Full wwPDB NMR Structure Validation Report (i)

Feb 16, 2022 – 09:49 AM EST

PDB ID	:	1NCV
Title	:	DETERMINATION CC-CHEMOKINE MCP-3, NMR, 7 STRUCTURES
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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 (i) symbol.

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

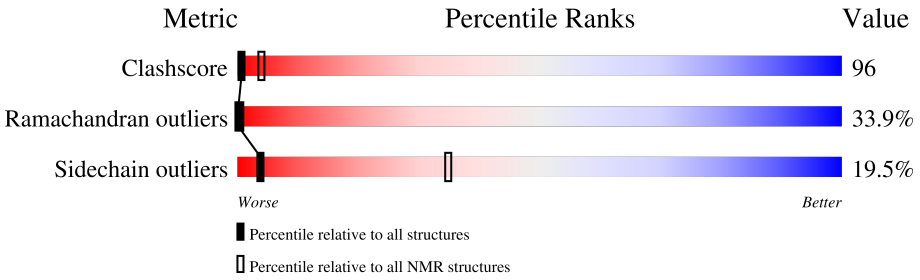
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	76	9% 41% 36% 14%
1	B	76	5% 49% 25% 21%

2 Ensemble composition and analysis (i)

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)	2.01	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	

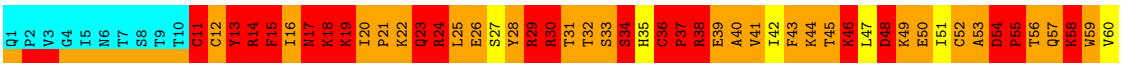
4 Residue-property plots

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.

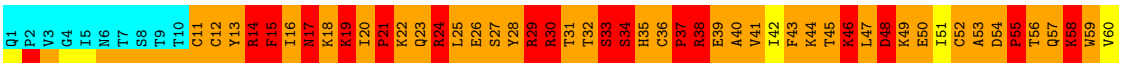
• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain A:



• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain B:



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

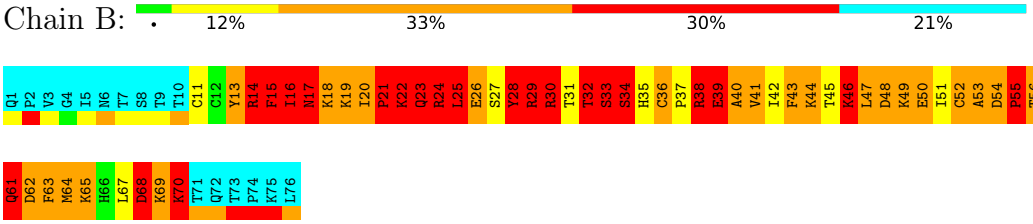
4.2.1 Score per residue for model 1

• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain A:

• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

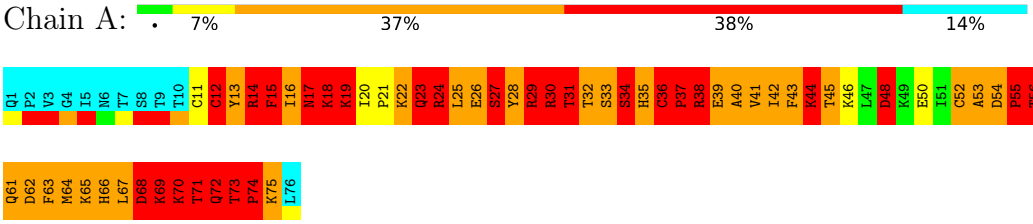
Chain B:



4.2.2 Score per residue for model 2

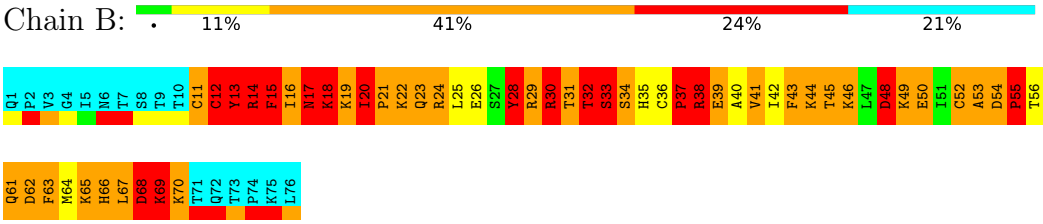
• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain A:



• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

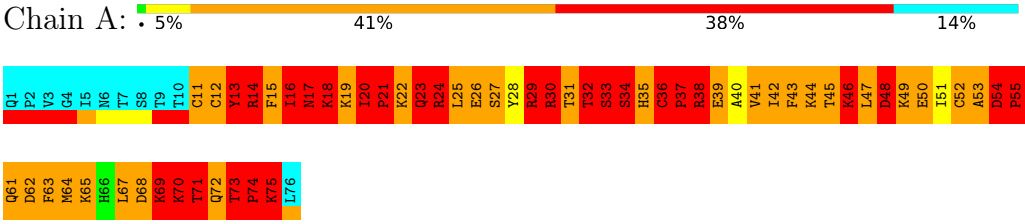
Chain B:



4.2.3 Score per residue for model 3

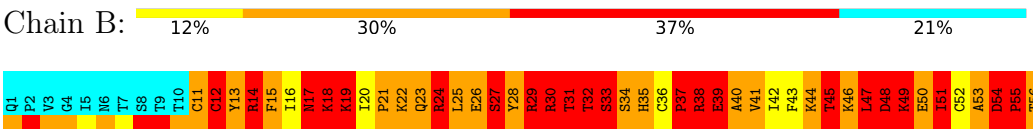
• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain A:



• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain B:



4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain A:

• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain B:

4.2.5 Score per residue for model 5

• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain A:

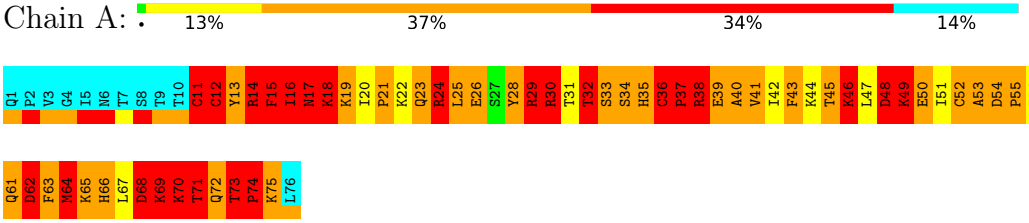
• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain B:

4.2.6 Score per residue for model 6

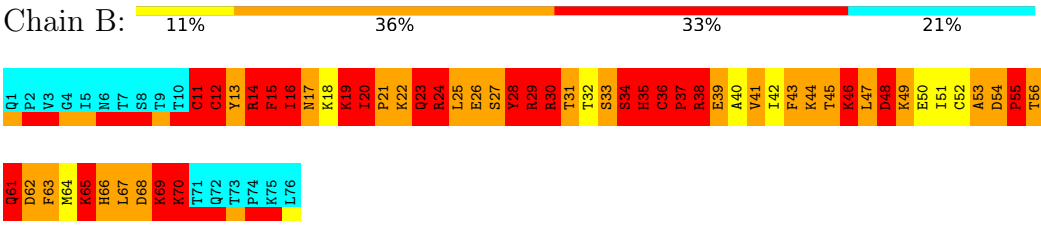
• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain A:



• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

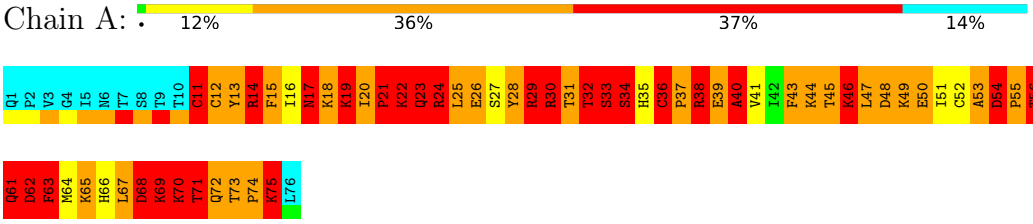
Chain B:



4.2.7 Score per residue for model 7

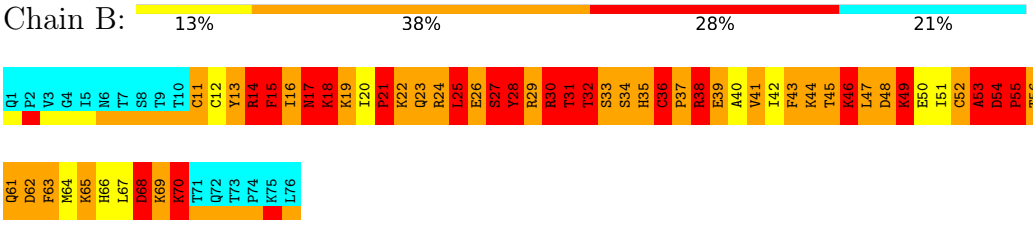
• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain A:



• Molecule 1: MONOCYTE CHEMOATTRACTANT PROTEIN 3

Chain B:



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	2.26±0.14	20±2/561 (3.5± 0.4%)	5.28±1.15	157±11/752 (20.9± 1.5%)
1	B	2.34±0.24	19±3/521 (3.7± 0.7%)	5.33±1.29	141±12/697 (20.3± 1.7%)
All	All	2.31	273/7574 (3.6%)	5.44	2089/10143 (20.6%)

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	B	28	TYR	CB-CG	25.21	1.89	1.51	7	1
1	A	15	PHE	CB-CG	23.64	1.91	1.51	7	1
1	B	28	TYR	CE1-CZ	20.54	1.65	1.38	7	1
1	B	28	TYR	CD2-CE2	16.76	1.64	1.39	7	1
1	B	28	TYR	CG-CD1	15.34	1.59	1.39	7	1
1	A	15	PHE	CD1-CE1	13.84	1.67	1.39	7	1
1	A	15	PHE	CE2-CZ	13.13	1.62	1.37	7	1
1	A	15	PHE	CG-CD2	12.83	1.57	1.38	7	1
1	B	28	TYR	CZ-OH	12.12	1.58	1.37	7	1
1	B	14	ARG	CZ-NH2	-10.79	1.19	1.33	2	7
1	A	30	ARG	CZ-NH1	-10.24	1.19	1.33	4	6
1	A	29	ARG	CZ-NH2	-10.18	1.19	1.33	6	7
1	B	29	ARG	CZ-NH1	-9.68	1.20	1.33	6	7
1	B	30	ARG	CZ-NH1	-9.61	1.20	1.33	4	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	38	ARG	CZ-NH1	-9.60	1.20	1.33	4	7
1	B	28	TYR	CD1-CE1	-9.53	1.25	1.39	7	1
1	A	29	ARG	CZ-NH1	-9.51	1.20	1.33	1	6
1	B	14	ARG	CZ-NH1	-9.50	1.20	1.33	4	7
1	A	38	ARG	CZ-NH2	-9.50	1.20	1.33	3	7
1	B	38	ARG	CZ-NH2	-9.47	1.20	1.33	6	7
1	A	14	ARG	CZ-NH2	-9.43	1.20	1.33	2	7
1	B	29	ARG	CZ-NH2	-9.33	1.21	1.33	6	7
1	B	30	ARG	CZ-NH2	-9.30	1.21	1.33	1	7
1	B	38	ARG	CZ-NH1	-9.24	1.21	1.33	5	7
1	A	14	ARG	CZ-NH1	-9.22	1.21	1.33	2	7
1	B	24	ARG	CZ-NH1	-9.22	1.21	1.33	5	7
1	A	30	ARG	CZ-NH2	-9.05	1.21	1.33	6	7
1	A	24	ARG	CZ-NH2	-8.75	1.21	1.33	2	7
1	B	24	ARG	CZ-NH2	-8.71	1.21	1.33	3	6
1	A	24	ARG	CZ-NH1	-8.64	1.21	1.33	6	7
1	A	30	ARG	NE-CZ	-8.04	1.22	1.33	4	6
1	B	38	ARG	NE-CZ	-7.85	1.22	1.33	3	7
1	A	24	ARG	NE-CZ	-7.70	1.23	1.33	7	7
1	B	14	ARG	NE-CZ	-7.56	1.23	1.33	2	7
1	A	14	ARG	CA-CB	7.37	1.70	1.53	3	1
1	A	40	ALA	N-CA	7.24	1.60	1.46	4	1
1	A	33	SER	CA-CB	7.18	1.63	1.52	5	1
1	B	30	ARG	NE-CZ	-7.14	1.23	1.33	5	7
1	A	14	ARG	NE-CZ	-7.07	1.23	1.33	6	7
1	A	38	ARG	NE-CZ	-7.05	1.23	1.33	3	7
1	B	24	ARG	NE-CZ	-7.02	1.24	1.33	2	6
1	B	29	ARG	NE-CZ	-6.94	1.24	1.33	6	7
1	A	29	ARG	NE-CZ	-6.83	1.24	1.33	2	6
1	B	27	SER	CA-CB	6.41	1.62	1.52	6	1
1	A	15	PHE	CD2-CE2	-6.38	1.26	1.39	7	1
1	B	27	SER	N-CA	6.30	1.58	1.46	3	1
1	A	34	SER	CA-CB	-6.20	1.43	1.52	7	1
1	B	59	TRP	NE1-CE2	-6.18	1.29	1.37	5	5
1	A	59	TRP	CG-CD2	-6.09	1.33	1.43	5	3
1	A	50	GLU	CA-CB	-6.03	1.40	1.53	5	1
1	A	39	GLU	CD-OE1	-5.90	1.19	1.25	5	2
1	B	69	LYS	CA-CB	-5.85	1.41	1.53	5	1
1	A	59	TRP	NE1-CE2	-5.79	1.30	1.37	2	2
1	A	26	GLU	CD-OE1	-5.78	1.19	1.25	3	1
1	B	25	LEU	N-CA	5.78	1.57	1.46	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	39	GLU	CD-OE2	-5.77	1.19	1.25	4	2
1	A	50	GLU	CD-OE1	-5.76	1.19	1.25	4	1
1	B	50	GLU	CD-OE1	-5.73	1.19	1.25	6	3
1	B	28	TYR	CE2-CZ	5.73	1.46	1.38	7	1
1	B	24	ARG	N-CA	5.56	1.57	1.46	3	1
1	B	34	SER	CA-CB	5.54	1.61	1.52	1	1
1	B	57	GLN	N-CA	5.54	1.57	1.46	3	1
1	B	39	GLU	CD-OE2	-5.49	1.19	1.25	5	2
1	A	73	THR	N-CA	5.49	1.57	1.46	4	1
1	A	26	GLU	CB-CG	5.42	1.62	1.52	4	1
1	A	26	GLU	CD-OE2	-5.40	1.19	1.25	5	3
1	A	12	CYS	N-CA	5.32	1.56	1.46	6	1
1	B	39	GLU	CB-CG	5.30	1.62	1.52	6	2
1	A	50	GLU	CB-CG	5.27	1.62	1.52	4	1
1	A	74	PRO	CA-C	5.27	1.63	1.52	3	1
1	B	44	LYS	CA-CB	-5.26	1.42	1.53	6	1
1	A	34	SER	N-CA	5.24	1.56	1.46	3	3
1	A	36	CYS	N-CA	5.23	1.56	1.46	6	1
1	A	38	ARG	N-CA	5.22	1.56	1.46	6	1
1	B	39	GLU	CD-OE1	-5.21	1.20	1.25	7	2
1	B	54	ASP	N-CA	5.20	1.56	1.46	3	1
1	B	26	GLU	CD-OE2	-5.16	1.20	1.25	7	1
1	A	55	PRO	CA-C	5.08	1.63	1.52	2	1
1	A	71	THR	N-CA	5.05	1.56	1.46	5	1
1	B	45	THR	N-CA	5.04	1.56	1.46	5	1
1	A	45	THR	CA-CB	-5.00	1.40	1.53	7	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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	28	TYR	CG-CD2-CE2	-115.55	28.86	121.30	7	1
1	B	28	TYR	CZ-CE2-CD2	-95.11	34.20	119.80	7	1
1	B	24	ARG	NE-CZ-NH2	-88.22	76.19	120.30	1	6
1	A	29	ARG	NE-CZ-NH1	-85.43	77.58	120.30	5	6
1	A	15	PHE	CG-CD1-CE1	-83.88	28.53	120.80	7	1
1	A	30	ARG	NE-CZ-NH1	-82.49	79.06	120.30	5	6
1	A	15	PHE	CD1-CE1-CZ	-73.46	31.95	120.10	7	1
1	B	24	ARG	NE-CZ-NH1	65.25	152.93	120.30	1	6
1	A	29	ARG	NE-CZ-NH2	54.51	147.56	120.30	5	6
1	B	28	TYR	CB-CG-CD2	52.38	152.43	121.00	7	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	28	TYR	CG-CD1-CE1	-52.10	79.62	121.30	7	1
1	A	30	ARG	NH1-CZ-NH2	-51.10	63.19	119.40	5	5
1	B	28	TYR	CD1-CG-CD2	-45.22	68.16	117.90	7	1
1	A	29	ARG	NH1-CZ-NH2	-44.90	70.01	119.40	5	4
1	A	30	ARG	NE-CZ-NH2	43.88	142.24	120.30	5	4
1	B	48	ASP	CB-CG-OD2	-40.37	81.97	118.30	4	6
1	B	24	ARG	NH1-CZ-NH2	-38.78	76.74	119.40	1	5
1	B	28	TYR	CD1-CE1-CZ	-38.56	85.09	119.80	7	1
1	A	15	PHE	CB-CG-CD1	37.76	147.23	120.80	7	5
1	A	15	PHE	CG-CD2-CE2	-37.38	79.69	120.80	7	1
1	A	15	PHE	CD1-CG-CD2	-37.26	69.87	118.30	7	1
1	B	28	TYR	CE1-CZ-CE2	-34.83	64.07	119.80	7	1
1	B	48	ASP	CB-CG-OD1	34.01	148.91	118.30	4	3
1	A	38	ARG	NE-CZ-NH2	31.56	136.08	120.30	1	5
1	A	15	PHE	CB-CG-CD2	31.54	142.88	120.80	7	5
1	A	15	PHE	CZ-CE2-CD2	-31.13	82.74	120.10	7	1
1	B	29	ARG	NE-CZ-NH1	-31.05	104.77	120.30	7	5
1	A	24	ARG	NE-CZ-NH1	-30.79	104.91	120.30	1	5
1	B	28	TYR	CB-CG-CD1	30.70	139.42	121.00	7	4
1	B	38	ARG	NE-CZ-NH1	-30.48	105.06	120.30	5	7
1	B	62	ASP	CB-CG-OD1	29.87	145.18	118.30	7	7
1	B	48	ASP	OD1-CG-OD2	-29.66	66.94	123.30	4	3
1	A	15	PHE	CE1-CZ-CE2	-29.32	67.23	120.00	7	1
1	B	30	ARG	NE-CZ-NH1	-28.98	105.81	120.30	5	5
1	A	62	ASP	CB-CG-OD1	28.51	143.96	118.30	6	6
1	A	38	ARG	NE-CZ-NH1	-26.83	106.89	120.30	3	5
1	B	57	GLN	OE1-CD-NE2	-25.34	63.63	121.90	3	3
1	B	14	ARG	NE-CZ-NH2	-25.07	107.77	120.30	5	2
1	B	29	ARG	NE-CZ-NH2	-24.07	108.26	120.30	5	5
1	A	14	ARG	NE-CZ-NH1	-23.57	108.52	120.30	5	5
1	B	30	ARG	NE-CZ-NH2	23.50	132.05	120.30	4	2
1	B	61	GLN	CG-CD-NE2	-23.22	60.98	116.70	4	2
1	B	62	ASP	CB-CG-OD2	22.62	138.66	118.30	4	4
1	A	53	ALA	N-CA-CB	-22.49	78.61	110.10	4	7
1	A	36	CYS	CA-CB-SG	21.30	152.35	114.00	6	4
1	B	31	THR	CA-CB-CG2	-21.01	82.99	112.40	3	3
1	A	14	ARG	NE-CZ-NH2	-20.30	110.15	120.30	6	4
1	A	61	GLN	CG-CD-OE1	-20.17	81.27	121.60	6	2
1	A	28	TYR	CB-CG-CD1	20.07	133.04	121.00	5	3
1	A	74	PRO	N-CA-CB	-19.75	79.60	103.30	3	4
1	A	24	ARG	NE-CZ-NH2	-19.48	110.56	120.30	7	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	14	ARG	NE-CZ-NH1	-18.89	110.85	120.30	1	4
1	A	62	ASP	CB-CG-OD2	18.69	135.12	118.30	1	5
1	A	33	SER	CA-C-N	17.58	155.87	117.20	5	3
1	A	61	GLN	OE1-CD-NE2	17.44	162.02	121.90	6	1
1	A	28	TYR	CB-CG-CD2	-17.40	110.56	121.00	5	4
1	A	52	CYS	CA-CB-SG	17.24	145.03	114.00	1	6
1	B	61	GLN	OE1-CD-NE2	16.83	160.61	121.90	4	3
1	B	53	ALA	N-CA-CB	-16.81	86.57	110.10	6	7
1	A	55	PRO	N-CA-CB	-16.40	83.62	103.30	2	4
1	B	57	GLN	CG-CD-NE2	16.39	156.04	116.70	3	3
1	A	24	ARG	NH1-CZ-NH2	15.81	136.80	119.40	1	6
1	A	54	ASP	CB-CG-OD1	15.64	132.38	118.30	3	2
1	B	38	ARG	NE-CZ-NH2	-15.62	112.49	120.30	4	6
1	A	13	TYR	CB-CG-CD1	-15.46	111.72	121.00	7	4
1	B	62	ASP	CA-CB-CG	15.43	147.35	113.40	7	4
1	A	31	THR	OG1-CB-CG2	-15.39	74.60	110.00	5	5
1	A	33	SER	O-C-N	-15.38	98.09	122.70	5	1
1	B	30	ARG	NH1-CZ-NH2	15.32	136.25	119.40	5	3
1	A	28	TYR	CA-CB-CG	15.31	142.49	113.40	2	4
1	B	57	GLN	N-CA-CB	-15.26	83.13	110.60	1	5
1	B	52	CYS	CA-CB-SG	15.22	141.39	114.00	6	4
1	B	43	PHE	CB-CG-CD2	-15.15	110.19	120.80	7	4
1	A	27	SER	N-CA-CB	-15.06	87.91	110.50	2	1
1	A	52	CYS	N-CA-CB	-15.01	83.59	110.60	6	3
1	A	61	GLN	CG-CD-NE2	-14.98	80.76	116.70	6	2
1	B	12	CYS	N-CA-C	14.88	151.18	111.00	4	3
1	A	17	ASN	N-CA-C	14.84	151.06	111.00	1	4
1	A	50	GLU	N-CA-C	14.82	151.01	111.00	7	2
1	B	25	LEU	N-CA-CB	-14.76	80.88	110.40	3	5
1	A	40	ALA	N-CA-CB	-14.62	89.63	110.10	7	4
1	A	45	THR	OG1-CB-CG2	-14.60	76.42	110.00	4	6
1	B	57	GLN	CG-CD-OE1	-14.59	92.42	121.60	3	1
1	B	32	THR	OG1-CB-CG2	-14.54	76.55	110.00	1	7
1	A	53	ALA	CB-CA-C	14.50	131.85	110.10	4	6
1	A	48	ASP	CB-CG-OD2	-14.39	105.35	118.30	7	3
1	A	14	ARG	NH1-CZ-NH2	14.39	135.23	119.40	5	5
1	A	21	PRO	N-CA-CB	-14.37	86.06	103.30	7	2
1	A	26	GLU	OE1-CD-OE2	-14.34	106.09	123.30	2	2
1	A	31	THR	N-CA-C	14.06	148.96	111.00	4	5
1	B	57	GLN	N-CA-C	14.01	148.84	111.00	3	3
1	A	41	VAL	N-CA-C	13.94	148.65	111.00	2	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	55	PRO	N-CD-CG	-13.91	82.33	103.20	4	6
1	B	62	ASP	OD1-CG-OD2	-13.79	97.09	123.30	4	5
1	B	30	ARG	CD-NE-CZ	13.77	142.88	123.60	1	6
1	A	75	LYS	N-CA-C	13.77	148.17	111.00	2	3
1	A	54	ASP	N-CA-C	13.75	148.13	111.00	4	3
1	B	45	THR	N-CA-C	13.68	147.93	111.00	3	5
1	A	11	CYS	CA-CB-SG	13.55	138.39	114.00	6	3
1	B	53	ALA	N-CA-C	13.53	147.54	111.00	4	4
1	A	26	GLU	C-N-CA	13.49	155.43	121.70	2	1
1	B	54	ASP	N-CA-CB	-13.47	86.36	110.60	5	6
1	B	44	LYS	N-CA-CB	-13.46	86.38	110.60	5	7
1	A	33	SER	C-N-CA	13.43	155.26	121.70	5	4
1	A	37	PRO	N-CA-C	13.43	147.01	112.10	3	2
1	A	39	GLU	OE1-CD-OE2	-13.41	107.21	123.30	2	5
1	A	12	CYS	CA-CB-SG	13.28	137.90	114.00	4	4
1	B	61	GLN	N-CA-CB	-12.97	87.26	110.60	2	2
1	B	25	LEU	CB-CA-C	12.86	134.63	110.20	3	3
1	B	28	TYR	OH-CZ-CE2	12.85	154.79	120.10	7	1
1	A	30	ARG	CA-CB-CG	12.79	141.54	113.40	7	1
1	A	50	GLU	OE1-CD-OE2	-12.78	107.97	123.30	3	3
1	A	43	PHE	CB-CG-CD2	-12.74	111.88	120.80	2	3
1	A	18	LYS	N-CA-CB	-12.59	87.93	110.60	4	5
1	A	68	ASP	CB-CG-OD2	12.58	129.63	118.30	7	5
1	B	70	LYS	N-CA-C	12.54	144.87	111.00	6	4
1	A	63	PHE	CB-CG-CD2	-12.50	112.05	120.80	6	2
1	B	33	SER	N-CA-C	12.45	144.62	111.00	3	3
1	B	28	TYR	CA-CB-CG	12.44	137.04	113.40	2	4
1	A	62	ASP	N-CA-CB	-12.41	88.25	110.60	7	4
1	B	36	CYS	CA-CB-SG	12.41	136.34	114.00	5	6
1	B	31	THR	OG1-CB-CG2	-12.39	81.50	110.00	3	6
1	A	62	ASP	CA-CB-CG	12.39	140.65	113.40	3	5
1	B	60	VAL	CA-CB-CG1	12.37	129.46	110.90	6	3
1	B	38	ARG	NH1-CZ-NH2	12.34	132.97	119.40	4	6
1	A	61	GLN	CB-CG-CD	12.33	143.66	111.60	6	5
1	A	72	GLN	N-CA-C	12.26	144.09	111.00	5	4
1	B	11	CYS	CA-CB-SG	12.23	136.01	114.00	6	2
1	B	57	GLN	CA-C-O	12.20	145.71	120.10	3	6
1	B	49	LYS	N-CA-CB	-12.17	88.69	110.60	2	2
1	B	55	PRO	N-CA-CB	-12.16	88.70	103.30	1	3
1	B	29	ARG	NH1-CZ-NH2	12.12	132.74	119.40	7	5
1	A	62	ASP	OD1-CG-OD2	-12.01	100.48	123.30	5	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	32	THR	N-CA-C	11.94	143.25	111.00	4	3
1	A	40	ALA	CB-CA-C	11.90	127.95	110.10	7	3
1	A	35	HIS	N-CA-C	11.87	143.04	111.00	6	3
1	B	49	LYS	CA-CB-CG	11.82	139.41	113.40	2	1
1	A	40	ALA	N-CA-C	11.80	142.86	111.00	6	3
1	A	23	GLN	C-N-CA	11.75	151.07	121.70	7	3
1	A	26	GLU	CG-CD-OE1	11.73	141.76	118.30	3	3
1	A	13	TYR	CB-CG-CD2	11.73	128.04	121.00	7	4
1	A	37	PRO	N-CA-CB	-11.65	89.31	103.30	2	3
1	B	68	ASP	N-CA-CB	-11.64	89.64	110.60	5	7
1	B	41	VAL	CA-CB-CG2	11.63	128.35	110.90	1	2
1	B	53	ALA	CB-CA-C	11.62	127.53	110.10	6	2
1	B	14	ARG	NH1-CZ-NH2	11.60	132.16	119.40	5	4
1	B	21	PRO	N-CA-CB	-11.60	89.39	103.30	1	3
1	A	21	PRO	N-CD-CG	-11.58	85.82	103.20	3	5
1	A	58	LYS	N-CA-CB	-11.57	89.77	110.60	5	4
1	A	38	ARG	NH1-CZ-NH2	-11.56	106.68	119.40	1	2
1	A	29	ARG	CD-NE-CZ	11.54	139.75	123.60	4	4
1	A	38	ARG	CA-CB-CG	11.53	138.76	113.40	5	2
1	A	73	THR	OG1-CB-CG2	-11.42	83.72	110.00	2	4
1	A	73	THR	CA-CB-CG2	11.40	128.36	112.40	4	2
1	A	15	PHE	N-CA-C	11.37	141.70	111.00	3	3
1	A	63	PHE	CB-CG-CD1	11.31	128.72	120.80	6	3
1	A	48	ASP	N-CA-CB	-11.28	90.29	110.60	3	7
1	B	30	ARG	CB-CG-CD	11.24	140.81	111.60	5	6
1	B	68	ASP	CA-CB-CG	11.18	137.99	113.40	2	2
1	B	56	THR	OG1-CB-CG2	-11.17	84.30	110.00	3	6
1	B	41	VAL	CG1-CB-CG2	-11.17	93.03	110.90	7	3
1	A	32	THR	OG1-CB-CG2	-11.13	84.39	110.00	7	5
1	B	58	LYS	N-CA-CB	-11.12	90.59	110.60	5	4
1	B	26	GLU	OE1-CD-OE2	-11.12	109.96	123.30	3	2
1	A	34	SER	N-CA-CB	11.12	127.18	110.50	5	1
1	B	43	PHE	CB-CG-CD1	11.11	128.58	120.80	7	2
1	A	74	PRO	N-CD-CG	-11.09	86.57	103.20	5	4
1	A	35	HIS	N-CA-CB	-11.07	90.68	110.60	6	5
1	B	24	ARG	O-C-N	-11.03	105.06	122.70	6	3
1	A	68	ASP	OD1-CG-OD2	-10.99	102.41	123.30	7	2
1	B	17	ASN	N-CA-C	10.99	140.66	111.00	6	6
1	B	61	GLN	CG-CD-OE1	-10.98	99.64	121.60	4	3
1	A	45	THR	N-CA-C	10.97	140.63	111.00	4	3
1	B	22	LYS	N-CA-CB	-10.96	90.88	110.60	5	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	68	ASP	N-CA-CB	-10.93	90.92	110.60	2	5
1	B	59	TRP	CG-CD1-NE1	-10.93	99.17	110.10	7	7
1	A	20	ILE	CA-CB-CG1	10.93	131.76	111.00	3	1
1	B	11	CYS	C-N-CA	10.93	149.02	121.70	3	4
1	A	54	ASP	N-CA-CB	-10.93	90.93	110.60	5	6
1	B	70	LYS	CA-C-N	10.90	141.17	117.20	7	1
1	A	52	CYS	CB-CA-C	10.89	132.19	110.40	6	1
1	B	24	ARG	CD-NE-CZ	10.86	138.81	123.60	2	4
1	B	14	ARG	N-CA-CB	-10.86	91.05	110.60	6	5
1	B	50	GLU	N-CA-CB	-10.85	91.07	110.60	5	7
1	A	72	GLN	C-N-CA	10.78	148.64	121.70	3	4
1	B	45	THR	CA-CB-CG2	10.76	127.46	112.40	3	3
1	A	56	THR	OG1-CB-CG2	-10.75	85.28	110.00	5	7
1	A	68	ASP	CB-CG-OD1	10.73	127.96	118.30	7	4
1	B	68	ASP	CB-CG-OD1	10.71	127.94	118.30	3	4
1	A	71	THR	OG1-CB-CG2	-10.70	85.38	110.00	7	7
1	B	59	TRP	CD1-NE1-CE2	10.69	118.62	109.00	5	6
1	B	39	GLU	N-CA-CB	-10.69	91.37	110.60	6	2
1	A	54	ASP	CB-CG-OD2	-10.66	108.70	118.30	2	5
1	A	55	PRO	N-CD-CG	-10.65	87.23	103.20	4	3
1	A	33	SER	N-CA-C	10.64	139.74	111.00	5	2
1	B	26	GLU	CG-CD-OE1	10.64	139.59	118.30	3	1
1	A	50	GLU	N-CA-CB	-10.60	91.52	110.60	5	5
1	B	23	GLN	N-CA-CB	-10.57	91.57	110.60	5	6
1	A	29	ARG	CA-CB-CG	10.54	136.58	113.40	5	1
1	A	60	VAL	CA-CB-CG1	10.52	126.68	110.90	2	2
1	B	13	TYR	CB-CG-CD2	-10.46	114.73	121.00	2	3
1	B	62	ASP	N-CA-CB	-10.45	91.79	110.60	1	3
1	B	48	ASP	N-CA-CB	-10.44	91.81	110.60	1	6
1	A	14	ARG	CG-CD-NE	-10.43	89.89	111.80	3	3
1	A	72	GLN	N-CA-CB	-10.41	91.87	110.60	5	5
1	A	31	THR	C-N-CA	10.40	147.69	121.70	3	3
1	B	15	PHE	O-C-N	-10.40	106.07	122.70	5	1
1	B	26	GLU	N-CA-C	10.38	139.02	111.00	1	3
1	B	14	ARG	CD-NE-CZ	10.37	138.12	123.60	7	3
1	A	57	GLN	N-CA-CB	-10.35	91.98	110.60	4	3
1	B	63	PHE	CB-CG-CD2	-10.32	113.58	120.80	5	3
1	A	43	PHE	CB-CG-CD1	10.30	128.01	120.80	2	2
1	B	54	ASP	CB-CG-OD1	10.29	127.56	118.30	1	3
1	B	44	LYS	CB-CA-C	10.28	130.96	110.40	5	5
1	B	26	GLU	N-CA-CB	-10.28	92.10	110.60	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	66	HIS	CA-CB-CG	-10.28	96.13	113.60	6	2
1	A	55	PRO	C-N-CA	10.27	147.38	121.70	2	1
1	B	43	PHE	CA-CB-CG	10.26	138.51	113.90	6	5
1	A	70	LYS	N-CA-CB	-10.25	92.16	110.60	3	6
1	A	19	LYS	N-CA-CB	-10.23	92.19	110.60	1	5
1	A	59	TRP	CD1-NE1-CE2	10.23	118.20	109.00	7	7
1	A	11	CYS	CA-C-N	10.21	139.66	117.20	7	2
1	B	23	GLN	N-CA-C	10.17	138.47	111.00	6	6
1	A	16	ILE	N-CA-C	10.17	138.45	111.00	2	2
1	B	24	ARG	N-CA-CB	-10.16	92.32	110.60	2	3
1	B	56	THR	O-C-N	-10.15	106.45	122.70	3	2
1	A	62	ASP	CB-CA-C	10.14	130.69	110.40	1	3
1	A	75	LYS	N-CA-CB	-10.08	92.45	110.60	6	4
1	A	48	ASP	N-CA-C	10.05	138.13	111.00	5	7
1	A	65	LYS	N-CA-CB	-9.99	92.61	110.60	7	3
1	A	31	THR	CA-C-N	-9.98	95.25	117.20	3	2
1	A	39	GLU	N-CA-C	9.97	137.92	111.00	1	4
1	B	13	TYR	CB-CG-CD1	9.97	126.98	121.00	2	3
1	A	48	ASP	CA-C-N	-9.96	95.29	117.20	1	7
1	A	30	ARG	CA-C-N	-9.90	95.42	117.20	5	1
1	A	30	ARG	C-N-CA	9.87	146.37	121.70	4	2
1	B	66	HIS	N-CA-CB	-9.86	92.86	110.60	3	4
1	A	38	ARG	CA-C-N	9.86	138.88	117.20	6	1
1	B	67	LEU	N-CA-CB	-9.79	90.82	110.40	1	3
1	A	17	ASN	N-CA-CB	-9.77	93.01	110.60	1	7
1	B	59	TRP	CD1-CG-CD2	9.77	114.12	106.30	7	6
1	A	41	VAL	CA-CB-CG2	-9.75	96.27	110.90	4	3
1	A	30	ARG	CB-CG-CD	9.75	136.95	111.60	4	3
1	B	55	PRO	N-CA-C	9.74	137.42	112.10	6	4
1	A	27	SER	CA-C-N	9.74	138.63	117.20	2	1
1	B	12	CYS	CA-CB-SG	9.73	131.52	114.00	3	3
1	B	65	LYS	N-CA-CB	-9.73	93.09	110.60	6	4
1	A	16	ILE	C-N-CA	9.73	146.02	121.70	5	1
1	B	19	LYS	N-CA-CB	-9.71	93.12	110.60	5	5
1	A	22	LYS	N-CA-CB	-9.71	93.13	110.60	3	5
1	B	45	THR	CA-CB-OG1	9.70	129.38	109.00	5	5
1	B	38	ARG	N-CA-CB	-9.70	93.14	110.60	3	1
1	A	47	LEU	N-CA-C	-9.69	84.83	111.00	1	2
1	A	50	GLU	CA-CB-CG	9.68	134.69	113.40	5	2
1	B	27	SER	N-CA-CB	-9.68	95.99	110.50	3	1
1	A	59	TRP	CB-CG-CD2	-9.66	114.05	126.60	6	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	62	ASP	CB-CA-C	9.65	129.70	110.40	1	3
1	B	11	CYS	N-CA-CB	-9.64	93.25	110.60	3	4
1	A	57	GLN	CA-C-O	9.63	140.33	120.10	5	6
1	A	59	TRP	CG-CD1-NE1	-9.62	100.48	110.10	6	7
1	B	32	THR	N-CA-C	9.61	136.96	111.00	2	3
1	B	50	GLU	OE1-CD-OE2	-9.61	111.77	123.30	4	2
1	A	72	GLN	CB-CG-CD	9.61	136.58	111.60	5	1
1	A	68	ASP	CB-CA-C	9.57	129.54	110.40	2	3
1	B	18	LYS	N-CA-CB	-9.57	93.37	110.60	1	2
1	A	69	LYS	N-CA-CB	-9.57	93.38	110.60	1	4
1	A	37	PRO	C-N-CA	9.54	145.56	121.70	5	2
1	A	53	ALA	N-CA-C	9.54	136.76	111.00	3	3
1	A	71	THR	N-CA-C	9.53	136.72	111.00	2	3
1	A	53	ALA	C-N-CA	9.48	145.40	121.70	4	2
1	B	37	PRO	N-CA-CB	-9.45	91.96	103.30	3	4
1	A	73	THR	N-CA-C	9.45	136.50	111.00	5	4
1	B	34	SER	N-CA-C	9.42	136.44	111.00	1	4
1	B	11	CYS	N-CA-C	9.37	136.29	111.00	3	2
1	A	38	ARG	CG-CD-NE	-9.34	92.20	111.80	3	3
1	B	50	GLU	N-CA-C	9.33	136.20	111.00	7	3
1	B	68	ASP	CB-CA-C	9.30	128.99	110.40	5	5
1	B	63	PHE	CB-CG-CD1	9.30	127.31	120.80	5	1
1	B	35	HIS	N-CA-C	9.28	136.05	111.00	3	4
1	B	22	LYS	N-CA-C	9.27	136.02	111.00	5	2
1	A	43	PHE	CA-CB-CG	9.26	136.13	113.90	3	6
1	A	64	MET	N-CA-CB	-9.22	94.00	110.60	2	1
1	A	29	ARG	N-CA-C	9.22	135.91	111.00	6	2
1	B	35	HIS	N-CA-CB	-9.21	94.03	110.60	5	5
1	B	25	LEU	N-CA-C	-9.20	86.15	111.00	3	1
1	A	57	GLN	OE1-CD-NE2	-9.19	100.77	121.90	4	3
1	A	39	GLU	N-CA-CB	-9.17	94.09	110.60	1	4
1	A	74	PRO	N-CA-C	9.17	135.95	112.10	6	4
1	B	54	ASP	CB-CG-OD2	-9.13	110.08	118.30	1	2
1	A	50	GLU	CB-CG-CD	9.11	138.81	114.20	3	3
1	B	20	ILE	CA-CB-CG1	9.11	128.31	111.00	2	1
1	A	12	CYS	CA-C-O	9.11	139.22	120.10	7	1
1	B	53	ALA	CA-C-O	-9.09	101.01	120.10	3	2
1	A	11	CYS	N-CA-CB	-9.07	94.27	110.60	1	3
1	A	14	ARG	C-N-CA	9.05	144.33	121.70	5	3
1	B	38	ARG	CG-CD-NE	-9.05	92.80	111.80	5	4
1	A	14	ARG	CD-NE-CZ	9.04	136.26	123.60	2	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	25	LEU	N-CA-CB	-9.04	92.31	110.40	1	5
1	A	30	ARG	CD-NE-CZ	9.01	136.22	123.60	2	2
1	B	21	PRO	N-CD-CG	-8.99	89.72	103.20	3	3
1	A	70	LYS	N-CA-C	8.98	135.25	111.00	6	4
1	A	31	THR	CA-CB-CG2	8.97	124.96	112.40	5	4
1	B	48	ASP	N-CA-C	8.96	135.19	111.00	5	4
1	B	18	LYS	N-CA-C	8.95	135.18	111.00	1	2
1	B	21	PRO	CA-N-CD	-8.95	98.97	111.50	4	1
1	B	26	GLU	C-N-CA	8.95	144.07	121.70	3	1
1	A	26	GLU	N-CA-CB	-8.93	94.53	110.60	4	5
1	A	44	LYS	N-CA-CB	-8.91	94.56	110.60	5	4
1	B	67	LEU	CB-CA-C	8.90	127.11	110.20	1	3
1	A	17	ASN	CA-CB-CG	8.86	132.88	113.40	1	2
1	B	40	ALA	N-CA-CB	-8.86	97.70	110.10	6	5
1	A	23	GLN	N-CA-C	8.85	134.89	111.00	3	3
1	B	36	CYS	N-CA-CB	-8.85	94.67	110.60	5	2
1	B	66	HIS	CA-C-N	-8.81	97.82	117.20	5	1
1	B	49	LYS	CB-CA-C	-8.80	92.79	110.40	5	2
1	A	73	THR	N-CA-CB	-8.79	93.60	110.30	3	1
1	B	39	GLU	CB-CG-CD	8.78	137.91	114.20	5	2
1	B	26	GLU	CB-CA-C	8.78	127.97	110.40	3	1
1	A	50	GLU	CG-CD-OE1	8.78	135.86	118.30	4	3
1	B	65	LYS	CG-CD-CE	8.77	138.20	111.90	3	1
1	B	69	LYS	CD-CE-NZ	-8.76	91.54	111.70	3	2
1	B	46	LYS	N-CA-CB	-8.75	94.84	110.60	1	4
1	A	75	LYS	C-N-CA	8.75	143.57	121.70	2	1
1	B	69	LYS	N-CA-C	8.73	134.58	111.00	2	2
1	A	27	SER	CA-C-O	-8.71	101.81	120.10	2	1
1	A	34	SER	CB-CA-C	-8.68	93.61	110.10	5	1
1	A	46	LYS	CA-CB-CG	8.67	132.47	113.40	5	2
1	B	13	TYR	N-CA-CB	-8.66	95.01	110.60	4	4
1	A	72	GLN	CA-CB-CG	8.65	132.42	113.40	2	2
1	B	61	GLN	CB-CA-C	8.64	127.69	110.40	2	2
1	B	50	GLU	C-N-CA	8.63	143.27	121.70	3	1
1	A	64	MET	CA-CB-CG	8.62	127.95	113.30	4	3
1	A	65	LYS	C-N-CA	8.62	143.25	121.70	2	1
1	A	70	LYS	C-N-CA	8.61	143.22	121.70	2	2
1	A	16	ILE	CA-C-N	8.61	136.14	117.20	2	2
1	A	14	ARG	CA-CB-CG	8.61	132.34	113.40	3	1
1	B	64	MET	N-CA-CB	-8.58	95.16	110.60	3	2
1	B	45	THR	N-CA-CB	-8.57	94.01	110.30	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	14	ARG	CG-CD-NE	-8.53	93.89	111.80	6	5
1	B	38	ARG	C-N-CA	8.53	143.02	121.70	3	3
1	A	39	GLU	CG-CD-OE1	8.52	135.34	118.30	2	2
1	B	24	ARG	CA-C-N	8.51	135.92	117.20	5	5
1	B	24	ARG	CB-CA-C	8.49	127.37	110.40	2	1
1	A	37	PRO	N-CD-CG	-8.47	90.49	103.20	1	5
1	A	32	THR	CA-CB-CG2	-8.47	100.53	112.40	5	2
1	A	60	VAL	CA-CB-CG2	-8.47	98.19	110.90	4	1
1	B	15	PHE	CB-CG-CD2	8.46	126.73	120.80	6	3
1	B	65	LYS	CB-CG-CD	8.45	133.56	111.60	7	1
1	B	56	THR	CA-CB-CG2	8.43	124.21	112.40	3	2
1	B	61	GLN	CA-C-N	-8.39	98.73	117.20	3	6
1	B	19	LYS	CD-CE-NZ	-8.39	92.40	111.70	4	2
1	B	25	LEU	CB-CG-CD1	8.37	125.22	111.00	7	1
1	B	39	GLU	OE1-CD-OE2	-8.35	113.29	123.30	7	4
1	A	46	LYS	CB-CG-CD	8.34	133.29	111.60	5	2
1	A	64	MET	CB-CA-C	8.33	127.06	110.40	2	1
1	B	54	ASP	CA-CB-CG	8.33	131.72	113.40	1	2
1	B	41	VAL	CA-CB-CG1	8.32	123.39	110.90	5	2
1	A	41	VAL	CA-CB-CG1	8.31	123.36	110.90	5	2
1	A	54	ASP	OD1-CG-OD2	-8.30	107.52	123.30	3	1
1	B	70	LYS	N-CA-CB	-8.26	95.73	110.60	4	3
1	B	57	GLN	CA-C-N	-8.23	99.10	117.20	4	2
1	A	59	TRP	CD1-CG-CD2	8.22	112.87	106.30	6	4
1	B	38	ARG	CD-NE-CZ	8.22	135.10	123.60	2	1
1	B	23	GLN	CB-CG-CD	8.20	132.91	111.60	2	2
1	A	48	ASP	CA-C-O	8.19	137.31	120.10	2	6
1	B	41	VAL	N-CA-C	8.19	133.12	111.00	6	3
1	B	70	LYS	CB-CG-CD	8.16	132.82	111.60	5	2
1	B	23	GLN	CG-CD-OE1	8.14	137.89	121.60	1	1
1	B	19	LYS	CG-CD-CE	8.14	136.31	111.90	6	2
1	A	48	ASP	O-C-N	-8.13	109.68	122.70	7	1
1	B	47	LEU	C-N-CA	8.13	142.03	121.70	4	4
1	A	25	LEU	CB-CA-C	8.13	125.64	110.20	4	3
1	A	23	GLN	N-CA-CB	-8.12	95.98	110.60	3	4
1	B	44	LYS	CG-CD-CE	8.11	136.24	111.90	4	1
1	B	56	THR	CA-C-N	8.10	135.01	117.20	3	2
1	B	39	GLU	N-CA-C	8.06	132.77	111.00	5	2
1	A	19	LYS	N-CA-C	8.06	132.76	111.00	2	1
1	A	18	LYS	N-CA-C	8.02	132.64	111.00	2	6
1	A	31	THR	O-C-N	8.00	135.51	122.70	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	22	LYS	CB-CA-C	8.00	126.40	110.40	2	3
1	B	47	LEU	N-CA-CB	-7.99	94.42	110.40	6	1
1	B	66	HIS	CB-CA-C	7.97	126.35	110.40	3	3
1	B	70	LYS	CD-CE-NZ	-7.97	93.36	111.70	6	1
1	A	15	PHE	C-N-CA	7.97	141.62	121.70	4	1
1	B	67	LEU	C-N-CA	7.97	141.62	121.70	5	1
1	A	41	VAL	CB-CA-C	-7.96	96.27	111.40	2	3
1	B	45	THR	OG1-CB-CG2	-7.96	91.69	110.00	4	4
1	B	70	LYS	CA-CB-CG	7.96	130.91	113.40	7	3
1	B	59	TRP	NE1-CE2-CZ2	7.96	139.16	130.40	2	2
1	B	17	ASN	N-CA-CB	-7.96	96.28	110.60	4	5
1	A	14	ARG	N-CA-C	7.95	132.45	111.00	2	2
1	B	61	GLN	CB-CG-CD	7.94	132.25	111.60	1	3
1	B	34	SER	N-CA-CB	-7.94	98.58	110.50	4	2
1	B	54	ASP	N-CA-C	7.93	132.40	111.00	7	3
1	A	31	THR	CA-CB-OG1	-7.92	92.37	109.00	2	2
1	A	24	ARG	CG-CD-NE	-7.91	95.20	111.80	2	2
1	A	29	ARG	C-N-CA	7.90	141.46	121.70	4	1
1	B	26	GLU	CA-CB-CG	7.88	130.73	113.40	5	3
1	B	54	ASP	CB-CA-C	7.87	126.15	110.40	5	3
1	A	58	LYS	CB-CA-C	7.87	126.14	110.40	6	3
1	B	15	PHE	CB-CG-CD1	7.87	126.31	120.80	2	4
1	A	57	GLN	O-C-N	-7.86	110.12	122.70	5	2
1	A	16	ILE	CB-CA-C	7.84	127.29	111.60	6	1
1	B	52	CYS	N-CA-CB	-7.84	96.49	110.60	6	3
1	A	27	SER	CB-CA-C	7.83	124.97	110.10	2	3
1	A	65	LYS	CB-CA-C	7.83	126.05	110.40	7	1
1	A	44	LYS	CA-CB-CG	7.80	130.56	113.40	5	2
1	B	19	LYS	CB-CG-CD	7.80	131.87	111.60	4	3
1	B	68	ASP	CA-C-N	-7.79	100.06	117.20	7	3
1	B	28	TYR	CE1-CZ-OH	7.79	141.14	120.10	7	1
1	B	58	LYS	CB-CA-C	7.79	125.98	110.40	5	3
1	A	75	LYS	CB-CA-C	7.79	125.97	110.40	6	2
1	B	46	LYS	CD-CE-NZ	-7.79	93.79	111.70	1	4
1	B	15	PHE	N-CA-C	7.78	132.01	111.00	6	3
1	B	28	TYR	C-N-CA	7.78	141.16	121.70	6	1
1	B	53	ALA	C-N-CA	7.78	141.14	121.70	4	2
1	A	35	HIS	C-N-CA	7.76	141.10	121.70	6	3
1	A	39	GLU	CB-CG-CD	7.76	135.15	114.20	2	3
1	B	29	ARG	CG-CD-NE	-7.75	95.52	111.80	4	2
1	B	12	CYS	CB-CA-C	-7.75	94.91	110.40	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	31	THR	N-CA-C	7.73	131.88	111.00	5	3
1	A	48	ASP	OD1-CG-OD2	7.73	137.99	123.30	7	1
1	B	41	VAL	CB-CA-C	-7.73	96.72	111.40	1	2
1	A	30	ARG	CA-C-O	7.72	136.32	120.10	5	1
1	A	31	THR	N-CA-CB	-7.72	95.64	110.30	4	1
1	A	70	LYS	CD-CE-NZ	-7.71	93.97	111.70	3	3
1	A	12	CYS	CA-C-N	-7.71	100.24	117.20	7	1
1	A	71	THR	C-N-CA	7.71	140.97	121.70	2	1
1	B	57	GLN	CB-CG-CD	7.69	131.59	111.60	2	2
1	A	12	CYS	N-CA-CB	-7.69	96.76	110.60	5	1
1	A	64	MET	O-C-N	7.67	134.97	122.70	5	1
1	B	21	PRO	C-N-CA	7.67	140.87	121.70	3	1
1	A	59	TRP	CB-CG-CD1	7.66	136.96	127.00	5	1
1	A	54	ASP	CB-CA-C	7.66	125.71	110.40	5	2
1	B	28	TYR	N-CA-CB	-7.64	96.85	110.60	5	2
1	A	74	PRO	C-N-CA	7.63	140.78	121.70	3	3
1	A	71	THR	O-C-N	-7.63	110.49	122.70	5	3
1	A	34	SER	C-N-CA	7.62	140.75	121.70	2	2
1	B	30	ARG	N-CA-C	-7.62	90.43	111.00	7	2
1	B	15	PHE	N-CA-CB	-7.61	96.90	110.60	7	4
1	B	28	TYR	CB-CA-C	7.61	125.61	110.40	5	1
1	B	59	TRP	CH2-CZ2-CE2	7.61	125.01	117.40	6	1
1	A	46	LYS	C-N-CA	7.57	140.63	121.70	5	2
1	A	18	LYS	CB-CA-C	7.57	125.53	110.40	6	2
1	A	38	ARG	CD-NE-CZ	7.56	134.18	123.60	2	2
1	B	33	SER	CB-CA-C	-7.55	95.75	110.10	3	1
1	B	66	HIS	CA-CB-CG	-7.55	100.77	113.60	6	2
1	B	19	LYS	N-CA-C	-7.55	90.62	111.00	4	5
1	A	75	LYS	CA-C-N	-7.52	100.66	117.20	2	1
1	A	22	LYS	CD-CE-NZ	-7.51	94.43	111.70	3	4
1	A	61	GLN	CA-C-N	-7.51	100.69	117.20	6	5
1	A	46	LYS	N-CA-CB	-7.50	97.10	110.60	6	3
1	A	36	CYS	N-CA-C	7.49	131.23	111.00	5	3
1	B	34	SER	C-N-CA	7.49	140.41	121.70	1	3
1	A	49	LYS	CD-CE-NZ	-7.48	94.50	111.70	3	3
1	B	29	ARG	CD-NE-CZ	7.47	134.06	123.60	3	4
1	A	27	SER	N-CA-C	7.47	131.16	111.00	2	1
1	B	70	LYS	CA-C-O	-7.45	104.45	120.10	7	1
1	B	11	CYS	CA-C-N	7.43	133.55	117.20	1	1
1	B	50	GLU	CB-CA-C	7.41	125.22	110.40	4	2
1	B	14	ARG	N-CA-C	7.41	131.01	111.00	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	17	ASN	CA-C-O	7.39	135.62	120.10	6	1
1	B	12	CYS	N-CA-CB	-7.39	97.30	110.60	2	3
1	B	32	THR	CA-CB-OG1	7.37	124.47	109.00	5	2
1	A	73	THR	CA-CB-OG1	7.35	124.43	109.00	7	1
1	A	44	LYS	CD-CE-NZ	-7.34	94.81	111.70	4	2
1	B	49	LYS	C-N-CA	7.34	140.05	121.70	2	1
1	B	39	GLU	CB-CA-C	7.34	125.07	110.40	6	2
1	B	61	GLN	CA-CB-CG	-7.33	97.28	113.40	3	3
1	A	17	ASN	OD1-CG-ND2	-7.31	105.09	121.90	6	3
1	B	44	LYS	CA-CB-CG	7.30	129.45	113.40	5	1
1	A	56	THR	N-CA-C	7.28	130.66	111.00	2	1
1	B	56	THR	CB-CA-C	-7.28	91.95	111.60	1	1
1	B	40	ALA	N-CA-C	7.27	130.63	111.00	6	3
1	A	28	TYR	N-CA-C	-7.26	91.40	111.00	5	4
1	A	15	PHE	CA-CB-CG	7.25	131.30	113.90	5	2
1	B	65	LYS	CD-CE-NZ	-7.21	95.12	111.70	7	1
1	A	36	CYS	O-C-N	-7.20	107.42	121.10	6	1
1	A	24	ARG	CD-NE-CZ	7.19	133.67	123.60	7	2
1	A	16	ILE	CA-CB-CG1	7.18	124.65	111.00	3	1
1	B	68	ASP	C-N-CA	7.18	139.65	121.70	5	1
1	A	33	SER	CA-C-O	7.18	135.17	120.10	2	3
1	A	15	PHE	CB-CA-C	-7.17	96.06	110.40	1	2
1	B	65	LYS	N-CA-C	7.14	130.28	111.00	5	1
1	A	19	LYS	CA-CB-CG	7.13	129.08	113.40	4	2
1	A	47	LEU	N-CA-CB	-7.12	96.16	110.40	6	1
1	A	16	ILE	N-CA-CB	-7.11	94.44	110.80	1	2
1	B	24	ARG	C-N-CA	7.11	139.48	121.70	6	3
1	A	39	GLU	CA-C-N	-7.11	101.57	117.20	3	2
1	A	47	LEU	C-N-CA	7.09	139.42	121.70	7	2
1	A	22	LYS	N-CA-C	7.08	130.12	111.00	3	2
1	B	66	HIS	O-C-N	7.08	134.03	122.70	5	1
1	A	17	ASN	CA-C-O	7.07	134.94	120.10	2	2
1	A	47	LEU	CA-C-N	-7.06	101.66	117.20	7	1
1	B	60	VAL	N-CA-C	-7.06	91.93	111.00	5	1
1	A	31	THR	CA-C-O	7.06	134.92	120.10	6	2
1	B	17	ASN	C-N-CA	7.05	139.32	121.70	3	2
1	A	40	ALA	CA-C-N	-7.05	101.69	117.20	7	1
1	B	37	PRO	N-CD-CG	-7.04	92.64	103.20	2	2
1	A	72	GLN	CA-C-N	-7.03	101.74	117.20	3	2
1	A	74	PRO	CB-CA-C	7.00	129.51	112.00	3	1
1	B	50	GLU	CA-C-O	7.00	134.80	120.10	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	75	LYS	CG-CD-CE	7.00	132.89	111.90	4	1
1	A	68	ASP	CA-C-N	-6.99	101.83	117.20	5	4
1	B	58	LYS	CB-CG-CD	-6.97	93.47	111.60	5	2
1	B	33	SER	CA-C-O	6.97	134.74	120.10	5	3
1	A	19	LYS	CG-CD-CE	6.97	132.81	111.90	7	1
1	A	67	LEU	N-CA-CB	-6.96	96.49	110.40	4	5
1	B	70	LYS	O-C-N	-6.96	111.57	122.70	5	3
1	B	28	TYR	N-CA-C	-6.95	92.24	111.00	5	2
1	B	49	LYS	CD-CE-NZ	-6.94	95.73	111.70	6	4
1	A	33	SER	CA-CB-OG	-6.93	92.48	111.20	1	3
1	B	24	ARG	N-CA-C	6.92	129.69	111.00	5	2
1	A	36	CYS	N-CA-CB	-6.92	98.15	110.60	5	3
1	B	23	GLN	OE1-CD-NE2	-6.91	106.01	121.90	1	1
1	A	75	LYS	CD-CE-NZ	-6.88	95.88	111.70	6	4
1	A	38	ARG	CA-C-O	-6.87	105.68	120.10	6	1
1	A	58	LYS	CD-CE-NZ	-6.86	95.91	111.70	3	1
1	A	69	LYS	N-CA-C	6.86	129.51	111.00	5	1
1	A	15	PHE	O-C-N	6.86	133.67	122.70	6	2
1	B	24	ARG	CA-CB-CG	6.85	128.47	113.40	7	1
1	B	48	ASP	CA-C-O	6.85	134.49	120.10	4	5
1	A	56	THR	N-CA-CB	6.85	123.31	110.30	1	1
1	B	28	TYR	CA-C-O	6.85	134.48	120.10	5	1
1	A	67	LEU	CB-CA-C	6.83	123.19	110.20	4	2
1	A	11	CYS	CA-C-O	-6.83	105.75	120.10	6	2
1	A	48	ASP	CB-CG-OD1	6.82	124.44	118.30	1	3
1	B	16	ILE	O-C-N	-6.82	111.78	122.70	2	4
1	A	16	ILE	CA-C-O	-6.82	105.77	120.10	2	2
1	A	49	LYS	CB-CA-C	-6.82	96.76	110.40	3	1
1	A	75	LYS	CA-CB-CG	6.81	128.38	113.40	1	3
1	B	38	ARG	CA-C-N	6.81	132.18	117.20	2	1
1	A	55	PRO	N-CA-C	6.81	129.80	112.10	5	4
1	A	11	CYS	O-C-N	-6.81	111.81	122.70	7	2
1	A	32	THR	C-N-CA	6.80	138.69	121.70	6	3
1	A	21	PRO	N-CA-C	6.80	129.77	112.10	7	1
1	A	57	GLN	CG-CD-OE1	6.79	135.18	121.60	5	1
1	A	29	ARG	CG-CD-NE	-6.79	97.55	111.80	5	2
1	B	18	LYS	CD-CE-NZ	-6.78	96.10	111.70	1	4
1	A	26	GLU	CA-C-N	-6.78	102.28	117.20	2	1
1	B	61	GLN	CA-C-O	6.78	134.33	120.10	3	3
1	A	30	ARG	N-CA-CB	-6.78	98.40	110.60	2	1
1	A	38	ARG	O-C-N	-6.78	111.86	122.70	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	46	LYS	CA-C-N	-6.77	102.30	117.20	3	3
1	B	18	LYS	CA-CB-CG	6.76	128.28	113.40	3	2
1	A	18	LYS	CB-CG-CD	6.76	129.17	111.60	5	2
1	A	55	PRO	CA-C-O	6.75	136.41	120.20	2	1
1	A	46	LYS	CG-CD-CE	6.73	132.09	111.90	5	1
1	B	56	THR	CA-C-O	6.73	134.23	120.10	5	2
1	A	29	ARG	CB-CG-CD	6.73	129.09	111.60	7	2
1	A	23	GLN	O-C-N	6.72	133.46	122.70	7	1
1	A	18	LYS	CG-CD-CE	6.72	132.07	111.90	7	2
1	A	61	GLN	CA-CB-CG	-6.72	98.61	113.40	3	3
1	B	68	ASP	CB-CG-OD2	6.71	124.34	118.30	6	3
1	A	23	GLN	CG-CD-OE1	6.69	134.98	121.60	6	1
1	B	45	THR	C-N-CA	6.69	138.42	121.70	4	3
1	A	18	LYS	CA-CB-CG	6.67	128.08	113.40	5	2
1	A	58	LYS	CA-CB-CG	6.66	128.06	113.40	2	1
1	B	29	ARG	CA-CB-CG	6.65	128.03	113.40	4	2
1	B	48	ASP	CB-CA-C	6.64	123.69	110.40	1	1
1	B	19	LYS	CB-CA-C	6.64	123.68	110.40	4	1
1	A	69	LYS	CB-CA-C	6.64	123.67	110.40	1	2
1	B	57	GLN	CA-CB-CG	-6.63	98.81	113.40	7	3
1	A	23	GLN	OE1-CD-NE2	-6.63	106.64	121.90	7	7
1	A	75	LYS	CB-CG-CD	-6.63	94.35	111.60	7	3
1	A	59	TRP	NE1-CE2-CZ2	6.63	137.69	130.40	3	5
1	A	68	ASP	C-N-CA	6.62	138.25	121.70	1	1
1	A	18	LYS	CD-CE-NZ	-6.62	96.48	111.70	7	2
1	A	21	PRO	C-N-CA	6.61	138.23	121.70	7	1
1	B	64	MET	CB-CA-C	6.55	123.51	110.40	3	1
1	B	47	LEU	CB-CA-C	6.55	122.65	110.20	6	1
1	A	66	HIS	N-CA-C	-6.55	93.31	111.00	2	2
1	A	17	ASN	CB-CA-C	6.54	123.48	110.40	2	1
1	B	54	ASP	CA-C-N	6.53	135.39	117.10	4	2
1	B	18	LYS	CB-CG-CD	6.52	128.54	111.60	2	1
1	B	46	LYS	CB-CG-CD	6.51	128.53	111.60	7	1
1	B	16	ILE	N-CA-CB	-6.51	95.82	110.80	4	4
1	B	39	GLU	CA-CB-CG	-6.51	99.08	113.40	1	1
1	B	65	LYS	CB-CA-C	6.51	123.42	110.40	6	1
1	B	39	GLU	C-N-CA	6.49	137.93	121.70	5	2
1	A	50	GLU	CB-CA-C	6.49	123.38	110.40	2	2
1	B	53	ALA	O-C-N	-6.47	112.34	122.70	7	2
1	A	72	GLN	CG-CD-NE2	6.47	132.24	116.70	5	1
1	A	25	LEU	N-CA-C	6.46	128.45	111.00	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	19	LYS	CA-CB-CG	6.46	127.61	113.40	4	3
1	A	70	LYS	O-C-N	-6.45	112.38	122.70	5	2
1	B	36	CYS	N-CA-C	6.45	128.42	111.00	7	2
1	B	32	THR	CA-CB-CG2	-6.45	103.37	112.40	1	2
1	A	74	PRO	CA-CB-CG	-6.45	91.74	104.00	4	1
1	B	23	GLN	CA-C-N	6.44	131.37	117.20	6	2
1	A	19	LYS	CB-CG-CD	6.43	128.33	111.60	1	2
1	B	28	TYR	CA-C-N	-6.43	103.04	117.20	5	1
1	A	14	ARG	CA-C-N	-6.43	103.04	117.20	7	1
1	A	33	SER	N-CA-CB	-6.42	100.86	110.50	5	2
1	A	38	ARG	N-CA-C	6.42	128.35	111.00	7	3
1	B	30	ARG	C-N-CA	6.42	137.75	121.70	7	1
1	A	70	LYS	CA-C-N	6.41	131.31	117.20	4	2
1	B	56	THR	N-CA-CB	6.41	122.48	110.30	1	2
1	A	57	GLN	CG-CD-NE2	6.41	132.07	116.70	4	1
1	A	61	GLN	CA-C-O	6.39	133.53	120.10	6	5
1	A	55	PRO	CA-CB-CG	-6.38	91.87	104.00	3	1
1	B	56	THR	N-CA-C	6.38	128.24	111.00	5	2
1	A	57	GLN	CA-C-N	-6.38	103.16	117.20	6	1
1	A	29	ARG	N-CA-CB	-6.38	99.11	110.60	6	2
1	B	20	ILE	N-CA-C	6.38	128.22	111.00	6	1
1	B	65	LYS	CA-C-N	-6.37	103.18	117.20	5	1
1	B	52	CYS	CA-C-O	-6.37	106.72	120.10	7	1
1	B	43	PHE	N-CA-C	-6.37	93.81	111.00	5	1
1	A	44	LYS	N-CA-C	-6.36	93.82	111.00	4	1
1	B	41	VAL	O-C-N	6.36	132.87	122.70	3	1
1	A	47	LEU	CB-CA-C	6.36	122.28	110.20	6	1
1	A	19	LYS	CB-CA-C	6.35	123.11	110.40	1	1
1	A	71	THR	N-CA-CB	-6.35	98.23	110.30	2	1
1	A	11	CYS	CB-CA-C	6.34	123.09	110.40	1	2
1	A	65	LYS	CD-CE-NZ	-6.34	97.12	111.70	2	2
1	A	14	ARG	CA-C-O	6.30	133.33	120.10	7	1
1	B	64	MET	CA-C-O	6.27	133.27	120.10	3	1
1	A	75	LYS	O-C-N	-6.25	112.69	122.70	1	2
1	A	57	GLN	CA-CB-CG	-6.25	99.65	113.40	2	2
1	A	74	PRO	CA-C-N	6.24	130.92	117.20	6	1
1	A	24	ARG	N-CA-C	-6.24	94.17	111.00	5	1
1	B	55	PRO	O-C-N	-6.24	112.72	122.70	7	1
1	B	23	GLN	C-N-CA	6.23	137.28	121.70	3	1
1	A	70	LYS	CB-CA-C	6.23	122.86	110.40	4	3
1	A	55	PRO	CB-CA-C	6.21	127.53	112.00	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	15	PHE	N-CA-CB	-6.21	99.43	110.60	3	2
1	A	32	THR	CB-CA-C	-6.20	94.85	111.60	4	1
1	B	27	SER	CB-CA-C	6.20	121.88	110.10	3	2
1	A	58	LYS	CG-CD-CE	6.20	130.49	111.90	1	2
1	B	31	THR	C-N-CA	6.19	137.18	121.70	3	1
1	B	22	LYS	CA-CB-CG	6.19	127.02	113.40	1	1
1	A	69	LYS	CD-CE-NZ	-6.18	97.47	111.70	7	4
1	B	65	LYS	CA-C-O	6.17	133.06	120.10	6	1
1	A	53	ALA	O-C-N	6.17	132.57	122.70	4	1
1	A	44	LYS	CB-CA-C	6.16	122.72	110.40	5	3
1	B	59	TRP	CG-CD2-CE3	6.14	139.43	133.90	5	2
1	B	66	HIS	C-N-CA	-6.14	106.35	121.70	5	1
1	A	18	LYS	C-N-CA	6.13	137.01	121.70	4	1
1	B	31	THR	O-C-N	6.12	132.50	122.70	5	2
1	B	33	SER	C-N-CA	6.12	137.00	121.70	1	2
1	A	41	VAL	CG1-CB-CG2	-6.12	101.11	110.90	6	3
1	B	19	LYS	C-N-CA	6.11	136.98	121.70	4	2
1	B	37	PRO	C-N-CA	6.11	136.97	121.70	5	2
1	B	32	THR	CA-C-N	-6.09	103.79	117.20	3	1
1	A	66	HIS	N-CA-CB	6.08	121.55	110.60	4	1
1	A	42	ILE	CA-CB-CG1	-6.08	99.45	111.00	2	2
1	B	12	CYS	C-N-CA	6.08	136.90	121.70	4	2
1	A	40	ALA	C-N-CA	6.07	136.87	121.70	7	1
1	A	51	ILE	C-N-CA	6.07	136.86	121.70	4	2
1	A	48	ASP	CA-CB-CG	-6.06	100.06	113.40	1	3
1	B	30	ARG	CA-C-O	6.05	132.81	120.10	5	2
1	B	59	TRP	O-C-N	6.04	132.36	122.70	7	1
1	B	57	GLN	O-C-N	-6.03	113.05	122.70	3	2
1	B	38	ARG	CB-CA-C	6.03	122.46	110.40	5	1
1	B	46	LYS	CB-CA-C	6.03	122.45	110.40	7	3
1	B	17	ASN	OD1-CG-ND2	-6.02	108.05	121.90	5	4
1	A	69	LYS	C-N-CA	6.02	136.75	121.70	1	2
1	B	33	SER	CA-C-N	-6.01	103.97	117.20	1	1
1	A	48	ASP	C-N-CA	6.01	136.73	121.70	1	2
1	A	26	GLU	CA-CB-CG	-6.01	100.18	113.40	5	1
1	A	55	PRO	CA-C-N	-6.00	103.99	117.20	2	2
1	A	26	GLU	CA-C-O	6.00	132.70	120.10	2	1
1	A	59	TRP	CH2-CZ2-CE2	6.00	123.40	117.40	1	2
1	B	13	TYR	CA-C-N	-6.00	104.01	117.20	5	2
1	B	56	THR	C-N-CA	5.99	136.68	121.70	4	1
1	B	59	TRP	C-N-CA	5.98	136.66	121.70	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	69	LYS	CA-C-O	5.98	132.66	120.10	1	1
1	B	49	LYS	N-CA-C	5.97	127.11	111.00	2	1
1	B	64	MET	O-C-N	-5.95	113.18	122.70	3	2
1	A	26	GLU	CB-CA-C	5.95	122.30	110.40	4	2
1	A	14	ARG	N-CA-CB	-5.95	99.90	110.60	1	1
1	B	50	GLU	CA-CB-CG	5.95	126.48	113.40	6	2
1	B	47	LEU	CB-CG-CD1	5.94	121.10	111.00	3	1
1	B	11	CYS	O-C-N	-5.94	113.20	122.70	1	1
1	A	20	ILE	N-CA-C	5.94	127.03	111.00	5	1
1	A	56	THR	O-C-N	-5.93	113.20	122.70	7	2
1	A	57	GLN	N-CA-C	5.92	126.98	111.00	2	1
1	B	70	LYS	CB-CA-C	-5.91	98.58	110.40	3	1
1	B	46	LYS	C-N-CA	5.91	136.47	121.70	3	3
1	B	31	THR	CB-CA-C	-5.89	95.70	111.60	3	1
1	B	58	LYS	CD-CE-NZ	-5.88	98.17	111.70	4	1
1	A	31	THR	CB-CA-C	-5.88	95.72	111.60	1	1
1	B	39	GLU	CG-CD-OE1	-5.88	106.54	118.30	4	1
1	B	29	ARG	N-CA-CB	-5.88	100.02	110.60	2	1
1	A	52	CYS	N-CA-C	5.88	126.86	111.00	4	1
1	A	56	THR	C-N-CA	5.86	136.36	121.70	2	2
1	A	61	GLN	O-C-N	5.86	132.07	122.70	7	1
1	B	53	ALA	CA-C-N	5.85	130.07	117.20	1	2
1	A	13	TYR	N-CA-C	-5.83	95.25	111.00	7	2
1	B	46	LYS	CG-CD-CE	5.83	129.40	111.90	1	2
1	B	35	HIS	CA-C-N	5.82	130.01	117.20	6	2
1	B	33	SER	CA-CB-OG	-5.81	95.50	111.20	7	1
1	A	43	PHE	N-CA-CB	-5.81	100.14	110.60	4	2
1	A	38	ARG	N-CA-CB	-5.81	100.15	110.60	1	1
1	B	48	ASP	CA-C-N	-5.81	104.43	117.20	6	2
1	A	44	LYS	O-C-N	5.79	131.97	122.70	7	1
1	A	19	LYS	CD-CE-NZ	-5.78	98.40	111.70	6	2
1	A	46	LYS	CD-CE-NZ	-5.78	98.42	111.70	4	1
1	B	34	SER	CA-CB-OG	-5.76	95.65	111.20	5	1
1	A	39	GLU	CA-C-O	5.76	132.19	120.10	3	1
1	A	67	LEU	CB-CG-CD2	-5.76	101.22	111.00	4	1
1	A	13	TYR	N-CA-CB	-5.75	100.24	110.60	2	1
1	B	22	LYS	C-N-CA	5.75	136.07	121.70	6	2
1	A	70	LYS	CA-CB-CG	5.74	126.03	113.40	2	2
1	A	25	LEU	CA-CB-CG	5.74	128.49	115.30	4	1
1	A	56	THR	CB-CA-C	-5.73	96.13	111.60	1	1
1	A	51	ILE	CA-CB-CG2	-5.73	99.44	110.90	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	45	THR	CB-CA-C	-5.73	96.14	111.60	1	1
1	A	30	ARG	N-CA-C	-5.73	95.54	111.00	5	1
1	B	59	TRP	CB-CG-CD2	-5.72	119.16	126.60	6	2
1	B	13	TYR	CA-C-O	5.71	132.08	120.10	4	2
1	A	71	THR	CA-C-O	5.70	132.08	120.10	5	1
1	A	68	ASP	CA-CB-CG	-5.70	100.86	113.40	2	1
1	B	31	THR	N-CA-CB	5.70	121.12	110.30	3	1
1	A	32	THR	CA-CB-OG1	-5.70	97.03	109.00	6	1
1	A	24	ARG	CB-CG-CD	5.68	126.37	111.60	6	1
1	A	22	LYS	CA-CB-CG	5.67	125.89	113.40	4	1
1	A	45	THR	CA-C-N	5.67	129.68	117.20	2	1
1	A	44	LYS	CG-CD-CE	5.67	128.91	111.90	1	1
1	A	71	THR	CA-CB-CG2	5.67	120.34	112.40	5	1
1	B	21	PRO	CB-CA-C	5.66	126.14	112.00	4	2
1	B	52	CYS	CB-CA-C	5.66	121.71	110.40	2	1
1	A	34	SER	CA-CB-OG	-5.65	95.94	111.20	7	2
1	B	25	LEU	CA-CB-CG	5.65	128.29	115.30	5	1
1	B	68	ASP	N-CA-C	-5.64	95.78	111.00	5	1
1	B	33	SER	N-CA-CB	5.63	118.95	110.50	4	1
1	A	63	PHE	CA-C-N	5.63	129.59	117.20	5	1
1	B	25	LEU	CA-C-N	-5.62	104.84	117.20	1	1
1	A	49	LYS	CA-CB-CG	5.62	125.76	113.40	6	1
1	A	38	ARG	C-N-CA	5.61	135.72	121.70	4	2
1	A	66	HIS	CB-CA-C	-5.60	99.19	110.40	4	1
1	B	17	ASN	CB-CG-ND2	5.60	130.14	116.70	6	2
1	A	19	LYS	CA-C-N	5.60	129.52	117.20	7	1
1	A	14	ARG	CB-CA-C	5.59	121.59	110.40	1	1
1	A	19	LYS	O-C-N	5.59	131.65	122.70	2	1
1	A	26	GLU	N-CA-C	-5.59	95.91	111.00	5	1
1	B	16	ILE	N-CA-C	5.58	126.07	111.00	4	1
1	A	51	ILE	CA-C-O	-5.58	108.38	120.10	1	1
1	B	63	PHE	CA-CB-CG	-5.58	100.51	113.90	6	1
1	B	69	LYS	N-CA-CB	-5.57	100.57	110.60	2	1
1	A	72	GLN	OE1-CD-NE2	-5.57	109.10	121.90	5	1
1	A	11	CYS	N-CA-C	5.56	126.02	111.00	3	1
1	B	37	PRO	CA-CB-CG	-5.55	93.45	104.00	3	1
1	A	59	TRP	O-C-N	5.55	131.58	122.70	2	1
1	A	58	LYS	CB-CG-CD	-5.55	97.18	111.60	4	3
1	A	49	LYS	C-N-CA	5.53	135.53	121.70	5	1
1	B	50	GLU	O-C-N	-5.53	113.86	122.70	2	1
1	B	66	HIS	CB-CG-ND1	5.53	137.02	123.20	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	29	ARG	N-CA-C	5.53	125.92	111.00	6	2
1	B	49	LYS	CG-CD-CE	5.52	128.46	111.90	7	1
1	A	56	THR	CA-CB-OG1	5.52	120.58	109.00	7	1
1	B	39	GLU	CA-C-N	-5.51	105.07	117.20	6	1
1	A	14	ARG	CB-CG-CD	5.51	125.92	111.60	3	1
1	B	18	LYS	CA-C-O	5.50	131.65	120.10	4	2
1	A	21	PRO	CA-N-CD	-5.50	103.80	111.50	7	1
1	B	58	LYS	CG-CD-CE	5.50	128.40	111.90	1	1
1	A	37	PRO	CA-CB-CG	-5.50	93.56	104.00	4	1
1	B	44	LYS	CB-CG-CD	-5.50	97.31	111.60	6	2
1	B	60	VAL	CG1-CB-CG2	-5.50	102.11	110.90	2	2
1	A	26	GLU	CG-CD-OE2	-5.49	107.32	118.30	7	2
1	B	32	THR	CA-C-O	5.49	131.62	120.10	3	1
1	B	14	ARG	CA-C-N	5.49	129.27	117.20	5	1
1	A	64	MET	CA-C-O	5.49	131.62	120.10	3	1
1	B	47	LEU	N-CA-C	-5.48	96.20	111.00	6	3
1	A	38	ARG	CB-CG-CD	5.48	125.84	111.60	4	1
1	A	45	THR	CA-CB-OG1	-5.47	97.50	109.00	6	1
1	B	62	ASP	N-CA-C	-5.47	96.23	111.00	2	1
1	A	39	GLU	CB-CA-C	-5.46	99.48	110.40	6	1
1	A	69	LYS	CA-C-N	-5.44	105.23	117.20	3	2
1	A	30	ARG	CB-CA-C	5.44	121.28	110.40	2	1
1	B	45	THR	CB-CA-C	-5.43	96.94	111.60	4	1
1	A	24	ARG	CA-C-O	5.42	131.49	120.10	4	1
1	A	54	ASP	CA-CB-CG	5.42	125.33	113.40	7	1
1	A	28	TYR	O-C-N	5.42	131.36	122.70	6	1
1	B	46	LYS	O-C-N	-5.41	114.05	122.70	5	1
1	A	37	PRO	CB-CA-C	5.40	125.51	112.00	2	1
1	B	32	THR	C-N-CA	5.40	135.21	121.70	3	2
1	A	41	VAL	CA-C-N	5.40	129.08	117.20	2	1
1	B	26	GLU	CG-CD-OE2	5.40	129.10	118.30	6	1
1	A	32	THR	CA-C-O	5.39	131.41	120.10	6	2
1	B	48	ASP	O-C-N	-5.39	114.08	122.70	7	1
1	B	13	TYR	CA-CB-CG	5.38	123.63	113.40	2	1
1	A	71	THR	CA-CB-OG1	5.38	120.30	109.00	4	1
1	B	52	CYS	N-CA-C	5.37	125.49	111.00	5	1
1	B	38	ARG	O-C-N	-5.36	114.12	122.70	2	1
1	A	51	ILE	N-CA-C	-5.36	96.53	111.00	7	1
1	B	70	LYS	C-N-CA	5.36	135.09	121.70	4	1
1	B	55	PRO	CA-N-CD	-5.35	104.00	111.50	3	2
1	A	57	GLN	CB-CA-C	5.35	121.10	110.40	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	51	ILE	CB-CA-C	-5.34	100.92	111.60	3	1
1	A	28	TYR	C-N-CA	5.34	135.04	121.70	6	2
1	B	22	LYS	CD-CE-NZ	-5.33	99.43	111.70	6	3
1	B	69	LYS	CA-C-N	-5.33	105.48	117.20	5	2
1	A	40	ALA	CA-C-O	5.33	131.28	120.10	7	1
1	B	35	HIS	CA-CB-CG	-5.32	104.55	113.60	4	1
1	A	49	LYS	N-CA-CB	5.32	120.18	110.60	3	1
1	A	12	CYS	C-N-CA	5.31	134.98	121.70	3	2
1	A	41	VAL	N-CA-CB	5.30	123.17	111.50	1	1
1	B	25	LEU	O-C-N	-5.30	114.22	122.70	5	1
1	A	41	VAL	CA-C-O	5.30	131.22	120.10	4	1
1	B	46	LYS	CA-CB-CG	5.29	125.04	113.40	7	1
1	A	65	LYS	CA-CB-CG	5.29	125.03	113.40	4	1
1	A	50	GLU	CA-C-O	5.29	131.20	120.10	7	1
1	B	26	GLU	O-C-N	-5.29	114.24	122.70	7	1
1	A	59	TRP	CA-CB-CG	-5.29	103.66	113.70	2	1
1	A	25	LEU	CB-CG-CD1	-5.27	102.04	111.00	7	1
1	B	69	LYS	O-C-N	5.26	131.12	122.70	5	1
1	A	68	ASP	O-C-N	5.26	131.11	122.70	1	1
1	B	24	ARG	CA-C-O	-5.26	109.06	120.10	7	1
1	B	68	ASP	OD1-CG-OD2	-5.25	113.32	123.30	7	2
1	B	32	THR	N-CA-CB	5.25	120.27	110.30	5	1
1	B	29	ARG	CB-CA-C	5.25	120.90	110.40	4	2
1	A	23	GLN	CA-C-N	5.25	128.74	117.20	1	1
1	A	74	PRO	O-C-N	-5.24	114.31	122.70	5	1
1	B	21	PRO	CA-CB-CG	-5.24	94.04	104.00	5	1
1	A	63	PHE	N-CA-CB	-5.24	101.17	110.60	5	1
1	A	48	ASP	CB-CA-C	5.24	120.87	110.40	7	2
1	B	57	GLN	CB-CA-C	5.23	120.86	110.40	2	1
1	A	58	LYS	CA-C-O	5.23	131.08	120.10	2	1
1	A	46	LYS	CA-C-O	5.23	131.09	120.10	7	1
1	B	13	TYR	N-CA-C	5.22	125.09	111.00	5	2
1	A	17	ASN	O-C-N	-5.22	114.35	122.70	2	1
1	A	17	ASN	CA-C-N	-5.22	105.72	117.20	6	1
1	A	50	GLU	CG-CD-OE2	-5.21	107.87	118.30	4	1
1	A	51	ILE	CA-CB-CG1	5.21	120.91	111.00	1	1
1	B	67	LEU	CB-CG-CD1	5.20	119.83	111.00	2	1
1	B	14	ARG	CA-CB-CG	5.19	124.82	113.40	1	1
1	B	14	ARG	CB-CA-C	5.19	120.78	110.40	6	1
1	A	26	GLU	CB-CG-CD	5.18	128.19	114.20	7	2
1	A	27	SER	CA-CB-OG	-5.18	97.22	111.20	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	44	LYS	CD-CE-NZ	-5.18	99.79	111.70	5	1
1	B	19	LYS	CA-C-N	-5.18	105.81	117.20	4	1
1	B	37	PRO	CA-C-O	5.17	132.61	120.20	6	1
1	A	56	THR	CA-C-O	5.17	130.95	120.10	6	1
1	B	12	CYS	O-C-N	-5.17	114.44	122.70	6	1
1	B	23	GLN	O-C-N	-5.16	114.44	122.70	7	1
1	B	28	TYR	O-C-N	5.16	130.95	122.70	6	1
1	B	38	ARG	N-CA-C	5.15	124.92	111.00	3	1
1	B	18	LYS	C-N-CA	5.15	134.57	121.70	4	1
1	A	18	LYS	O-C-N	-5.14	114.47	122.70	2	1
1	A	69	LYS	CB-CG-CD	-5.14	98.23	111.60	7	1
1	B	54	ASP	O-C-N	-5.14	111.33	121.10	1	1
1	A	28	TYR	CA-C-N	-5.14	105.89	117.20	6	1
1	A	21	PRO	CB-CA-C	5.13	124.83	112.00	1	2
1	A	13	TYR	C-N-CA	5.13	134.52	121.70	1	1
1	B	65	LYS	CA-CB-CG	5.13	124.68	113.40	3	1
1	A	22	LYS	CB-CA-C	5.13	120.65	110.40	5	1
1	A	45	THR	CA-C-O	-5.11	109.37	120.10	2	1
1	A	62	ASP	N-CA-C	-5.10	97.24	111.00	2	1
1	A	39	GLU	C-N-CA	5.10	134.44	121.70	4	1
1	A	49	LYS	CB-CG-CD	-5.09	98.36	111.60	1	1
1	A	12	CYS	CB-CA-C	5.09	120.58	110.40	5	1
1	A	49	LYS	N-CA-C	-5.09	97.26	111.00	6	1
1	A	43	PHE	N-CA-C	-5.08	97.28	111.00	7	1
1	B	47	LEU	O-C-N	5.08	130.83	122.70	5	1
1	B	23	GLN	CB-CA-C	5.07	120.55	110.40	5	1
1	A	13	TYR	CA-CB-CG	-5.07	103.77	113.40	7	1
1	A	44	LYS	CB-CG-CD	5.06	124.76	111.60	2	1
1	B	13	TYR	CB-CA-C	5.06	120.51	110.40	4	1
1	B	11	CYS	CB-CA-C	5.05	120.51	110.40	2	1
1	B	35	HIS	CB-CG-ND1	5.05	135.83	123.20	6	1
1	A	34	SER	CA-C-N	5.05	128.32	117.20	7	1
1	B	26	GLU	CB-CG-CD	5.05	127.84	114.20	3	1
1	B	59	TRP	CD2-CE2-CZ2	-5.04	116.26	122.30	6	1
1	A	72	GLN	O-C-N	5.02	130.73	122.70	3	1
1	A	35	HIS	CA-C-N	-5.01	106.17	117.20	7	1
1	A	69	LYS	O-C-N	5.01	130.72	122.70	6	1
1	A	55	PRO	O-C-N	-5.00	114.70	122.70	3	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
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	560	128±35
1	B	509	522	521	116±23
All	All	7399	7602	7567	1432

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 96.

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
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	0.96	1.80	5	1
1:A:29:ARG:HH22	1:A:50:GLU:HG2	0.95	1.20	4	1
1:A:58:LYS:HD2	1:A:58:LYS:C	0.93	1.82	4	3
1:B:26:GLU:HG2	1:B:45:THR:N	0.93	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:HD3	1:A:41:VAL:C	0.87	1.89	4	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: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: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:26:GLU:HB2	1:A:44:LYS:HZ2	0.76	1.39	4	1
1:A:30:ARG:NH2	1:A:31:THR:C	0.76	2.39	5	1
1:A:42:ILE:HA	1:A:51:ILE:O	0.75	1.82	1	3
1:A:16:ILE:C	1:A:17:ASN:HD22	0.75	1.84	6	1
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:A:24:ARG:HH12	1:B:35:HIS:CG	0.74	2.00	1	1
1:A:32:THR:HA	1:B:27:SER:HB2	0.74	1.56	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:SER:CA	1:B:27:SER:HB3	0.74	2.12	3	1
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: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: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: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:B:69:LYS:HD3	1:B:69:LYS:C	0.70	2.06	4	1
1:A:34:SER:N	1:B:27:SER:CB	0.70	2.54	3	1
1:A:31:THR:C	1:B:68:ASP:HA	0.70	2.08	7	1
1:B:30:ARG:HD2	1:B:64:MET:SD	0.69	2.27	2	1
1:B:65:LYS:HD2	1:B:65:LYS:O	0.69	1.87	6	2
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:28:TYR:CD1	1:A:30:ARG:HD3	0.68	2.24	2	1
1:B:64:MET:O	1:B:68:ASP:HB2	0.68	1.89	5	3
1:A:30:ARG:NH2	1:A:39:GLU:C	0.68	2.47	4	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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:36:CYS:SG	1:A:37:PRO:HD2	0.66	2.31	4	4
1:B:57:GLN:CD	1:B:57:GLN:N	0.66	2.49	3	1
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:58:LYS:C	1:A:58:LYS:CD	0.66	2.62	4	2
1:A:51:ILE:HG22	1:A:59:TRP:CZ2	0.66	2.25	5	1
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:A:44:LYS:HD3	1:A:44:LYS:C	0.66	2.11	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:B:30:ARG:HG2	1:B:41:VAL:HB	0.65	1.68	4	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
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:B:52:CYS:SG	1:B:53:ALA:N	0.65	2.70	3	3
1:A:74:PRO:HD3	1:B:15:PHE:CD2	0.65	2.26	4	1
1:B:11:CYS:SG	1:B:12:CYS:N	0.65	2.70	5	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:67:LEU:C	1:B:69:LYS:N	0.65	2.51	5	1
1:A:43:PHE:CZ	1:A:59:TRP:CZ3	0.65	2.84	3	6
1:B:58:LYS:HD3	1:B:58:LYS:C	0.65	2.11	2	1
1:A:26:GLU:CB	1:A:44:LYS:HZ2	0.65	2.05	4	1
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: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:57:GLN:C	1:A:61:GLN:NE2	0.64	2.51	7	6
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: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	1
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:75:LYS:HB3	1:B:18:LYS:H	0.63	1.51	3	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
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:33:SER:N	1:B:26:GLU:HG3	0.62	2.09	2	1
1:A:30:ARG:HG3	1:A:40:ALA:C	0.62	2.15	4	1
1:A:48:ASP:O	1:A:49:LYS:HE3	0.62	1.92	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:58:LYS:HD3	1:A:58:LYS:C	0.62	2.15	6	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:19:LYS:HZ3	1:A:66:HIS:CE1	0.61	2.13	2	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:NZ	1:A:18:LYS:HB3	0.61	2.10	4	1
1:A:30:ARG:CD	1:A:64:MET:SD	0.61	2.89	7	1
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:B:57:GLN:N	1:B:61:GLN:NE2	0.61	2.49	5	1
1:A:54:ASP:CG	1:A:55:PRO:HD2	0.61	2.15	5	1
1:A:18:LYS:HD2	1:A:57:GLN:OE1	0.61	1.95	7	1
1:B:23:GLN:HA	1:B:67:LEU:HD22	0.61	1.72	5	1
1:A:17:ASN:C	1:A:59:TRP:CD1	0.61	2.74	3	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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ASN:N	1:A:52:CYS:O	0.60	2.34	6	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: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:A:70:LYS:HE3	1:A:70:LYS:C	0.59	2.17	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: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: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: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	4
1:A:29:ARG:NH2	1:A:42:ILE:HG21	0.58	2.13	2	1
1:A:39:GLU:CD	1:A:39:GLU:N	0.58	2.57	3	1
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:A:17:ASN:H	1:A:57:GLN:HG2	0.57	1.58	3	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: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:27:SER:OG	1:B:32:THR:N	0.57	2.37	2	2
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: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: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:B:26:GLU:CD	1:B:44:LYS:HZ2	0.57	2.02	2	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ARG:HD2	1:A:41:VAL:HG22	0.56	1.77	2	2
1:A:30:ARG:CD	1:A:41:VAL:C	0.56	2.71	4	1
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:B:19:LYS:HZ3	1:B:25:LEU:CB	0.56	2.13	1	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: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: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
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:59:TRP:CE2	1:B:60:VAL:HG23	0.56	2.36	3	2
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: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:B:45:THR:HB	1:B:49:LYS:HB2	0.56	1.76	7	1
1:A:26:GLU:CD	1:A:44:LYS:HZ2	0.55	2.03	3	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: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:75:LYS:C	1:B:57:GLN:NE2	0.55	2.60	3	1
1:B:28:TYR:CE2	1:B:30:ARG:CD	0.55	2.90	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:MET:HE2	1:B:65:LYS:HG2	0.55	1.79	2	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
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:B:28:TYR:CD1	1:B:28:TYR:C	0.55	2.80	3	2
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:66:HIS:HA	1:A:69:LYS:HZ3	0.54	1.62	2	1
1:A:19:LYS:NZ	1:A:21:PRO:O	0.54	2.38	6	1
1:B:57:GLN:C	1:B:61:GLN:NE2	0.54	2.60	6	2
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:A:54:ASP:C	1:A:56:THR:N	0.54	2.60	7	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:19:LYS:HD2	1:A:19:LYS:O	0.54	2.03	7	1
1:A:75:LYS:H	1:B:54:ASP:HB3	0.54	1.62	3	1
1:A:26:GLU:CB	1:A:44:LYS:NZ	0.54	2.70	4	1
1:A:28:TYR:CZ	1:A:67:LEU:HD12	0.54	2.38	1	1
1:A:64:MET:HE2	1:B:65:LYS:CG	0.54	2.33	2	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
1:A:29:ARG:NH2	1:A:42:ILE:CD1	0.53	2.72	2	1
1:A:73:THR:O	1:B:18:LYS:NZ	0.53	2.39	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:A:63:PHE:O	1:A:64:MET:C	0.53	2.46	5	4
1:A:23:GLN:CD	1:A:23:GLN:H	0.53	2.06	4	2
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:65:LYS:O	1:A:69:LYS:NZ	0.53	2.41	2	1
1:A:18:LYS:HB3	1:A:18:LYS:HZ2	0.53	1.64	4	1
1:A:30:ARG:CG	1:A:42:ILE:HG13	0.53	2.34	4	1
1:B:63:PHE:O	1:B:64:MET:C	0.53	2.43	5	5
1:A:46:LYS:CE	1:B:34:SER:O	0.53	2.57	2	1
1:A:41:VAL:CG2	1:A:42:ILE:N	0.53	2.71	5	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:LYS:NZ	1:B:33:SER:O	0.53	2.41	1	1
1:A:71:THR:CG2	1:B:40:ALA:C	0.53	2.77	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:44:LYS:HZ3	1:A:48:ASP:CG	0.53	2.06	6	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: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
1:B:23:GLN:OE1	1:B:24:ARG:NH1	0.53	2.41	5	1
1:A:67:LEU:O	1:A:68:ASP:C	0.53	2.47	2	6
1:A:40:ALA:HA	1:B:68:ASP:CB	0.53	2.34	4	1
1:A:40:ALA:HA	1:B:68:ASP:CG	0.53	2.24	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:B:19:LYS:HE3	1:B:63:PHE:HA	0.52	1.79	5	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:54:ASP:OD2	1:B:70:LYS:NZ	0.52	2.42	1	1
1:A:65:LYS:NZ	1:A:68:ASP:OD2	0.52	2.43	2	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:ARG:NH2	1:A:14:ARG:C	0.52	2.63	7	1
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:41:VAL:O	1:A:53:ALA:HB3	0.52	2.04	6	1
1:B:17:ASN:HA	1:B:57:GLN:NE2	0.52	2.19	1	1
1:B:62:ASP:O	1:B:63:PHE:C	0.52	2.48	4	6
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:17:ASN:O	1:A:18:LYS:NZ	0.52	2.42	6	1
1:A:13:TYR:O	1:A:14:ARG:HB2	0.52	2.04	2	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:A:11:CYS:O	1:A:12:CYS:C	0.52	2.48	6	1
1:B:68:ASP:CG	1:B:69:LYS:HZ3	0.52	2.07	7	1
1:A:29:ARG:CZ	1:A:42:ILE:HD13	0.52	2.35	4	1
1:A:42:ILE:HG12	1:A:52:CYS:CA	0.51	2.35	4	1
1:A:58:LYS:CE	1:A:58:LYS:C	0.51	2.78	5	1
1:A:16:ILE:C	1:A:17:ASN:ND2	0.51	2.60	6	1
1:B:62:ASP:OD2	1:B:65:LYS:NZ	0.51	2.43	3	1
1:B:22:LYS:HZ1	1:B:62:ASP:CB	0.51	2.18	7	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: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:59:TRP:N	1:A:59:TRP:CD1	0.51	2.79	2	1
1:A:67:LEU:HB2	1:B:30:ARG:NH1	0.51	2.19	2	1
1:A:47:LEU:O	1:A:49:LYS:NZ	0.51	2.42	3	2
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:A:19:LYS:O	1:A:20:ILE:C	0.51	2.49	7	2
1:B:14:ARG:NH1	1:B:50:GLU:O	0.51	2.44	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:CYS:O	1:A:15:PHE:N	0.51	2.43	6	2
1:A:32:THR:C	1:A:39:GLU:HG2	0.51	2.25	5	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:A:75:LYS:C	1:B:57:GLN:CD	0.51	2.69	3	1
1:A:58:LYS:HZ1	1:A:62:ASP:CG	0.51	2.08	5	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:68:ASP:CG	1:A:69:LYS:H	0.51	2.09	1	1
1:A:44:LYS:NZ	1:A:48:ASP:CG	0.51	2.64	4	1
1:A:70:LYS:O	1:A:70:LYS:HE3	0.51	2.05	4	1
1:B:30:ARG:CG	1:B:41:VAL:CG2	0.51	2.87	5	2
1:B:15:PHE:CD2	1:B:16:ILE:N	0.51	2.79	6	2
1:A:30:ARG:NE	1:B:64:MET:HE2	0.51	2.21	7	1
1:B:58:LYS:H	1:B:58:LYS:CD	0.51	2.19	4	2
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: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:11:CYS:SG	1:A:37:PRO:HG2	0.51	2.46	4	2
1:A:62:ASP:O	1:A:63:PHE:C	0.51	2.49	2	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:39:GLU:CB	1:B:68:ASP:O	0.51	2.59	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:13:TYR:CD1	1:A:13:TYR:C	0.50	2.85	4	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:30:ARG:HH22	1:A:31:THR:C	0.50	2.10	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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
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: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:A:30:ARG:C	1:B:27:SER:OG	0.50	2.50	5	1
1:A:34:SER:HA	1:B:68:ASP:C	0.50	2.27	5	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:29:ARG:NH1	1:A:35:HIS:O	0.50	2.44	3	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:64:MET:SD	1:B:65:LYS:NZ	0.50	2.72	7	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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: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:21:PRO:O	1:A:22:LYS:HE3	0.49	2.07	4	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:B:20:ILE:HD12	1:B:20:ILE:H	0.49	1.67	6	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: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:26:GLU:CD	1:B:44:LYS:NZ	0.49	2.66	2	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:B:44:LYS:HD3	1:B:44:LYS:C	0.49	2.27	2	1
1:A:23:GLN:O	1:A:24:ARG:CB	0.49	2.60	5	1
1:B:46:LYS:O	1:B:46:LYS:CG	0.49	2.60	5	1
1:B:65:LYS:O	1:B:69:LYS:NZ	0.49	2.43	7	1
1:B:30:ARG:HA	1:B:40:ALA:O	0.49	2.07	1	1
1:B:23:GLN:CA	1:B:25:LEU:HD13	0.49	2.37	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:14:ARG:NH1	1:B:14:ARG:CB	0.49	2.75	1	1
1:B:22:LYS:C	1:B:23:GLN:HG3	0.49	2.28	2	1
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:B:16:ILE:O	1:B:17:ASN:C	0.49	2.50	4	1
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:A:11:CYS:O	1:A:38:ARG:NH2	0.49	2.46	4	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:70:LYS:HE3	1:B:61:GLN:OE1	0.48	2.08	2	1
1:B:57:GLN:NE2	1:B:57:GLN:N	0.48	2.61	3	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:43:PHE:HE2	1:B:63:PHE:CG	0.48	2.26	1	1
1:A:26:GLU:O	1:B:32:THR:CA	0.48	2.62	1	1
1:B:57:GLN:O	1:B:58:LYS:C	0.48	2.51	2	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
1:A:75:LYS:CD	1:B:17:ASN:H	0.48	2.21	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:44:LYS:HZ1	1:A:48:ASP:CG	0.48	2.12	2	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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:19:LYS:HZ3	1:B:25:LEU:HB2	0.48	1.67	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:A:59:TRP:NE1	1:A:60:VAL:HG23	0.48	2.24	3	1
1:A:74:PRO:HB2	1:B:53:ALA:C	0.48	2.29	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: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:58:LYS:CG	1:A:59:TRP:N	0.48	2.76	7	2
1:A:57:GLN:O	1:A:60:VAL:HB	0.48	2.09	5	1
1:A:54:ASP:H	1:A:57:GLN:CD	0.48	2.12	6	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
1:A:71:THR:HG21	1:B:54:ASP:CG	0.48	2.30	4	1
1:B:35:HIS:ND1	1:B:36:CYS:HB3	0.48	2.23	5	1
1:A:70:LYS:HD2	1:B:39:GLU:CD	0.48	2.28	6	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:B:43:PHE:CE2	1:B:59:TRP:HZ3	0.47	2.27	7	2
1:A:26:GLU:OE2	1:A:46:LYS:NZ	0.47	2.37	2	1
1:B:28:TYR:HH	1:B:67:LEU:HB3	0.47	1.69	2	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ASN:HB3	1:A:57:GLN:CD	0.47	2.30	6	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:B:32:THR:O	1:B:33:SER:CB	0.47	2.62	4	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: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:24:ARG:NH1	1:B:34:SER:C	0.47	2.68	1	2
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:64:MET:C	1:B:68:ASP:HB2	0.47	2.30	2	1
1:A:26:GLU:OE1	1:A:44:LYS:NZ	0.47	2.47	4	1
1:A:29:ARG:HH22	1:A:50:GLU:CD	0.47	2.13	4	1
1:A:75:LYS:CE	1:B:14:ARG:O	0.47	2.63	5	1
1:B:29:ARG:HH12	1:B:50:GLU:CD	0.47	2.13	1	1
1:A:16:ILE:O	1:A:17:ASN:C	0.47	2.53	2	1
1:A:75:LYS:HZ3	1:B:57:GLN:CD	0.47	2.13	5	1
1:A:28:TYR:CD1	1:B:30:ARG:HB2	0.47	2.44	5	2
1:A:57:GLN:C	1:A:61:GLN:HE22	0.47	2.13	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
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:A:16:ILE:HA	1:A:57:GLN:CD	0.47	2.30	3	1
1:B:59:TRP:CZ2	1:B:60:VAL:CG2	0.47	2.98	3	1
1:B:66:HIS:O	1:B:69:LYS:HE2	0.47	2.10	6	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:SER:CA	1:B:26:GLU:HG3	0.46	2.40	2	1
1:A:34:SER:HA	1:A:39:GLU:CD	0.46	2.31	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:B:57:GLN:HG2	1:B:59:TRP:HE1	0.46	1.70	7	1
1:A:22:LYS:NZ	1:A:23:GLN:O	0.46	2.48	1	1
1:A:36:CYS:O	1:A:38:ARG:N	0.46	2.49	5	2
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:A:74:PRO:HD3	1:B:53:ALA:HB1	0.46	1.86	1	1
1:A:57:GLN:O	1:A:58:LYS:C	0.46	2.54	3	3
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: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:67:LEU:O	1:A:70:LYS:HG2	0.46	2.11	6	1
1:A:32:THR:N	1:A:39:GLU:CD	0.46	2.69	1	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:A:44:LYS:NZ	1:A:48:ASP:OD1	0.46	2.48	3	3
1:B:22:LYS:NZ	1:B:50:GLU:O	0.46	2.48	3	1
1:A:30:ARG:HE	1:A:40:ALA:C	0.46	2.14	4	1
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:A:22:LYS:HD3	1:A:66:HIS:CE1	0.46	2.46	1	1
1:A:16:ILE:O	1:A:17:ASN:CG	0.46	2.55	2	1
1:A:26:GLU:HG2	1:A:45:THR:C	0.46	2.31	3	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ARG:CZ	1:B:68:ASP:CG	0.46	2.84	6	1
1:B:14:ARG:HH12	1:B:16:ILE:HG21	0.46	1.71	6	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: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: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:A:19:LYS:NZ	1:A:19:LYS:O	0.45	2.46	5	1
1:B:26:GLU:CB	1:B:44:LYS:HG3	0.45	2.41	5	1
1:A:66:HIS:CE1	1:A:69:LYS:HZ1	0.45	2.29	6	1
1:B:25:LEU:C	1:B:70:LYS:HE2	0.45	2.31	7	1
1:B:45:THR:HB	1:B:49:LYS:CB	0.45	2.41	7	1
1:B:59:TRP:CH2	1:B:60:VAL:HG22	0.45	2.46	2	1
1:A:28:TYR:CD1	1:A:28:TYR:C	0.45	2.89	3	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:22:LYS:HZ1	1:B:62:ASP:HB3	0.45	1.70	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: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:B:52:CYS:O	1:B:53:ALA:HB3	0.45	2.11	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:23:GLN:CD	1:B:24:ARG:H	0.45	2.15	4	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:60:VAL:O	1:B:61:GLN:C	0.45	2.53	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:57:GLN:N	1:B:57:GLN:CD	0.45	2.69	6	1
1:A:60:VAL:O	1:A:61:GLN:C	0.45	2.52	4	1
1:A:11:CYS:SG	1:A:37:PRO:HD2	0.45	2.52	5	1
1:A:30:ARG:HH22	1:A:39:GLU:CD	0.45	2.15	6	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:25:LEU:HG	1:B:44:LYS:O	0.45	2.12	6	2
1:A:44:LYS:NZ	1:A:50:GLU:OE1	0.45	2.49	7	1
1:B:19:LYS:HZ3	1:B:25:LEU:CD1	0.45	2.25	1	1
1:A:30:ARG:CD	1:A:41:VAL:N	0.45	2.79	4	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:A:74:PRO:C	1:B:57:GLN:HE22	0.45	2.15	3	1
1:B:25:LEU:CD1	1:B:45:THR:HB	0.45	2.42	4	1
1:A:58:LYS:C	1:A:58:LYS:HE3	0.45	2.32	5	1
1:B:19:LYS:HZ1	1:B:66:HIS:CG	0.45	2.30	5	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
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:26:GLU:HB2	1:A:45:THR:C	0.45	2.32	6	1
1:A:32:THR:H	1:A:39:GLU:CD	0.44	2.16	1	1
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:A:26:GLU:HG2	1:A:44:LYS:HZ2	0.44	1.72	2	1
1:A:65:LYS:CG	1:B:65:LYS:HG3	0.44	2.43	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:67:LEU:O	1:B:68:ASP:C	0.44	2.56	4	4
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:B:28:TYR:CE2	1:B:30:ARG:HD3	0.44	2.47	1	1
1:B:69:LYS:C	1:B:70:LYS:HE3	0.44	2.33	1	1
1:A:15:PHE:CD2	1:A:55:PRO:HB2	0.44	2.48	2	1
1:A:26:GLU:CG	1:A:44:LYS:HZ2	0.44	2.24	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:B:24:ARG:HH22	1:B:26:GLU:CD	0.44	2.15	3	1
1:B:62:ASP:CG	1:B:65:LYS:NZ	0.44	2.71	4	1
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:38:ARG:HH12	1:A:54:ASP:CG	0.44	2.16	3	1
1:A:31:THR:OG1	1:B:27:SER:HA	0.44	2.12	4	1
1:A:51:ILE:CG2	1:A:59:TRP:CZ2	0.44	2.99	5	1
1:B:19:LYS:NZ	1:B:19:LYS:O	0.44	2.44	7	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
1:B:14:ARG:CZ	1:B:14:ARG:CB	0.44	2.96	1	1
1:B:69:LYS:O	1:B:70:LYS:C	0.44	2.55	1	2
1:A:30:ARG:CD	1:A:41:VAL:HG22	0.44	2.41	2	2
1:A:64:MET:SD	1:A:65:LYS:HB3	0.44	2.51	4	1
1:B:63:PHE:CD1	1:B:63:PHE:C	0.44	2.90	5	1
1:A:12:CYS:SG	1:A:16:ILE:HB	0.44	2.53	6	1
1:B:44:LYS:NZ	1:B:48:ASP:OD1	0.44	2.44	1	3
1:A:65:LYS:HB2	1:A:65:LYS:HZ2	0.44	1.73	3	1
1:B:17:ASN:O	1:B:18:LYS:NZ	0.44	2.48	3	1
1:A:30:ARG:O	1:B:28:TYR:CD1	0.44	2.71	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:29:ARG:HH21	1:A:50:GLU:CD	0.44	2.16	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: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: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: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:A:71:THR:C	1:A:73:THR:N	0.44	2.71	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:A:31:THR:HG22	1:B:27:SER:CA	0.44	2.41	7	1
1:A:60:VAL:CG1	1:A:61:GLN:N	0.43	2.80	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
1:A:26:GLU:HB2	1:A:44:LYS:NZ	0.43	2.20	4	1
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:B:58:LYS:HD2	1:B:58:LYS:C	0.43	2.33	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:24:ARG:O	1:B:46:LYS:NZ	0.43	2.48	4	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:30:ARG:NH1	1:B:64:MET:HE3	0.43	2.28	1	1
1:B:14:ARG:NH2	1:B:50:GLU:CD	0.43	2.72	2	1
1:B:49:LYS:NZ	1:B:49:LYS:HB2	0.43	2.29	2	1
1:B:15:PHE:CE2	1:B:54:ASP:CG	0.43	2.92	3	1
1:B:55:PRO:O	1:B:61:GLN:NE2	0.43	2.52	4	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: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
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: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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:LYS:HB2	1:B:59:TRP:NE1	0.43	2.28	3	1
1:B:62:ASP:CG	1:B:65:LYS:HZ3	0.43	2.17	4	1
1:A:33:SER:H	1:B:68:ASP:CG	0.43	2.17	5	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:29:ARG:CZ	1:A:42:ILE:CD1	0.43	2.97	4	1
1:A:58:LYS:HD2	1:A:58:LYS:O	0.43	2.09	4	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:B:14:ARG:HH12	1:B:50:GLU:CD	0.43	2.17	4	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:A:39:GLU:O	1:A:40:ALA:C	0.43	2.57	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
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:59:TRP:O	1:B:63:PHE:HB2	0.42	2.14	5	1
1:B:66:HIS:CD2	1:B:69:LYS:HZ1	0.42	2.31	6	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:HG3	1:B:25:LEU:C	0.42	2.35	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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: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:B:54:ASP:CG	1:B:57:GLN:HE22	0.42	2.18	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
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: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: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:41:VAL:CG1	1:B:64:MET:CE	0.42	2.97	2	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:17:ASN:C	1:A:57:GLN:NE2	0.42	2.73	7	1
1:B:22:LYS:HE3	1:B:66:HIS:HB3	0.42	1.91	7	1
1:B:16:ILE:HD13	1:B:17:ASN:N	0.42	2.30	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:A:66:HIS:CA	1:A:69:LYS:HZ2	0.41	2.27	2	1
1:B:32:THR:HG22	1:B:33:SER:N	0.41	2.29	2	1
1:A:28:TYR:HH	1:B:30:ARG:NH1	0.41	2.13	3	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
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: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:B:47:LEU:O	1:B:48:ASP:HB3	0.41	2.16	3	1
1:B:64:MET:HE2	1:B:68:ASP:CB	0.41	2.45	3	1
1:A:54:ASP:N	1:A:57:GLN:NE2	0.41	2.68	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: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:31:THR:C	1:B:34:SER:OG	0.41	2.59	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:A:26:GLU:HA	1:B:35:HIS:ND1	0.41	2.30	4	1
1:A:52:CYS:O	1:A:59:TRP:CZ2	0.41	2.72	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:43:PHE:CE1	1:A:59:TRP:CZ3	0.41	3.09	2	2
1:A:26:GLU:HG2	1:A:44:LYS:HZ1	0.41	1.75	4	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:69:LYS:NZ	1:A:69:LYS:HB2	0.41	2.31	1	1
1:B:35:HIS:H	1:B:39:GLU:CD	0.41	2.19	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: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:26:GLU:CB	1:B:44:LYS:C	0.41	2.89	7	1
1:B:57:GLN:CG	1:B:59:TRP:NE1	0.41	2.84	7	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:30:ARG:NH2	1:B:68:ASP:CG	0.41	2.74	6	1
1:B:25:LEU:C	1:B:70:LYS:CE	0.41	2.89	7	1
1:A:44:LYS:HZ2	1:A:48:ASP:CG	0.41	2.19	1	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: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:27:SER:O	1:A:44:LYS:N	0.41	2.54	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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:32:THR:CG2	1:A:39:GLU:H	0.41	2.27	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:75:LYS:CD	1:B:17:ASN:N	0.41	2.84	5	1
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:A:45:THR:O	1:A:46:LYS:C	0.41	2.59	7	1
1:A:70:LYS:HZ2	1:B:39:GLU:CG	0.41	2.28	2	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:A:33:SER:C	1:B:27:SER:OG	0.41	2.60	3	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:B:37:PRO:O	1:B:38:ARG:HB3	0.41	2.16	5	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:A:70:LYS:HZ2	1:B:39:GLU:HG3	0.40	1.76	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:A:26:GLU:CD	1:A:46:LYS:N	0.40	2.74	7	1
1:B:25:LEU:H	1:B:70:LYS:CB	0.40	2.29	7	1
1:A:22:LYS:O	1:A:23:GLN:C	0.40	2.59	1	1
1:A:70:LYS:HB3	1:A:70:LYS:HZ3	0.40	1.75	1	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:A:30:ARG:HH11	1:A:40:ALA:C	0.40	2.19	6	1
1:A:44:LYS:NZ	1:A:48:ASP:OD2	0.40	2.54	6	1
1:B:36:CYS:HA	1:B:37:PRO:HD2	0.40	1.64	6	1
1:A:35:HIS:CD2	1:A:36:CYS:H	0.40	2.35	2	1
1:A:62:ASP:O	1:A:65:LYS:C	0.40	2.60	2	1
1:A:31:THR:HB	1:B:70:LYS:HZ1	0.40	1.76	3	1
1:A:44:LYS:CE	1:A:48:ASP:OD2	0.40	2.69	4	1
1:A:71:THR:HG23	1:B:39:GLU:C	0.40	2.35	4	1
1:B:25:LEU:CD1	1:B:44:LYS:O	0.40	2.68	5	1
1:A:25:LEU:O	1:B:34:SER:HA	0.40	2.16	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: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:29:ARG:C	1:B:41:VAL:HG23	0.40	2.37	4	1
1:B:30:ARG:NH2	1:B:54:ASP:O	0.40	2.55	4	1
1:B:19:LYS:HZ1	1:B:66:HIS:CD2	0.40	2.34	5	1
1:A:46:LYS:C	1:A:47:LEU:HD12	0.40	2.36	3	1
1:B:19:LYS:NZ	1:B:23:GLN:OE1	0.40	2.53	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:B:54:ASP:C	1:B:57:GLN:NE2	0.40	2.75	6	1
1:A:41:VAL:HG22	1:A:64:MET:SD	0.40	2.57	7	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Res	Type	Models (Total)
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
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

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Mol	Chain	Res	Type	Models (Total)
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%)	50±1 (80±2%)	13±1 (20±2%)	3	33
1	B	58/73 (79%)	47±2 (81±4%)	11±2 (19±4%)	4	36
All	All	847/1022 (83%)	682 (81%)	165 (19%)	4	35

All 75 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	7
1	A	48	ASP	5
1	B	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	15	PHE	4
1	B	21	PRO	4
1	B	28	TYR	4
1	B	37	PRO	4
1	B	24	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	44	LYS	3
1	A	46	LYS	3
1	A	61	GLN	3
1	A	74	PRO	3
1	B	14	ARG	3
1	A	55	PRO	3
1	B	17	ASN	3
1	B	65	LYS	3
1	A	14	ARG	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	B	20	ILE	2
1	B	55	PRO	2
1	B	61	GLN	2
1	B	70	LYS	2
1	A	23	GLN	2
1	A	37	PRO	2
1	A	63	PHE	2
1	B	13	TYR	2
1	B	69	LYS	2
1	A	20	ILE	2
1	A	70	LYS	2
1	B	45	THR	2
1	B	49	LYS	2
1	A	28	TYR	2
1	B	35	HIS	2
1	B	38	ARG	2
1	B	44	LYS	2
1	A	15	PHE	2
1	A	49	LYS	2
1	A	13	TYR	1
1	A	29	ARG	1
1	A	66	HIS	1
1	A	67	LEU	1
1	A	75	LYS	1
1	B	16	ILE	1
1	B	22	LYS	1
1	B	52	CYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	30	ARG	1
1	A	60	VAL	1
1	A	68	ASP	1
1	B	63	PHE	1
1	A	16	ILE	1
1	A	54	ASP	1
1	B	57	GLN	1
1	B	64	MET	1
1	A	50	GLU	1
1	A	65	LYS	1
1	B	26	GLU	1
1	B	29	ARG	1
1	A	31	THR	1
1	A	41	VAL	1
1	A	17	ASN	1
1	A	62	ASP	1
1	A	64	MET	1
1	B	23	GLN	1
1	B	67	LEU	1
1	A	36	CYS	1
1	B	25	LEU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided