	1:A:56:THR:N	0.67	2.28	2	1
1:A:30:ARG:HG3	1:A:40:ALA:C	0.67	2.15	4	1
1:A:61:GLN:HE21	1:A:61:GLN:N	0.67	1.88	4	1
1:B:67:LEU:O	1:B:69:LYS:N	0.67	2.28	5	1
1:B:57:GLN:HA	1:B:58:LYS:HD3	0.67	1.67	6	1
1:B:28:TYR:CZ	1:B:30:ARG:HD3	0.67	2.25	1	1
1:A:54:ASP:CG	1:A:55:PRO:HD2	0.67	2.15	5	1
1:A:11:CYS:HB3	1:A:37:PRO:CG	0.67	2.20	7	1
1:B:12:CYS:HB2	1:B:40:ALA:CB	0.67	2.20	4	1
1:B:13:TYR:N	1:B:52:CYS:SG	0.66	2.68	5	1
1:A:75:LYS:N	1:B:57:GLN:HE22	0.66	1.88	3	1
1:A:33:SER:H	1:B:26:GLU:HG3	0.66	1.50	2	1
1:A:26:GLU:CD	1:A:44:LYS:HZ2	0.66	1.97	3	2
1:A:36:CYS:SG	1:A:37:PRO:HD2	0.66	2.31	4	4
1:A:32:THR:HB	1:B:68:ASP:HB2	0.66	1.66	7	1
1:A:43:PHE:CE2	1:A:63:PHE:CD2	0.66	2.84	3	3
1:A:51:ILE:HG22	1:A:59:TRP:CZ2	0.66	2.25	5	1
1:B:26:GLU:CD	1:B:46:LYS:H	0.66	1.98	5	2
1:A:58:LYS:HD3	1:A:59:TRP:N	0.66	2.04	6	1
1:A:34:SER:CB	1:A:39:GLU:HB2	0.66	2.20	7	1
1:B:25:LEU:H	1:B:27:SER:H	0.66	1.30	3	1
1:A:20:ILE:HG12	1:A:21:PRO:HD3	0.66	1.67	3	1
1:A:74:PRO:HD3	1:B:15:PHE:CE2	0.66	2.26	4	1
1:B:43:PHE:CD2	1:B:63:PHE:CZ	0.66	2.84	7	1
1:A:15:PHE:CB	1:A:52:CYS:SG	0.66	2.84	5	1
1:A:62:ASP:O	1:A:66:HIS:N	0.65	2.29	4	5
1:A:66:HIS:HA	1:A:69:LYS:HZ3	0.65	1.51	2	1
1:B:30:ARG:HG2	1:B:41:VAL:HB	0.65	1.68	4	2
1:A:17:ASN:C	1:A:59:TRP:CD1	0.65	2.74	3	2
1:B:49:LYS:H	1:B:49:LYS:CD	0.65	2.04	3	1
1:B:25:LEU:HB3	1:B:44:LYS:O	0.65	1.89	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:LYS:HD3	1:A:58:LYS:C	0.65	2.15	6	1
1:A:57:GLN:N	1:A:61:GLN:HE22	0.65	1.89	5	2
1:A:34:SER:CB	1:B:70:LYS:HE3	0.65	2.21	7	1
1:A:74:PRO:HD3	1:B:15:PHE:CD2	0.65	2.26	4	1
1:B:28:TYR:CG	1:B:28:TYR:CA	0.65	2.76	7	1
1:A:58:LYS:H	1:A:58:LYS:CD	0.65	2.03	1	1
1:A:43:PHE:CZ	1:A:59:TRP:CZ3	0.65	2.84	3	6
1:A:68:ASP:HA	1:B:30:ARG:NH2	0.65	2.07	4	1
1:A:66:HIS:HA	1:A:69:LYS:NZ	0.65	2.06	2	1
1:B:52:CYS:SG	1:B:53:ALA:N	0.64	2.70	3	3
1:A:28:TYR:CG	1:A:30:ARG:HD3	0.64	2.26	2	1
1:A:71:THR:HG22	1:A:72:GLN:N	0.64	2.07	4	1
1:B:57:GLN:HG2	1:B:59:TRP:CD1	0.64	2.27	1	1
1:A:39:GLU:HG2	1:B:70:LYS:CB	0.64	2.22	3	1
1:A:28:TYR:CE1	1:B:30:ARG:HB2	0.64	2.28	5	1
1:B:57:GLN:N	1:B:57:GLN:OE1	0.64	2.30	6	2
1:A:54:ASP:HB3	1:A:55:PRO:CD	0.64	2.23	4	1
1:B:41:VAL:HG21	1:B:64:MET:SD	0.64	2.33	2	1
1:A:16:ILE:HB	1:A:52:CYS:SG	0.64	2.33	6	1
1:A:73:THR:O	1:B:56:THR:N	0.64	2.30	3	2
1:B:62:ASP:O	1:B:66:HIS:N	0.64	2.31	6	4
1:A:70:LYS:HE3	1:A:70:LYS:C	0.64	2.17	4	1
1:B:28:TYR:CD1	1:B:41:VAL:HG21	0.64	2.27	5	1
1:B:63:PHE:CD1	1:B:67:LEU:HG	0.64	2.28	7	1
1:B:58:LYS:HD3	1:B:58:LYS:H	0.63	1.51	1	2
1:A:30:ARG:HH12	1:A:31:THR:HG22	0.63	1.53	5	1
1:B:64:MET:O	1:B:68:ASP:CB	0.63	2.46	5	3
1:B:29:ARG:CD	1:B:42:ILE:HB	0.63	2.23	6	1
1:B:46:LYS:O	1:B:46:LYS:HD3	0.63	1.93	1	1
1:B:59:TRP:CE2	1:B:60:VAL:CG2	0.63	2.81	3	1
1:A:43:PHE:CZ	1:A:63:PHE:CD2	0.63	2.87	4	2
1:B:43:PHE:CE2	1:B:59:TRP:CZ3	0.63	2.86	1	2
1:A:61:GLN:HA	1:A:64:MET:SD	0.63	2.33	6	2
1:A:39:GLU:CD	1:A:39:GLU:N	0.63	2.57	3	1
1:A:75:LYS:HB3	1:B:18:LYS:H	0.63	1.51	3	1
1:B:67:LEU:C	1:B:69:LYS:N	0.63	2.51	5	1
1:B:32:THR:HG21	1:B:35:HIS:ND1	0.63	2.08	1	1
1:B:23:GLN:N	1:B:25:LEU:CD1	0.63	2.61	3	1
1:A:70:LYS:CD	1:B:39:GLU:HG3	0.63	2.22	5	1
1:A:28:TYR:CE2	1:A:67:LEU:HB2	0.62	2.29	5	1
1:B:19:LYS:NZ	1:B:25:LEU:HB2	0.62	2.08	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LYS:HZ3	1:A:48:ASP:CG	0.62	2.02	4	2
1:B:28:TYR:CE2	1:B:30:ARG:HD2	0.62	2.30	5	1
1:A:31:THR:HG22	1:B:27:SER:HA	0.62	1.71	7	1
1:B:25:LEU:H	1:B:70:LYS:CG	0.62	2.07	7	1
1:A:26:GLU:CB	1:A:44:LYS:HZ1	0.62	2.07	4	1
1:A:33:SER:N	1:B:26:GLU:HG3	0.62	2.09	2	1
1:A:48:ASP:O	1:A:49:LYS:HE3	0.62	1.92	7	1
1:B:36:CYS:SG	1:B:37:PRO:CG	0.62	2.87	7	1
1:A:75:LYS:N	1:B:57:GLN:NE2	0.62	2.48	3	1
1:A:61:GLN:H	1:A:61:GLN:NE2	0.62	1.92	4	1
1:A:18:LYS:CA	1:A:59:TRP:CE2	0.62	2.82	6	1
1:A:53:ALA:HB1	1:A:60:VAL:CG2	0.62	2.24	6	1
1:B:58:LYS:HD2	1:B:59:TRP:N	0.62	2.10	7	1
1:A:70:LYS:O	1:A:71:THR:HB	0.62	1.93	4	1
1:A:19:LYS:HB2	1:A:59:TRP:HB2	0.62	1.70	2	1
1:B:15:PHE:CD2	1:B:54:ASP:HB2	0.62	2.30	3	1
1:B:25:LEU:N	1:B:69:LYS:HB2	0.62	2.10	5	1
1:A:39:GLU:CG	1:B:70:LYS:HB2	0.61	2.23	3	1
1:A:70:LYS:NZ	1:A:71:THR:OG1	0.61	2.32	3	2
1:B:19:LYS:NZ	1:B:21:PRO:O	0.61	2.32	7	1
1:B:26:GLU:OE1	1:B:26:GLU:HA	0.61	1.95	7	1
1:B:47:LEU:O	1:B:49:LYS:NZ	0.61	2.32	7	4
1:A:18:LYS:HB3	1:A:18:LYS:NZ	0.61	2.10	4	1
1:A:30:ARG:CD	1:A:64:MET:SD	0.61	2.89	7	1
1:B:26:GLU:CD	1:B:44:LYS:HZ2	0.61	2.02	2	2
1:B:15:PHE:CD1	1:B:16:ILE:N	0.61	2.68	5	1
1:A:18:LYS:N	1:A:59:TRP:CE2	0.61	2.69	6	1
1:A:15:PHE:CG	1:A:15:PHE:CA	0.61	2.81	7	1
1:A:30:ARG:CD	1:A:41:VAL:C	0.61	2.71	4	1
1:B:11:CYS:SG	1:B:12:CYS:N	0.61	2.70	5	1
1:B:57:GLN:N	1:B:61:GLN:NE2	0.61	2.49	5	1
1:A:18:LYS:HD2	1:A:57:GLN:OE1	0.61	1.95	7	1
1:A:75:LYS:C	1:B:57:GLN:CD	0.61	2.69	3	1
1:B:23:GLN:HA	1:B:67:LEU:HD22	0.61	1.72	5	1
1:A:44:LYS:HZ1	1:A:48:ASP:CG	0.61	2.04	2	2
1:B:64:MET:O	1:B:68:ASP:HB3	0.61	1.95	7	1
1:A:71:THR:CB	1:B:30:ARG:NH2	0.60	2.64	1	1
1:B:33:SER:O	1:B:35:HIS:N	0.60	2.34	6	1
1:A:46:LYS:NZ	1:A:47:LEU:O	0.60	2.33	1	1
1:A:71:THR:HG23	1:B:40:ALA:N	0.60	2.12	4	1
1:B:25:LEU:O	1:B:70:LYS:NZ	0.60	2.34	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:GLN:CA	1:B:55:PRO:HG3	0.60	2.26	5	1
1:B:23:GLN:HG2	1:B:63:PHE:CD2	0.60	2.32	2	1
1:A:34:SER:H	1:B:27:SER:HB3	0.60	1.56	3	1
1:A:34:SER:O	1:B:70:LYS:NZ	0.60	2.35	6	2
1:B:30:ARG:HG2	1:B:41:VAL:CB	0.60	2.26	7	2
1:A:46:LYS:NZ	1:A:46:LYS:O	0.60	2.35	5	1
1:A:17:ASN:CA	1:A:59:TRP:CD1	0.60	2.73	3	1
1:B:46:LYS:O	1:B:46:LYS:HG2	0.60	1.97	5	1
1:A:17:ASN:N	1:A:52:CYS:O	0.60	2.34	6	1
1:A:75:LYS:C	1:B:57:GLN:NE2	0.60	2.60	3	1
1:A:34:SER:OG	1:B:70:LYS:HE3	0.60	1.96	7	1
1:A:71:THR:N	1:B:39:GLU:HB2	0.60	2.11	3	1
1:A:31:THR:HG22	1:A:32:THR:N	0.59	2.12	4	1
1:A:75:LYS:HG2	1:B:17:ASN:H	0.59	1.56	5	1
1:A:15:PHE:CE1	1:A:51:ILE:HG23	0.59	2.32	4	1
1:A:71:THR:HG22	1:A:72:GLN:H	0.59	1.55	4	1
1:B:55:PRO:O	1:B:57:GLN:N	0.59	2.34	4	2
1:A:15:PHE:CA	1:A:52:CYS:SG	0.59	2.90	5	1
1:B:28:TYR:CD1	1:B:28:TYR:C	0.59	2.80	3	3
1:A:19:LYS:HZ1	1:A:66:HIS:CE1	0.59	2.15	2	1
1:B:44:LYS:HD3	1:B:48:ASP:O	0.59	1.98	3	1
1:B:30:ARG:NH1	1:B:64:MET:SD	0.59	2.74	4	1
1:A:18:LYS:HA	1:A:59:TRP:CD2	0.59	2.32	6	1
1:A:70:LYS:HB3	1:B:38:ARG:O	0.59	1.97	1	1
1:A:55:PRO:O	1:A:57:GLN:N	0.59	2.35	3	1
1:A:71:THR:HG22	1:A:73:THR:HA	0.59	1.75	3	1
1:A:26:GLU:CG	1:A:44:LYS:NZ	0.59	2.66	4	1
1:A:30:ARG:NH1	1:A:40:ALA:O	0.59	2.35	5	1
1:B:37:PRO:O	1:B:38:ARG:NH1	0.59	2.36	7	1
1:A:27:SER:HB2	1:B:34:SER:CB	0.59	2.28	2	1
1:B:56:THR:HG23	1:B:57:GLN:HE21	0.59	1.58	3	1
1:B:41:VAL:CG1	1:B:54:ASP:H	0.59	2.11	4	1
1:B:61:GLN:HA	1:B:64:MET:HE2	0.59	1.75	4	1
1:A:24:ARG:HH22	1:B:35:HIS:CD2	0.59	2.15	1	1
1:A:70:LYS:CE	1:B:30:ARG:HB3	0.59	2.27	3	1
1:A:71:THR:HG21	1:B:40:ALA:HA	0.59	1.73	4	1
1:B:43:PHE:HB2	1:B:51:ILE:HB	0.59	1.75	5	3
1:B:57:GLN:C	1:B:61:GLN:NE2	0.59	2.60	6	4
1:B:59:TRP:CZ2	1:B:60:VAL:HG22	0.59	2.33	3	1
1:A:34:SER:HA	1:B:70:LYS:CG	0.59	2.26	7	1
1:A:54:ASP:C	1:A:56:THR:N	0.59	2.60	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:MET:O	1:A:68:ASP:N	0.59	2.36	3	1
1:A:30:ARG:CZ	1:A:31:THR:O	0.59	2.51	5	1
1:A:16:ILE:C	1:A:17:ASN:ND2	0.58	2.60	6	1
1:A:29:ARG:HE	1:A:42:ILE:CG2	0.58	2.10	6	1
1:A:58:LYS:NZ	1:A:62:ASP:OD2	0.58	2.36	4	3
1:A:29:ARG:NH2	1:A:42:ILE:HG21	0.58	2.13	2	1
1:A:23:GLN:CD	1:A:23:GLN:H	0.58	2.06	4	2
1:B:12:CYS:SG	1:B:13:TYR:N	0.58	2.75	6	2
1:B:43:PHE:CD2	1:B:63:PHE:CE1	0.58	2.92	7	1
1:A:11:CYS:HB3	1:A:38:ARG:CA	0.58	2.28	1	1
1:A:30:ARG:HG3	1:A:41:VAL:HA	0.58	1.76	4	1
1:B:43:PHE:CZ	1:B:59:TRP:CZ3	0.58	2.91	1	3
1:A:63:PHE:O	1:A:64:MET:C	0.58	2.46	5	5
1:A:75:LYS:N	1:B:54:ASP:HB3	0.58	2.13	3	1
1:A:32:THR:CB	1:B:68:ASP:HB2	0.58	2.28	7	1
1:A:59:TRP:CE2	1:A:60:VAL:HG23	0.58	2.33	3	2
1:A:73:THR:HG1	1:B:57:GLN:HA	0.58	1.57	3	1
1:B:23:GLN:O	1:B:24:ARG:HG2	0.58	1.99	3	1
1:A:32:THR:N	1:B:68:ASP:OD2	0.58	2.37	5	1
1:A:15:PHE:CG	1:A:16:ILE:N	0.58	2.71	7	1
1:A:70:LYS:O	1:B:38:ARG:NH1	0.58	2.37	2	1
1:A:17:ASN:HA	1:A:59:TRP:HD1	0.58	1.50	3	1
1:A:38:ARG:CZ	1:A:50:GLU:HG2	0.58	2.28	7	1
1:B:63:PHE:O	1:B:64:MET:C	0.58	2.43	5	6
1:B:36:CYS:SG	1:B:37:PRO:HD2	0.58	2.39	7	2
1:A:31:THR:HB	1:A:34:SER:HB3	0.58	1.76	5	1
1:A:30:ARG:CG	1:A:41:VAL:HG22	0.58	2.29	6	3
1:A:12:CYS:SG	1:A:16:ILE:N	0.58	2.77	5	1
1:B:64:MET:SD	1:B:65:LYS:NZ	0.58	2.72	7	1
1:A:71:THR:CG2	1:B:40:ALA:C	0.57	2.77	1	1
1:A:17:ASN:H	1:A:57:GLN:HG2	0.57	1.58	3	1
1:A:58:LYS:HZ1	1:A:62:ASP:CG	0.57	2.07	5	1
1:B:29:ARG:HD2	1:B:42:ILE:HB	0.57	1.74	6	1
1:B:44:LYS:HD3	1:B:45:THR:N	0.57	2.14	2	1
1:A:73:THR:O	1:A:75:LYS:NZ	0.57	2.37	6	1
1:A:64:MET:O	1:A:68:ASP:HB2	0.57	1.99	5	3
1:A:75:LYS:CG	1:B:18:LYS:H	0.57	2.12	3	1
1:A:54:ASP:H	1:A:57:GLN:NE2	0.57	1.96	4	1
1:A:12:CYS:SG	1:A:38:ARG:HD3	0.57	2.39	7	1
1:A:29:ARG:HG2	1:B:27:SER:HB2	0.57	1.76	7	1
1:A:67:LEU:O	1:A:68:ASP:C	0.57	2.47	2	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:SER:OG	1:B:32:THR:N	0.57	2.37	2	2
1:A:40:ALA:HA	1:B:68:ASP:CG	0.57	2.24	4	1
1:A:64:MET:O	1:A:68:ASP:CB	0.57	2.52	3	1
1:A:71:THR:CA	1:B:39:GLU:HB2	0.57	2.26	3	1
1:A:31:THR:HB	1:B:68:ASP:HA	0.57	1.76	4	1
1:A:70:LYS:NZ	1:B:31:THR:O	0.57	2.36	5	2
1:B:26:GLU:HG3	1:B:44:LYS:CG	0.57	2.30	5	1
1:A:59:TRP:CG	1:A:60:VAL:N	0.57	2.72	2	2
1:B:57:GLN:NE2	1:B:57:GLN:H	0.57	1.97	3	1
1:A:30:ARG:HB2	1:A:31:THR:HA	0.57	1.75	4	1
1:B:19:LYS:HZ1	1:B:25:LEU:CB	0.57	2.13	1	1
1:B:44:LYS:HA	1:B:49:LYS:O	0.57	2.00	4	5
1:A:67:LEU:HB2	1:B:30:ARG:HH12	0.57	1.59	2	1
1:A:75:LYS:HB2	1:B:56:THR:OG1	0.57	2.00	2	1
1:B:28:TYR:CG	1:B:30:ARG:HD2	0.57	2.33	5	1
1:B:24:ARG:HG3	1:B:25:LEU:O	0.57	2.00	3	1
1:B:41:VAL:HG12	1:B:54:ASP:H	0.57	1.60	4	1
1:A:14:ARG:NH2	1:A:14:ARG:C	0.57	2.63	7	1
1:A:34:SER:OG	1:B:70:LYS:HG3	0.57	1.98	7	1
1:A:38:ARG:O	1:A:38:ARG:NH2	0.57	2.38	1	1
1:A:62:ASP:O	1:A:66:HIS:HB2	0.57	2.00	4	2
1:A:30:ARG:HG2	1:A:42:ILE:HG13	0.57	1.75	4	1
1:A:65:LYS:HB2	1:A:65:LYS:NZ	0.57	2.15	3	1
1:A:57:GLN:O	1:A:61:GLN:NE2	0.57	2.38	4	1
1:A:73:THR:OG1	1:B:57:GLN:CA	0.56	2.53	1	2
1:B:62:ASP:O	1:B:63:PHE:C	0.56	2.48	4	6
1:A:30:ARG:HD2	1:A:41:VAL:HG22	0.56	1.77	2	2
1:A:31:THR:CG2	1:A:32:THR:N	0.56	2.67	4	1
1:B:19:LYS:HB2	1:B:59:TRP:CZ3	0.56	2.35	7	1
1:B:22:LYS:HE3	1:B:51:ILE:CG1	0.56	2.30	3	1
1:B:19:LYS:NZ	1:B:63:PHE:CE1	0.56	2.71	4	1
1:A:58:LYS:HD2	1:A:59:TRP:N	0.56	2.16	3	1
1:B:12:CYS:SG	1:B:40:ALA:HB1	0.56	2.40	3	1
1:B:24:ARG:CG	1:B:25:LEU:CA	0.56	2.84	3	1
1:A:14:ARG:CA	1:A:14:ARG:HH11	0.56	2.14	5	1
1:A:11:CYS:O	1:A:12:CYS:C	0.56	2.48	6	1
1:B:12:CYS:SG	1:B:40:ALA:HB3	0.56	2.40	3	1
1:A:40:ALA:CA	1:B:68:ASP:HB3	0.56	2.30	4	1
1:A:58:LYS:CE	1:A:58:LYS:C	0.56	2.78	5	1
1:B:24:ARG:HD2	1:B:24:ARG:N	0.56	2.15	6	1
1:A:36:CYS:SG	1:A:37:PRO:HD3	0.56	2.40	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:THR:HG21	1:A:34:SER:OG	0.56	2.00	7	1
1:A:36:CYS:SG	1:A:37:PRO:CG	0.56	2.94	5	2
1:A:61:GLN:N	1:A:61:GLN:NE2	0.56	2.54	4	1
1:B:57:GLN:HA	1:B:59:TRP:CD1	0.56	2.36	2	1
1:A:30:ARG:NH2	1:A:53:ALA:O	0.56	2.39	4	1
1:A:29:ARG:NH2	1:B:27:SER:OG	0.56	2.39	7	1
1:B:68:ASP:CG	1:B:69:LYS:HZ3	0.56	2.08	7	1
1:B:59:TRP:CE2	1:B:60:VAL:HG23	0.56	2.36	3	2
1:A:19:LYS:O	1:A:20:ILE:C	0.56	2.49	7	2
1:A:32:THR:C	1:A:39:GLU:HG2	0.56	2.25	5	1
1:B:57:GLN:N	1:B:61:GLN:HE22	0.56	1.98	5	1
1:A:41:VAL:CB	1:A:64:MET:HB3	0.56	2.30	4	1
1:A:68:ASP:CG	1:A:69:LYS:H	0.56	2.09	1	1
1:A:17:ASN:CA	1:A:59:TRP:NE1	0.56	2.69	2	1
1:A:19:LYS:HE3	1:A:63:PHE:CE2	0.56	2.36	2	1
1:A:27:SER:CB	1:B:34:SER:OG	0.56	2.54	2	1
1:A:70:LYS:HE2	1:B:30:ARG:HB3	0.56	1.78	3	1
1:A:44:LYS:NZ	1:A:48:ASP:CG	0.56	2.64	4	1
1:B:45:THR:HB	1:B:49:LYS:HB2	0.56	1.76	7	1
1:A:72:GLN:OE1	1:B:38:ARG:NH2	0.55	2.40	1	1
1:B:44:LYS:NZ	1:B:48:ASP:OD2	0.55	2.39	4	1
1:A:59:TRP:CE2	1:A:60:VAL:HG22	0.55	2.35	6	1
1:B:46:LYS:O	1:B:46:LYS:CE	0.55	2.54	7	1
1:A:62:ASP:O	1:A:63:PHE:C	0.55	2.49	2	2
1:A:19:LYS:CB	1:A:59:TRP:HB2	0.55	2.32	2	1
1:A:30:ARG:HD2	1:A:41:VAL:CG2	0.55	2.31	2	2
1:B:14:ARG:HB3	1:B:14:ARG:CZ	0.55	2.31	1	1
1:A:59:TRP:CE2	1:A:60:VAL:CG2	0.55	2.90	3	2
1:B:52:CYS:O	1:B:53:ALA:CB	0.55	2.54	7	1
1:A:13:TYR:CD1	1:A:13:TYR:C	0.55	2.85	4	1
1:B:28:TYR:CE2	1:B:30:ARG:CD	0.55	2.90	5	1
1:A:30:ARG:HG2	1:A:41:VAL:HG22	0.55	1.76	3	2
1:A:75:LYS:CB	1:B:18:LYS:H	0.55	2.15	3	1
1:A:28:TYR:O	1:B:29:ARG:HA	0.55	2.01	4	1
1:A:32:THR:HG21	1:B:70:LYS:HB3	0.55	1.79	4	1
1:A:12:CYS:SG	1:A:38:ARG:CD	0.55	2.94	7	1
1:B:41:VAL:HG12	1:B:42:ILE:N	0.55	2.17	6	2
1:B:43:PHE:CE1	1:B:60:VAL:HG13	0.55	2.37	2	1
1:A:64:MET:SD	1:A:65:LYS:HG3	0.55	2.42	4	1
1:A:33:SER:O	1:A:34:SER:CB	0.55	2.55	7	1
1:A:58:LYS:N	1:A:61:GLN:OE1	0.55	2.39	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:PHE:CE2	1:B:63:PHE:CG	0.55	2.95	1	3
1:B:62:ASP:OD1	1:B:65:LYS:NZ	0.55	2.39	4	3
1:A:70:LYS:O	1:A:71:THR:CB	0.55	2.55	4	2
1:A:30:ARG:C	1:B:27:SER:OG	0.55	2.50	5	1
1:B:47:LEU:O	1:B:49:LYS:CE	0.55	2.55	1	1
1:B:60:VAL:O	1:B:63:PHE:HB3	0.55	2.01	2	2
1:A:30:ARG:HH11	1:A:41:VAL:HB	0.55	1.62	5	1
1:B:57:GLN:O	1:B:60:VAL:HG12	0.55	2.02	6	2
1:A:74:PRO:O	1:A:75:LYS:CB	0.55	2.55	7	1
1:B:25:LEU:H	1:B:70:LYS:HD3	0.55	1.62	7	1
1:B:57:GLN:HG3	1:B:59:TRP:CD1	0.55	2.37	7	1
1:A:29:ARG:NH2	1:A:50:GLU:OE2	0.54	2.40	6	1
1:B:18:LYS:NZ	1:B:19:LYS:O	0.54	2.39	1	1
1:B:24:ARG:HG3	1:B:25:LEU:CA	0.54	2.32	3	1
1:A:30:ARG:HE	1:A:40:ALA:CA	0.54	2.15	4	1
1:B:58:LYS:H	1:B:58:LYS:HD3	0.54	1.61	4	1
1:A:34:SER:HA	1:B:68:ASP:C	0.54	2.27	5	1
1:A:26:GLU:CB	1:A:44:LYS:NZ	0.54	2.70	4	1
1:A:19:LYS:NZ	1:A:21:PRO:O	0.54	2.38	6	1
1:A:43:PHE:CE1	1:A:59:TRP:CH2	0.54	2.96	6	2
1:A:44:LYS:HB2	1:A:50:GLU:HG3	0.54	1.78	3	1
1:A:30:ARG:NH1	1:A:38:ARG:O	0.54	2.40	4	1
1:A:12:CYS:SG	1:A:15:PHE:HA	0.54	2.42	6	2
1:A:38:ARG:O	1:A:38:ARG:NH1	0.54	2.40	5	1
1:B:25:LEU:H	1:B:70:LYS:CD	0.54	2.16	7	1
1:A:44:LYS:HG2	1:A:45:THR:N	0.54	2.18	3	2
1:A:59:TRP:CH2	1:A:60:VAL:CG2	0.54	2.90	4	1
1:A:31:THR:CB	1:B:68:ASP:OD1	0.54	2.56	5	1
1:B:25:LEU:O	1:B:70:LYS:HD3	0.54	2.02	7	1
1:A:12:CYS:SG	1:A:38:ARG:NH2	0.54	2.80	1	1
1:A:71:THR:HB	1:B:30:ARG:NH2	0.54	2.18	1	1
1:B:12:CYS:HB3	1:B:32:THR:CG2	0.54	2.33	3	1
1:B:28:TYR:CE1	1:B:30:ARG:NE	0.54	2.75	3	1
1:A:30:ARG:HH22	1:A:31:THR:C	0.54	2.10	5	1
1:A:19:LYS:O	1:A:19:LYS:HD2	0.54	2.03	7	1
1:B:26:GLU:CD	1:B:44:LYS:NZ	0.54	2.66	2	1
1:A:75:LYS:H	1:B:54:ASP:HB3	0.54	1.62	3	1
1:A:28:TYR:CZ	1:A:67:LEU:HD12	0.54	2.38	1	1
1:A:68:ASP:O	1:B:30:ARG:NH2	0.54	2.41	5	2
1:B:19:LYS:NZ	1:B:66:HIS:CD2	0.54	2.76	5	1
1:B:28:TYR:HB3	1:B:63:PHE:CE2	0.53	2.38	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:ARG:NH2	1:A:42:ILE:CD1	0.53	2.72	2	1
1:B:57:GLN:O	1:B:60:VAL:HB	0.53	2.03	2	2
1:A:18:LYS:HD2	1:A:18:LYS:O	0.53	2.03	4	1
1:A:30:ARG:HD3	1:A:41:VAL:O	0.53	2.03	4	1
1:B:23:GLN:CG	1:B:24:ARG:H	0.53	2.16	4	1
1:B:69:LYS:O	1:B:69:LYS:CD	0.53	2.52	4	1
1:B:56:THR:N	1:B:57:GLN:OE1	0.53	2.41	6	1
1:B:22:LYS:C	1:B:23:GLN:HG3	0.53	2.28	2	1
1:A:30:ARG:HG3	1:A:41:VAL:CA	0.53	2.32	4	1
1:A:36:CYS:SG	1:A:37:PRO:HG2	0.53	2.44	5	1
1:A:18:LYS:N	1:A:59:TRP:CZ2	0.53	2.77	6	1
1:A:58:LYS:O	1:A:62:ASP:HB2	0.53	2.03	7	1
1:B:24:ARG:HD3	1:B:47:LEU:N	0.53	2.18	1	1
1:A:33:SER:HA	1:B:26:GLU:HA	0.53	1.79	2	1
1:A:38:ARG:H	1:A:38:ARG:HD2	0.53	1.63	3	1
1:B:26:GLU:CG	1:B:45:THR:N	0.53	2.66	5	1
1:B:25:LEU:O	1:B:70:LYS:CE	0.53	2.56	7	1
1:B:46:LYS:O	1:B:46:LYS:CD	0.53	2.56	1	1
1:A:30:ARG:CG	1:A:42:ILE:HG13	0.53	2.34	4	1
1:A:46:LYS:CE	1:B:34:SER:O	0.53	2.57	2	1
1:B:16:ILE:O	1:B:17:ASN:C	0.53	2.50	4	1
1:A:41:VAL:CG2	1:A:42:ILE:N	0.53	2.71	5	1
1:B:57:GLN:O	1:B:58:LYS:C	0.53	2.51	2	3
1:B:20:ILE:HB	1:B:21:PRO:HD3	0.53	1.79	4	1
1:A:15:PHE:HA	1:A:52:CYS:SG	0.53	2.44	5	1
1:A:11:CYS:CB	1:A:38:ARG:HA	0.53	2.32	1	1
1:A:22:LYS:NZ	1:B:33:SER:O	0.53	2.41	1	1
1:B:58:LYS:HD3	1:B:58:LYS:N	0.53	2.18	1	1
1:B:17:ASN:O	1:B:59:TRP:CD1	0.53	2.62	5	1
1:B:28:TYR:CG	1:B:28:TYR:N	0.53	2.76	7	1
1:A:64:MET:O	1:A:68:ASP:HB3	0.53	2.03	1	1
1:A:75:LYS:HE2	1:A:75:LYS:O	0.53	2.03	1	1
1:A:34:SER:CA	1:B:27:SER:CB	0.53	2.87	3	1
1:A:18:LYS:NZ	1:A:18:LYS:CB	0.53	2.71	4	1
1:A:43:PHE:CE2	1:A:63:PHE:CG	0.53	2.97	1	3
1:B:13:TYR:CD1	1:B:15:PHE:CZ	0.53	2.96	2	1
1:B:44:LYS:HD3	1:B:44:LYS:C	0.53	2.27	2	1
1:A:74:PRO:HB2	1:B:53:ALA:C	0.53	2.29	3	1
1:B:66:HIS:O	1:B:69:LYS:NZ	0.53	2.42	3	1
1:A:26:GLU:HB3	1:B:35:HIS:CE1	0.53	2.38	4	1
1:A:33:SER:HB3	1:A:39:GLU:CG	0.53	2.34	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:23:GLN:OE1	1:B:24:ARG:NH1	0.53	2.41	5	1
1:B:22:LYS:HZ1	1:B:62:ASP:CB	0.53	2.17	7	1
1:A:40:ALA:HA	1:B:68:ASP:CB	0.53	2.34	4	1
1:B:44:LYS:NZ	1:B:48:ASP:O	0.52	2.42	3	1
1:A:30:ARG:O	1:B:28:TYR:CG	0.52	2.62	4	1
1:A:31:THR:HB	1:B:68:ASP:CA	0.52	2.34	4	1
1:A:59:TRP:CZ2	1:A:60:VAL:CG2	0.52	2.92	4	1
1:A:70:LYS:NZ	1:B:39:GLU:OE1	0.52	2.41	4	2
1:A:26:GLU:HG2	1:B:29:ARG:CZ	0.52	2.34	5	1
1:A:28:TYR:CZ	1:A:67:LEU:CB	0.52	2.92	5	1
1:A:30:ARG:HA	1:A:30:ARG:NE	0.52	2.19	5	1
1:A:42:ILE:HG12	1:A:52:CYS:HA	0.52	1.80	1	2
1:A:46:LYS:O	1:A:46:LYS:HG2	0.52	2.03	4	2
1:B:42:ILE:HA	1:B:51:ILE:O	0.52	2.05	4	5
1:B:14:ARG:NH2	1:B:50:GLU:OE1	0.52	2.42	2	1
1:A:68:ASP:O	1:B:30:ARG:NH1	0.52	2.42	3	2
1:A:75:LYS:HZ3	1:B:59:TRP:CG	0.52	2.22	4	1
1:B:19:LYS:HE3	1:B:63:PHE:HA	0.52	1.79	5	1
1:A:70:LYS:HD2	1:B:39:GLU:CD	0.52	2.28	6	1
1:B:15:PHE:CD1	1:B:15:PHE:N	0.52	2.77	6	1
1:A:28:TYR:CZ	1:A:67:LEU:CD1	0.52	2.92	1	1
1:A:16:ILE:HD13	1:A:16:ILE:N	0.52	2.19	3	1
1:A:30:ARG:NE	1:A:64:MET:HE2	0.52	2.18	3	1
1:A:54:ASP:OD2	1:B:70:LYS:NZ	0.52	2.42	1	1
1:A:58:LYS:CD	1:A:59:TRP:N	0.52	2.73	6	2
1:A:68:ASP:OD2	1:A:69:LYS:NZ	0.52	2.42	4	1
1:B:57:GLN:O	1:B:59:TRP:N	0.52	2.41	5	2
1:A:27:SER:HA	1:B:31:THR:HB	0.52	1.81	3	1
1:B:31:THR:O	1:B:39:GLU:HB2	0.52	2.03	5	1
1:A:18:LYS:HA	1:A:59:TRP:CE2	0.52	2.39	6	1
1:B:28:TYR:CE1	1:B:30:ARG:HD3	0.52	2.40	1	2
1:B:26:GLU:CB	1:B:44:LYS:HD2	0.52	2.35	3	1
1:B:41:VAL:HG12	1:B:54:ASP:HB2	0.52	1.79	4	1
1:A:57:GLN:O	1:A:60:VAL:N	0.52	2.43	7	2
1:A:17:ASN:O	1:A:18:LYS:NZ	0.52	2.42	6	1
1:A:41:VAL:O	1:A:53:ALA:HB3	0.52	2.04	6	1
1:A:24:ARG:NH1	1:B:34:SER:C	0.52	2.68	1	2
1:B:17:ASN:HA	1:B:57:GLN:NE2	0.52	2.19	1	1
1:A:53:ALA:HB1	1:A:60:VAL:HG13	0.52	1.81	5	1
1:B:36:CYS:O	1:B:38:ARG:N	0.52	2.43	5	1
1:A:13:TYR:O	1:A:14:ARG:HB2	0.52	2.04	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:64:MET:C	1:B:68:ASP:HB2	0.52	2.30	2	1
1:A:29:ARG:HH22	1:A:50:GLU:CD	0.52	2.13	4	1
1:A:32:THR:HG22	1:A:39:GLU:H	0.52	1.64	4	1
1:A:34:SER:HB3	1:B:70:LYS:HE3	0.52	1.81	7	1
1:A:31:THR:HG21	1:B:68:ASP:HA	0.52	1.82	3	1
1:A:31:THR:O	1:A:39:GLU:HA	0.52	2.05	4	1
1:A:15:PHE:CE2	1:A:59:TRP:NE1	0.52	2.78	5	1
1:B:29:ARG:HH12	1:B:50:GLU:CD	0.52	2.13	1	1
1:B:57:GLN:CD	1:B:57:GLN:H	0.52	2.13	3	1
1:A:29:ARG:CZ	1:A:42:ILE:HD13	0.52	2.35	4	1
1:A:71:THR:HG21	1:B:54:ASP:CG	0.52	2.30	4	1
1:B:67:LEU:C	1:B:69:LYS:H	0.52	2.04	5	1
1:A:42:ILE:HG12	1:A:52:CYS:CA	0.51	2.35	4	1
1:B:62:ASP:OD2	1:B:65:LYS:NZ	0.51	2.43	3	1
1:A:57:GLN:C	1:A:61:GLN:HE22	0.51	2.13	5	2
1:A:32:THR:N	1:A:39:GLU:CD	0.51	2.69	1	1
1:B:17:ASN:CA	1:B:57:GLN:NE2	0.51	2.73	1	1
1:B:53:ALA:HB1	1:B:60:VAL:CG2	0.51	2.35	4	2
1:A:16:ILE:HA	1:A:57:GLN:CD	0.51	2.30	3	1
1:A:38:ARG:HH11	1:A:38:ARG:HG3	0.51	1.65	3	1
1:A:41:VAL:HB	1:A:64:MET:HB3	0.51	1.81	4	1
1:A:34:SER:HA	1:A:39:GLU:CD	0.51	2.31	2	1
1:A:54:ASP:C	1:A:56:THR:H	0.51	2.14	2	2
1:A:59:TRP:CD1	1:A:59:TRP:N	0.51	2.79	2	1
1:A:67:LEU:HB2	1:B:30:ARG:NH1	0.51	2.19	2	1
1:B:38:ARG:CZ	1:B:54:ASP:O	0.51	2.58	3	1
1:A:73:THR:OG1	1:A:75:LYS:NZ	0.51	2.41	6	1
1:A:68:ASP:OD1	1:A:69:LYS:NZ	0.51	2.42	5	2
1:A:16:ILE:HB	1:A:59:TRP:CH2	0.51	2.41	2	1
1:B:14:ARG:NH1	1:B:50:GLU:O	0.51	2.44	4	1
1:A:12:CYS:O	1:A:15:PHE:N	0.51	2.43	6	2
1:A:17:ASN:HB3	1:A:57:GLN:CD	0.51	2.30	6	1
1:B:11:CYS:O	1:B:38:ARG:NH2	0.51	2.43	6	1
1:A:62:ASP:OD1	1:A:65:LYS:NZ	0.51	2.39	1	1
1:A:71:THR:CB	1:B:30:ARG:HH21	0.51	2.18	1	1
1:A:13:TYR:O	1:A:14:ARG:CB	0.51	2.58	2	1
1:B:66:HIS:CE1	1:B:69:LYS:NZ	0.51	2.79	6	1
1:B:31:THR:OG1	1:B:32:THR:N	0.51	2.44	7	1
1:A:57:GLN:O	1:A:58:LYS:C	0.51	2.54	3	4
1:A:70:LYS:HE3	1:A:70:LYS:O	0.51	2.05	4	1
1:B:30:ARG:CG	1:B:41:VAL:CG2	0.51	2.87	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:15:PHE:CD2	1:B:16:ILE:N	0.51	2.79	6	2
1:B:58:LYS:H	1:B:58:LYS:CD	0.51	2.19	4	3
1:B:57:GLN:O	1:B:60:VAL:N	0.51	2.44	2	3
1:B:24:ARG:CG	1:B:25:LEU:HA	0.51	2.35	3	1
1:A:12:CYS:O	1:A:14:ARG:N	0.51	2.44	5	1
1:A:28:TYR:CE2	1:A:67:LEU:CB	0.51	2.94	5	1
1:A:43:PHE:CD1	1:A:59:TRP:CZ3	0.51	2.98	5	1
1:A:16:ILE:O	1:A:17:ASN:C	0.51	2.53	2	2
1:A:16:ILE:HD13	1:A:16:ILE:H	0.51	1.65	3	1
1:A:65:LYS:NZ	1:A:65:LYS:CB	0.51	2.74	3	1
1:A:75:LYS:HZ3	1:B:57:GLN:CD	0.51	2.14	5	1
1:A:11:CYS:SG	1:A:37:PRO:HG2	0.51	2.46	4	2
1:B:54:ASP:O	1:B:61:GLN:NE2	0.51	2.43	2	1
1:B:64:MET:O	1:B:66:HIS:N	0.51	2.44	2	1
1:B:64:MET:O	1:B:68:ASP:N	0.51	2.44	5	3
1:A:30:ARG:HE	1:A:40:ALA:C	0.51	2.14	4	1
1:A:39:GLU:CB	1:B:68:ASP:O	0.51	2.59	4	1
1:B:62:ASP:CG	1:B:65:LYS:HZ3	0.51	2.14	4	1
1:B:20:ILE:H	1:B:20:ILE:CD1	0.51	2.19	5	2
1:A:23:GLN:O	1:A:24:ARG:NE	0.50	2.43	7	2
1:A:29:ARG:HG2	1:B:27:SER:CB	0.50	2.36	7	1
1:A:16:ILE:O	1:A:17:ASN:CG	0.50	2.55	2	1
1:A:26:GLU:HG2	1:A:45:THR:C	0.50	2.31	3	1
1:A:70:LYS:HA	1:B:38:ARG:CZ	0.50	2.36	2	1
1:B:13:TYR:O	1:B:15:PHE:N	0.50	2.44	7	2
1:A:71:THR:O	1:A:73:THR:N	0.50	2.45	3	1
1:A:41:VAL:CG2	1:A:64:MET:CB	0.50	2.88	4	1
1:A:26:GLU:HG2	1:B:29:ARG:NH2	0.50	2.20	5	1
1:A:30:ARG:NH2	1:A:31:THR:O	0.50	2.45	5	1
1:A:43:PHE:CD1	1:A:59:TRP:CH2	0.50	2.99	5	1
1:B:30:ARG:HG2	1:B:41:VAL:HG23	0.50	1.79	5	1
1:A:25:LEU:HD23	1:A:26:GLU:N	0.50	2.22	6	1
1:A:44:LYS:NZ	1:A:48:ASP:O	0.50	2.44	7	1
1:B:25:LEU:C	1:B:70:LYS:HE2	0.50	2.31	7	1
1:A:59:TRP:CH2	1:A:60:VAL:HG23	0.50	2.42	2	1
1:A:28:TYR:OH	1:B:30:ARG:NH1	0.50	2.43	3	2
1:B:25:LEU:CB	1:B:44:LYS:O	0.50	2.60	3	1
1:A:19:LYS:O	1:A:19:LYS:NZ	0.50	2.44	7	2
1:A:27:SER:HB3	1:B:31:THR:HB	0.50	1.82	5	1
1:A:75:LYS:CG	1:B:17:ASN:H	0.50	2.19	5	1
1:B:32:THR:HA	1:B:39:GLU:HB3	0.50	1.83	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:TYR:CD1	1:A:28:TYR:C	0.50	2.89	3	1
1:A:30:ARG:HB2	1:B:28:TYR:CZ	0.50	2.42	3	1
1:B:20:ILE:HG22	1:B:21:PRO:CD	0.50	2.37	3	1
1:A:44:LYS:HA	1:A:49:LYS:O	0.50	2.06	4	1
1:A:75:LYS:HD3	1:B:59:TRP:CD1	0.50	2.42	4	1
1:A:30:ARG:NH1	1:A:30:ARG:HA	0.50	2.20	5	1
1:A:43:PHE:HB2	1:A:51:ILE:HB	0.50	1.82	5	1
1:A:58:LYS:HG3	1:A:59:TRP:N	0.50	2.21	7	2
1:A:30:ARG:CZ	1:B:68:ASP:CG	0.50	2.84	6	1
1:B:29:ARG:HD2	1:B:42:ILE:CB	0.50	2.37	6	1
1:A:28:TYR:HA	1:A:42:ILE:O	0.50	2.07	3	1
1:A:38:ARG:NH1	1:A:52:CYS:SG	0.50	2.80	4	1
1:B:44:LYS:NZ	1:B:50:GLU:OE2	0.50	2.44	5	1
1:B:14:ARG:NH1	1:B:16:ILE:CG2	0.50	2.75	6	1
1:A:38:ARG:HD3	1:A:38:ARG:O	0.50	2.07	7	1
1:A:56:THR:H	1:A:61:GLN:NE2	0.50	2.05	1	1
1:A:65:LYS:O	1:A:69:LYS:NZ	0.50	2.41	2	1
1:A:29:ARG:NH1	1:A:35:HIS:O	0.50	2.44	3	1
1:A:26:GLU:HB2	1:A:44:LYS:NZ	0.50	2.20	4	1
1:A:16:ILE:O	1:A:17:ASN:ND2	0.50	2.45	6	1
1:A:53:ALA:HB1	1:A:60:VAL:HG22	0.50	1.84	6	1
1:B:60:VAL:O	1:B:61:GLN:C	0.50	2.53	7	1
1:A:60:VAL:O	1:A:61:GLN:C	0.50	2.52	4	2
1:B:49:LYS:HD2	1:B:49:LYS:N	0.50	2.22	1	1
1:B:26:GLU:CG	1:B:44:LYS:HG3	0.50	2.34	5	1
1:B:14:ARG:HH12	1:B:16:ILE:CG2	0.50	2.20	6	1
1:A:26:GLU:HG2	1:A:47:LEU:H	0.50	1.65	7	1
1:B:17:ASN:O	1:B:18:LYS:HG2	0.50	2.06	3	1
1:A:12:CYS:HB2	1:A:38:ARG:NE	0.50	2.22	4	1
1:A:30:ARG:NH2	1:A:38:ARG:O	0.50	2.44	4	1
1:A:30:ARG:N	1:B:28:TYR:O	0.50	2.45	4	1
1:A:31:THR:HG22	1:A:32:THR:H	0.50	1.66	4	1
1:A:14:ARG:HH11	1:A:14:ARG:HA	0.50	1.67	5	1
1:A:34:SER:HA	1:B:69:LYS:N	0.50	2.22	5	1
1:A:30:ARG:HH22	1:A:39:GLU:CD	0.50	2.15	6	1
1:A:48:ASP:O	1:A:49:LYS:CE	0.50	2.60	7	1
1:A:57:GLN:O	1:A:59:TRP:N	0.50	2.45	7	1
1:A:63:PHE:HA	1:A:66:HIS:CB	0.49	2.36	2	1
1:A:68:ASP:CA	1:A:70:LYS:HE2	0.49	2.36	2	1
1:A:30:ARG:HB2	1:A:31:THR:CA	0.49	2.37	4	1
1:B:19:LYS:HG3	1:B:59:TRP:CZ3	0.49	2.41	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:26:GLU:OE2	1:B:45:THR:HA	0.49	2.07	4	1
1:A:30:ARG:O	1:B:27:SER:HB3	0.49	2.07	7	1
1:B:18:LYS:NZ	1:B:56:THR:OG1	0.49	2.45	2	1
1:A:13:TYR:CD1	1:A:14:ARG:N	0.49	2.79	3	1
1:A:74:PRO:CG	1:B:60:VAL:HG21	0.49	2.35	3	1
1:A:28:TYR:HB2	1:A:42:ILE:O	0.49	2.06	4	1
1:B:23:GLN:CD	1:B:24:ARG:H	0.49	2.15	4	1
1:B:14:ARG:O	1:B:14:ARG:NE	0.49	2.45	7	1
1:A:32:THR:HB	1:A:35:HIS:HA	0.49	1.82	2	1
1:A:74:PRO:C	1:B:57:GLN:HE22	0.49	2.15	3	1
1:A:21:PRO:O	1:A:22:LYS:HE3	0.49	2.07	4	1
1:A:58:LYS:C	1:A:58:LYS:HE3	0.49	2.32	5	1
1:A:73:THR:HB	1:B:56:THR:OG1	0.49	2.07	7	1
1:B:28:TYR:CE1	1:B:64:MET:HA	0.49	2.43	7	1
1:A:53:ALA:HB1	1:A:57:GLN:NE2	0.49	2.22	1	1
1:B:24:ARG:O	1:B:27:SER:HA	0.49	2.08	3	1
1:B:59:TRP:NE1	1:B:60:VAL:HG23	0.49	2.22	3	1
1:A:43:PHE:O	1:A:51:ILE:N	0.49	2.45	5	1
1:A:17:ASN:HB3	1:A:57:GLN:OE1	0.49	2.07	6	1
1:A:26:GLU:HB2	1:A:45:THR:C	0.49	2.32	6	1
1:B:20:ILE:HD12	1:B:20:ILE:H	0.49	1.67	6	1
1:A:32:THR:H	1:A:39:GLU:CD	0.49	2.16	1	1
1:B:68:ASP:OD1	1:B:69:LYS:NZ	0.49	2.44	1	2
1:A:13:TYR:O	1:A:14:ARG:NH2	0.49	2.45	3	2
1:A:58:LYS:O	1:A:61:GLN:HB2	0.49	2.06	3	2
1:B:38:ARG:HE	1:B:55:PRO:CA	0.49	2.20	3	1
1:A:30:ARG:NH2	1:A:31:THR:CG2	0.49	2.75	5	1
1:A:75:LYS:HE2	1:B:14:ARG:O	0.49	2.06	5	1
1:B:57:GLN:N	1:B:57:GLN:CD	0.49	2.69	6	1
1:B:19:LYS:HZ1	1:B:25:LEU:HB2	0.49	1.66	1	1
1:A:31:THR:HB	1:B:26:GLU:O	0.49	2.07	2	1
1:A:62:ASP:O	1:A:65:LYS:N	0.49	2.45	2	1
1:B:67:LEU:O	1:B:68:ASP:C	0.49	2.56	4	4
1:A:75:LYS:HZ1	1:B:54:ASP:CG	0.49	2.16	5	1
1:A:43:PHE:CE2	1:A:59:TRP:CH2	0.49	3.00	7	1
1:A:28:TYR:OH	1:B:30:ARG:NH2	0.49	2.46	1	1
1:B:34:SER:HA	1:B:39:GLU:OE2	0.49	2.07	1	1
1:A:38:ARG:HH12	1:A:54:ASP:CG	0.49	2.16	3	1
1:B:24:ARG:HH22	1:B:26:GLU:CD	0.49	2.15	3	1
1:B:62:ASP:CG	1:B:65:LYS:NZ	0.49	2.71	4	1
1:A:23:GLN:O	1:A:24:ARG:CB	0.49	2.60	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:46:LYS:O	1:B:46:LYS:CG	0.49	2.60	5	1
1:B:30:ARG:HA	1:B:40:ALA:O	0.49	2.07	1	1
1:B:69:LYS:C	1:B:70:LYS:HE3	0.49	2.33	1	1
1:B:23:GLN:CA	1:B:25:LEU:HD13	0.49	2.37	3	1
1:A:59:TRP:CD2	1:A:60:VAL:HG23	0.49	2.41	4	1
1:A:68:ASP:HA	1:B:30:ARG:CZ	0.49	2.36	4	1
1:A:30:ARG:HH22	1:A:32:THR:N	0.49	2.05	5	1
1:B:30:ARG:CG	1:B:41:VAL:HG23	0.49	2.37	5	1
1:B:14:ARG:NH1	1:B:16:ILE:HG21	0.49	2.22	6	1
1:B:61:GLN:HE21	1:B:61:GLN:N	0.49	2.05	6	1
1:A:28:TYR:CE2	1:A:63:PHE:CE1	0.49	3.00	7	1
1:B:22:LYS:NZ	1:B:62:ASP:HB2	0.49	2.22	7	1
1:B:65:LYS:O	1:B:69:LYS:NZ	0.49	2.43	7	1
1:B:14:ARG:NH1	1:B:14:ARG:CB	0.49	2.75	1	1
1:A:47:LEU:O	1:A:49:LYS:NZ	0.49	2.44	4	2
1:B:49:LYS:HE3	1:B:49:LYS:N	0.49	2.22	3	1
1:A:70:LYS:HD2	1:B:39:GLU:OE1	0.49	2.08	6	2
1:A:15:PHE:HB2	1:A:52:CYS:SG	0.49	2.47	5	1
1:A:61:GLN:HG3	1:A:65:LYS:HZ1	0.49	1.65	7	1
1:B:69:LYS:O	1:B:70:LYS:C	0.49	2.55	1	2
1:B:28:TYR:HH	1:B:67:LEU:HB3	0.49	1.68	2	1
1:A:71:THR:C	1:A:73:THR:N	0.49	2.71	3	1
1:A:11:CYS:O	1:A:38:ARG:NH2	0.49	2.46	4	1
1:B:63:PHE:CD1	1:B:63:PHE:C	0.49	2.90	5	1
1:A:17:ASN:HB3	1:A:57:GLN:NE2	0.49	2.23	6	1
1:A:28:TYR:CD1	1:A:28:TYR:N	0.49	2.81	7	1
1:B:25:LEU:HD13	1:B:27:SER:H	0.49	1.67	7	1
1:A:29:ARG:HH21	1:A:50:GLU:CD	0.48	2.16	6	1
1:A:70:LYS:HE3	1:B:61:GLN:OE1	0.48	2.08	2	1
1:A:43:PHE:CE2	1:A:63:PHE:CE2	0.48	3.02	4	1
1:A:29:ARG:NE	1:A:42:ILE:HB	0.48	2.23	6	1
1:B:22:LYS:NZ	1:B:62:ASP:CB	0.48	2.76	7	1
1:A:73:THR:CA	1:B:53:ALA:O	0.48	2.62	1	1
1:B:19:LYS:HG2	1:B:20:ILE:H	0.48	1.68	1	1
1:B:43:PHE:HE2	1:B:63:PHE:CG	0.48	2.26	1	1
1:A:16:ILE:C	1:A:17:ASN:CG	0.48	2.81	2	1
1:A:31:THR:HG1	1:A:39:GLU:C	0.48	2.16	7	1
1:B:58:LYS:HD2	1:B:58:LYS:C	0.48	2.33	7	1
1:A:26:GLU:O	1:B:32:THR:CA	0.48	2.62	1	1
1:A:29:ARG:HB2	1:A:33:SER:O	0.48	2.09	3	1
1:A:72:GLN:HA	1:B:55:PRO:CG	0.48	2.36	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:LYS:CD	1:B:17:ASN:H	0.48	2.21	5	1
1:B:19:LYS:HZ1	1:B:66:HIS:CG	0.48	2.26	5	1
1:A:34:SER:CB	1:B:70:LYS:CE	0.48	2.92	7	1
1:A:73:THR:CB	1:B:61:GLN:HE22	0.48	2.21	1	1
1:A:41:VAL:O	1:A:53:ALA:N	0.48	2.47	6	2
1:A:30:ARG:O	1:B:28:TYR:CD2	0.48	2.66	4	1
1:A:40:ALA:HB3	1:A:54:ASP:HB2	0.48	1.84	4	1
1:B:64:MET:O	1:B:68:ASP:CA	0.48	2.61	5	1
1:A:30:ARG:HE	1:B:64:MET:HE2	0.48	1.68	7	1
1:B:22:LYS:NZ	1:B:23:GLN:OE1	0.48	2.47	1	1
1:B:49:LYS:H	1:B:49:LYS:HE3	0.48	1.65	3	1
1:A:71:THR:CG2	1:A:72:GLN:N	0.48	2.76	4	1
1:A:57:GLN:CA	1:A:61:GLN:HE22	0.48	2.21	5	1
1:B:14:ARG:O	1:B:14:ARG:HD3	0.48	2.09	6	1
1:A:61:GLN:O	1:A:64:MET:SD	0.48	2.71	1	1
1:B:57:GLN:O	1:B:61:GLN:NE2	0.48	2.47	3	3
1:A:13:TYR:CE2	1:A:14:ARG:CZ	0.48	2.97	2	1
1:B:14:ARG:NH2	1:B:50:GLU:CD	0.48	2.72	2	1
1:A:59:TRP:NE1	1:A:60:VAL:HG23	0.48	2.24	3	1
1:B:15:PHE:CE2	1:B:54:ASP:CG	0.48	2.92	3	1
1:B:24:ARG:HG2	1:B:25:LEU:HA	0.48	1.85	3	1
1:A:30:ARG:CZ	1:A:38:ARG:O	0.48	2.61	4	1
1:A:39:GLU:O	1:A:40:ALA:CB	0.48	2.62	4	2
1:B:14:ARG:HH12	1:B:50:GLU:CD	0.48	2.17	4	1
1:A:24:ARG:NH1	1:B:32:THR:CG2	0.48	2.77	1	1
1:A:42:ILE:CA	1:A:51:ILE:O	0.48	2.60	1	2
1:A:32:THR:O	1:A:38:ARG:N	0.48	2.47	3	1
1:A:30:ARG:HD3	1:A:41:VAL:CA	0.48	2.38	4	1
1:B:28:TYR:CD2	1:B:30:ARG:CD	0.48	2.95	5	1
1:A:67:LEU:CD2	1:B:32:THR:HB	0.48	2.38	2	1
1:B:26:GLU:OE1	1:B:44:LYS:NZ	0.48	2.46	6	2
1:B:41:VAL:HG11	1:B:64:MET:CE	0.48	2.39	2	1
1:B:15:PHE:CG	1:B:54:ASP:HB2	0.48	2.44	3	1
1:A:16:ILE:O	1:A:18:LYS:N	0.48	2.47	7	2
1:A:57:GLN:O	1:A:60:VAL:HB	0.48	2.09	5	1
1:A:54:ASP:HB3	1:A:57:GLN:NE2	0.48	2.24	6	1
1:A:71:THR:HG23	1:A:72:GLN:N	0.48	2.23	7	2
1:A:31:THR:CA	1:A:39:GLU:HB3	0.48	2.39	1	1
1:A:29:ARG:CB	1:B:29:ARG:HG2	0.48	2.39	3	1
1:A:75:LYS:CB	1:B:17:ASN:HA	0.48	2.39	3	1
1:B:28:TYR:CD1	1:B:30:ARG:HG3	0.48	2.43	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:69:LYS:C	1:B:69:LYS:CD	0.48	2.86	4	1
1:B:35:HIS:ND1	1:B:36:CYS:HB3	0.48	2.23	5	1
1:B:30:ARG:CA	1:B:41:VAL:HG22	0.48	2.34	6	1
1:A:34:SER:HB2	1:A:39:GLU:HB2	0.48	1.84	7	1
1:B:54:ASP:OD1	1:B:55:PRO:HD3	0.47	2.08	3	1
1:A:33:SER:H	1:B:68:ASP:CG	0.47	2.17	5	1
1:A:30:ARG:NE	1:B:64:MET:HE2	0.47	2.24	7	1
1:B:43:PHE:CE2	1:B:59:TRP:HZ3	0.47	2.27	7	2
1:B:20:ILE:HB	1:B:21:PRO:CD	0.47	2.39	6	2
1:A:70:LYS:HG2	1:B:38:ARG:NH1	0.47	2.23	5	1
1:A:70:LYS:HZ3	1:B:39:GLU:CD	0.47	2.17	7	1
1:A:25:LEU:O	1:B:32:THR:HG22	0.47	2.09	1	1
1:B:69:LYS:N	1:B:69:LYS:HD2	0.47	2.23	1	1
1:B:62:ASP:O	1:B:65:LYS:N	0.47	2.47	2	3
1:A:27:SER:OG	1:B:32:THR:HA	0.47	2.08	3	1
1:A:30:ARG:NH2	1:A:39:GLU:O	0.47	2.47	4	1
1:A:58:LYS:CG	1:A:59:TRP:N	0.47	2.76	7	2
1:B:32:THR:O	1:B:33:SER:CB	0.47	2.62	4	1
1:A:39:GLU:O	1:A:40:ALA:C	0.47	2.57	7	1
1:A:45:THR:HB	1:A:49:LYS:HB2	0.47	1.86	7	1
1:A:71:THR:O	1:A:72:GLN:HG3	0.47	2.09	2	1
1:B:17:ASN:O	1:B:18:LYS:NZ	0.47	2.48	3	1
1:A:43:PHE:CZ	1:A:63:PHE:CG	0.47	3.02	4	1
1:A:71:THR:CG2	1:A:72:GLN:H	0.47	2.22	4	1
1:A:34:SER:N	1:B:26:GLU:O	0.47	2.47	6	1
1:A:34:SER:CB	1:B:24:ARG:HH22	0.47	2.23	1	1
1:A:57:GLN:NE2	1:A:59:TRP:CZ2	0.47	2.83	1	1
1:B:25:LEU:HD12	1:B:45:THR:HB	0.47	1.85	4	1
1:A:17:ASN:CB	1:A:57:GLN:OE1	0.47	2.63	6	1
1:B:19:LYS:HE3	1:B:20:ILE:O	0.47	2.09	1	1
1:A:67:LEU:CD2	1:B:32:THR:CB	0.47	2.93	2	1
1:B:11:CYS:SG	1:B:40:ALA:HB3	0.47	2.50	2	1
1:B:28:TYR:CD2	1:B:64:MET:HE3	0.47	2.45	2	1
1:B:24:ARG:HG3	1:B:25:LEU:C	0.47	2.35	3	1
1:A:26:GLU:OE1	1:A:44:LYS:NZ	0.47	2.47	4	1
1:A:75:LYS:CE	1:B:14:ARG:O	0.47	2.63	5	1
1:A:28:TYR:CD1	1:B:30:ARG:HB2	0.47	2.44	5	2
1:B:54:ASP:CG	1:B:57:GLN:HE22	0.47	2.18	5	1
1:B:44:LYS:HG2	1:B:45:THR:N	0.47	2.25	6	1
1:B:45:THR:HB	1:B:49:LYS:CG	0.47	2.40	7	1
1:A:57:GLN:O	1:A:60:VAL:HG12	0.47	2.09	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:PHE:CZ	1:B:60:VAL:HA	0.47	2.45	2	1
1:A:26:GLU:CB	1:B:35:HIS:CE1	0.47	2.97	4	1
1:B:25:LEU:HB2	1:B:67:LEU:HD12	0.47	1.87	7	1
1:A:73:THR:HB	1:A:74:PRO:CD	0.47	2.40	2	1
1:B:59:TRP:CZ2	1:B:60:VAL:CG2	0.47	2.98	3	1
1:A:26:GLU:CG	1:A:44:LYS:HZ1	0.47	2.22	4	1
1:B:66:HIS:O	1:B:69:LYS:HE2	0.47	2.10	6	1
1:A:28:TYR:CD2	1:A:64:MET:HE1	0.47	2.45	7	1
1:A:16:ILE:CG2	1:A:59:TRP:CH2	0.46	2.97	2	1
1:A:26:GLU:HG2	1:A:44:LYS:NZ	0.46	2.25	4	2
1:A:33:SER:CA	1:B:26:GLU:HG3	0.46	2.40	2	1
1:A:60:VAL:O	1:A:64:MET:HG2	0.46	2.10	2	1
1:A:75:LYS:HB2	1:B:59:TRP:HE1	0.46	1.70	3	1
1:A:17:ASN:C	1:A:57:GLN:NE2	0.46	2.73	7	1
1:B:57:GLN:HG2	1:B:59:TRP:HE1	0.46	1.70	7	1
1:A:73:THR:HG21	1:B:61:GLN:NE2	0.46	2.25	1	1
1:A:67:LEU:HD22	1:B:32:THR:CB	0.46	2.40	2	1
1:A:67:LEU:CD1	1:B:32:THR:HB	0.46	2.40	2	1
1:A:35:HIS:O	1:A:36:CYS:HB2	0.46	2.09	3	1
1:B:23:GLN:CG	1:B:24:ARG:N	0.46	2.78	4	1
1:A:59:TRP:CZ2	1:A:60:VAL:HG22	0.46	2.45	6	2
1:B:11:CYS:O	1:B:32:THR:HB	0.46	2.11	3	1
1:A:70:LYS:NZ	1:B:39:GLU:OE2	0.46	2.48	6	2
1:B:22:LYS:HZ1	1:B:62:ASP:HB3	0.46	1.69	7	1
1:A:74:PRO:HD3	1:B:53:ALA:HB1	0.46	1.86	1	1
1:B:22:LYS:O	1:B:24:ARG:NE	0.46	2.49	6	1
1:B:25:LEU:N	1:B:70:LYS:HD3	0.46	2.25	7	1
1:B:31:THR:C	1:B:34:SER:OG	0.46	2.59	2	1
1:A:41:VAL:CG2	1:A:64:MET:HB3	0.46	2.41	4	1
1:A:59:TRP:CZ3	1:A:60:VAL:HG22	0.46	2.45	4	1
1:A:75:LYS:HZ3	1:B:59:TRP:CD1	0.46	2.28	4	1
1:A:67:LEU:O	1:A:70:LYS:HG2	0.46	2.11	6	1
1:B:19:LYS:NZ	1:B:19:LYS:O	0.46	2.44	7	1
1:A:65:LYS:NZ	1:A:68:ASP:OD2	0.46	2.43	2	1
1:A:30:ARG:HE	1:A:64:MET:HE2	0.46	1.70	3	1
1:A:71:THR:CG2	1:B:40:ALA:N	0.46	2.78	4	1
1:A:26:GLU:HA	1:B:34:SER:N	0.46	2.25	7	1
1:A:68:ASP:O	1:A:70:LYS:N	0.46	2.49	2	1
1:A:20:ILE:CG1	1:A:21:PRO:HD3	0.46	2.40	3	1
1:A:39:GLU:OE2	1:B:70:LYS:NZ	0.46	2.48	3	1
1:B:22:LYS:NZ	1:B:50:GLU:O	0.46	2.48	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:VAL:CG1	1:A:42:ILE:N	0.46	2.77	4	1
1:A:33:SER:H	1:B:26:GLU:CG	0.46	2.23	2	1
1:A:28:TYR:CZ	1:A:67:LEU:HB2	0.46	2.45	5	1
1:B:55:PRO:N	1:B:57:GLN:HE22	0.46	2.09	6	1
1:B:26:GLU:CB	1:B:44:LYS:C	0.46	2.89	7	1
1:A:22:LYS:HD3	1:A:66:HIS:CE1	0.46	2.46	1	1
1:B:49:LYS:H	1:B:49:LYS:HD2	0.46	1.71	3	1
1:A:73:THR:CG2	1:A:74:PRO:HD2	0.46	2.41	4	1
1:A:61:GLN:O	1:A:64:MET:HG2	0.46	2.10	5	1
1:A:30:ARG:NH2	1:B:68:ASP:CG	0.46	2.74	6	1
1:B:14:ARG:HH12	1:B:16:ILE:HG21	0.46	1.71	6	1
1:B:25:LEU:C	1:B:70:LYS:CE	0.46	2.89	7	1
1:B:30:ARG:HD3	1:B:64:MET:HE3	0.46	1.86	7	1
1:A:73:THR:HB	1:A:74:PRO:HD2	0.46	1.86	2	1
1:A:29:ARG:CG	1:A:42:ILE:HB	0.46	2.41	3	1
1:B:63:PHE:CE1	1:B:67:LEU:HD22	0.46	2.46	3	1
1:A:71:THR:HB	1:B:55:PRO:CG	0.46	2.41	4	1
1:A:33:SER:HB3	1:A:39:GLU:HG2	0.46	1.88	5	1
1:A:38:ARG:NH1	1:A:38:ARG:C	0.46	2.74	5	1
1:B:44:LYS:HE3	1:B:49:LYS:O	0.46	2.11	5	1
1:A:26:GLU:HB2	1:A:44:LYS:O	0.45	2.11	7	2
1:B:35:HIS:H	1:B:39:GLU:CD	0.45	2.19	1	1
1:A:38:ARG:HG2	1:A:40:ALA:CB	0.45	2.41	3	1
1:A:59:TRP:O	1:A:63:PHE:HB2	0.45	2.11	3	2
1:A:32:THR:OG1	1:B:70:LYS:HG2	0.45	2.10	4	1
1:B:26:GLU:CB	1:B:44:LYS:HG3	0.45	2.41	5	1
1:A:45:THR:O	1:A:46:LYS:C	0.45	2.59	7	1
1:B:45:THR:HB	1:B:49:LYS:CB	0.45	2.41	7	1
1:A:62:ASP:O	1:A:65:LYS:C	0.45	2.60	2	1
1:B:59:TRP:CH2	1:B:60:VAL:HG22	0.45	2.46	2	1
1:A:29:ARG:HB3	1:B:29:ARG:HG2	0.45	1.88	3	1
1:A:28:TYR:OH	1:B:30:ARG:NE	0.45	2.49	4	1
1:B:11:CYS:O	1:B:14:ARG:NH1	0.45	2.49	5	1
1:B:18:LYS:HD2	1:B:59:TRP:HB3	0.45	1.88	5	1
1:A:40:ALA:HB1	1:A:53:ALA:O	0.45	2.12	7	1
1:B:61:GLN:O	1:B:65:LYS:HB3	0.45	2.11	1	1
1:A:39:GLU:OE2	1:B:46:LYS:NZ	0.45	2.50	2	1
1:A:17:ASN:OD1	1:A:18:LYS:CE	0.45	2.64	3	1
1:A:32:THR:OG1	1:B:27:SER:CB	0.45	2.64	3	1
1:A:33:SER:C	1:B:27:SER:OG	0.45	2.60	3	1
1:A:65:LYS:HB2	1:A:65:LYS:HZ2	0.45	1.71	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:LEU:O	1:A:69:LYS:N	0.45	2.49	6	3
1:A:43:PHE:CD2	1:A:63:PHE:CE2	0.45	3.04	4	1
1:A:30:ARG:HG2	1:A:40:ALA:O	0.45	2.11	6	1
1:A:33:SER:O	1:A:34:SER:HB2	0.45	2.10	7	1
1:A:75:LYS:O	1:A:75:LYS:CE	0.45	2.64	1	1
1:A:52:CYS:SG	1:A:53:ALA:N	0.45	2.89	2	1
1:B:41:VAL:CG1	1:B:64:MET:HE1	0.45	2.41	2	1
1:B:25:LEU:H	1:B:69:LYS:HB2	0.45	1.71	5	1
1:A:71:THR:HG22	1:B:55:PRO:CD	0.45	2.41	6	1
1:A:19:LYS:O	1:A:19:LYS:CD	0.45	2.64	7	1
1:B:58:LYS:CD	1:B:59:TRP:N	0.45	2.79	2	1
1:B:25:LEU:HD11	1:B:43:PHE:HB3	0.45	1.88	5	1
1:A:30:ARG:HH11	1:A:40:ALA:C	0.45	2.19	6	1
1:A:26:GLU:CD	1:A:46:LYS:N	0.45	2.74	7	1
1:B:56:THR:C	1:B:58:LYS:H	0.45	2.20	2	1
1:A:71:THR:HG23	1:B:39:GLU:C	0.45	2.35	4	1
1:A:11:CYS:SG	1:A:37:PRO:HD2	0.45	2.52	5	1
1:A:58:LYS:NZ	1:A:62:ASP:OD1	0.45	2.49	7	1
1:A:55:PRO:O	1:A:57:GLN:HG3	0.45	2.12	3	1
1:A:22:LYS:O	1:A:24:ARG:N	0.45	2.50	4	1
1:A:31:THR:CB	1:B:68:ASP:HA	0.45	2.41	4	1
1:A:75:LYS:CD	1:B:17:ASN:O	0.45	2.63	4	1
1:B:29:ARG:C	1:B:41:VAL:HG23	0.45	2.37	4	1
1:B:25:LEU:HG	1:B:44:LYS:O	0.45	2.12	6	2
1:B:54:ASP:C	1:B:57:GLN:NE2	0.45	2.75	6	1
1:A:44:LYS:NZ	1:A:50:GLU:OE1	0.45	2.49	7	1
1:A:46:LYS:C	1:A:47:LEU:HD12	0.45	2.36	3	1
1:A:30:ARG:CD	1:A:41:VAL:N	0.45	2.79	4	1
1:A:22:LYS:O	1:A:23:GLN:C	0.45	2.59	1	1
1:B:15:PHE:CZ	1:B:54:ASP:O	0.45	2.70	1	1
1:A:27:SER:HB2	1:B:34:SER:OG	0.45	2.12	2	1
1:B:25:LEU:CD1	1:B:45:THR:HB	0.45	2.42	4	1
1:A:24:ARG:HB2	1:A:46:LYS:CE	0.45	2.42	6	1
1:A:34:SER:HB3	1:B:70:LYS:CE	0.45	2.41	7	1
1:A:64:MET:SD	1:A:65:LYS:N	0.45	2.90	1	1
1:A:66:HIS:CA	1:A:69:LYS:NZ	0.45	2.78	2	1
1:A:26:GLU:OE2	1:A:44:LYS:NZ	0.45	2.50	5	2
1:B:48:ASP:HB3	1:B:49:LYS:NZ	0.45	2.27	3	1
1:A:40:ALA:HB3	1:A:53:ALA:O	0.45	2.11	4	1
1:B:21:PRO:HB2	1:B:66:HIS:CE1	0.45	2.47	4	1
1:B:22:LYS:H	1:B:66:HIS:CD2	0.45	2.29	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:29:ARG:HB2	1:B:44:LYS:HB2	0.45	1.88	5	1
1:A:15:PHE:O	1:A:15:PHE:CD1	0.45	2.69	6	1
1:A:36:CYS:O	1:A:38:ARG:N	0.44	2.49	5	2
1:B:68:ASP:HB3	1:B:69:LYS:HD2	0.44	1.89	1	1
1:A:13:TYR:N	1:A:13:TYR:CD1	0.44	2.84	5	1
1:A:14:ARG:HA	1:A:14:ARG:NH1	0.44	2.27	5	1
1:B:55:PRO:O	1:B:57:GLN:HG3	0.44	2.12	5	1
1:B:63:PHE:CZ	1:B:67:LEU:HD12	0.44	2.47	5	1
1:B:54:ASP:CG	1:B:57:GLN:NE2	0.44	2.76	6	1
1:A:26:GLU:HG3	1:B:33:SER:C	0.44	2.36	7	1
1:A:65:LYS:CG	1:B:65:LYS:HG3	0.44	2.43	2	1
1:A:53:ALA:O	1:A:57:GLN:NE2	0.44	2.49	3	1
1:B:23:GLN:O	1:B:24:ARG:CG	0.44	2.64	3	1
1:A:26:GLU:OE1	1:A:45:THR:HA	0.44	2.11	4	1
1:B:41:VAL:CG2	1:B:42:ILE:N	0.44	2.80	7	2
1:A:39:GLU:OE1	1:B:65:LYS:NZ	0.44	2.50	5	1
1:A:71:THR:HG22	1:B:54:ASP:CG	0.44	2.36	7	1
1:B:28:TYR:CE2	1:B:30:ARG:HD3	0.44	2.47	1	1
1:A:15:PHE:CD2	1:A:55:PRO:HB2	0.44	2.48	2	1
1:A:75:LYS:HG3	1:B:56:THR:HG21	0.44	1.89	2	1
1:B:12:CYS:O	1:B:13:TYR:CB	0.44	2.65	2	2
1:A:34:SER:HA	1:B:70:LYS:CD	0.44	2.42	7	1
1:A:70:LYS:CE	1:B:39:GLU:OE1	0.44	2.65	7	1
1:A:24:ARG:HH22	1:B:35:HIS:CE1	0.44	2.31	1	1
1:A:32:THR:N	1:A:39:GLU:HG3	0.44	2.27	1	1
1:B:30:ARG:NE	1:B:64:MET:SD	0.44	2.91	2	1
1:A:44:LYS:NZ	1:A:48:ASP:OD1	0.44	2.48	3	2
1:B:57:GLN:N	1:B:57:GLN:NE2	0.44	2.61	3	1
1:A:31:THR:OG1	1:B:27:SER:HA	0.44	2.12	4	1
1:A:44:LYS:CE	1:A:48:ASP:CG	0.44	2.90	4	1
1:A:33:SER:N	1:B:68:ASP:CG	0.44	2.75	5	1
1:A:51:ILE:CG2	1:A:59:TRP:CZ2	0.44	2.99	5	1
1:A:75:LYS:C	1:B:57:GLN:HG2	0.44	2.36	6	1
1:B:54:ASP:HB3	1:B:55:PRO:HD3	0.44	1.88	7	1
1:A:72:GLN:HB2	1:B:54:ASP:CB	0.44	2.43	1	1
1:A:30:ARG:NE	1:B:68:ASP:OD2	0.44	2.50	2	1
1:B:33:SER:O	1:B:34:SER:CB	0.44	2.66	3	1
1:A:54:ASP:OD1	1:A:55:PRO:HD2	0.44	2.13	5	1
1:B:32:THR:O	1:B:34:SER:N	0.44	2.50	5	1
1:B:46:LYS:NZ	1:B:48:ASP:OD2	0.44	2.50	6	1
1:B:53:ALA:O	1:B:60:VAL:HG11	0.44	2.13	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:14:ARG:CZ	1:B:14:ARG:CB	0.44	2.96	1	1
1:A:30:ARG:CD	1:A:41:VAL:HG22	0.44	2.41	2	2
1:A:68:ASP:CG	1:B:30:ARG:NH1	0.44	2.76	3	1
1:A:64:MET:SD	1:A:65:LYS:HB3	0.44	2.51	4	1
1:A:12:CYS:SG	1:A:16:ILE:HB	0.44	2.53	6	1
1:B:52:CYS:O	1:B:53:ALA:HB3	0.44	2.11	7	1
1:B:44:LYS:NZ	1:B:48:ASP:OD1	0.44	2.44	1	3
1:A:30:ARG:O	1:B:28:TYR:CD1	0.44	2.71	4	1
1:A:40:ALA:HA	1:B:68:ASP:HB3	0.44	1.89	4	1
1:A:33:SER:N	1:A:39:GLU:HG2	0.44	2.28	5	1
1:B:57:GLN:HB3	1:B:59:TRP:NE1	0.44	2.28	5	1
1:A:25:LEU:HG	1:A:44:LYS:O	0.44	2.13	6	1
1:A:34:SER:OG	1:B:70:LYS:CG	0.44	2.66	7	1
1:B:63:PHE:CE1	1:B:67:LEU:HG	0.44	2.47	7	1
1:A:28:TYR:CE2	1:A:67:LEU:HD12	0.44	2.48	1	1
1:B:44:LYS:NZ	1:B:45:THR:O	0.44	2.49	2	1
1:B:48:ASP:OD2	1:B:49:LYS:NZ	0.44	2.51	2	1
1:B:63:PHE:C	1:B:63:PHE:CD1	0.44	2.96	2	1
1:A:53:ALA:C	1:A:57:GLN:NE2	0.44	2.76	3	1
1:B:45:THR:O	1:B:48:ASP:N	0.44	2.50	3	1
1:A:15:PHE:CZ	1:A:18:LYS:HE3	0.44	2.48	5	1
1:A:30:ARG:NH1	1:A:31:THR:H	0.44	2.11	5	1
1:A:43:PHE:CG	1:A:59:TRP:CZ3	0.44	3.06	5	1
1:A:70:LYS:O	1:B:55:PRO:HD3	0.44	2.12	5	1
1:A:74:PRO:C	1:A:75:LYS:HG3	0.44	2.38	5	1
1:A:68:ASP:OD2	1:B:65:LYS:NZ	0.44	2.43	7	1
1:B:13:TYR:O	1:B:14:ARG:HB3	0.44	2.12	1	1
1:A:30:ARG:CZ	1:A:30:ARG:HB2	0.44	2.43	2	1
1:A:34:SER:N	1:B:27:SER:OG	0.44	2.51	3	1
1:A:34:SER:O	1:B:44:LYS:HD2	0.44	2.13	3	1
1:B:12:CYS:O	1:B:38:ARG:NH1	0.44	2.51	3	1
1:A:58:LYS:O	1:A:62:ASP:CB	0.44	2.66	4	1
1:B:19:LYS:HZ1	1:B:66:HIS:CD2	0.44	2.31	5	1
1:A:31:THR:HG22	1:B:27:SER:CA	0.44	2.41	7	1
1:B:68:ASP:CG	1:B:69:LYS:NZ	0.43	2.76	1	1
1:A:60:VAL:CG1	1:A:61:GLN:N	0.43	2.80	2	1
1:A:62:ASP:OD1	1:A:69:LYS:NZ	0.43	2.41	2	1
1:B:13:TYR:O	1:B:15:PHE:CD2	0.43	2.71	2	1
1:B:64:MET:HB3	1:B:68:ASP:OD2	0.43	2.13	2	1
1:A:36:CYS:CB	1:A:37:PRO:HD2	0.43	2.42	3	1
1:A:21:PRO:O	1:A:22:LYS:CE	0.43	2.66	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ARG:HE	1:A:40:ALA:N	0.43	2.10	4	1
1:A:60:VAL:O	1:A:63:PHE:N	0.43	2.51	4	1
1:A:65:LYS:HE2	1:A:65:LYS:O	0.43	2.13	4	1
1:A:61:GLN:CA	1:A:64:MET:SD	0.43	3.06	6	1
1:B:59:TRP:CH2	1:B:60:VAL:HG23	0.43	2.47	6	1
1:B:60:VAL:HG12	1:B:61:GLN:NE2	0.43	2.27	6	1
1:A:54:ASP:OD1	1:A:56:THR:HA	0.43	2.13	7	1
1:A:32:THR:CA	1:B:27:SER:HB2	0.43	2.34	1	1
1:A:18:LYS:N	1:A:18:LYS:CD	0.43	2.81	2	1
1:B:28:TYR:OH	1:B:67:LEU:CB	0.43	2.64	2	1
1:A:65:LYS:O	1:A:65:LYS:CE	0.43	2.66	4	1
1:B:30:ARG:NH2	1:B:54:ASP:C	0.43	2.76	4	1
1:A:58:LYS:NZ	1:A:62:ASP:CG	0.43	2.76	5	1
1:B:28:TYR:CD2	1:B:64:MET:HB3	0.43	2.47	5	1
1:A:41:VAL:CG2	1:A:64:MET:SD	0.43	3.06	7	1
1:A:13:TYR:O	1:A:14:ARG:NE	0.43	2.52	2	1
1:A:28:TYR:CE1	1:A:43:PHE:CE1	0.43	3.06	2	1
1:A:35:HIS:O	1:A:36:CYS:CB	0.43	2.67	3	1
1:A:73:THR:OG1	1:B:57:GLN:N	0.43	2.51	3	1
1:B:29:ARG:HB2	1:B:42:ILE:HB	0.43	1.90	3	1
1:A:31:THR:HG21	1:B:67:LEU:HG	0.43	1.90	4	1
1:A:15:PHE:O	1:A:17:ASN:ND2	0.43	2.52	5	1
1:B:44:LYS:HA	1:B:44:LYS:HE3	0.43	1.90	5	1
1:A:18:LYS:O	1:A:18:LYS:HE2	0.43	2.13	6	1
1:B:49:LYS:NZ	1:B:49:LYS:HB2	0.43	2.29	2	1
1:B:55:PRO:O	1:B:61:GLN:NE2	0.43	2.52	4	1
1:A:23:GLN:O	1:A:46:LYS:NZ	0.43	2.50	6	1
1:B:55:PRO:C	1:B:57:GLN:OE1	0.43	2.61	6	1
1:B:66:HIS:O	1:B:69:LYS:CE	0.43	2.67	6	1
1:B:68:ASP:O	1:B:70:LYS:N	0.43	2.52	6	1
1:A:27:SER:HB3	1:B:31:THR:HA	0.43	1.90	2	1
1:A:29:ARG:HD3	1:B:29:ARG:NH2	0.43	2.28	3	1
1:A:29:ARG:HA	1:B:28:TYR:O	0.43	2.14	4	1
1:A:74:PRO:HD3	1:B:15:PHE:CG	0.43	2.48	4	1
1:A:30:ARG:NH1	1:A:31:THR:OG1	0.43	2.52	5	1
1:A:30:ARG:O	1:B:28:TYR:HB3	0.43	2.13	5	1
1:B:59:TRP:HA	1:B:62:ASP:HB3	0.43	1.91	5	1
1:A:29:ARG:NH2	1:A:50:GLU:CD	0.43	2.77	6	1
1:B:26:GLU:HB2	1:B:45:THR:CA	0.43	2.44	7	1
1:A:30:ARG:HD3	1:B:28:TYR:CE2	0.43	2.48	1	1
1:A:12:CYS:HB2	1:A:38:ARG:CG	0.43	2.43	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:SER:H	1:B:26:GLU:HA	0.43	1.73	4	1
1:A:31:THR:N	1:B:27:SER:OG	0.43	2.52	5	1
1:A:42:ILE:HG23	1:A:51:ILE:O	0.43	2.13	6	1
1:A:28:TYR:CD2	1:A:43:PHE:CD1	0.43	3.06	7	1
1:B:18:LYS:HA	1:B:59:TRP:CE2	0.43	2.48	7	1
1:A:17:ASN:N	1:A:59:TRP:NE1	0.43	2.67	2	1
1:A:64:MET:C	1:A:68:ASP:HB2	0.43	2.39	3	1
1:A:57:GLN:C	1:A:61:GLN:OE1	0.43	2.62	4	1
1:A:62:ASP:O	1:A:66:HIS:CB	0.43	2.67	4	1
1:A:74:PRO:HD3	1:B:15:PHE:CZ	0.43	2.48	4	1
1:A:70:LYS:NZ	1:B:39:GLU:CD	0.43	2.77	6	1
1:A:34:SER:HA	1:B:70:LYS:HD2	0.43	1.91	7	1
1:B:34:SER:OG	1:B:35:HIS:N	0.43	2.52	7	1
1:B:58:LYS:O	1:B:61:GLN:HB2	0.43	2.13	1	1
1:A:28:TYR:HE1	1:A:43:PHE:CE1	0.43	2.31	2	1
1:A:75:LYS:HB2	1:B:59:TRP:NE1	0.43	2.28	3	1
1:A:43:PHE:CG	1:A:59:TRP:HZ3	0.43	2.32	5	1
1:B:43:PHE:HE2	1:B:59:TRP:CH2	0.43	2.32	6	1
1:A:56:THR:O	1:A:58:LYS:NZ	0.43	2.52	1	1
1:B:57:GLN:HG2	1:B:59:TRP:NE1	0.43	2.28	1	1
1:A:26:GLU:OE2	1:A:46:LYS:NZ	0.43	2.37	2	1
1:A:29:ARG:CZ	1:A:42:ILE:CD1	0.43	2.97	4	1
1:A:44:LYS:C	1:A:44:LYS:CD	0.43	2.88	4	1
1:A:58:LYS:HD2	1:A:58:LYS:O	0.43	2.09	4	1
1:A:66:HIS:CE1	1:A:69:LYS:HZ1	0.43	2.31	6	1
1:B:23:GLN:N	1:B:23:GLN:CD	0.43	2.76	6	1
1:A:26:GLU:HG2	1:A:47:LEU:N	0.43	2.29	7	1
1:B:13:TYR:O	1:B:13:TYR:CD2	0.43	2.72	7	1
1:A:29:ARG:NH1	1:A:32:THR:OG1	0.43	2.52	1	1
1:A:16:ILE:HG22	1:A:59:TRP:CZ2	0.43	2.49	2	1
1:A:12:CYS:O	1:A:14:ARG:NH2	0.43	2.52	3	1
1:A:75:LYS:HG3	1:B:59:TRP:CZ2	0.43	2.49	3	1
1:B:43:PHE:CZ	1:B:59:TRP:CH2	0.43	3.07	3	1
1:A:26:GLU:HG2	1:A:47:LEU:CA	0.43	2.44	7	1
1:A:30:ARG:HD2	1:A:64:MET:SD	0.43	2.53	7	1
1:B:28:TYR:CB	1:B:28:TYR:OH	0.43	2.66	7	1
1:B:25:LEU:H	1:B:27:SER:N	0.42	2.04	3	1
1:A:33:SER:HA	1:B:26:GLU:CB	0.42	2.40	4	1
1:B:64:MET:CG	1:B:65:LYS:N	0.42	2.82	5	1
1:A:41:VAL:HB	1:A:53:ALA:HB3	0.42	1.90	6	1
1:A:74:PRO:HA	1:B:54:ASP:OD2	0.42	2.14	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:68:ASP:OD1	1:B:68:ASP:N	0.42	2.52	7	1
1:A:22:LYS:HE3	1:A:23:GLN:N	0.42	2.28	1	1
1:A:17:ASN:OD1	1:A:18:LYS:NZ	0.42	2.51	3	1
1:A:28:TYR:CZ	1:B:30:ARG:HB2	0.42	2.49	3	1
1:B:22:LYS:CE	1:B:51:ILE:HG12	0.42	2.44	3	1
1:B:50:GLU:O	1:B:51:ILE:HG12	0.42	2.14	3	1
1:B:49:LYS:C	1:B:50:GLU:HG3	0.42	2.39	5	1
1:B:59:TRP:CD2	1:B:59:TRP:C	0.42	2.97	5	1
1:B:59:TRP:O	1:B:63:PHE:HB2	0.42	2.14	5	1
1:A:41:VAL:HG11	1:A:43:PHE:CE2	0.42	2.49	7	1
1:A:29:ARG:HD3	1:B:29:ARG:CZ	0.42	2.45	3	1
1:A:29:ARG:HA	1:B:29:ARG:HA	0.42	1.91	3	1
1:A:34:SER:HA	1:B:27:SER:CA	0.42	2.44	3	1
1:B:24:ARG:NH2	1:B:25:LEU:O	0.42	2.52	3	1
1:A:32:THR:HG22	1:A:38:ARG:HB3	0.42	1.92	4	1
1:A:71:THR:CG2	1:B:40:ALA:HA	0.42	2.44	4	1
1:A:74:PRO:O	1:B:57:GLN:HG3	0.42	2.14	4	1
1:A:70:LYS:HG2	1:B:55:PRO:HA	0.42	1.92	2	1
1:A:31:THR:HB	1:B:70:LYS:HZ1	0.42	1.74	3	1
1:B:48:ASP:HB3	1:B:49:LYS:HZ1	0.42	1.75	3	1
1:A:28:TYR:CA	1:A:42:ILE:O	0.42	2.67	4	1
1:A:32:THR:H	1:B:68:ASP:CG	0.42	2.22	5	1
1:A:54:ASP:OD1	1:A:55:PRO:CD	0.42	2.68	5	1
1:B:33:SER:HB3	1:B:35:HIS:CD2	0.42	2.50	5	1
1:A:24:ARG:O	1:A:25:LEU:HB2	0.42	2.13	7	1
1:B:36:CYS:C	1:B:38:ARG:N	0.42	2.76	1	1
1:A:29:ARG:HD2	1:A:34:SER:OG	0.42	2.15	3	1
1:A:27:SER:OG	1:B:29:ARG:HG3	0.42	2.14	5	1
1:B:25:LEU:O	1:B:69:LYS:CB	0.42	2.67	5	1
1:A:19:LYS:NZ	1:A:66:HIS:CE1	0.42	2.86	2	1
1:A:33:SER:CA	1:B:26:GLU:HA	0.42	2.45	2	1
1:B:13:TYR:CD1	1:B:15:PHE:CE2	0.42	3.07	2	1
1:A:29:ARG:CZ	1:A:42:ILE:HD12	0.42	2.44	3	1
1:B:59:TRP:CE2	1:B:60:VAL:HG22	0.42	2.48	3	1
1:A:28:TYR:CD1	1:A:41:VAL:HG13	0.42	2.49	4	1
1:B:41:VAL:O	1:B:52:CYS:SG	0.42	2.77	4	1
1:B:20:ILE:H	1:B:20:ILE:HD12	0.42	1.74	5	1
1:A:35:HIS:ND1	1:A:36:CYS:N	0.42	2.68	6	1
1:A:34:SER:OG	1:B:70:LYS:CE	0.42	2.67	7	1
1:A:43:PHE:CE2	1:A:59:TRP:CZ3	0.42	3.08	7	1
1:A:56:THR:HB	1:A:60:VAL:HB	0.42	1.92	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ARG:HB2	1:B:28:TYR:CE2	0.42	2.50	1	1
1:A:24:ARG:HD3	1:A:24:ARG:N	0.42	2.30	3	1
1:B:66:HIS:C	1:B:67:LEU:HD12	0.42	2.39	3	1
1:A:24:ARG:NH1	1:B:34:SER:O	0.42	2.53	4	2
1:B:41:VAL:CG1	1:B:54:ASP:HB2	0.42	2.44	4	1
1:A:28:TYR:CZ	1:A:67:LEU:HB3	0.42	2.50	5	1
1:A:62:ASP:HA	1:A:65:LYS:HE3	0.42	1.90	5	1
1:A:67:LEU:N	1:A:67:LEU:CD2	0.42	2.83	5	1
1:A:71:THR:HG22	1:B:54:ASP:CB	0.42	2.45	7	1
1:B:26:GLU:OE2	1:B:44:LYS:NZ	0.42	2.51	1	1
1:A:31:THR:OG1	1:A:40:ALA:N	0.42	2.52	2	1
1:A:65:LYS:C	1:A:69:LYS:HZ2	0.42	2.22	2	1
1:A:70:LYS:C	1:B:38:ARG:NH1	0.42	2.78	2	1
1:B:58:LYS:C	1:B:58:LYS:CD	0.42	2.86	2	1
1:A:23:GLN:O	1:A:24:ARG:HB2	0.42	2.14	3	1
1:B:50:GLU:OE2	1:B:51:ILE:HA	0.42	2.15	3	1
1:B:29:ARG:HD2	1:B:42:ILE:CG2	0.42	2.45	6	1
1:B:32:THR:O	1:B:33:SER:C	0.42	2.62	1	1
1:B:41:VAL:CG1	1:B:64:MET:CE	0.42	2.97	2	1
1:B:45:THR:H	1:B:49:LYS:C	0.42	2.23	3	1
1:A:46:LYS:O	1:A:46:LYS:CG	0.42	2.67	4	1
1:A:67:LEU:HD21	1:B:32:THR:HG21	0.42	1.92	4	1
1:B:26:GLU:OE2	1:B:46:LYS:N	0.42	2.52	4	1
1:B:63:PHE:O	1:B:67:LEU:N	0.42	2.52	4	1
1:A:31:THR:HG23	1:B:68:ASP:OD1	0.42	2.14	5	1
1:A:13:TYR:CD1	1:A:13:TYR:N	0.42	2.88	6	1
1:A:29:ARG:O	1:A:41:VAL:HA	0.42	2.15	6	1
1:B:22:LYS:HE3	1:B:66:HIS:HB3	0.42	1.91	7	1
1:B:35:HIS:ND1	1:B:35:HIS:C	0.42	2.77	7	1
1:B:16:ILE:HD13	1:B:17:ASN:N	0.42	2.30	1	1
1:B:36:CYS:O	1:B:37:PRO:C	0.42	2.63	1	1
1:A:27:SER:HA	1:B:31:THR:CB	0.42	2.44	3	1
1:B:18:LYS:H	1:B:18:LYS:HD3	0.42	1.74	4	1
1:A:71:THR:HG23	1:B:14:ARG:HE	0.42	1.75	5	1
1:A:14:ARG:O	1:A:14:ARG:HD3	0.42	2.14	6	1
1:A:37:PRO:O	1:A:38:ARG:HB2	0.42	2.15	6	1
1:B:32:THR:HG22	1:B:33:SER:N	0.41	2.29	2	1
1:A:32:THR:HA	1:A:38:ARG:CA	0.41	2.45	3	1
1:A:67:LEU:O	1:A:70:LYS:HB3	0.41	2.15	3	1
1:A:64:MET:SD	1:A:65:LYS:CG	0.41	3.08	4	1
1:A:14:ARG:HH11	1:A:14:ARG:CB	0.41	2.28	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:LYS:O	1:A:49:LYS:NZ	0.41	2.52	5	1
1:A:61:GLN:HA	1:A:64:MET:HG2	0.41	1.91	5	1
1:B:21:PRO:C	1:B:22:LYS:HG2	0.41	2.40	5	1
1:B:19:LYS:O	1:B:19:LYS:HG2	0.41	2.15	7	1
1:A:24:ARG:NH1	1:B:35:HIS:CG	0.41	2.79	1	1
1:A:25:LEU:O	1:B:34:SER:CB	0.41	2.68	2	1
1:A:70:LYS:HD3	1:B:39:GLU:HG2	0.41	1.92	2	1
1:A:34:SER:HA	1:B:27:SER:N	0.41	2.29	3	1
1:A:71:THR:HA	1:B:39:GLU:CB	0.41	2.34	3	1
1:A:15:PHE:C	1:A:16:ILE:CD1	0.41	2.93	4	1
1:A:62:ASP:HA	1:A:65:LYS:CD	0.41	2.45	4	1
1:A:42:ILE:HG22	1:A:43:PHE:N	0.41	2.30	5	1
1:B:43:PHE:CG	1:B:63:PHE:CZ	0.41	3.08	7	1
1:B:17:ASN:HA	1:B:57:GLN:CD	0.41	2.41	1	1
1:A:30:ARG:CZ	1:A:30:ARG:CB	0.41	2.98	2	1
1:B:28:TYR:CE2	1:B:64:MET:HA	0.41	2.50	2	1
1:B:65:LYS:HE2	1:B:66:HIS:HB2	0.41	1.90	2	1
1:A:75:LYS:HB3	1:B:17:ASN:HA	0.41	1.92	3	1
1:A:75:LYS:CD	1:B:18:LYS:H	0.41	2.27	3	1
1:B:47:LEU:O	1:B:48:ASP:HB3	0.41	2.16	3	1
1:A:26:GLU:HA	1:B:35:HIS:ND1	0.41	2.30	4	1
1:A:30:ARG:C	1:A:40:ALA:O	0.41	2.63	4	1
1:A:52:CYS:O	1:A:59:TRP:CZ2	0.41	2.72	5	1
1:B:35:HIS:CG	1:B:36:CYS:H	0.41	2.32	5	1
1:A:14:ARG:O	1:A:14:ARG:CD	0.41	2.68	6	1
1:A:14:ARG:NH2	1:A:15:PHE:O	0.41	2.53	7	1
1:B:26:GLU:C	1:B:70:LYS:HE2	0.41	2.40	7	1
1:A:43:PHE:CE1	1:A:59:TRP:CZ3	0.41	3.09	2	2
1:A:64:MET:HE3	1:B:65:LYS:CA	0.41	2.45	2	1
1:A:32:THR:C	1:A:38:ARG:O	0.41	2.64	3	1
1:B:54:ASP:N	1:B:60:VAL:HG11	0.41	2.30	4	1
1:B:38:ARG:HB3	1:B:38:ARG:HH21	0.41	1.75	5	1
1:B:38:ARG:HB3	1:B:38:ARG:NH2	0.41	2.29	5	1
1:A:28:TYR:CE2	1:A:43:PHE:CD1	0.41	3.09	7	1
1:A:36:CYS:C	1:A:38:ARG:N	0.41	2.77	1	1
1:A:69:LYS:NZ	1:A:69:LYS:HB2	0.41	2.31	1	1
1:A:70:LYS:HG2	1:B:55:PRO:CA	0.41	2.46	2	1
1:B:58:LYS:HD3	1:B:59:TRP:N	0.41	2.30	2	1
1:B:46:LYS:O	1:B:47:LEU:CB	0.41	2.69	5	1
1:A:29:ARG:HB2	1:A:42:ILE:H	0.41	1.76	6	1
1:B:13:TYR:O	1:B:14:ARG:C	0.41	2.64	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:ILE:CG2	1:A:50:GLU:HG2	0.41	2.46	3	1
1:A:17:ASN:O	1:A:59:TRP:NE1	0.41	2.53	4	1
1:B:57:GLN:CG	1:B:59:TRP:NE1	0.41	2.84	7	1
1:B:64:MET:C	1:B:66:HIS:N	0.41	2.79	2	1
1:A:31:THR:C	1:B:27:SER:HB2	0.41	2.40	3	1
1:A:55:PRO:O	1:A:56:THR:C	0.41	2.62	3	1
1:A:58:LYS:CE	1:A:58:LYS:O	0.41	2.68	5	1
1:B:19:LYS:O	1:B:22:LYS:HE3	0.41	2.16	5	1
1:B:59:TRP:CZ2	1:B:60:VAL:HG23	0.41	2.50	5	1
1:A:73:THR:CB	1:B:61:GLN:NE2	0.41	2.83	1	1
1:A:70:LYS:HD3	1:B:39:GLU:CG	0.41	2.45	2	1
1:B:14:ARG:O	1:B:14:ARG:HG2	0.41	2.15	2	1
1:A:38:ARG:HH11	1:A:52:CYS:CB	0.41	2.27	4	1
1:B:21:PRO:O	1:B:22:LYS:C	0.41	2.64	4	1
1:A:32:THR:HB	1:B:68:ASP:OD2	0.41	2.15	5	1
1:B:19:LYS:CE	1:B:63:PHE:HA	0.41	2.46	5	1
1:B:23:GLN:HA	1:B:67:LEU:CD2	0.41	2.44	5	1
1:B:49:LYS:HG2	1:B:50:GLU:N	0.41	2.30	5	1
1:A:54:ASP:HB3	1:A:57:GLN:HE21	0.41	1.76	6	1
1:A:14:ARG:C	1:A:14:ARG:CZ	0.41	2.94	7	1
1:A:27:SER:O	1:A:44:LYS:N	0.41	2.54	7	1
1:A:30:ARG:NH1	1:A:31:THR:C	0.41	2.79	7	1
1:A:38:ARG:NH2	1:A:50:GLU:HG2	0.41	2.31	7	1
1:B:68:ASP:OD2	1:B:69:LYS:NZ	0.41	2.52	7	1
1:A:43:PHE:CE2	1:A:59:TRP:HZ3	0.41	2.34	1	1
1:A:73:THR:HG23	1:B:57:GLN:N	0.41	2.30	1	1
1:A:75:LYS:HE2	1:A:75:LYS:C	0.41	2.41	1	1
1:B:36:CYS:HB3	1:B:39:GLU:CA	0.41	2.45	1	1
1:A:26:GLU:CB	1:A:45:THR:O	0.41	2.68	2	1
1:A:70:LYS:HD3	1:B:39:GLU:H	0.41	1.76	2	1
1:B:16:ILE:O	1:B:18:LYS:N	0.41	2.54	2	1
1:A:30:ARG:HD3	1:A:41:VAL:N	0.41	2.31	4	1
1:A:30:ARG:NH2	1:A:53:ALA:C	0.41	2.78	4	1
1:A:32:THR:CG2	1:A:39:GLU:H	0.41	2.27	4	1
1:A:54:ASP:N	1:A:57:GLN:NE2	0.41	2.68	4	1
1:A:73:THR:HA	1:B:15:PHE:CE2	0.41	2.50	4	1
1:A:23:GLN:O	1:A:24:ARG:HB3	0.41	2.15	5	1
1:A:25:LEU:N	1:B:33:SER:O	0.41	2.54	5	1
1:A:58:LYS:HE3	1:A:58:LYS:O	0.41	2.16	5	1
1:A:61:GLN:O	1:A:62:ASP:C	0.41	2.63	5	1
1:A:75:LYS:CD	1:B:17:ASN:N	0.41	2.84	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ARG:HB2	1:A:38:ARG:NH2	0.41	2.30	6	1
1:A:49:LYS:HE3	1:A:49:LYS:CA	0.41	2.46	6	1
1:A:19:LYS:NZ	1:A:59:TRP:CZ3	0.41	2.89	7	1
1:B:23:GLN:HG2	1:B:63:PHE:CE2	0.41	2.51	2	1
1:B:28:TYR:CZ	1:B:64:MET:HA	0.41	2.51	2	1
1:B:22:LYS:HD3	1:B:45:THR:HG21	0.41	1.92	3	1
1:A:31:THR:HB	1:B:68:ASP:OD1	0.41	2.16	4	1
1:A:29:ARG:C	1:B:27:SER:OG	0.41	2.64	5	1
1:B:37:PRO:O	1:B:38:ARG:HB3	0.41	2.16	5	1
1:A:44:LYS:NZ	1:A:48:ASP:OD2	0.41	2.54	6	1
1:A:24:ARG:HH12	1:B:35:HIS:CB	0.40	2.29	1	1
1:B:28:TYR:HB3	1:B:63:PHE:CZ	0.40	2.51	1	1
1:A:30:ARG:HG2	1:A:41:VAL:HG13	0.40	1.92	2	1
1:A:39:GLU:O	1:B:70:LYS:N	0.40	2.54	2	1
1:B:20:ILE:HD13	1:B:21:PRO:CD	0.40	2.46	2	1
1:B:32:THR:CG2	1:B:33:SER:N	0.40	2.84	2	1
1:B:22:LYS:CE	1:B:51:ILE:CG1	0.40	2.99	3	1
1:A:20:ILE:O	1:A:22:LYS:NZ	0.40	2.54	4	1
1:B:21:PRO:HB2	1:B:66:HIS:ND1	0.40	2.31	4	1
1:B:61:GLN:HE22	1:B:61:GLN:H	0.40	1.59	4	1
1:A:26:GLU:HB2	1:A:46:LYS:N	0.40	2.31	6	1
1:A:65:LYS:NZ	1:B:61:GLN:OE1	0.40	2.55	6	1
1:B:19:LYS:NZ	1:B:63:PHE:CE2	0.40	2.84	6	1
1:B:63:PHE:HA	1:B:66:HIS:CB	0.40	2.46	6	1
1:B:25:LEU:H	1:B:70:LYS:CB	0.40	2.29	7	1
1:A:17:ASN:C	1:A:18:LYS:HD3	0.40	2.41	2	1
1:A:64:MET:HE3	1:B:65:LYS:HA	0.40	1.93	2	1
1:A:65:LYS:HD3	1:B:65:LYS:HG3	0.40	1.94	2	1
1:B:23:GLN:HE21	1:B:66:HIS:CD2	0.40	2.34	2	1
1:B:58:LYS:CG	1:B:59:TRP:N	0.40	2.84	2	1
1:A:32:THR:OG1	1:A:33:SER:N	0.40	2.53	3	1
1:A:68:ASP:CG	1:B:30:ARG:HH12	0.40	2.24	3	1
1:A:75:LYS:O	1:B:18:LYS:CE	0.40	2.69	3	1
1:B:11:CYS:N	1:B:39:GLU:HA	0.40	2.31	3	1
1:A:43:PHE:CD2	1:A:59:TRP:HZ3	0.40	2.34	5	1
1:B:36:CYS:HA	1:B:37:PRO:HD2	0.40	1.64	6	1
1:B:65:LYS:HD2	1:B:65:LYS:C	0.40	2.40	6	1
1:A:31:THR:C	1:B:26:GLU:O	0.40	2.64	2	1
1:A:35:HIS:CD2	1:A:36:CYS:H	0.40	2.35	2	1
1:A:44:LYS:CE	1:A:48:ASP:OD2	0.40	2.69	4	1
1:B:25:LEU:CD1	1:B:44:LYS:O	0.40	2.68	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:LEU:O	1:B:34:SER:HA	0.40	2.16	7	1
1:A:56:THR:C	1:A:61:GLN:HE22	0.40	2.25	7	1
1:A:12:CYS:CB	1:A:38:ARG:HH21	0.40	2.30	1	1
1:B:14:ARG:O	1:B:14:ARG:HD2	0.40	2.17	1	1
1:B:32:THR:HG21	1:B:35:HIS:CE1	0.40	2.51	1	1
1:A:11:CYS:O	1:A:12:CYS:CB	0.40	2.69	2	1
1:A:26:GLU:HG2	1:A:44:LYS:HZ2	0.40	1.74	2	1
1:A:27:SER:CB	1:B:31:THR:HA	0.40	2.46	2	1
1:B:41:VAL:O	1:B:52:CYS:HA	0.40	2.16	2	1
1:A:25:LEU:HA	1:A:45:THR:HA	0.40	1.93	3	1
1:B:20:ILE:CG2	1:B:21:PRO:CD	0.40	2.99	3	1
1:A:34:SER:N	1:B:26:GLU:HA	0.40	2.30	4	1
1:B:30:ARG:NH2	1:B:54:ASP:O	0.40	2.55	4	1
1:B:61:GLN:O	1:B:62:ASP:C	0.40	2.63	6	1
1:A:58:LYS:O	1:A:59:TRP:C	0.40	2.65	3	1
1:B:35:HIS:O	1:B:35:HIS:ND1	0.40	2.54	3	1
1:B:67:LEU:O	1:B:70:LYS:CE	0.40	2.69	3	1
1:A:30:ARG:CG	1:A:41:VAL:CA	0.40	2.99	4	1
1:B:26:GLU:HB2	1:B:44:LYS:HE3	0.40	1.93	4	1
1:A:14:ARG:C	1:A:14:ARG:HH21	0.40	2.22	7	1
1:A:41:VAL:HG22	1:A:64:MET:SD	0.40	2.57	7	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	65/76 (86%)	29±2 (44±3%)	12±2 (18±2%)	24±2 (37±3%)	0	0
1	B	60/76 (79%)	30±3 (50±5%)	12±2 (20±4%)	18±3 (30±6%)	0	1
All	All	875/1064 (82%)	410 (47%)	168 (19%)	297 (34%)	0	0

All 80 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	20	ILE	7
1	A	71	THR	7
1	B	33	SER	7
1	B	55	PRO	7
1	B	70	LYS	7
1	A	11	CYS	6
1	A	15	PHE	6
1	A	23	GLN	6
1	A	37	PRO	6
1	A	48	ASP	6
1	A	68	ASP	6
1	A	69	LYS	6
1	B	17	ASN	6
1	B	34	SER	6
1	B	68	ASP	6
1	A	17	ASN	6
1	A	24	ARG	6
1	A	34	SER	6
1	B	48	ASP	6
1	A	13	TYR	5
1	A	55	PRO	5
1	A	58	LYS	5
1	A	74	PRO	5
1	B	14	ARG	5
1	B	46	LYS	5
1	A	36	CYS	5
1	A	70	LYS	5
1	A	73	THR	5
1	A	46	LYS	4
1	A	56	THR	4
1	A	75	LYS	4
1	B	32	THR	4
1	B	47	LEU	4
1	B	58	LYS	4
1	B	12	CYS	4
1	B	20	ILE	4
1	B	37	PRO	4
1	A	33	SER	4
1	B	69	LYS	4
1	A	16	ILE	3
1	A	21	PRO	3
1	A	31	THR	3
1	A	38	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	B	23	GLN	3
1	B	39	GLU	3
1	A	14	ARG	3
1	A	18	LYS	3
1	A	19	LYS	3
1	B	13	TYR	3
1	B	19	LYS	3
1	A	32	THR	3
1	A	54	ASP	3
1	B	27	SER	3
1	B	31	THR	3
1	B	54	ASP	3
1	A	40	ALA	3
1	B	11	CYS	3
1	B	15	PHE	3
1	A	47	LEU	2
1	B	21	PRO	2
1	A	12	CYS	2
1	A	27	SER	2
1	A	72	GLN	2
1	B	18	LYS	2
1	A	22	LYS	2
1	A	39	GLU	2
1	B	56	THR	2
1	B	36	CYS	2
1	A	49	LYS	1
1	B	25	LEU	1
1	A	35	HIS	1
1	B	24	ARG	1
1	B	49	LYS	1
1	B	51	ILE	1
1	B	22	LYS	1
1	B	40	ALA	1
1	B	38	ARG	1
1	B	16	ILE	1
1	A	62	ASP	1
1	B	53	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	63/73 (86%)	51±2 (81±4%)	12±2 (19±4%)	3	35
1	B	58/73 (79%)	48±3 (82±4%)	10±3 (18±4%)	4	37
All	All	847/1022 (83%)	693 (82%)	154 (18%)	3	36

All 70 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	58	LYS	5
1	A	18	LYS	5
1	A	19	LYS	4
1	A	22	LYS	4
1	A	38	ARG	4
1	B	21	PRO	4
1	B	28	TYR	4
1	B	37	PRO	4
1	B	58	LYS	4
1	B	24	ARG	4
1	A	44	LYS	3
1	A	46	LYS	3
1	A	48	ASP	3
1	A	61	GLN	3
1	A	74	PRO	3
1	A	55	PRO	3
1	B	15	PHE	3
1	B	17	ASN	3
1	B	49	LYS	3
1	B	65	LYS	3
1	A	24	ARG	3
1	A	72	GLN	3
1	B	18	LYS	3
1	B	19	LYS	3
1	B	46	LYS	3
1	A	21	PRO	2
1	A	67	LEU	2
1	A	69	LYS	2
1	B	14	ARG	2
1	B	20	ILE	2
1	B	26	GLU	2
1	B	55	PRO	2

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Mol	Chain	Res	Type	Models (Total)
1	B	61	GLN	2
1	B	67	LEU	2
1	B	70	LYS	2
1	A	23	GLN	2
1	A	30	ARG	2
1	A	37	PRO	2
1	A	14	ARG	2
1	A	20	ILE	2
1	A	65	LYS	2
1	A	70	LYS	2
1	B	45	THR	2
1	B	57	GLN	2
1	B	44	LYS	2
1	A	15	PHE	2
1	A	49	LYS	2
1	A	66	HIS	1
1	A	75	LYS	1
1	B	16	ILE	1
1	B	22	LYS	1
1	B	52	CYS	1
1	A	60	VAL	1
1	A	63	PHE	1
1	B	63	PHE	1
1	A	16	ILE	1
1	B	31	THR	1
1	B	64	MET	1
1	A	25	LEU	1
1	A	50	GLU	1
1	B	38	ARG	1
1	B	69	LYS	1
1	A	28	TYR	1
1	A	31	THR	1
1	A	41	VAL	1
1	A	17	ASN	1
1	B	23	GLN	1
1	B	35	HIS	1
1	A	36	CYS	1
1	B	25	LEU	1

6.3.3 RNA ⓘ

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](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided