



Full wwPDB NMR Structure Validation Report ⓘ

Feb 16, 2022 – 06:19 AM EST

PDB ID : 1MPZ
Title : NMR solution structure of native Viperidae lebetina obtusa protein
Authors : Moreno-Murciano, M.P.; Monleon, D.; Marcinkiewicz, C.; Calvete, J.J.; Celda, B.
Deposited on : 2002-09-13

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

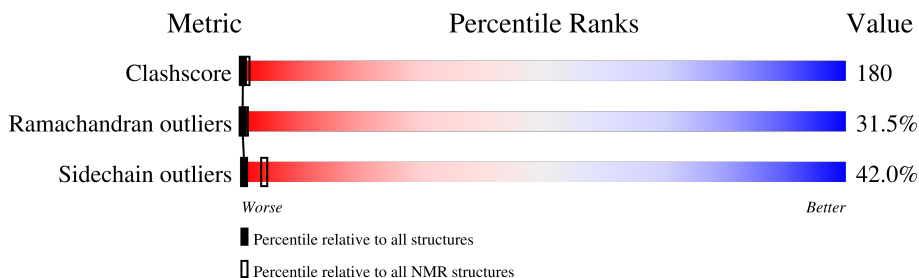
1 Overall quality at a glance

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	41	

2 Ensemble composition and analysis

This entry contains 22 models. Model 22 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:2-A:39 (38)	0.46	22

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 588 atoms, of which 288 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Obtustatin.

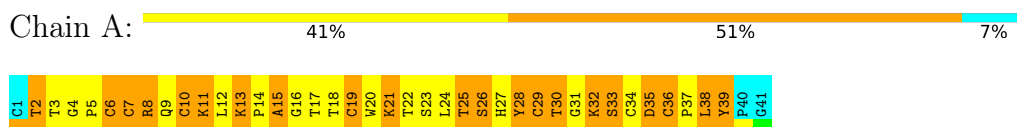
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	41	588	184	288	52	56	8	0

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Obtustatin

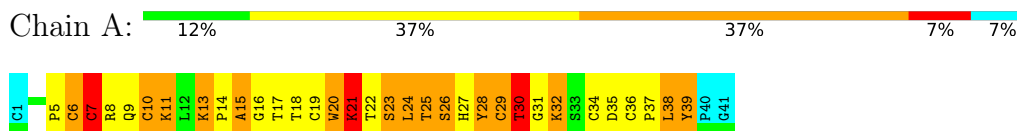


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

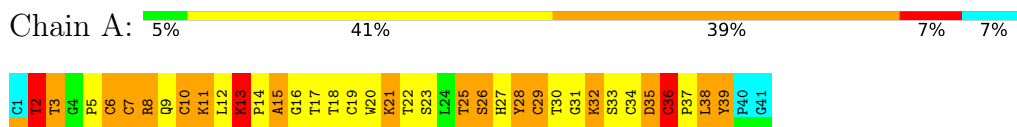
4.2.1 Score per residue for model 1

- Molecule 1: Obtustatin



4.2.2 Score per residue for model 2

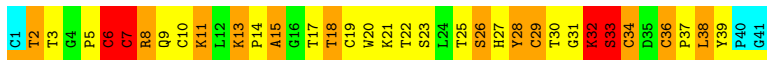
- Molecule 1: Obtustatin



4.2.3 Score per residue for model 3

- Molecule 1: Obtustatin

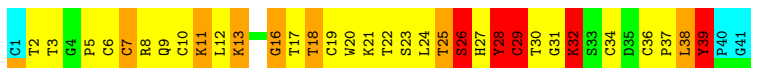
Chain A: 12% 41% 29% 10% 7%



4.2.4 Score per residue for model 4

- Molecule 1: Obtustatin

Chain A: 12% 51% 17% 12% 7%



4.2.5 Score per residue for model 5

- Molecule 1: Obtustatin

Chain A: 54% 24% 15% 7%



4.2.6 Score per residue for model 6

- Molecule 1: Obtustatin

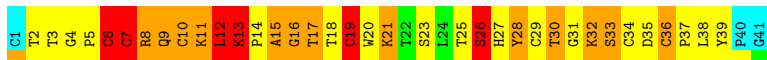
Chain A: 5% 32% 41% 15% 7%



4.2.7 Score per residue for model 7

- Molecule 1: Obtustatin

Chain A: 5% 41% 32% 15% 7%



4.2.8 Score per residue for model 8

- Molecule 1: Obtustatin

Chain A: 7% 34% 34% 17% 7%



4.2.9 Score per residue for model 9

- Molecule 1: Obtustatin

Chain A: 5% 37% 39% 12% 7%



4.2.10 Score per residue for model 10

- Molecule 1: Obtustatin

Chain A: 5% 39% 37% 12% 7%



4.2.11 Score per residue for model 11

- Molecule 1: Obtustatin

Chain A: 54% 29% 7% 7%



4.2.12 Score per residue for model 12

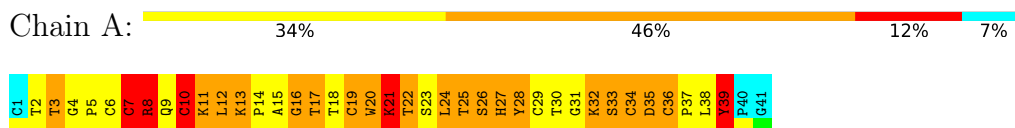
- Molecule 1: Obtustatin

Chain A: 34% 44% 15% 7%



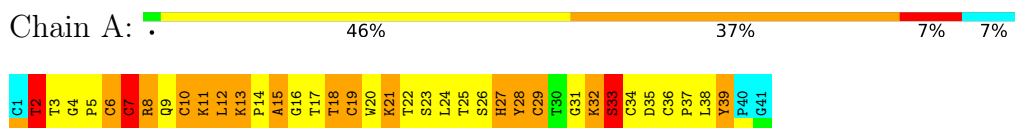
4.2.13 Score per residue for model 13

- Molecule 1: Obtustatin



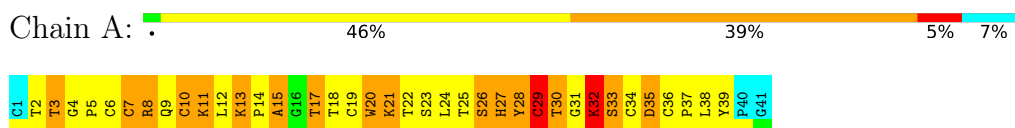
4.2.14 Score per residue for model 14

- Molecule 1: Obtustatin



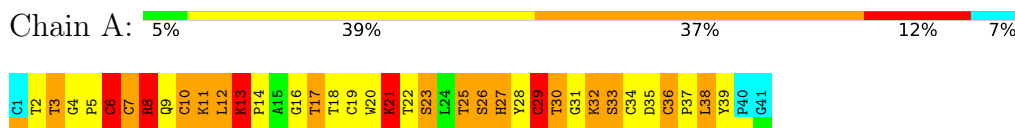
4.2.15 Score per residue for model 15

- Molecule 1: Obtustatin



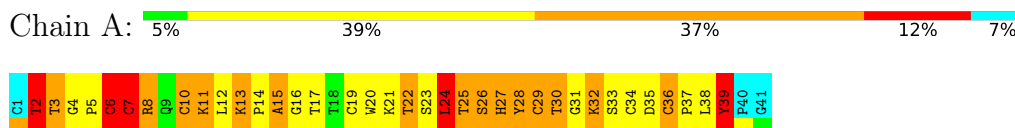
4.2.16 Score per residue for model 16

- Molecule 1: Obtustatin



4.2.17 Score per residue for model 17

- Molecule 1: Obtustatin



4.2.18 Score per residue for model 18

- Molecule 1: Obtustatin

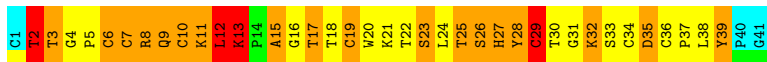
Chain A: 41% 37% 12% 7%



4.2.19 Score per residue for model 19

- Molecule 1: Obtustatin

Chain A: 37% 44% 10% 7%



4.2.20 Score per residue for model 20

- Molecule 1: Obtustatin

Chain A: 34% 46% 10% 7%



4.2.21 Score per residue for model 21

- Molecule 1: Obtustatin

Chain A: 54% 24% 15% 7%



4.2.22 Score per residue for model 22 (medoid)

- Molecule 1: Obtustatin

Chain A: 5% 12% 32% 44% 7%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Manual assignment by Wuthrich protocols and automatic NOESY assignment extension by NOAH.*

Of the 500 calculated structures, 22 were deposited, based on the following criterion: *structures with the lowest energy, target function.*

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

Software name	Classification	Version
DYANA	structure solution	1.5
DYANA	refinement	

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.54±3.85	6±26/291 (1.9± 8.8%)	1.69±3.05	5±24/397 (1.3± 6.0%)
All	All	4.14	123/6402 (1.9%)	3.48	114/8734 (1.3%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	39	TYR	CE2-CZ	-71.67	0.45	1.38	22	1
1	A	39	TYR	CG-CD1	-70.27	0.47	1.39	22	1
1	A	20	TRP	NE1-CE2	-69.48	0.47	1.37	22	1
1	A	20	TRP	CD2-CE3	-61.09	0.48	1.40	22	1
1	A	39	TYR	CE1-CZ	-59.71	0.60	1.38	22	1
1	A	39	TYR	CG-CD2	-58.16	0.63	1.39	22	1
1	A	28	TYR	CE1-CZ	-55.62	0.66	1.38	22	1
1	A	28	TYR	CE2-CZ	-55.34	0.66	1.38	22	1
1	A	8	ARG	CZ-NH2	-54.00	0.62	1.33	22	1
1	A	28	TYR	CG-CD2	-53.08	0.70	1.39	22	1
1	A	28	TYR	CG-CD1	-52.67	0.70	1.39	22	1
1	A	8	ARG	CZ-NH1	-51.06	0.66	1.33	22	1
1	A	27	HIS	CE1-NE2	-50.74	0.15	1.32	22	1
1	A	20	TRP	CZ2-CH2	-47.09	0.47	1.37	22	1
1	A	10	CYS	CB-SG	-45.72	1.04	1.82	22	1
1	A	32	LYS	C-O	-44.77	0.38	1.23	22	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	2	THR	CB-OG1	-44.09	0.55	1.43	22	1
1	A	32	LYS	CE-NZ	-43.69	0.39	1.49	22	1
1	A	34	CYS	CB-SG	-42.83	1.09	1.82	22	1
1	A	20	TRP	CG-CD1	-42.39	0.77	1.36	22	1
1	A	8	ARG	CD-NE	-41.91	0.75	1.46	22	1
1	A	35	ASP	CG-OD1	-41.45	0.30	1.25	22	1
1	A	22	THR	C-O	-38.22	0.50	1.23	22	1
1	A	27	HIS	CG-ND1	-38.13	0.54	1.38	22	1
1	A	25	THR	C-O	-37.34	0.52	1.23	22	1
1	A	30	THR	CB-OG1	-36.58	0.70	1.43	22	1
1	A	27	HIS	C-O	-36.56	0.53	1.23	22	1
1	A	27	HIS	CG-CD2	-36.38	0.73	1.35	22	1
1	A	32	LYS	CG-CD	-35.02	0.33	1.52	22	1
1	A	33	SER	CB-OG	-34.97	0.96	1.42	22	1
1	A	11	LYS	CE-NZ	-34.00	0.64	1.49	22	1
1	A	29	CYS	CB-SG	-32.28	1.27	1.82	22	1
1	A	9	GLN	CD-OE1	-32.00	0.53	1.24	22	1
1	A	2	THR	N-CA	-31.92	0.82	1.46	22	1
1	A	26	SER	CB-OG	-31.64	1.01	1.42	22	1
1	A	21	LYS	CE-NZ	-31.57	0.70	1.49	22	1
1	A	16	GLY	C-O	-31.13	0.73	1.23	22	1
1	A	9	GLN	C-O	-31.01	0.64	1.23	22	1
1	A	39	TYR	CB-CG	-29.08	1.08	1.51	22	1
1	A	32	LYS	CB-CG	-28.98	0.74	1.52	22	1
1	A	6	CYS	C-O	-28.70	0.68	1.23	22	1
1	A	13	LYS	CD-CE	-28.40	0.80	1.51	22	1
1	A	21	LYS	CG-CD	-28.14	0.56	1.52	22	1
1	A	20	TRP	CG-CD2	-27.04	0.97	1.43	22	1
1	A	24	LEU	CB-CG	-26.57	0.75	1.52	22	1
1	A	2	THR	CA-CB	-25.71	0.86	1.53	22	1
1	A	8	ARG	NE-CZ	-25.33	1.00	1.33	22	1
1	A	35	ASP	CB-CG	-25.23	0.98	1.51	22	1
1	A	39	TYR	CD2-CE2	-25.20	1.01	1.39	22	1
1	A	39	TYR	CD1-CE1	-25.11	1.01	1.39	22	1
1	A	23	SER	CA-CB	-24.92	1.15	1.52	22	1
1	A	39	TYR	CZ-OH	-24.58	0.96	1.37	22	1
1	A	24	LEU	CG-CD2	-23.68	0.64	1.51	22	1
1	A	23	SER	CB-OG	-23.66	1.11	1.42	22	1
1	A	35	ASP	CG-OD2	-23.05	0.72	1.25	22	1
1	A	32	LYS	C-N	-22.82	0.81	1.34	22	1
1	A	25	THR	C-N	-22.52	0.82	1.34	22	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	22	THR	C-N	-22.17	0.83	1.34	22	1
1	A	8	ARG	CB-CG	-21.36	0.94	1.52	22	1
1	A	22	THR	CB-OG1	-20.91	1.01	1.43	22	1
1	A	27	HIS	CD2-NE2	-20.05	0.93	1.38	22	1
1	A	18	THR	C-O	-19.98	0.85	1.23	22	1
1	A	30	THR	CB-CG2	-19.72	0.87	1.52	22	1
1	A	27	HIS	C-N	-19.41	0.89	1.34	22	1
1	A	9	GLN	CD-NE2	-19.10	0.85	1.32	22	1
1	A	2	THR	C-O	-18.28	0.88	1.23	22	1
1	A	9	GLN	C-N	-18.23	0.92	1.34	22	1
1	A	27	HIS	CB-CG	-18.06	1.17	1.50	22	1
1	A	20	TRP	CD2-CE2	-17.16	1.20	1.41	22	1
1	A	22	THR	CA-CB	-16.66	1.10	1.53	22	1
1	A	23	SER	C-N	-16.56	0.95	1.34	22	1
1	A	9	GLN	CG-CD	-15.82	1.14	1.51	22	1
1	A	6	CYS	C-N	-15.81	0.97	1.34	22	1
1	A	14	PRO	C-O	-15.45	0.92	1.23	22	1
1	A	13	LYS	CE-NZ	-15.42	1.10	1.49	22	1
1	A	20	TRP	CE2-CZ2	-15.40	1.13	1.39	22	1
1	A	21	LYS	CB-CG	-15.03	1.11	1.52	22	1
1	A	24	LEU	CG-CD1	-14.95	0.96	1.51	22	1
1	A	18	THR	C-N	-14.85	0.99	1.34	22	1
1	A	13	LYS	CB-CG	-14.78	1.12	1.52	22	1
1	A	23	SER	C-O	-14.70	0.95	1.23	22	1
1	A	23	SER	N-CA	-14.38	1.17	1.46	22	1
1	A	20	TRP	CE3-CZ3	-14.21	1.14	1.38	22	1
1	A	39	TYR	C-O	-14.02	0.96	1.23	22	1
1	A	2	THR	C-N	-13.99	1.01	1.34	22	1
1	A	33	SER	C-O	-13.93	0.96	1.23	22	1
1	A	16	GLY	C-N	-13.62	1.02	1.34	22	1
1	A	2	THR	CB-CG2	-13.52	1.07	1.52	22	1
1	A	39	TYR	C-N	-13.44	1.08	1.34	22	1
1	A	27	HIS	ND1-CE1	-13.42	1.01	1.34	22	1
1	A	14	PRO	C-N	-12.72	1.04	1.34	22	1
1	A	22	THR	CA-C	-12.21	1.21	1.52	22	1
1	A	11	LYS	CD-CE	-11.86	1.21	1.51	22	1
1	A	20	TRP	C-O	-11.74	1.01	1.23	22	1
1	A	33	SER	C-N	-11.24	1.08	1.34	22	1
1	A	20	TRP	CZ3-CH2	-11.23	1.22	1.40	22	1
1	A	24	LEU	C-N	-11.04	1.08	1.34	22	1
1	A	39	TYR	CA-CB	-10.98	1.29	1.53	22	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	32	LYS	CD-CE	-10.75	1.24	1.51	22	1
1	A	11	LYS	CG-CD	-10.70	1.16	1.52	22	1
1	A	21	LYS	CD-CE	-10.07	1.26	1.51	22	1
1	A	17	THR	C-O	-10.00	1.04	1.23	22	1
1	A	24	LEU	C-O	-9.43	1.05	1.23	22	1
1	A	39	TYR	CA-C	-8.52	1.30	1.52	22	1
1	A	24	LEU	CA-CB	-8.25	1.34	1.53	22	1
1	A	10	CYS	C-O	-8.13	1.07	1.23	22	1
1	A	19	CYS	CB-SG	-7.92	1.68	1.82	22	1
1	A	38	LEU	CG-CD1	-7.91	1.22	1.51	22	1
1	A	38	LEU	CG-CD2	-7.70	1.23	1.51	22	1
1	A	13	LYS	CG-CD	-7.33	1.27	1.52	22	1
1	A	3	THR	CB-OG1	-7.18	1.28	1.43	22	1
1	A	8	ARG	CG-CD	-7.07	1.34	1.51	22	1
1	A	24	LEU	N-CA	-7.02	1.32	1.46	22	1
1	A	18	THR	CB-OG1	-6.81	1.29	1.43	22	1
1	A	33	SER	CA-CB	-6.79	1.42	1.52	22	1
1	A	17	THR	C-N	-6.69	1.18	1.34	22	1
1	A	11	LYS	CB-CG	-6.63	1.34	1.52	22	1
1	A	21	LYS	CA-CB	-6.54	1.39	1.53	22	1
1	A	20	TRP	CD1-NE1	-5.73	1.28	1.38	22	1
1	A	32	LYS	CA-CB	-5.62	1.41	1.53	22	1
1	A	20	TRP	C-N	-5.34	1.21	1.34	22	1
1	A	7	CYS	C-O	-5.16	1.13	1.23	22	1
1	A	38	LEU	CB-CG	-5.03	1.38	1.52	22	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	28	TYR	CD1-CG-CD2	-82.41	27.25	117.90	22	1
1	A	28	TYR	CB-CG-CD1	75.72	166.43	121.00	22	1
1	A	28	TYR	CB-CG-CD2	75.54	166.32	121.00	22	1
1	A	20	TRP	CD1-CG-CD2	-71.57	49.05	106.30	22	1
1	A	27	HIS	ND1-CG-CD2	-65.12	14.83	106.00	22	1
1	A	39	TYR	CB-CG-CD2	57.78	155.67	121.00	22	1
1	A	28	TYR	CE1-CZ-CE2	-56.80	28.91	119.80	22	1
1	A	28	TYR	CG-CD1-CE1	56.38	166.40	121.30	22	1
1	A	28	TYR	CG-CD2-CE2	56.31	166.35	121.30	22	1
1	A	39	TYR	CD1-CG-CD2	-54.47	57.99	117.90	22	1
1	A	20	TRP	CE2-CD2-CG	54.04	150.53	107.30	22	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	32	LYS	O-C-N	-52.81	38.20	122.70	22	1
1	A	28	TYR	CZ-CE2-CD2	50.91	165.62	119.80	22	1
1	A	28	TYR	CD1-CE1-CZ	50.75	165.47	119.80	22	1
1	A	20	TRP	CG-CD2-CE3	-49.31	89.52	133.90	22	1
1	A	27	HIS	CG-ND1-CE1	43.86	169.61	108.20	22	1
1	A	39	TYR	CG-CD2-CE2	42.98	155.68	121.30	22	1
1	A	39	TYR	CB-CG-CD1	42.24	146.34	121.00	22	1
1	A	35	ASP	CB-CG-OD2	42.02	156.12	118.30	22	1
1	A	8	ARG	NE-CZ-NH1	40.84	140.72	120.30	22	1
1	A	25	THR	O-C-N	-39.87	58.90	122.70	22	1
1	A	39	TYR	CD1-CE1-CZ	38.30	154.27	119.80	22	1
1	A	20	TRP	CG-CD1-NE1	37.90	148.00	110.10	22	1
1	A	39	TYR	CE1-CZ-CE2	-36.60	61.24	119.80	22	1
1	A	8	ARG	NE-CZ-NH2	36.25	138.42	120.30	22	1
1	A	8	ARG	NH1-CZ-NH2	-35.04	80.85	119.40	22	1
1	A	20	TRP	CE3-CZ3-CH2	34.76	159.44	121.20	22	1
1	A	20	TRP	CH2-CZ2-CE2	-33.70	83.70	117.40	22	1
1	A	27	HIS	CG-CD2-NE2	33.02	171.94	109.20	22	1
1	A	27	HIS	O-C-N	-32.33	70.98	122.70	22	1
1	A	39	TYR	CG-CD1-CE1	31.36	146.39	121.30	22	1
1	A	20	TRP	CD2-CE2-CZ2	30.44	158.83	122.30	22	1
1	A	20	TRP	CD2-CE3-CZ3	-29.16	80.90	118.80	22	1
1	A	39	TYR	CZ-CE2-CD2	27.37	144.43	119.80	22	1
1	A	20	TRP	NE1-CE2-CD2	-26.76	80.54	107.30	22	1
1	A	27	HIS	CE1-NE2-CD2	-25.90	41.86	106.60	22	1
1	A	20	TRP	CB-CG-CD2	23.54	157.21	126.60	22	1
1	A	9	GLN	O-C-N	-22.76	86.29	122.70	22	1
1	A	32	LYS	CA-C-N	22.60	166.92	117.20	22	1
1	A	20	TRP	CB-CG-CD1	20.57	153.75	127.00	22	1
1	A	21	LYS	CG-CD-CE	20.41	173.14	111.90	22	1
1	A	22	THR	O-C-N	-20.04	90.64	122.70	22	1
1	A	6	CYS	O-C-N	-19.96	90.76	122.70	22	1
1	A	21	LYS	CB-CG-CD	19.18	161.46	111.60	22	1
1	A	27	HIS	CB-CG-ND1	19.10	170.95	123.20	22	1
1	A	35	ASP	OD1-CG-OD2	-18.89	87.40	123.30	22	1
1	A	10	CYS	CA-CB-SG	18.77	147.78	114.00	22	1
1	A	32	LYS	C-N-CA	18.49	167.92	121.70	22	1
1	A	32	LYS	CA-CB-CG	18.06	153.12	113.40	22	1
1	A	13	LYS	CB-CG-CD	17.67	157.55	111.60	22	1
1	A	25	THR	CA-C-N	17.52	155.74	117.20	22	1
1	A	28	TYR	OH-CZ-CE2	16.88	165.68	120.10	22	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	28	TYR	CE1-CZ-OH	16.78	165.40	120.10	22	1
1	A	32	LYS	CA-C-O	16.56	154.88	120.10	22	1
1	A	30	THR	CA-CB-CG2	16.34	135.28	112.40	22	1
1	A	27	HIS	CA-C-N	15.96	152.32	117.20	22	1
1	A	16	GLY	O-C-N	-15.04	98.63	122.70	22	1
1	A	8	ARG	CD-NE-CZ	14.66	144.12	123.60	22	1
1	A	27	HIS	ND1-CE1-NE2	14.49	141.77	109.90	22	1
1	A	25	THR	C-N-CA	14.31	157.47	121.70	22	1
1	A	27	HIS	CB-CG-CD2	14.01	174.22	130.80	22	1
1	A	24	LEU	CB-CG-CD1	13.84	134.53	111.00	22	1
1	A	18	THR	O-C-N	-13.72	100.75	122.70	22	1
1	A	29	CYS	CA-CB-SG	13.50	138.30	114.00	22	1
1	A	24	LEU	CA-CB-CG	13.25	145.78	115.30	22	1
1	A	27	HIS	C-N-CA	13.08	154.40	121.70	22	1
1	A	22	THR	CA-C-N	12.73	145.20	117.20	22	1
1	A	30	THR	OG1-CB-CG2	-12.71	80.77	110.00	22	1
1	A	39	TYR	CE1-CZ-OH	12.66	154.29	120.10	22	1
1	A	11	LYS	CD-CE-NZ	12.54	140.54	111.70	22	1
1	A	32	LYS	CB-CG-CD	-12.24	79.79	111.60	22	1
1	A	32	LYS	CG-CD-CE	-12.04	75.77	111.90	22	1
1	A	25	THR	CA-C-O	12.03	145.36	120.10	22	1
1	A	9	GLN	CA-C-N	11.78	143.11	117.20	22	1
1	A	2	THR	O-C-N	-11.76	103.89	122.70	22	1
1	A	2	THR	N-CA-CB	-11.68	88.11	110.30	22	1
1	A	6	CYS	CA-C-N	10.86	141.10	117.20	22	1
1	A	22	THR	C-N-CA	10.58	148.15	121.70	22	1
1	A	2	THR	CA-CB-CG2	10.13	126.58	112.40	22	1
1	A	9	GLN	OE1-CD-NE2	-10.02	98.86	121.90	22	1
1	A	14	PRO	O-C-N	-9.95	106.78	122.70	22	1
1	A	9	GLN	CG-CD-NE2	9.91	140.49	116.70	22	1
1	A	9	GLN	C-N-CA	9.69	145.91	121.70	22	1
1	A	13	LYS	CD-CE-NZ	-9.42	90.03	111.70	22	1
1	A	16	GLY	CA-C-N	9.24	137.53	117.20	22	1
1	A	24	LEU	CD1-CG-CD2	-9.20	82.91	110.50	22	1
1	A	39	TYR	OH-CZ-CE2	9.02	144.46	120.10	22	1
1	A	6	CYS	C-N-CA	8.99	144.17	121.70	22	1
1	A	20	TRP	NE1-CE2-CZ2	-8.88	120.63	130.40	22	1
1	A	35	ASP	CA-CB-CG	8.71	132.56	113.40	22	1
1	A	32	LYS	CD-CE-NZ	8.29	130.77	111.70	22	1
1	A	33	SER	O-C-N	-8.20	109.57	122.70	22	1
1	A	8	ARG	CG-CD-NE	8.16	128.94	111.80	22	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	LYS	CG-CD-CE	8.06	136.07	111.90	22	1
1	A	27	HIS	CA-CB-CG	7.91	127.04	113.60	22	1
1	A	27	HIS	CA-C-O	7.91	136.71	120.10	22	1
1	A	11	LYS	CB-CG-CD	7.82	131.94	111.60	22	1
1	A	16	GLY	C-N-CA	7.75	141.06	121.70	22	1
1	A	8	ARG	CA-CB-CG	7.50	129.91	113.40	22	1
1	A	23	SER	O-C-N	-7.32	110.98	122.70	22	1
1	A	13	LYS	CG-CD-CE	-6.92	91.15	111.90	22	1
1	A	30	THR	CA-CB-OG1	6.29	122.20	109.00	22	1
1	A	18	THR	CA-C-N	6.23	130.90	117.20	22	1
1	A	33	SER	CA-CB-OG	6.11	127.69	111.20	22	1
1	A	13	LYS	CA-CB-CG	5.98	126.55	113.40	22	1
1	A	2	THR	CB-CA-C	5.88	127.48	111.60	22	1
1	A	2	THR	N-CA-C	5.64	126.23	111.00	22	1
1	A	24	LEU	CB-CG-CD2	5.54	120.41	111.00	22	1
1	A	8	ARG	CB-CG-CD	5.41	125.66	111.60	22	1
1	A	34	CYS	CA-CB-SG	5.39	123.71	114.00	22	1
1	A	38	LEU	CB-CG-CD1	5.31	120.03	111.00	22	1
1	A	2	THR	CA-C-N	5.20	128.65	117.20	22	1
1	A	18	THR	C-N-CA	5.20	134.70	121.70	22	1
1	A	2	THR	OG1-CB-CG2	-5.10	98.26	110.00	22	1

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

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	2	THR	CA,CB	1
1	A	30	THR	CB	1

There are no planarity outliers.

6.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	283	274	250	100±15
All	All	6226	6028	5974	2192

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 180.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LYS:NZ	1:A:21:LYS:CD	1.50	1.74	22	1
1:A:32:LYS:CB	1:A:32:LYS:CE	1.47	1.93	22	1
1:A:11:LYS:NZ	1:A:11:LYS:CD	1.44	1.75	22	1
1:A:28:TYR:CZ	1:A:28:TYR:CD2	1.43	2.07	22	1
1:A:28:TYR:CZ	1:A:28:TYR:CD1	1.42	2.06	22	1
1:A:28:TYR:CG	1:A:28:TYR:CE1	1.39	2.11	22	1
1:A:32:LYS:CD	1:A:32:LYS:CA	1.39	2.01	22	1
1:A:28:TYR:CG	1:A:28:TYR:CE2	1.38	2.10	22	1
1:A:29:CYS:SG	1:A:34:CYS:SG	1.36	1.38	16	7
1:A:32:LYS:CA	1:A:32:LYS:O	1.30	1.77	22	1
1:A:32:LYS:CA	1:A:32:LYS:HD3	1.30	1.54	22	1
1:A:28:TYR:CD1	1:A:28:TYR:CB	1.25	2.20	22	1
1:A:28:TYR:CD2	1:A:28:TYR:CB	1.24	2.19	22	1
1:A:25:THR:O	1:A:26:SER:CA	1.22	1.87	22	1
1:A:32:LYS:O	1:A:33:SER:CA	1.21	1.86	22	1
1:A:34:CYS:SG	1:A:34:CYS:CA	1.19	2.29	22	1
1:A:34:CYS:SG	1:A:34:CYS:CB	1.18	1.09	22	1
1:A:26:SER:O	1:A:38:LEU:HD23	1.18	1.39	15	2
1:A:30:THR:CG2	1:A:30:THR:CA	1.17	2.20	22	1
1:A:28:TYR:CE2	1:A:28:TYR:OH	1.16	1.99	22	1
1:A:6:CYS:SG	1:A:34:CYS:SG	1.16	2.44	18	4
1:A:28:TYR:CE1	1:A:28:TYR:OH	1.14	1.98	22	1
1:A:25:THR:O	1:A:25:THR:CA	1.13	1.94	22	1
1:A:30:THR:CA	1:A:30:THR:OG1	1.12	1.96	22	1
1:A:32:LYS:C	1:A:33:SER:CA	1.12	2.18	22	1
1:A:38:LEU:HD23	1:A:38:LEU:N	1.10	1.61	6	2
1:A:25:THR:C	1:A:26:SER:CA	1.08	2.21	22	1
1:A:30:THR:CG2	1:A:30:THR:HB	1.04	1.59	22	1
1:A:9:GLN:O	1:A:10:CYS:HB2	1.03	1.54	18	2
1:A:32:LYS:CA	1:A:33:SER:N	1.01	2.22	22	1
1:A:11:LYS:HA	1:A:38:LEU:HD12	1.01	1.32	6	2
1:A:5:PRO:O	1:A:7:CYS:N	1.01	1.91	1	13
1:A:6:CYS:HA	1:A:10:CYS:CB	1.00	1.85	18	14
1:A:13:LYS:CD	1:A:38:LEU:HD22	1.00	1.85	2	12
1:A:29:CYS:SG	1:A:34:CYS:CB	1.00	2.49	18	9
1:A:34:CYS:SG	1:A:34:CYS:HB2	0.99	1.65	22	1
1:A:25:THR:CA	1:A:26:SER:N	0.99	2.26	22	1
1:A:6:CYS:HA	1:A:10:CYS:HB3	0.98	1.33	21	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:CYS:SG	1:A:34:CYS:HB3	0.98	1.65	22	1
1:A:32:LYS:CA	1:A:32:LYS:CG	0.97	2.10	22	1
1:A:30:THR:CB	1:A:30:THR:HG22	0.97	1.50	22	1
1:A:7:CYS:O	1:A:32:LYS:N	0.97	1.97	7	3
1:A:6:CYS:SG	1:A:36:CYS:O	0.96	2.23	12	13
1:A:6:CYS:HB2	1:A:38:LEU:HD12	0.95	1.34	15	4
1:A:21:LYS:NZ	1:A:21:LYS:HD2	0.95	1.72	22	1
1:A:30:THR:CB	1:A:30:THR:HG21	0.95	1.50	22	1
1:A:11:LYS:HA	1:A:38:LEU:HD13	0.95	1.34	15	12
1:A:9:GLN:O	1:A:10:CYS:SG	0.94	2.25	20	1
1:A:21:LYS:NZ	1:A:21:LYS:HE2	0.94	1.34	22	1
1:A:30:THR:CB	1:A:30:THR:HG23	0.94	1.50	22	1
1:A:13:LYS:H	1:A:13:LYS:HE2	0.94	1.22	22	1
1:A:21:LYS:NZ	1:A:21:LYS:HE3	0.93	1.35	22	1
1:A:10:CYS:O	1:A:38:LEU:HD11	0.93	1.63	1	3
1:A:19:CYS:HA	1:A:28:TYR:CG	0.93	1.99	11	22
1:A:32:LYS:CB	1:A:32:LYS:HG3	0.93	1.46	22	1
1:A:13:LYS:HD3	1:A:38:LEU:HD22	0.92	1.40	2	13
1:A:7:CYS:SG	1:A:34:CYS:CB	0.91	2.58	22	3
1:A:32:LYS:CB	1:A:32:LYS:HG2	0.91	1.46	22	1
1:A:13:LYS:NZ	1:A:25:THR:HG23	0.90	1.82	20	3
1:A:9:GLN:O	1:A:10:CYS:HB3	0.89	1.68	13	2
1:A:29:CYS:SG	1:A:38:LEU:HD11	0.88	2.09	11	6
1:A:6:CYS:CB	1:A:10:CYS:SG	0.88	2.61	19	9
1:A:10:CYS:O	1:A:38:LEU:HD13	0.88	1.69	7	4
1:A:23:SER:C	1:A:24:LEU:HD13	0.88	1.88	21	1
1:A:29:CYS:HB2	1:A:38:LEU:HD21	0.88	1.44	22	9
1:A:6:CYS:HA	1:A:10:CYS:SG	0.87	2.10	15	2
1:A:28:TYR:O	1:A:29:CYS:SG	0.87	2.32	1	5
1:A:25:THR:C	1:A:26:SER:N	0.87	0.82	22	1
1:A:30:THR:CG2	1:A:30:THR:CB	0.87	0.87	22	1
1:A:13:LYS:HD3	1:A:38:LEU:HD13	0.87	1.45	16	4
1:A:2:THR:HG21	1:A:12:LEU:HD23	0.87	1.45	14	2
1:A:29:CYS:CB	1:A:38:LEU:HD21	0.86	2.00	13	10
1:A:26:SER:O	1:A:38:LEU:HB3	0.86	1.69	22	13
1:A:29:CYS:CB	1:A:34:CYS:SG	0.86	2.63	12	5
1:A:29:CYS:SG	1:A:38:LEU:HD21	0.86	2.10	4	4
1:A:6:CYS:CA	1:A:10:CYS:HB3	0.86	2.00	21	11
1:A:13:LYS:CD	1:A:38:LEU:HD13	0.86	2.01	16	4
1:A:37:PRO:C	1:A:38:LEU:HD23	0.86	1.90	6	2
1:A:11:LYS:NZ	1:A:11:LYS:HE2	0.86	1.26	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LYS:O	1:A:11:LYS:CG	0.86	2.24	9	16
1:A:4:GLY:O	1:A:10:CYS:SG	0.86	2.33	7	1
1:A:11:LYS:NZ	1:A:11:LYS:HE3	0.86	1.26	22	1
1:A:6:CYS:HB2	1:A:38:LEU:CD1	0.86	2.01	8	14
1:A:11:LYS:CD	1:A:11:LYS:O	0.86	2.24	22	1
1:A:6:CYS:O	1:A:9:GLN:N	0.85	2.09	20	14
1:A:2:THR:N	1:A:10:CYS:SG	0.85	2.49	21	9
1:A:25:THR:O	1:A:26:SER:N	0.85	0.71	22	1
1:A:7:CYS:SG	1:A:34:CYS:N	0.85	2.49	19	19
1:A:29:CYS:HB3	1:A:38:LEU:HD21	0.85	1.47	21	4
1:A:21:LYS:O	1:A:22:THR:CB	0.85	2.25	18	1
1:A:21:LYS:NZ	1:A:21:LYS:CE	0.85	0.70	22	1
1:A:11:LYS:O	1:A:11:LYS:CE	0.84	2.25	22	7
1:A:38:LEU:N	1:A:38:LEU:CD2	0.84	2.36	6	1
1:A:32:LYS:C	1:A:33:SER:N	0.84	0.81	22	1
1:A:6:CYS:SG	1:A:38:LEU:HD11	0.84	2.13	2	6
1:A:17:THR:O	1:A:30:THR:HG23	0.83	1.73	18	1
1:A:27:HIS:O	1:A:38:LEU:HD22	0.83	1.73	20	5
1:A:36:CYS:O	1:A:38:LEU:CD2	0.83	2.27	6	2
1:A:7:CYS:SG	1:A:29:CYS:SG	0.83	2.76	12	2
1:A:12:LEU:HD12	1:A:12:LEU:O	0.83	1.74	11	1
1:A:29:CYS:SG	1:A:38:LEU:CD2	0.82	2.67	10	4
1:A:6:CYS:O	1:A:8:ARG:N	0.82	2.13	5	7
1:A:28:TYR:HB3	1:A:36:CYS:HB3	0.82	1.50	15	5
1:A:5:PRO:O	1:A:6:CYS:SG	0.81	2.38	6	18
1:A:28:TYR:N	1:A:38:LEU:HD23	0.81	1.89	4	4
1:A:3:THR:HG21	1:A:9:GLN:HB3	0.81	1.52	11	7
1:A:7:CYS:C	1:A:32:LYS:H	0.81	1.78	7	6
1:A:7:CYS:SG	1:A:32:LYS:N	0.81	2.54	8	19
1:A:11:LYS:NZ	1:A:11:LYS:O	0.80	2.14	22	1
1:A:11:LYS:O	1:A:11:LYS:HG3	0.80	1.77	9	6
1:A:13:LYS:HD2	1:A:38:LEU:HD22	0.80	1.54	15	4
1:A:6:CYS:CB	1:A:38:LEU:HD21	0.80	2.07	6	1
1:A:3:THR:N	1:A:10:CYS:SG	0.79	2.55	7	5
1:A:6:CYS:O	1:A:34:CYS:SG	0.79	2.40	17	3
1:A:27:HIS:O	1:A:29:CYS:N	0.79	2.16	19	9
1:A:11:LYS:O	1:A:11:LYS:CD	0.78	2.31	9	12
1:A:23:SER:O	1:A:24:LEU:CB	0.78	2.32	18	1
1:A:3:THR:HG21	1:A:9:GLN:CB	0.78	2.08	11	3
1:A:21:LYS:O	1:A:22:THR:HB	0.78	1.77	18	2
1:A:34:CYS:CB	1:A:34:CYS:HG	0.78	1.87	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:CYS:O	1:A:8:ARG:CG	0.78	2.31	5	4
1:A:31:GLY:O	1:A:32:LYS:CB	0.78	2.31	5	5
1:A:19:CYS:HA	1:A:28:TYR:CD2	0.78	2.14	22	16
1:A:11:LYS:NZ	1:A:11:LYS:CE	0.78	0.64	22	1
1:A:7:CYS:CB	1:A:34:CYS:SG	0.77	2.72	4	2
1:A:32:LYS:HD3	1:A:32:LYS:C	0.77	1.99	22	1
1:A:7:CYS:O	1:A:8:ARG:CB	0.77	2.33	14	19
1:A:13:LYS:HE2	1:A:13:LYS:N	0.77	1.92	22	1
1:A:32:LYS:O	1:A:33:SER:CB	0.76	2.33	20	11
1:A:11:LYS:HA	1:A:38:LEU:CD1	0.76	2.10	20	7
1:A:36:CYS:O	1:A:38:LEU:HD21	0.76	1.80	6	1
1:A:6:CYS:HA	1:A:10:CYS:HB2	0.76	1.56	20	1
1:A:32:LYS:CG	1:A:32:LYS:HB2	0.76	1.30	22	1
1:A:22:THR:CG2	1:A:27:HIS:CG	0.76	2.69	5	6
1:A:34:CYS:O	1:A:35:ASP:CB	0.76	2.33	13	5
1:A:25:THR:HG22	1:A:26:SER:N	0.76	1.95	4	4
1:A:31:GLY:O	1:A:32:LYS:HG3	0.76	1.81	10	2
1:A:25:THR:O	1:A:26:SER:CB	0.76	2.33	16	12
1:A:26:SER:O	1:A:38:LEU:CB	0.76	2.34	16	7
1:A:13:LYS:HZ2	1:A:25:THR:HG23	0.75	1.37	20	1
1:A:6:CYS:HA	1:A:10:CYS:N	0.75	1.96	5	7
1:A:6:CYS:HB2	1:A:38:LEU:HD11	0.75	1.59	18	9
1:A:11:LYS:CA	1:A:38:LEU:HD13	0.74	2.11	15	10
1:A:9:GLN:O	1:A:10:CYS:CB	0.74	2.35	8	5
1:A:15:ALA:HB1	1:A:30:THR:HA	0.74	1.56	18	1
1:A:8:ARG:O	1:A:8:ARG:CD	0.73	2.36	9	3
1:A:6:CYS:O	1:A:7:CYS:HB2	0.73	1.84	16	5
1:A:21:LYS:O	1:A:22:THR:CG2	0.73	2.36	18	1
1:A:3:THR:H	1:A:10:CYS:HB2	0.73	1.43	5	2
1:A:3:THR:HG21	1:A:9:GLN:CD	0.73	2.03	11	1
1:A:20:TRP:CB	1:A:27:HIS:CE1	0.73	2.72	19	2
1:A:22:THR:CG2	1:A:27:HIS:CE1	0.73	2.72	9	6
1:A:13:LYS:HZ3	1:A:25:THR:CG2	0.73	1.97	10	2
1:A:30:THR:OG1	1:A:30:THR:CB	0.73	0.70	22	1
1:A:29:CYS:SG	1:A:34:CYS:HB2	0.73	2.23	9	7
1:A:5:PRO:O	1:A:6:CYS:C	0.73	2.26	3	2
1:A:6:CYS:HB2	1:A:10:CYS:O	0.72	1.84	10	3
1:A:6:CYS:O	1:A:7:CYS:CB	0.72	2.37	16	5
1:A:6:CYS:HB2	1:A:10:CYS:SG	0.72	2.24	17	8
1:A:6:CYS:CB	1:A:10:CYS:HB3	0.72	2.14	21	6
1:A:28:TYR:CD2	1:A:37:PRO:O	0.72	2.43	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:CYS:HA	1:A:11:LYS:HG2	0.72	1.58	4	12
1:A:29:CYS:HB2	1:A:38:LEU:HD11	0.72	1.62	7	5
1:A:15:ALA:HB1	1:A:30:THR:HG23	0.72	1.62	12	1
1:A:3:THR:CG2	1:A:9:GLN:HB3	0.71	2.14	11	5
1:A:10:CYS:SG	1:A:38:LEU:HD12	0.71	2.25	14	4
1:A:8:ARG:CG	1:A:8:ARG:O	0.71	2.38	19	2
1:A:19:CYS:HA	1:A:28:TYR:CD1	0.71	2.19	22	4
1:A:25:THR:O	1:A:25:THR:C	0.71	0.52	22	1
1:A:6:CYS:HA	1:A:10:CYS:CA	0.71	2.16	14	7
1:A:10:CYS:SG	1:A:10:CYS:O	0.71	2.49	16	2
1:A:10:CYS:O	1:A:38:LEU:CD1	0.71	2.39	16	6
1:A:7:CYS:SG	1:A:32:LYS:C	0.70	2.70	13	14
1:A:29:CYS:HB2	1:A:34:CYS:SG	0.70	2.25	10	2
1:A:9:GLN:O	1:A:12:LEU:N	0.70	2.24	5	2
1:A:14:PRO:O	1:A:15:ALA:O	0.70	2.09	22	8
1:A:28:TYR:O	1:A:29:CYS:HB2	0.70	1.84	19	8
1:A:4:GLY:N	1:A:10:CYS:SG	0.70	2.65	11	2
1:A:13:LYS:NZ	1:A:25:THR:CG2	0.70	2.55	10	3
1:A:7:CYS:O	1:A:8:ARG:HB3	0.70	1.86	13	10
1:A:6:CYS:HB3	1:A:10:CYS:SG	0.70	2.27	13	8
1:A:32:LYS:CB	1:A:32:LYS:CD	0.70	0.75	22	1
1:A:32:LYS:CB	1:A:32:LYS:CG	0.70	0.74	22	1
1:A:12:LEU:HD12	1:A:12:LEU:C	0.69	2.07	7	2
1:A:11:LYS:HA	1:A:13:LYS:HD2	0.69	1.63	5	11
1:A:5:PRO:O	1:A:6:CYS:O	0.69	2.11	17	3
1:A:11:LYS:CE	1:A:11:LYS:O	0.69	2.40	19	1
1:A:32:LYS:O	1:A:33:SER:N	0.69	0.56	22	1
1:A:19:CYS:SG	1:A:28:TYR:CE2	0.69	2.86	13	7
1:A:32:LYS:CD	1:A:32:LYS:C	0.69	2.60	22	1
1:A:29:CYS:CB	1:A:38:LEU:HD11	0.69	2.18	15	5
1:A:6:CYS:CA	1:A:10:CYS:SG	0.69	2.81	15	5
1:A:13:LYS:CE	1:A:38:LEU:HD13	0.68	2.19	10	2
1:A:3:THR:H	1:A:10:CYS:HA	0.68	1.46	7	1
1:A:3:THR:CB	1:A:9:GLN:HB3	0.68	2.18	11	5
1:A:3:THR:N	1:A:10:CYS:HB2	0.68	2.04	13	5
1:A:6:CYS:HB2	1:A:11:LYS:HB3	0.68	1.64	10	2
1:A:6:CYS:CA	1:A:10:CYS:CB	0.68	2.72	7	7
1:A:30:THR:HG22	1:A:34:CYS:HB3	0.68	1.64	15	1
1:A:8:ARG:O	1:A:8:ARG:CG	0.68	2.41	9	4
1:A:22:THR:HG21	1:A:27:HIS:CE1	0.68	2.24	9	5
1:A:27:HIS:O	1:A:38:LEU:CG	0.68	2.42	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:TYR:H	1:A:38:LEU:HD23	0.68	1.48	3	4
1:A:27:HIS:ND1	1:A:27:HIS:C	0.67	2.47	19	1
1:A:27:HIS:O	1:A:29:CYS:SG	0.67	2.53	2	1
1:A:29:CYS:SG	1:A:38:LEU:CD1	0.67	2.83	2	3
1:A:29:CYS:HB2	1:A:38:LEU:CD2	0.67	2.18	1	8
1:A:2:THR:O	1:A:3:THR:O	0.67	2.13	20	2
1:A:13:LYS:CB	1:A:14:PRO:CD	0.67	2.72	15	6
1:A:6:CYS:CB	1:A:38:LEU:CD1	0.67	2.72	2	7
1:A:31:GLY:O	1:A:32:LYS:CG	0.67	2.44	4	1
1:A:20:TRP:HB3	1:A:27:HIS:CE1	0.66	2.25	19	3
1:A:11:LYS:CA	1:A:38:LEU:CD1	0.66	2.74	20	5
1:A:17:THR:HB	1:A:27:HIS:HE2	0.66	1.49	19	1
1:A:6:CYS:SG	1:A:29:CYS:CB	0.66	2.83	20	1
1:A:3:THR:N	1:A:10:CYS:HG	0.66	1.88	22	1
1:A:6:CYS:C	1:A:11:LYS:HB3	0.66	2.10	1	7
1:A:21:LYS:O	1:A:22:THR:HG22	0.66	1.90	18	1
1:A:7:CYS:O	1:A:8:ARG:HB2	0.66	1.91	6	11
1:A:20:TRP:N	1:A:28:TYR:CD1	0.66	2.64	20	15
1:A:24:LEU:HG	1:A:24:LEU:C	0.66	1.84	22	1
1:A:20:TRP:O	1:A:21:LYS:CG	0.65	2.44	10	4
1:A:22:THR:HG23	1:A:27:HIS:CD2	0.65	2.26	11	2
1:A:11:LYS:O	1:A:13:LYS:N	0.65	2.29	16	9
1:A:25:THR:O	1:A:27:HIS:N	0.65	2.29	12	5
1:A:6:CYS:SG	1:A:6:CYS:O	0.65	2.55	3	4
1:A:17:THR:O	1:A:29:CYS:O	0.65	2.15	22	10
1:A:6:CYS:CB	1:A:38:LEU:HD11	0.65	2.22	2	4
1:A:14:PRO:O	1:A:15:ALA:C	0.65	2.35	14	3
1:A:27:HIS:O	1:A:28:TYR:CD1	0.65	2.50	4	1
1:A:27:HIS:O	1:A:28:TYR:HD1	0.65	1.73	4	1
1:A:2:THR:OG1	1:A:39:TYR:CD1	0.65	2.50	14	1
1:A:27:HIS:C	1:A:38:LEU:CD2	0.64	2.65	15	1
1:A:19:CYS:SG	1:A:28:TYR:CD2	0.64	2.91	13	8
1:A:20:TRP:O	1:A:21:LYS:CB	0.64	2.45	10	6
1:A:38:LEU:HD12	1:A:38:LEU:N	0.64	2.07	2	1
1:A:7:CYS:SG	1:A:33:SER:C	0.64	2.76	13	4
1:A:27:HIS:C	1:A:38:LEU:HD23	0.64	2.13	13	4
1:A:11:LYS:HZ3	1:A:11:LYS:C	0.64	1.95	6	1
1:A:3:THR:HB	1:A:9:GLN:O	0.64	1.93	12	4
1:A:3:THR:OG1	1:A:10:CYS:CA	0.64	2.45	17	1
1:A:6:CYS:CB	1:A:10:CYS:HB2	0.64	2.23	11	4
1:A:14:PRO:O	1:A:15:ALA:HB3	0.64	1.92	13	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:THR:HG21	1:A:20:TRP:CE3	0.64	2.27	15	1
1:A:10:CYS:SG	1:A:38:LEU:HD11	0.63	2.33	12	1
1:A:31:GLY:O	1:A:32:LYS:HB3	0.63	1.91	13	5
1:A:16:GLY:HA3	1:A:27:HIS:CD2	0.63	2.27	19	5
1:A:31:GLY:O	1:A:32:LYS:CD	0.63	2.46	12	3
1:A:13:LYS:HZ3	1:A:25:THR:HG23	0.63	1.52	14	1
1:A:11:LYS:HD3	1:A:31:GLY:CA	0.63	2.24	22	10
1:A:27:HIS:O	1:A:38:LEU:HD23	0.63	1.92	13	1
1:A:11:LYS:NZ	1:A:11:LYS:HD2	0.63	2.02	22	1
1:A:11:LYS:CB	1:A:38:LEU:HD11	0.63	2.24	9	2
1:A:22:THR:CG2	1:A:27:HIS:CD2	0.63	2.82	11	7
1:A:22:THR:HG23	1:A:27:HIS:CG	0.63	2.28	14	2
1:A:15:ALA:HB1	1:A:30:THR:CA	0.63	2.23	18	1
1:A:2:THR:HB	1:A:10:CYS:O	0.63	1.94	14	2
1:A:33:SER:O	1:A:34:CYS:C	0.63	2.37	13	2
1:A:10:CYS:O	1:A:38:LEU:CG	0.62	2.47	16	1
1:A:6:CYS:CB	1:A:11:LYS:HB3	0.62	2.25	10	3
1:A:6:CYS:CB	1:A:38:LEU:HD12	0.62	2.18	15	2
1:A:6:CYS:CA	1:A:10:CYS:HB2	0.62	2.23	20	2
1:A:6:CYS:SG	1:A:7:CYS:N	0.62	2.73	19	12
1:A:28:TYR:CD2	1:A:36:CYS:SG	0.62	2.93	20	3
1:A:24:LEU:HD22	1:A:24:LEU:N	0.62	2.10	21	1
1:A:19:CYS:C	1:A:28:TYR:CD1	0.62	2.73	18	3
1:A:28:TYR:CB	1:A:37:PRO:O	0.62	2.48	2	16
1:A:31:GLY:O	1:A:32:LYS:O	0.62	2.17	10	2
1:A:11:LYS:CE	1:A:31:GLY:HA2	0.62	2.25	10	1
1:A:29:CYS:CB	1:A:38:LEU:CD2	0.62	2.78	12	3
1:A:22:THR:O	1:A:23:SER:CB	0.61	2.48	2	4
1:A:6:CYS:N	1:A:10:CYS:HB2	0.61	2.09	7	1
1:A:19:CYS:HB3	1:A:28:TYR:CE2	0.61	2.30	11	3
1:A:29:CYS:O	1:A:30:THR:CB	0.61	2.47	1	2
1:A:22:THR:HG22	1:A:27:HIS:CD2	0.61	2.30	8	3
1:A:24:LEU:C	1:A:24:LEU:CD1	0.61	2.69	9	1
1:A:10:CYS:C	1:A:12:LEU:H	0.61	1.97	20	3
1:A:13:LYS:HD3	1:A:38:LEU:CD2	0.61	2.24	17	9
1:A:29:CYS:SG	1:A:38:LEU:CG	0.61	2.89	2	3
1:A:10:CYS:C	1:A:12:LEU:N	0.61	2.55	20	3
1:A:11:LYS:HZ2	1:A:13:LYS:HG2	0.60	1.56	14	2
1:A:18:THR:O	1:A:19:CYS:C	0.60	2.39	6	15
1:A:27:HIS:O	1:A:38:LEU:CD2	0.60	2.50	13	6
1:A:7:CYS:CB	1:A:32:LYS:N	0.60	2.65	17	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:CYS:O	1:A:28:TYR:CE1	0.60	2.55	18	1
1:A:16:GLY:HA3	1:A:27:HIS:CG	0.60	2.31	16	10
1:A:10:CYS:O	1:A:13:LYS:CE	0.60	2.50	8	2
1:A:11:LYS:O	1:A:12:LEU:C	0.60	2.40	16	7
1:A:13:LYS:HB2	1:A:14:PRO:HD2	0.60	1.72	18	6
1:A:21:LYS:CE	1:A:21:LYS:HZ2	0.60	1.30	22	1
1:A:28:TYR:CD1	1:A:28:TYR:CG	0.60	0.70	22	1
1:A:28:TYR:O	1:A:36:CYS:CB	0.60	2.50	17	11
1:A:26:SER:O	1:A:28:TYR:N	0.60	2.33	11	3
1:A:17:THR:HG22	1:A:18:THR:H	0.59	1.56	13	7
1:A:26:SER:O	1:A:38:LEU:HB2	0.59	1.96	16	3
1:A:7:CYS:CA	1:A:32:LYS:H	0.59	2.09	7	5
1:A:26:SER:O	1:A:38:LEU:HA	0.59	1.97	12	8
1:A:24:LEU:O	1:A:25:THR:CB	0.59	2.50	18	1
1:A:21:LYS:CE	1:A:21:LYS:HZ1	0.59	1.30	22	1
1:A:34:CYS:SG	1:A:34:CYS:N	0.59	2.73	22	1
1:A:29:CYS:CB	1:A:34:CYS:HB2	0.59	2.26	2	1
1:A:7:CYS:O	1:A:32:LYS:CA	0.59	2.49	7	2
1:A:3:THR:N	1:A:10:CYS:CB	0.59	2.65	19	1
1:A:7:CYS:CA	1:A:11:LYS:HG2	0.59	2.26	16	2
1:A:38:LEU:O	1:A:39:TYR:CB	0.59	2.49	4	4
1:A:29:CYS:HB2	1:A:34:CYS:CB	0.59	2.27	10	2
1:A:32:LYS:O	1:A:33:SER:HB2	0.59	1.96	20	2
1:A:29:CYS:HB2	1:A:38:LEU:HD23	0.59	1.74	12	2
1:A:25:THR:O	1:A:26:SER:OG	0.59	2.20	16	6
1:A:10:CYS:O	1:A:13:LYS:HE3	0.59	1.98	8	4
1:A:6:CYS:O	1:A:29:CYS:SG	0.59	2.60	17	2
1:A:6:CYS:HB3	1:A:10:CYS:HB2	0.59	1.74	11	1
1:A:27:HIS:O	1:A:28:TYR:C	0.59	2.41	6	7
1:A:10:CYS:O	1:A:12:LEU:N	0.58	2.36	20	2
1:A:28:TYR:CG	1:A:37:PRO:O	0.58	2.57	2	3
1:A:30:THR:HG23	1:A:34:CYS:SG	0.58	2.38	8	2
1:A:31:GLY:O	1:A:32:LYS:HB2	0.58	1.98	4	4
1:A:5:PRO:O	1:A:6:CYS:CB	0.58	2.52	7	2
1:A:27:HIS:O	1:A:38:LEU:HG	0.58	1.97	13	1
1:A:7:CYS:HB3	1:A:32:LYS:HA	0.58	1.73	10	4
1:A:10:CYS:O	1:A:38:LEU:HD21	0.58	1.99	16	1
1:A:32:LYS:C	1:A:32:LYS:CD	0.58	2.71	14	3
1:A:25:THR:O	1:A:26:SER:HB2	0.58	1.97	10	6
1:A:29:CYS:HB3	1:A:34:CYS:SG	0.58	2.39	4	2
1:A:3:THR:CB	1:A:9:GLN:CB	0.58	2.81	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LYS:CE	1:A:21:LYS:HZ3	0.58	1.30	22	1
1:A:19:CYS:CA	1:A:28:TYR:CD2	0.58	2.87	11	2
1:A:32:LYS:CD	1:A:32:LYS:O	0.58	2.51	14	1
1:A:32:LYS:HB3	1:A:32:LYS:HD2	0.58	0.60	22	1
1:A:7:CYS:HB3	1:A:32:LYS:CA	0.58	2.29	6	10
1:A:21:LYS:O	1:A:21:LYS:HG2	0.58	1.98	9	4
1:A:28:TYR:CD2	1:A:28:TYR:CG	0.58	0.70	22	1
1:A:6:CYS:SG	1:A:38:LEU:HD21	0.57	2.38	6	4
1:A:11:LYS:O	1:A:11:LYS:HG2	0.57	1.98	7	3
1:A:6:CYS:HA	1:A:10:CYS:H	0.57	1.59	1	6
1:A:11:LYS:CD	1:A:11:LYS:C	0.57	2.73	7	5
1:A:13:LYS:NZ	1:A:13:LYS:HB3	0.57	2.14	20	4
1:A:37:PRO:C	1:A:38:LEU:CD2	0.57	2.70	6	1
1:A:3:THR:CG2	1:A:9:GLN:CB	0.57	2.78	11	1
1:A:13:LYS:HB2	1:A:14:PRO:CD	0.57	2.29	18	2
1:A:13:LYS:CB	1:A:14:PRO:HD2	0.57	2.29	15	3
1:A:11:LYS:N	1:A:38:LEU:HD13	0.57	2.14	11	1
1:A:29:CYS:CB	1:A:34:CYS:CB	0.56	2.83	2	1
1:A:11:LYS:O	1:A:11:LYS:HE2	0.56	2.00	2	4
1:A:11:LYS:CA	1:A:38:LEU:HD11	0.56	2.30	9	3
1:A:21:LYS:CD	1:A:21:LYS:C	0.56	2.73	14	2
1:A:11:LYS:O	1:A:11:LYS:HD2	0.56	1.99	4	12
1:A:6:CYS:HB2	1:A:10:CYS:HB2	0.56	1.77	4	1
1:A:6:CYS:CB	1:A:10:CYS:CB	0.56	2.84	5	2
1:A:11:LYS:O	1:A:11:LYS:NZ	0.56	2.35	6	3
1:A:8:ARG:N	1:A:11:LYS:HD2	0.56	2.16	10	2
1:A:27:HIS:ND1	1:A:28:TYR:N	0.56	2.53	19	1
1:A:30:THR:O	1:A:30:THR:CG2	0.56	2.54	6	1
1:A:28:TYR:CZ	1:A:28:TYR:CE2	0.56	0.66	22	1
1:A:5:PRO:C	1:A:7:CYS:N	0.56	2.58	10	10
1:A:13:LYS:NZ	1:A:16:GLY:N	0.56	2.53	11	1
1:A:19:CYS:CB	1:A:28:TYR:CD2	0.56	2.89	11	2
1:A:2:THR:CG2	1:A:12:LEU:HD23	0.56	2.28	14	1
1:A:21:LYS:C	1:A:22:THR:OG1	0.56	2.44	6	1
1:A:31:GLY:C	1:A:32:LYS:CD	0.56	2.74	16	2
1:A:18:THR:O	1:A:19:CYS:SG	0.56	2.64	13	2
1:A:34:CYS:O	1:A:35:ASP:HB2	0.56	2.00	13	4
1:A:32:LYS:O	1:A:32:LYS:CG	0.56	2.53	14	1
1:A:27:HIS:O	1:A:38:LEU:HD21	0.56	2.01	15	1
1:A:39:TYR:CD1	1:A:39:TYR:C	0.56	2.78	21	1
1:A:28:TYR:C	1:A:29:CYS:SG	0.56	2.84	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:THR:OG1	1:A:39:TYR:CE1	0.55	2.59	14	1
1:A:17:THR:O	1:A:29:CYS:N	0.55	2.39	3	7
1:A:31:GLY:C	1:A:32:LYS:HG3	0.55	2.22	12	2
1:A:28:TYR:CZ	1:A:28:TYR:CE1	0.55	0.66	22	1
1:A:26:SER:O	1:A:38:LEU:CA	0.55	2.55	13	4
1:A:17:THR:O	1:A:29:CYS:C	0.55	2.44	18	7
1:A:11:LYS:CD	1:A:30:THR:O	0.55	2.54	20	1
1:A:11:LYS:CE	1:A:11:LYS:HZ2	0.55	1.25	22	1
1:A:11:LYS:CE	1:A:11:LYS:HZ1	0.55	1.25	22	1
1:A:22:THR:CG2	1:A:27:HIS:NE2	0.55	2.70	9	3
1:A:17:THR:HG22	1:A:18:THR:N	0.55	2.16	19	4
1:A:28:TYR:O	1:A:29:CYS:CB	0.55	2.54	16	6
1:A:38:LEU:HD12	1:A:38:LEU:H	0.55	1.61	2	1
1:A:27:HIS:C	1:A:29:CYS:N	0.55	2.60	2	2
1:A:15:ALA:CB	1:A:30:THR:O	0.55	2.55	8	5
1:A:13:LYS:CD	1:A:38:LEU:CD1	0.55	2.85	9	1
1:A:15:ALA:O	1:A:27:HIS:CE1	0.55	2.60	18	1
1:A:28:TYR:HB2	1:A:37:PRO:O	0.55	2.02	19	7
1:A:8:ARG:O	1:A:9:GLN:CG	0.55	2.55	12	2
1:A:11:LYS:C	1:A:13:LYS:N	0.54	2.58	20	14
1:A:8:ARG:O	1:A:8:ARG:HG3	0.54	2.01	9	6
1:A:28:TYR:HB3	1:A:36:CYS:CB	0.54	2.29	15	2
1:A:23:SER:O	1:A:24:LEU:HB3	0.54	2.00	18	2
1:A:11:LYS:CE	1:A:11:LYS:HZ3	0.54	1.25	22	1
1:A:30:THR:CB	1:A:30:THR:HG1	0.54	1.26	22	1
1:A:7:CYS:C	1:A:8:ARG:CG	0.54	2.75	2	2
1:A:11:LYS:HB2	1:A:38:LEU:HD21	0.54	1.78	1	2
1:A:21:LYS:HB3	1:A:28:TYR:CD1	0.54	2.38	15	3
1:A:32:LYS:CD	1:A:33:SER:N	0.54	2.70	13	2
1:A:21:LYS:HA	1:A:26:SER:HA	0.54	1.79	14	3
1:A:11:LYS:HZ3	1:A:30:THR:CA	0.54	2.15	19	1
1:A:11:LYS:CE	1:A:13:LYS:O	0.54	2.56	9	1
1:A:11:LYS:CB	1:A:38:LEU:HD21	0.54	2.32	10	1
1:A:32:LYS:CG	1:A:32:LYS:HB3	0.54	1.30	22	1
1:A:25:THR:CG2	1:A:26:SER:N	0.54	2.65	4	2
1:A:29:CYS:SG	1:A:36:CYS:O	0.54	2.65	3	4
1:A:6:CYS:HA	1:A:11:LYS:N	0.54	2.18	14	2
1:A:20:TRP:O	1:A:21:LYS:CD	0.54	2.56	10	1
1:A:17:THR:OG1	1:A:20:TRP:CG	0.54	2.55	15	1
1:A:7:CYS:HB3	1:A:32:LYS:O	0.54	2.03	5	3
1:A:11:LYS:HA	1:A:13:LYS:HD3	0.54	1.79	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:CYS:HA	1:A:28:TYR:HA	0.54	1.79	15	2
1:A:22:THR:O	1:A:25:THR:O	0.54	2.25	18	2
1:A:32:LYS:CD	1:A:32:LYS:HB3	0.54	1.23	22	1
1:A:25:THR:HG22	1:A:26:SER:H	0.53	1.63	8	3
1:A:11:LYS:NZ	1:A:13:LYS:O	0.53	2.41	9	1
1:A:23:SER:O	1:A:24:LEU:HB2	0.53	2.02	18	1
1:A:36:CYS:HB3	1:A:37:PRO:HD2	0.53	1.81	15	2
1:A:32:LYS:O	1:A:32:LYS:C	0.53	0.38	22	1
1:A:4:GLY:N	1:A:10:CYS:HB2	0.53	2.17	16	2
1:A:20:TRP:HA	1:A:20:TRP:CE3	0.53	2.38	13	1
1:A:13:LYS:HZ3	1:A:13:LYS:HB3	0.53	1.62	14	1
1:A:2:THR:CA	1:A:10:CYS:HB2	0.53	2.33	19	1
1:A:26:SER:HB3	1:A:39:TYR:CD1	0.53	2.38	4	1
1:A:13:LYS:NZ	1:A:13:LYS:HB2	0.53	2.18	9	2
1:A:32:LYS:CB	1:A:32:LYS:HD3	0.53	1.07	22	1
1:A:11:LYS:CD	1:A:30:THR:C	0.53	2.77	2	2
1:A:2:THR:N	1:A:10:CYS:HB3	0.53	2.18	11	1
1:A:7:CYS:N	1:A:11:LYS:HB3	0.53	2.18	16	1
1:A:20:TRP:HB2	1:A:27:HIS:CE1	0.53	2.39	19	1
1:A:7:CYS:SG	1:A:33:SER:N	0.53	2.82	5	8
1:A:29:CYS:HB3	1:A:38:LEU:CD2	0.53	2.34	12	1
1:A:13:LYS:HD2	1:A:38:LEU:CD1	0.53	2.34	20	2
1:A:22:THR:OG1	1:A:23:SER:N	0.52	2.42	10	7
1:A:17:THR:HB	1:A:20:TRP:CB	0.52	2.34	8	4
1:A:3:THR:HB	1:A:10:CYS:CB	0.52	2.34	9	2
1:A:3:THR:HB	1:A:9:GLN:C	0.52	2.24	18	2
1:A:19:CYS:HA	1:A:28:TYR:CE1	0.52	2.40	4	1
1:A:13:LYS:NZ	1:A:25:THR:O	0.52	2.42	14	1
1:A:26:SER:HB2	1:A:39:TYR:N	0.52	2.19	5	2
1:A:39:TYR:CD1	1:A:39:TYR:O	0.52	2.62	21	1
1:A:28:TYR:O	1:A:38:LEU:CD2	0.52	2.57	9	1
1:A:32:LYS:O	1:A:33:SER:OG	0.52	2.27	20	1
1:A:6:CYS:CB	1:A:38:LEU:CD2	0.52	2.86	6	1
1:A:30:THR:CG2	1:A:34:CYS:SG	0.52	2.98	8	2
1:A:13:LYS:HD3	1:A:38:LEU:HB3	0.52	1.80	13	2
1:A:17:THR:HG21	1:A:20:TRP:CZ3	0.52	2.39	15	1
1:A:12:LEU:O	1:A:13:LYS:O	0.52	2.27	12	6
1:A:7:CYS:C	1:A:8:ARG:HG2	0.52	2.25	21	4
1:A:11:LYS:N	1:A:11:LYS:HD3	0.52	2.20	10	1
1:A:26:SER:C	1:A:28:TYR:N	0.52	2.62	15	2
1:A:3:THR:OG1	1:A:10:CYS:N	0.52	2.43	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LYS:HD3	1:A:31:GLY:HA2	0.52	1.81	22	2
1:A:2:THR:H	1:A:10:CYS:HB3	0.52	1.63	15	2
1:A:10:CYS:SG	1:A:38:LEU:CD1	0.52	2.98	12	1
1:A:11:LYS:HE3	1:A:38:LEU:HD21	0.51	1.83	2	1
1:A:11:LYS:HD3	1:A:30:THR:C	0.51	2.26	13	6
1:A:11:LYS:N	1:A:38:LEU:CD1	0.51	2.73	20	2
1:A:22:THR:HG22	1:A:27:HIS:CE1	0.51	2.39	16	1
1:A:6:CYS:SG	1:A:29:CYS:HB2	0.51	2.45	20	1
1:A:11:LYS:HZ2	1:A:31:GLY:HA2	0.51	1.64	21	1
1:A:16:GLY:O	1:A:17:THR:OG1	0.51	2.27	17	3
1:A:27:HIS:O	1:A:38:LEU:HB3	0.51	2.04	16	2
1:A:17:THR:O	1:A:29:CYS:CA	0.51	2.57	10	2
1:A:9:GLN:C	1:A:11:LYS:N	0.51	2.62	14	2
1:A:11:LYS:C	1:A:11:LYS:HD3	0.51	2.25	7	2
1:A:29:CYS:SG	1:A:38:LEU:HD23	0.51	2.42	10	1
1:A:2:THR:N	1:A:10:CYS:HB2	0.51	2.19	19	1
1:A:24:LEU:HD22	1:A:24:LEU:H	0.51	1.64	21	1
1:A:32:LYS:CB	1:A:32:LYS:HD2	0.51	1.10	22	1
1:A:7:CYS:CB	1:A:32:LYS:H	0.51	2.19	17	9
1:A:13:LYS:HD3	1:A:38:LEU:CB	0.51	2.35	13	4
1:A:25:THR:HG22	1:A:27:HIS:HD2	0.51	1.66	7	1
1:A:8:ARG:H	1:A:11:LYS:HD2	0.51	1.65	10	1
1:A:22:THR:HG23	1:A:27:HIS:ND1	0.51	2.20	14	1
1:A:39:TYR:CG	1:A:39:TYR:O	0.51	2.63	1	1
1:A:38:LEU:O	1:A:39:TYR:HB2	0.51	2.06	6	3
1:A:17:THR:HB	1:A:27:HIS:NE2	0.51	2.20	19	1
1:A:17:THR:N	1:A:29:CYS:O	0.51	2.43	21	4
1:A:26:SER:CB	1:A:39:TYR:HA	0.51	2.35	6	1
1:A:25:THR:HG22	1:A:27:HIS:CD2	0.51	2.41	7	1
1:A:11:LYS:C	1:A:13:LYS:H	0.51	2.09	4	3
1:A:7:CYS:SG	1:A:31:GLY:C	0.51	2.89	11	7
1:A:28:TYR:HB3	1:A:37:PRO:O	0.51	2.05	13	3
1:A:11:LYS:CA	1:A:13:LYS:HD2	0.50	2.34	5	3
1:A:22:THR:CG2	1:A:27:HIS:ND1	0.50	2.73	5	1
1:A:6:CYS:HA	1:A:9:GLN:O	0.50	2.06	20	1
1:A:3:THR:CB	1:A:9:GLN:O	0.50	2.59	12	1
1:A:3:THR:CG2	1:A:9:GLN:O	0.50	2.59	12	1
1:A:3:THR:OG1	1:A:4:GLY:N	0.50	2.44	17	1
1:A:21:LYS:HB2	1:A:28:TYR:CD1	0.50	2.41	5	1
1:A:7:CYS:HA	1:A:11:LYS:HG3	0.50	1.83	10	1
1:A:32:LYS:C	1:A:32:LYS:HD3	0.50	2.26	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:PRO:O	1:A:15:ALA:CB	0.50	2.58	13	1
1:A:6:CYS:O	1:A:11:LYS:CB	0.50	2.58	14	1
1:A:16:GLY:O	1:A:17:THR:CB	0.50	2.59	4	1
1:A:11:LYS:CD	1:A:31:GLY:HA2	0.50	2.37	16	2
1:A:26:SER:CB	1:A:39:TYR:O	0.50	2.59	3	1
1:A:6:CYS:O	1:A:7:CYS:SG	0.50	2.69	12	2
1:A:10:CYS:O	1:A:38:LEU:CD2	0.50	2.60	16	1
1:A:24:LEU:HD13	1:A:24:LEU:N	0.50	2.21	21	1
1:A:11:LYS:NZ	1:A:30:THR:O	0.50	2.41	9	2
1:A:28:TYR:O	1:A:36:CYS:O	0.50	2.30	2	3
1:A:11:LYS:HD2	1:A:31:GLY:N	0.50	2.22	2	2
1:A:29:CYS:HB3	1:A:34:CYS:CB	0.50	2.37	4	3
1:A:13:LYS:HB3	1:A:14:PRO:CD	0.50	2.34	15	2
1:A:34:CYS:O	1:A:35:ASP:HB3	0.50	2.06	13	1
1:A:30:THR:CG2	1:A:31:GLY:N	0.50	2.74	19	1
1:A:28:TYR:O	1:A:36:CYS:HB2	0.50	2.07	4	5
1:A:22:THR:HG22	1:A:27:HIS:CG	0.50	2.42	5	1
1:A:3:THR:HG21	1:A:9:GLN:HG2	0.50	1.83	6	1
1:A:13:LYS:HD2	1:A:38:LEU:HD13	0.50	1.82	16	2
1:A:6:CYS:N	1:A:10:CYS:SG	0.50	2.85	11	1
1:A:21:LYS:HB3	1:A:28:TYR:CE1	0.49	2.42	15	5
1:A:3:THR:HG22	1:A:9:GLN:OE1	0.49	2.08	10	2
1:A:13:LYS:HB3	1:A:13:LYS:NZ	0.49	2.19	17	1
1:A:24:LEU:C	1:A:24:LEU:HD13	0.49	2.28	9	1
1:A:6:CYS:N	1:A:10:CYS:HB3	0.49	2.22	16	3
1:A:11:LYS:HG2	1:A:31:GLY:HA2	0.49	1.82	20	4
1:A:13:LYS:HD2	1:A:38:LEU:HD12	0.49	1.84	20	1
1:A:13:LYS:HG3	1:A:25:THR:CG2	0.49	2.38	1	1
1:A:4:GLY:N	1:A:9:GLN:OE1	0.49	2.46	10	1
1:A:11:LYS:CE	1:A:31:GLY:CA	0.49	2.90	16	3
1:A:6:CYS:CB	1:A:10:CYS:O	0.49	2.61	1	1
1:A:3:THR:HG22	1:A:4:GLY:N	0.49	2.22	5	4
1:A:26:SER:CB	1:A:38:LEU:C	0.49	2.81	18	1
1:A:30:THR:N	1:A:34:CYS:HB3	0.49	2.22	6	1
1:A:22:THR:HG23	1:A:23:SER:N	0.49	2.22	18	1
1:A:3:THR:HG22	1:A:9:GLN:HB3	0.49	1.85	8	1
1:A:11:LYS:O	1:A:13:LYS:HE3	0.49	2.07	16	1
1:A:30:THR:O	1:A:31:GLY:O	0.48	2.30	6	1
1:A:3:THR:C	1:A:10:CYS:SG	0.48	2.92	7	1
1:A:7:CYS:HB3	1:A:32:LYS:N	0.48	2.23	16	4
1:A:3:THR:HB	1:A:10:CYS:HB2	0.48	1.84	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LYS:CE	1:A:31:GLY:HA3	0.48	2.38	4	3
1:A:28:TYR:O	1:A:36:CYS:HB3	0.48	2.09	17	4
1:A:11:LYS:HB2	1:A:38:LEU:HD11	0.48	1.84	9	1
1:A:9:GLN:O	1:A:12:LEU:HB3	0.48	2.08	11	1
1:A:23:SER:O	1:A:24:LEU:HD13	0.48	2.05	21	1
1:A:22:THR:HG21	1:A:27:HIS:CD2	0.48	2.43	4	1
1:A:36:CYS:O	1:A:38:LEU:HD23	0.48	2.09	9	1
1:A:6:CYS:SG	1:A:38:LEU:CD1	0.48	3.02	5	1
1:A:24:LEU:CD2	1:A:24:LEU:O	0.48	2.62	12	1
1:A:3:THR:OG1	1:A:10:CYS:SG	0.48	2.72	2	1
1:A:26:SER:CB	1:A:38:LEU:HA	0.48	2.38	11	1
1:A:19:CYS:C	1:A:28:TYR:CE1	0.48	2.87	18	3
1:A:13:LYS:NZ	1:A:38:LEU:HB2	0.48	2.24	13	1
1:A:2:THR:OG1	1:A:38:LEU:O	0.48	2.32	16	1
1:A:29:CYS:SG	1:A:38:LEU:HG	0.48	2.48	4	2
1:A:8:ARG:O	1:A:8:ARG:NE	0.48	2.47	16	3
1:A:2:THR:CG2	1:A:39:TYR:O	0.48	2.62	4	1
1:A:9:GLN:O	1:A:11:LYS:N	0.48	2.46	14	2
1:A:3:THR:OG1	1:A:10:CYS:CB	0.48	2.62	17	1
1:A:26:SER:O	1:A:38:LEU:C	0.48	2.52	6	1
1:A:27:HIS:CG	1:A:27:HIS:O	0.48	2.67	11	1
1:A:6:CYS:O	1:A:7:CYS:C	0.48	2.53	11	3
1:A:28:TYR:CD2	1:A:36:CYS:HB3	0.48	2.44	4	1
1:A:13:LYS:CD	1:A:38:LEU:HB3	0.48	2.38	11	1
1:A:22:THR:O	1:A:25:THR:N	0.48	2.43	12	1
1:A:32:LYS:O	1:A:32:LYS:HG3	0.48	2.08	14	1
1:A:11:LYS:NZ	1:A:31:GLY:CA	0.48	2.76	21	1
1:A:13:LYS:HZ3	1:A:16:GLY:CA	0.47	2.21	11	1
1:A:17:THR:CG2	1:A:20:TRP:CE3	0.47	2.97	15	1
1:A:5:PRO:O	1:A:34:CYS:O	0.47	2.33	11	2
1:A:17:THR:CB	1:A:20:TRP:CE3	0.47	2.96	15	1
1:A:20:TRP:O	1:A:21:LYS:HB3	0.47	2.09	22	7
1:A:28:TYR:CG	1:A:28:TYR:HD1	0.47	1.23	22	1
1:A:17:THR:O	1:A:27:HIS:O	0.47	2.32	8	3
1:A:33:SER:O	1:A:34:CYS:O	0.47	2.32	20	3
1:A:28:TYR:CG	1:A:28:TYR:HD2	0.47	1.23	22	1
1:A:11:LYS:CD	1:A:31:GLY:CA	0.47	2.92	16	4
1:A:19:CYS:N	1:A:28:TYR:HA	0.47	2.25	4	5
1:A:10:CYS:C	1:A:38:LEU:CD1	0.47	2.83	4	1
1:A:22:THR:HG22	1:A:27:HIS:ND1	0.47	2.23	5	1
1:A:31:GLY:C	1:A:33:SER:N	0.47	2.68	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:THR:HG22	1:A:27:HIS:NE2	0.47	2.25	9	1
1:A:2:THR:HB	1:A:10:CYS:CA	0.47	2.40	13	1
1:A:32:LYS:CD	1:A:32:LYS:N	0.47	2.78	16	1
1:A:10:CYS:C	1:A:38:LEU:HD12	0.47	2.30	20	1
1:A:11:LYS:NZ	1:A:31:GLY:HA2	0.47	2.24	21	1
1:A:11:LYS:O	1:A:13:LYS:O	0.47	2.32	6	2
1:A:11:LYS:N	1:A:38:LEU:HD12	0.47	2.25	20	1
1:A:26:SER:O	1:A:37:PRO:O	0.47	2.32	15	1
1:A:11:LYS:O	1:A:11:LYS:HE3	0.47	2.10	4	3
1:A:26:SER:CB	1:A:39:TYR:HB2	0.47	2.40	4	1
1:A:6:CYS:HB2	1:A:38:LEU:HD21	0.47	1.83	6	2
1:A:13:LYS:HB2	1:A:13:LYS:HZ2	0.47	1.70	9	1
1:A:16:GLY:O	1:A:17:THR:C	0.47	2.52	16	1
1:A:21:LYS:HB2	1:A:28:TYR:CE1	0.47	2.45	16	1
1:A:34:CYS:O	1:A:35:ASP:CG	0.47	2.53	20	1
1:A:8:ARG:CG	1:A:9:GLN:N	0.46	2.78	1	1
1:A:18:THR:O	1:A:36:CYS:SG	0.46	2.74	7	3
1:A:6:CYS:O	1:A:11:LYS:N	0.46	2.37	15	2
1:A:21:LYS:N	1:A:27:HIS:CD2	0.46	2.83	11	1
1:A:32:LYS:HD3	1:A:33:SER:N	0.46	2.25	13	1
1:A:22:THR:HG21	1:A:27:HIS:NE2	0.46	2.26	16	3
1:A:26:SER:O	1:A:38:LEU:O	0.46	2.33	6	1
1:A:13:LYS:NZ	1:A:16:GLY:CA	0.46	2.79	11	1
1:A:17:THR:O	1:A:20:TRP:CB	0.46	2.63	8	1
1:A:38:LEU:O	1:A:39:TYR:CD2	0.46	2.68	17	1
1:A:27:HIS:HA	1:A:38:LEU:HD23	0.46	1.87	2	1
1:A:13:LYS:CE	1:A:38:LEU:HB2	0.46	2.40	21	1
1:A:28:TYR:O	1:A:38:LEU:HD23	0.46	2.10	1	1
1:A:5:PRO:C	1:A:7:CYS:H	0.46	2.11	4	1
1:A:30:THR:O	1:A:30:THR:HG22	0.46	2.10	6	1
1:A:26:SER:OG	1:A:38:LEU:HA	0.46	2.11	8	1
1:A:10:CYS:C	1:A:38:LEU:HD11	0.46	2.30	16	1
1:A:32:LYS:CB	1:A:32:LYS:O	0.46	2.55	22	1
1:A:37:PRO:HB2	1:A:39:TYR:CD2	0.46	2.46	21	1
1:A:32:LYS:HD2	1:A:32:LYS:C	0.46	2.31	1	1
1:A:10:CYS:O	1:A:13:LYS:HE2	0.46	2.11	21	1
1:A:3:THR:HB	1:A:10:CYS:CA	0.46	2.41	16	2
1:A:2:THR:O	1:A:2:THR:OG1	0.46	2.33	6	2
1:A:3:THR:N	1:A:10:CYS:HA	0.46	2.21	7	1
1:A:6:CYS:O	1:A:34:CYS:HB2	0.46	2.11	3	1
1:A:28:TYR:CZ	1:A:28:TYR:HE2	0.46	1.21	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LYS:HE3	1:A:38:LEU:HD13	0.45	1.86	1	1
1:A:11:LYS:HA	1:A:13:LYS:CD	0.45	2.41	4	5
1:A:37:PRO:CA	1:A:38:LEU:HD23	0.45	2.41	6	1
1:A:6:CYS:O	1:A:11:LYS:HD2	0.45	2.10	10	1
1:A:31:GLY:O	1:A:33:SER:N	0.45	2.49	15	3
1:A:2:THR:HG23	1:A:10:CYS:O	0.45	2.09	19	1
1:A:17:THR:C	1:A:29:CYS:O	0.45	2.55	15	2
1:A:10:CYS:SG	1:A:38:LEU:HG	0.45	2.51	9	1
1:A:7:CYS:HA	1:A:11:LYS:HD2	0.45	1.87	10	1
1:A:3:THR:CG2	1:A:9:GLN:OE1	0.45	2.64	15	1
1:A:32:LYS:N	1:A:32:LYS:HD2	0.45	2.27	16	1
1:A:17:THR:O	1:A:18:THR:C	0.45	2.55	8	1
1:A:3:THR:H	1:A:10:CYS:CB	0.45	2.20	5	2
1:A:5:PRO:O	1:A:6:CYS:HB3	0.45	2.12	7	2
1:A:15:ALA:HB1	1:A:30:THR:O	0.45	2.12	8	1
1:A:13:LYS:CD	1:A:13:LYS:H	0.45	2.24	13	2
1:A:3:THR:OG1	1:A:10:CYS:HB2	0.45	2.12	17	1
1:A:30:THR:OG1	1:A:31:GLY:N	0.45	2.50	20	1
1:A:24:LEU:N	1:A:24:LEU:CD2	0.45	2.78	21	1
1:A:27:HIS:O	1:A:38:LEU:HD13	0.45	2.10	6	1
1:A:8:ARG:O	1:A:8:ARG:HD2	0.45	2.11	9	1
1:A:29:CYS:HA	1:A:34:CYS:CB	0.45	2.42	12	1
1:A:27:HIS:O	1:A:28:TYR:HB2	0.45	2.10	13	2
1:A:28:TYR:CZ	1:A:28:TYR:HE1	0.45	1.21	22	1
1:A:15:ALA:HB1	1:A:30:THR:OG1	0.45	2.12	2	1
1:A:26:SER:OG	1:A:39:TYR:CG	0.45	2.69	4	1
1:A:20:TRP:O	1:A:21:LYS:HB2	0.45	2.11	5	1
1:A:29:CYS:HA	1:A:34:CYS:HB2	0.45	1.89	13	1
1:A:11:LYS:HZ3	1:A:30:THR:N	0.45	2.09	19	1
1:A:11:LYS:O	1:A:13:LYS:HG2	0.45	2.12	10	1
1:A:16:GLY:HA3	1:A:27:HIS:HB3	0.45	1.89	22	2
1:A:30:THR:CG2	1:A:30:THR:C	0.45	2.84	22	1
1:A:11:LYS:HZ3	1:A:30:THR:C	0.44	2.15	1	2
1:A:19:CYS:HA	1:A:28:TYR:CZ	0.44	2.47	4	1
1:A:7:CYS:CA	1:A:11:LYS:HD2	0.44	2.42	7	2
1:A:32:LYS:O	1:A:32:LYS:CD	0.44	2.65	8	2
1:A:21:LYS:CB	1:A:28:TYR:CD1	0.44	3.00	15	1
1:A:18:THR:O	1:A:19:CYS:CB	0.44	2.66	20	1
1:A:6:CYS:SG	1:A:34:CYS:HB2	0.44	2.52	21	1
1:A:26:SER:HB3	1:A:38:LEU:C	0.44	2.32	1	2
1:A:19:CYS:HA	1:A:28:TYR:CA	0.44	2.43	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:THR:O	1:A:27:HIS:CD2	0.44	2.70	7	1
1:A:11:LYS:NZ	1:A:30:THR:C	0.44	2.71	1	1
1:A:13:LYS:CG	1:A:25:THR:CG2	0.44	2.94	1	1
1:A:11:LYS:CD	1:A:31:GLY:N	0.44	2.81	19	3
1:A:32:LYS:O	1:A:33:SER:HB3	0.44	2.12	10	1
1:A:12:LEU:O	1:A:13:LYS:C	0.44	2.56	7	4
1:A:11:LYS:CA	1:A:38:LEU:HD12	0.44	2.22	6	1
1:A:21:LYS:O	1:A:21:LYS:CD	0.44	2.66	7	1
1:A:16:GLY:C	1:A:17:THR:OG1	0.44	2.56	20	4
1:A:8:ARG:HG2	1:A:9:GLN:N	0.44	2.27	1	1
1:A:6:CYS:O	1:A:11:LYS:HB3	0.44	2.13	14	1
1:A:16:GLY:C	1:A:29:CYS:O	0.44	2.56	11	2
1:A:29:CYS:CB	1:A:38:LEU:HD23	0.44	2.38	12	1
1:A:31:GLY:C	1:A:32:LYS:CG	0.44	2.86	12	2
1:A:26:SER:OG	1:A:39:TYR:HB2	0.44	2.12	4	1
1:A:27:HIS:O	1:A:28:TYR:CB	0.44	2.66	4	1
1:A:13:LYS:HZ3	1:A:16:GLY:HA3	0.44	1.73	11	1
1:A:32:LYS:N	1:A:32:LYS:CD	0.44	2.77	18	1
1:A:6:CYS:SG	1:A:36:CYS:N	0.44	2.91	7	2
1:A:16:GLY:CA	1:A:27:HIS:CG	0.44	3.01	21	1
1:A:5:PRO:O	1:A:34:CYS:SG	0.44	2.76	4	2
1:A:6:CYS:N	1:A:10:CYS:CB	0.44	2.79	7	1
1:A:11:LYS:CG	1:A:31:GLY:HA2	0.44	2.43	10	1
1:A:28:TYR:CE2	1:A:36:CYS:SG	0.44	3.11	21	1
1:A:11:LYS:HD3	1:A:30:THR:O	0.43	2.13	15	3
1:A:13:LYS:NZ	1:A:38:LEU:HD13	0.43	2.28	10	1
1:A:32:LYS:O	1:A:32:LYS:HD3	0.43	2.12	22	1
1:A:11:LYS:CB	1:A:29:CYS:SG	0.43	3.05	8	2
1:A:3:THR:HG21	1:A:9:GLN:CG	0.43	2.42	20	2
1:A:6:CYS:CA	1:A:11:LYS:N	0.43	2.81	14	1
1:A:13:LYS:N	1:A:13:LYS:HE2	0.43	2.28	20	1
1:A:17:THR:HB	1:A:20:TRP:CG	0.43	2.49	8	2
1:A:11:LYS:HD3	1:A:31:GLY:HA3	0.43	1.89	6	1
1:A:30:THR:N	1:A:34:CYS:CB	0.43	2.82	6	1
1:A:7:CYS:HA	1:A:11:LYS:CG	0.43	2.41	20	1
1:A:6:CYS:O	1:A:11:LYS:CG	0.43	2.66	5	1
1:A:7:CYS:SG	1:A:32:LYS:CA	0.43	3.07	8	1
1:A:20:TRP:C	1:A:28:TYR:CE1	0.43	2.92	11	1
1:A:6:CYS:HB2	1:A:38:LEU:CD2	0.43	2.43	6	1
1:A:19:CYS:CA	1:A:28:TYR:HA	0.43	2.43	11	3
1:A:16:GLY:O	1:A:17:THR:O	0.43	2.36	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:SER:CB	1:A:38:LEU:O	0.43	2.67	10	1
1:A:11:LYS:HB2	1:A:13:LYS:HE2	0.43	1.91	16	1
1:A:11:LYS:HA	1:A:38:LEU:CD2	0.43	2.44	16	1
1:A:5:PRO:O	1:A:7:CYS:HB2	0.43	2.14	3	1
1:A:13:LYS:HZ1	1:A:16:GLY:N	0.43	2.12	11	1
1:A:21:LYS:N	1:A:28:TYR:HD1	0.43	2.10	13	1
1:A:26:SER:C	1:A:28:TYR:H	0.43	2.17	15	1
1:A:2:THR:C	1:A:10:CYS:HB2	0.43	2.34	19	1
1:A:8:ARG:H	1:A:11:LYS:CG	0.43	2.27	6	1
1:A:19:CYS:CA	1:A:28:TYR:CG	0.43	2.88	11	1
1:A:13:LYS:HG2	1:A:14:PRO:N	0.43	2.29	16	1
1:A:2:THR:HG23	1:A:10:CYS:CB	0.43	2.44	19	1
1:A:11:LYS:CE	1:A:38:LEU:HD21	0.43	2.44	2	1
1:A:21:LYS:CA	1:A:27:HIS:CD2	0.43	3.02	11	1
1:A:8:ARG:H	1:A:11:LYS:HG2	0.43	1.74	6	1
1:A:29:CYS:HB2	1:A:38:LEU:CD1	0.43	2.42	13	2
1:A:22:THR:HG21	1:A:27:HIS:HE1	0.43	1.73	22	1
1:A:7:CYS:O	1:A:8:ARG:HG2	0.43	2.11	5	1
1:A:3:THR:HB	1:A:9:GLN:CB	0.43	2.44	11	1
1:A:16:GLY:HA3	1:A:27:HIS:HB2	0.43	1.91	14	1
1:A:21:LYS:NZ	1:A:21:LYS:HD3	0.43	2.05	22	1
1:A:7:CYS:CB	1:A:34:CYS:N	0.42	2.82	5	1
1:A:15:ALA:HB2	1:A:30:THR:O	0.42	2.14	5	2
1:A:17:THR:CG2	1:A:20:TRP:HB2	0.42	2.44	17	2
1:A:17:THR:CG2	1:A:18:THR:N	0.42	2.81	9	1
1:A:31:GLY:O	1:A:32:LYS:C	0.42	2.57	16	2
1:A:13:LYS:HZ1	1:A:25:THR:HG23	0.42	1.73	6	1
1:A:22:THR:HG22	1:A:26:SER:OG	0.42	2.14	6	1
1:A:31:GLY:O	1:A:32:LYS:HD2	0.42	2.13	15	2
1:A:10:CYS:O	1:A:13:LYS:NZ	0.42	2.50	21	1
1:A:7:CYS:HB2	1:A:34:CYS:SG	0.42	2.50	4	1
1:A:2:THR:HB	1:A:10:CYS:HA	0.42	1.91	13	3
1:A:22:THR:HG23	1:A:27:HIS:N	0.42	2.29	5	1
1:A:11:LYS:O	1:A:30:THR:O	0.42	2.37	10	1
1:A:11:LYS:HA	1:A:13:LYS:HE2	0.42	1.90	11	1
1:A:21:LYS:HA	1:A:26:SER:CA	0.42	2.44	14	1
1:A:11:LYS:HE2	1:A:30:THR:C	0.42	2.33	17	1
1:A:2:THR:HG23	1:A:39:TYR:O	0.42	2.14	4	1
1:A:2:THR:CB	1:A:10:CYS:HA	0.42	2.43	5	1
1:A:21:LYS:HA	1:A:27:HIS:N	0.42	2.29	11	2
1:A:11:LYS:CA	1:A:13:LYS:HE2	0.42	2.45	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:CYS:HA	1:A:11:LYS:CD	0.42	2.44	10	1
1:A:21:LYS:CB	1:A:26:SER:HA	0.42	2.44	11	1
1:A:33:SER:O	1:A:34:CYS:HB3	0.42	2.15	17	1
1:A:6:CYS:N	1:A:9:GLN:O	0.42	2.51	18	1
1:A:35:ASP:O	1:A:35:ASP:OD1	0.42	2.37	19	1
1:A:6:CYS:HB2	1:A:38:LEU:CG	0.42	2.44	6	1
1:A:10:CYS:HB2	1:A:38:LEU:HD12	0.42	1.91	11	1
1:A:3:THR:CA	1:A:10:CYS:HB2	0.42	2.45	16	1
1:A:31:GLY:O	1:A:32:LYS:NZ	0.42	2.50	9	1
1:A:13:LYS:H	1:A:13:LYS:HG3	0.42	1.30	12	1
1:A:28:TYR:HB2	1:A:38:LEU:HA	0.42	1.92	4	1
1:A:29:CYS:SG	1:A:34:CYS:HB3	0.42	2.54	7	1
1:A:20:TRP:O	1:A:21:LYS:HG2	0.42	2.14	9	2
1:A:26:SER:CB	1:A:39:TYR:N	0.42	2.83	7	1
1:A:11:LYS:CE	1:A:15:ALA:HA	0.42	2.45	17	1
1:A:19:CYS:CB	1:A:28:TYR:CE2	0.42	3.03	19	1
1:A:32:LYS:C	1:A:32:LYS:HD2	0.42	2.36	5	1
1:A:15:ALA:HA	1:A:30:THR:O	0.42	2.15	8	1
1:A:15:ALA:HA	1:A:30:THR:CB	0.42	2.45	10	1
1:A:17:THR:C	1:A:19:CYS:N	0.42	2.72	15	1
1:A:22:THR:O	1:A:23:SER:HB3	0.42	2.15	16	1
1:A:34:CYS:O	1:A:35:ASP:OD2	0.41	2.38	12	1
1:A:28:TYR:HB2	1:A:38:LEU:CA	0.41	2.45	4	1
1:A:5:PRO:C	1:A:6:CYS:SG	0.41	2.99	6	1
1:A:17:THR:CB	1:A:20:TRP:HB2	0.41	2.45	8	1
1:A:12:LEU:C	1:A:13:LYS:O	0.41	2.58	12	1
1:A:30:THR:HG22	1:A:33:SER:O	0.41	2.15	17	1
1:A:10:CYS:O	1:A:13:LYS:HD2	0.41	2.15	20	1
1:A:13:LYS:H	1:A:13:LYS:CE	0.41	2.10	22	1
1:A:3:THR:OG1	1:A:10:CYS:HA	0.41	2.15	17	1
1:A:21:LYS:CD	1:A:26:SER:HA	0.41	2.45	5	1
1:A:16:GLY:CA	1:A:27:HIS:CD2	0.41	3.03	6	1
1:A:3:THR:HG22	1:A:9:GLN:CD	0.41	2.36	10	1
1:A:11:LYS:CB	1:A:38:LEU:CD1	0.41	2.98	15	1
1:A:29:CYS:HB3	1:A:34:CYS:HB2	0.41	1.91	2	1
1:A:13:LYS:HG2	1:A:25:THR:CG2	0.41	2.45	7	1
1:A:21:LYS:C	1:A:27:HIS:CE1	0.41	2.93	14	1
1:A:32:LYS:CA	1:A:32:LYS:HD2	0.41	2.04	22	1
1:A:26:SER:CB	1:A:39:TYR:CD1	0.41	3.03	4	1
1:A:29:CYS:HB2	1:A:38:LEU:HD22	0.41	1.92	9	2
1:A:11:LYS:HB2	1:A:29:CYS:CB	0.41	2.45	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:CYS:HB3	1:A:32:LYS:C	0.41	2.35	13	1
1:A:8:ARG:O	1:A:9:GLN:OE1	0.41	2.38	19	1
1:A:11:LYS:HD3	1:A:31:GLY:N	0.41	2.30	22	1
1:A:11:LYS:C	1:A:11:LYS:NZ	0.41	2.70	6	1
1:A:36:CYS:HB3	1:A:37:PRO:CD	0.41	2.44	15	1
1:A:13:LYS:HD2	1:A:38:LEU:CD2	0.41	2.42	3	1
1:A:13:LYS:CA	1:A:13:LYS:HE3	0.41	2.44	11	1
1:A:13:LYS:HB3	1:A:14:PRO:HD2	0.41	1.91	15	1
1:A:21:LYS:CD	1:A:26:SER:OG	0.41	2.68	2	1
1:A:12:LEU:C	1:A:12:LEU:HD12	0.41	2.37	8	1
1:A:11:LYS:HE2	1:A:31:GLY:CA	0.41	2.46	9	1
1:A:21:LYS:O	1:A:21:LYS:HG3	0.41	2.15	14	1
1:A:15:ALA:O	1:A:27:HIS:CG	0.41	2.74	18	1
1:A:25:THR:O	1:A:27:HIS:ND1	0.41	2.54	18	1
1:A:6:CYS:O	1:A:9:GLN:C	0.41	2.58	20	1
1:A:12:LEU:C	1:A:12:LEU:CD1	0.41	2.81	7	1
1:A:13:LYS:HE3	1:A:13:LYS:N	0.41	2.31	11	1
1:A:20:TRP:HB3	1:A:27:HIS:NE2	0.41	2.30	11	1
1:A:24:LEU:HG	1:A:25:THR:N	0.41	2.30	17	2
1:A:11:LYS:HD2	1:A:11:LYS:C	0.41	2.36	20	1
1:A:38:LEU:CD1	1:A:38:LEU:N	0.40	2.77	2	1
1:A:25:THR:C	1:A:26:SER:OG	0.40	2.58	4	1
1:A:3:THR:HB	1:A:10:CYS:N	0.40	2.32	5	1
1:A:24:LEU:HD23	1:A:25:THR:N	0.40	2.31	8	1
1:A:25:THR:O	1:A:25:THR:HG22	0.40	2.16	11	1
1:A:30:THR:CG2	1:A:33:SER:O	0.40	2.69	15	1
1:A:30:THR:HG22	1:A:34:CYS:SG	0.40	2.57	21	1
1:A:22:THR:OG1	1:A:25:THR:O	0.40	2.38	3	1
1:A:22:THR:HG21	1:A:27:HIS:CG	0.40	2.48	5	1
1:A:10:CYS:C	1:A:38:LEU:HG	0.40	2.36	6	1
1:A:35:ASP:O	1:A:36:CYS:SG	0.40	2.78	6	1
1:A:17:THR:HG22	1:A:20:TRP:HB2	0.40	1.93	8	1
1:A:13:LYS:C	1:A:15:ALA:H	0.40	2.19	13	2
1:A:13:LYS:HB3	1:A:13:LYS:HZ3	0.40	1.73	20	1
1:A:11:LYS:HB2	1:A:38:LEU:CD1	0.40	2.46	9	1
1:A:2:THR:CG2	1:A:10:CYS:HA	0.40	2.46	13	1
1:A:21:LYS:O	1:A:21:LYS:CG	0.40	2.69	14	1
1:A:3:THR:HG1	1:A:10:CYS:N	0.40	2.14	17	1
1:A:11:LYS:HB2	1:A:38:LEU:CD2	0.40	2.45	1	1
1:A:19:CYS:HA	1:A:28:TYR:CB	0.40	2.45	11	1
1:A:17:THR:HG21	1:A:20:TRP:CG	0.40	2.51	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:HIS:C	1:A:29:CYS:H	0.40	2.19	21	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	38/41 (93%)	12±3 (31±9%)	14±3 (37±7%)	12±3 (31±7%)	0 0
All	All	836/902 (93%)	260 (31%)	313 (37%)	263 (31%)	0 0

All 33 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	35	ASP	20
1	A	26	SER	19
1	A	21	LYS	18
1	A	7	CYS	16
1	A	15	ALA	16
1	A	8	ARG	14
1	A	2	THR	13
1	A	33	SER	12
1	A	6	CYS	11
1	A	28	TYR	11
1	A	29	CYS	11
1	A	32	LYS	10
1	A	3	THR	10
1	A	22	THR	8
1	A	19	CYS	8
1	A	12	LEU	6
1	A	10	CYS	6
1	A	27	HIS	6
1	A	24	LEU	5
1	A	39	TYR	5
1	A	13	LYS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	16	GLY	5
1	A	23	SER	4
1	A	9	GLN	4
1	A	17	THR	4
1	A	11	LYS	4
1	A	30	THR	3
1	A	34	CYS	3
1	A	25	THR	2
1	A	36	CYS	1
1	A	20	TRP	1
1	A	31	GLY	1
1	A	4	GLY	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	34/36 (94%)	20±2 (58±6%)	14±2 (42±6%)	0 4
All	All	748/792 (94%)	434 (58%)	314 (42%)	0 4

All 30 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	11	LYS	22
1	A	13	LYS	22
1	A	32	LYS	18
1	A	21	LYS	16
1	A	23	SER	16
1	A	28	TYR	16
1	A	7	CYS	14
1	A	10	CYS	14
1	A	25	THR	14
1	A	24	LEU	13
1	A	30	THR	13
1	A	2	THR	13
1	A	36	CYS	13

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Mol	Chain	Res	Type	Models (Total)
1	A	38	LEU	12
1	A	39	TYR	12
1	A	29	CYS	11
1	A	18	THR	10
1	A	12	LEU	10
1	A	8	ARG	9
1	A	33	SER	8
1	A	6	CYS	8
1	A	26	SER	6
1	A	20	TRP	5
1	A	35	ASP	5
1	A	19	CYS	4
1	A	27	HIS	4
1	A	34	CYS	2
1	A	9	GLN	2
1	A	22	THR	1
1	A	17	THR	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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	22-A	17

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
22	A	17:THR	C	18:THR	N	1.18
22	A	24:LEU	C	25:THR	N	1.08
22	A	33:SER	C	34:CYS	N	1.08
22	A	39:TYR	C	40:PRO	N	1.08
22	A	1:CYS	C	2:THR	N	1.04
22	A	14:PRO	C	15:ALA	N	1.04
22	A	16:GLY	C	17:THR	N	1.02
22	A	2:THR	C	3:THR	N	1.01
22	A	18:THR	C	19:CYS	N	0.99
22	A	6:CYS	C	7:CYS	N	0.97
22	A	23:SER	C	24:LEU	N	0.96
22	A	9:GLN	C	10:CYS	N	0.92
22	A	27:HIS	C	28:TYR	N	0.89
22	A	22:THR	C	23:SER	N	0.83
22	A	25:THR	C	26:SER	N	0.82
22	A	32:LYS	C	33:SER	N	0.81
22	A	40:PRO	C	41:GLY	N	0.78

7 Chemical shift validation

No chemical shift data were provided