



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1IKC / pdb_00001ike
Title : NMR Structure of alpha-Bungarotoxin
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Deposited on : 2001-05-03

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

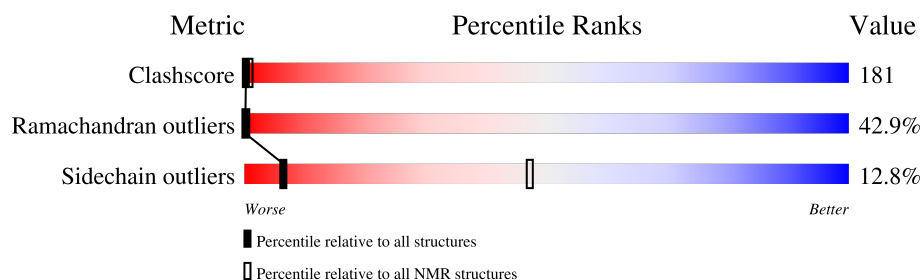
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	74	9% 34% 26% 23% 8%

2 Ensemble composition and analysis

This entry contains 30 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 10 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:2-A:16, A:22-A:74 (68)	0.27	10

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 3 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 18, 19, 22, 23, 24, 26, 29
2	20, 21
3	17, 25
Single-model clusters	27; 28; 30

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 694 atoms, of which 143 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called long neurotoxin 1.

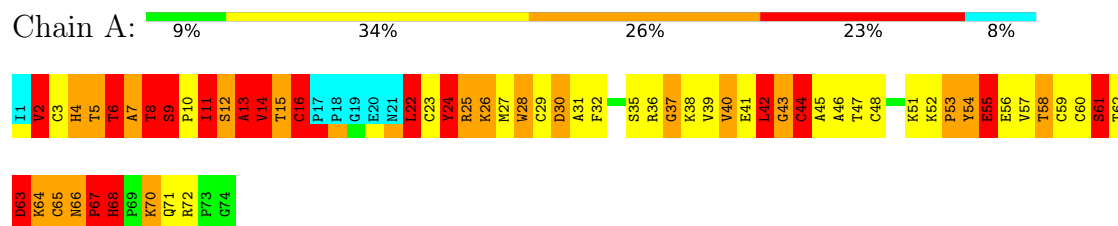
Mol	Chain	Residues	Atoms						Trace
1	A	74	Total	C	H	N	O	S	0
			694	338	143	97	105	11	

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: long neurotoxin 1

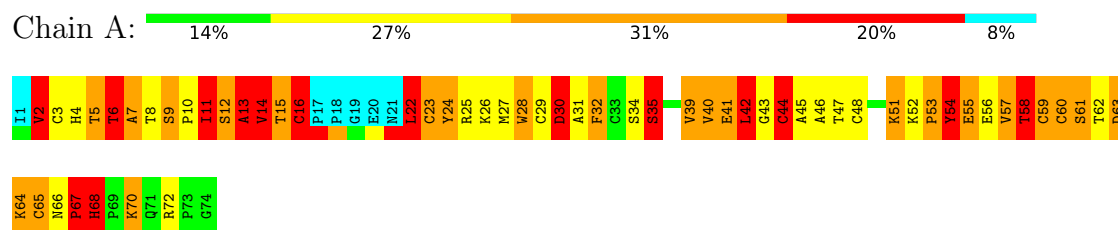


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

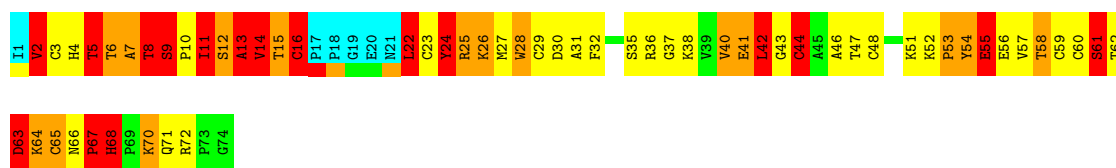
- Molecule 1: long neurotoxin 1



4.2.2 Score per residue for model 2

- Molecule 1: long neurotoxin 1

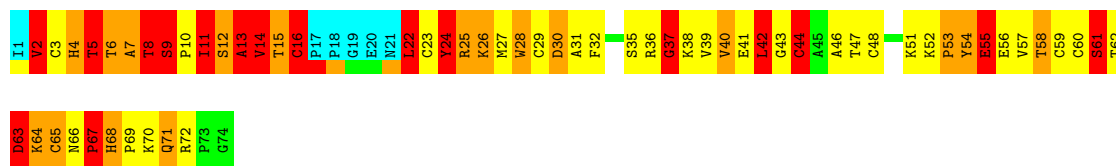




4.2.3 Score per residue for model 3

- Molecule 1: long neurotoxin 1

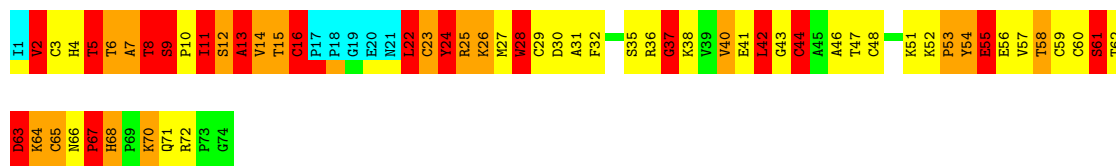
Chain A: 9% 36% 23% 23% 8%



4.2.4 Score per residue for model 4

- Molecule 1: long neurotoxin 1

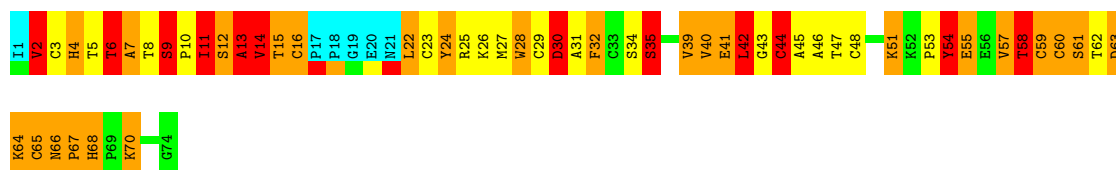
Chain A: 12% 35% 22% 23% 8%



4.2.5 Score per residue for model 5

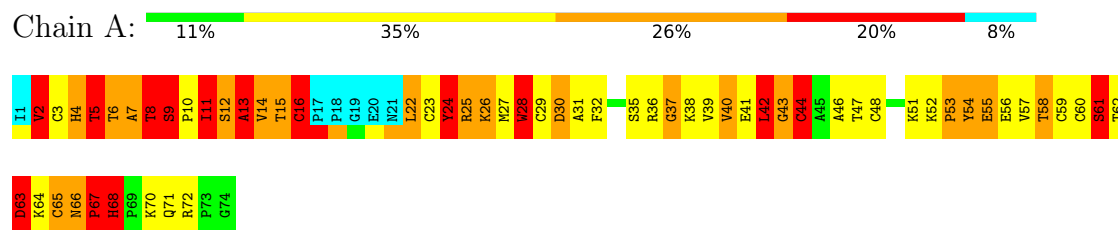
- Molecule 1: long neurotoxin 1

Chain A: 18% 24% 34% 16% 8%



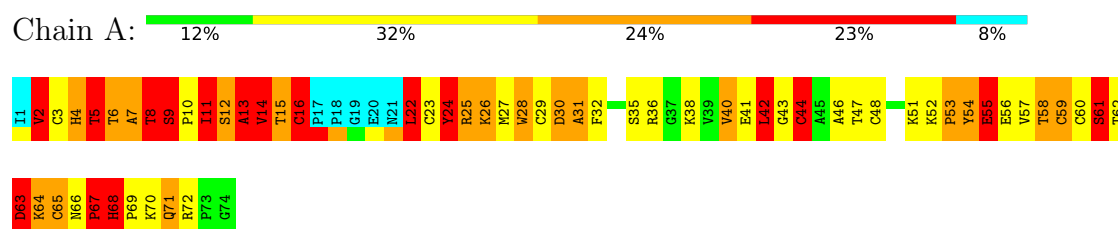
4.2.6 Score per residue for model 6

- Molecule 1: long neurotoxin 1



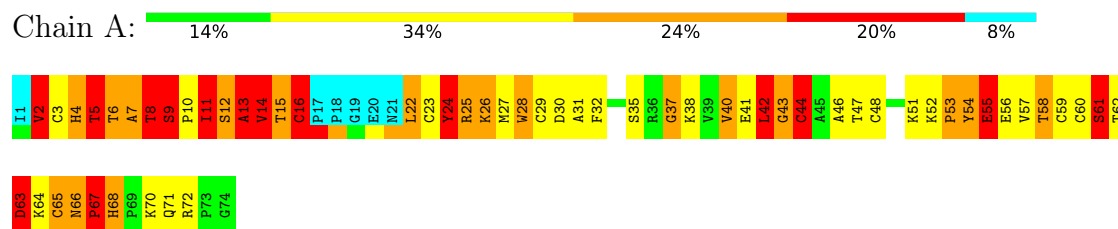
4.2.7 Score per residue for model 7

- Molecule 1: long neurotoxin 1



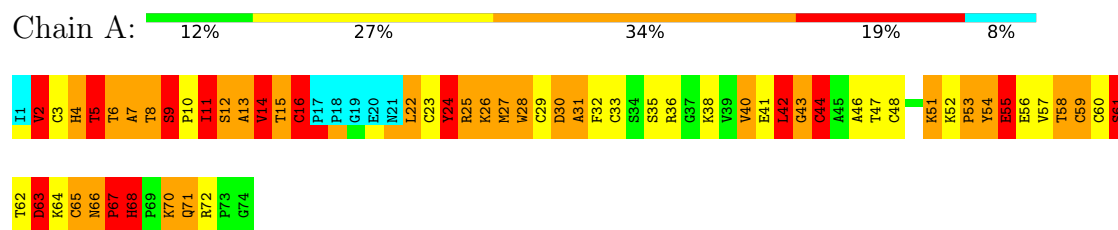
4.2.8 Score per residue for model 8

- Molecule 1: long neurotoxin 1



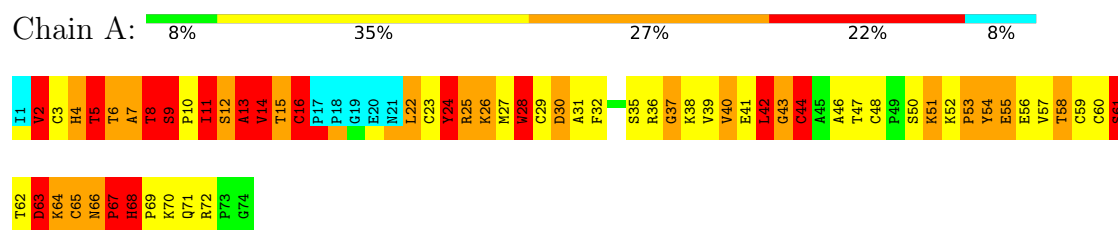
4.2.9 Score per residue for model 9

- Molecule 1: long neurotoxin 1



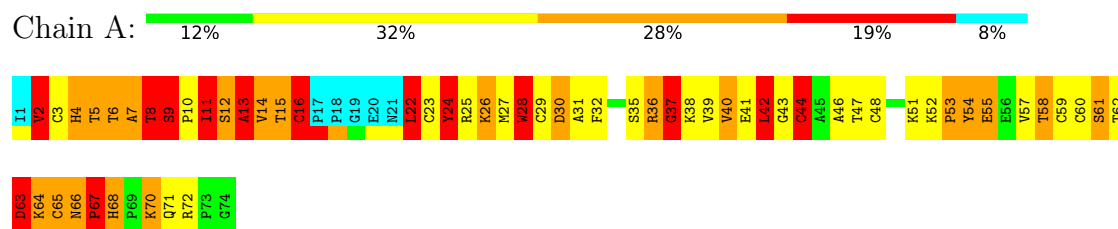
4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: long neurotoxin 1



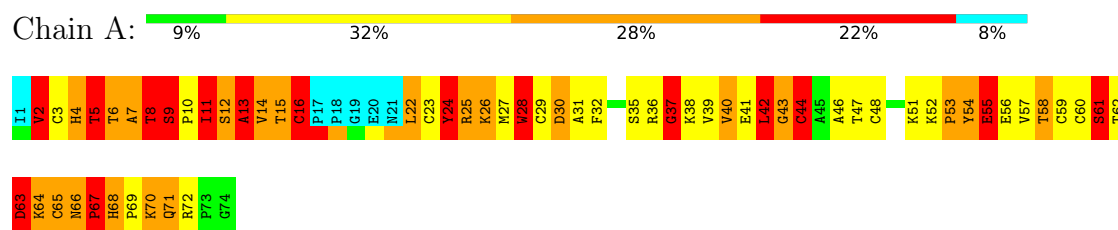
4.2.11 Score per residue for model 11

- Molecule 1: long neurotoxin 1



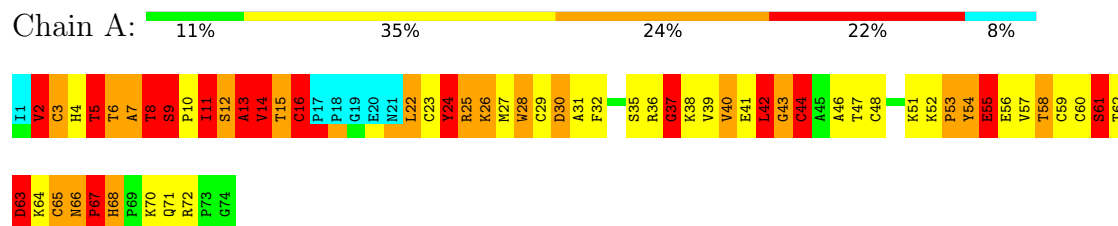
4.2.12 Score per residue for model 12

- Molecule 1: long neurotoxin 1



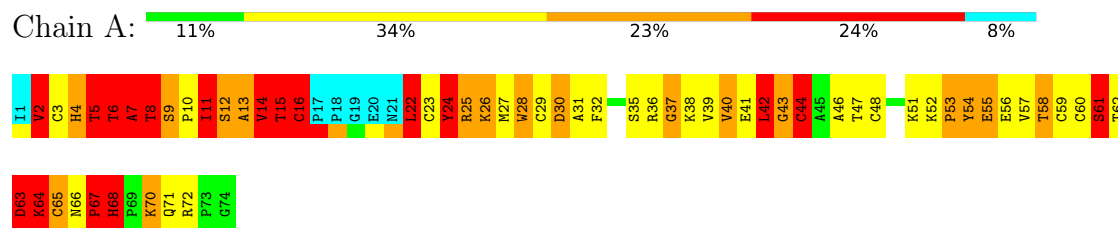
4.2.13 Score per residue for model 13

- Molecule 1: long neurotoxin 1



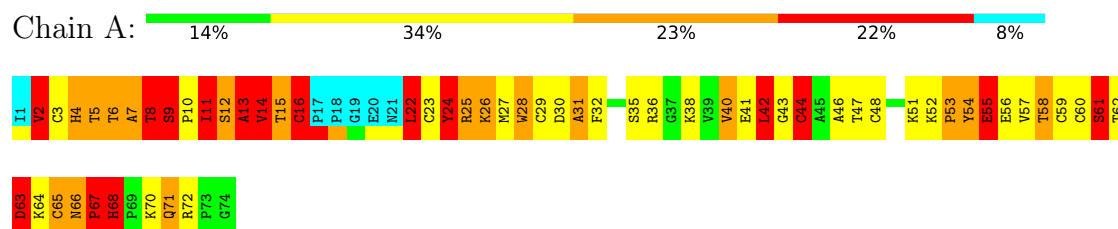
4.2.14 Score per residue for model 14

- Molecule 1: long neurotoxin 1



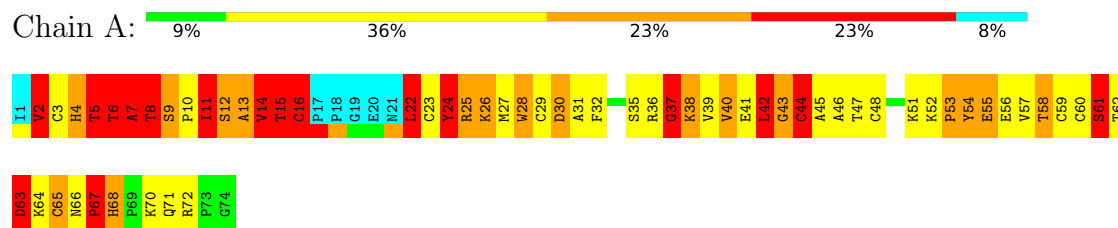
4.2.15 Score per residue for model 15

- Molecule 1: long neurotoxin 1



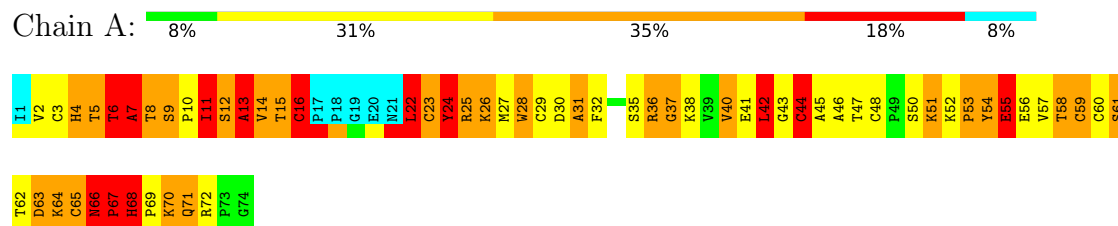
4.2.16 Score per residue for model 16

- Molecule 1: long neurotoxin 1



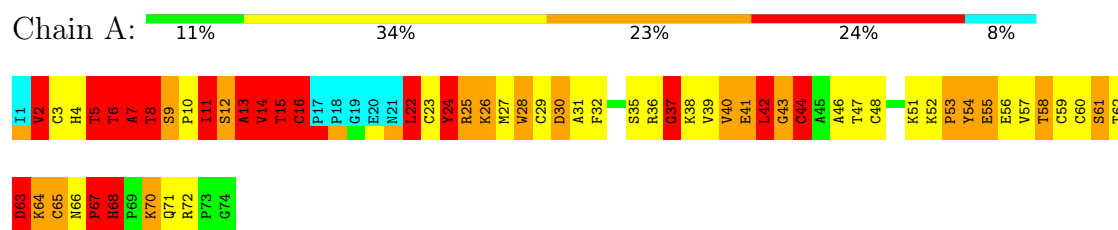
4.2.17 Score per residue for model 17

- Molecule 1: long neurotoxin 1



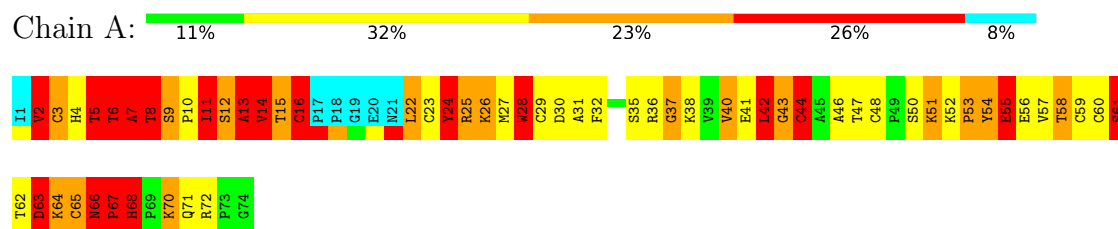
4.2.18 Score per residue for model 18

- Molecule 1: long neurotoxin 1



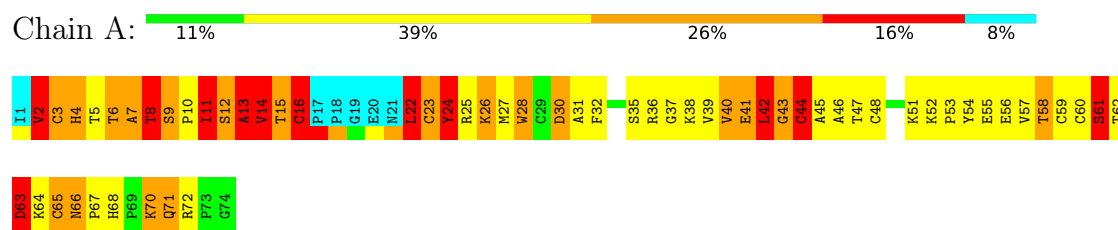
4.2.19 Score per residue for model 19

- Molecule 1: long neurotoxin 1



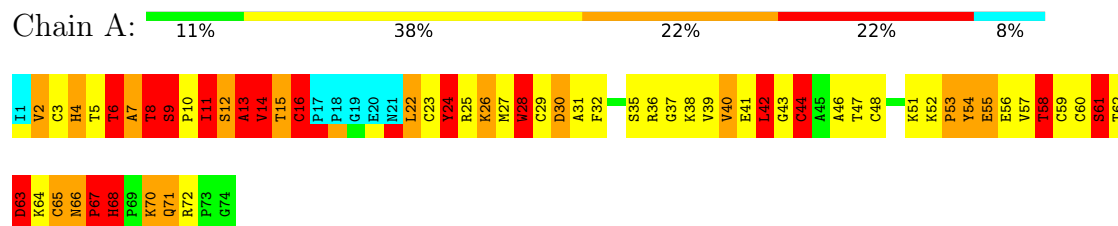
4.2.20 Score per residue for model 20

- Molecule 1: long neurotoxin 1



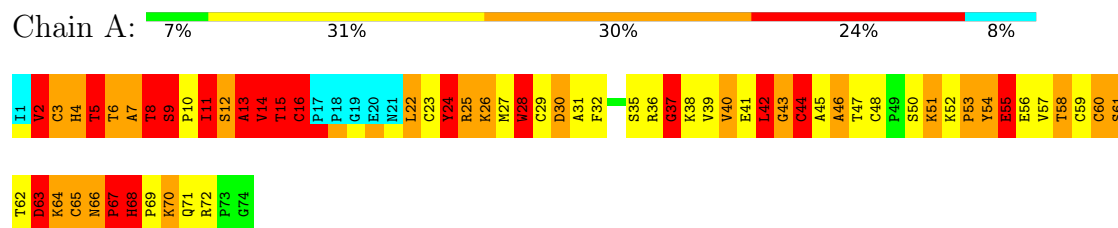
4.2.21 Score per residue for model 21

- Molecule 1: long neurotoxin 1



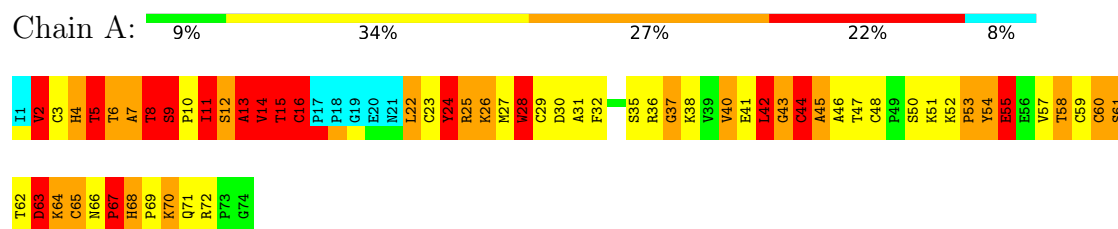
4.2.22 Score per residue for model 22

- Molecule 1: long neurotoxin 1



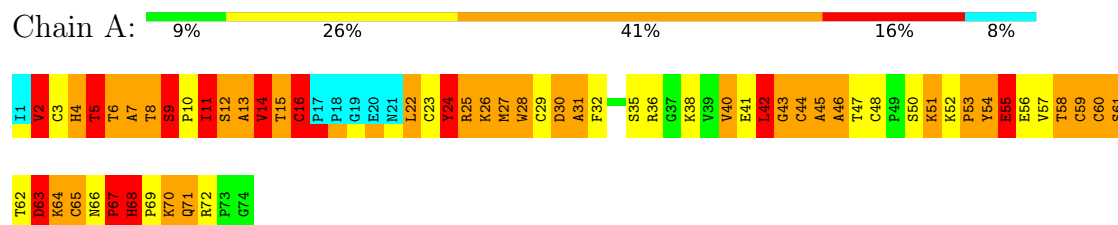
4.2.23 Score per residue for model 23

- Molecule 1: long neurotoxin 1



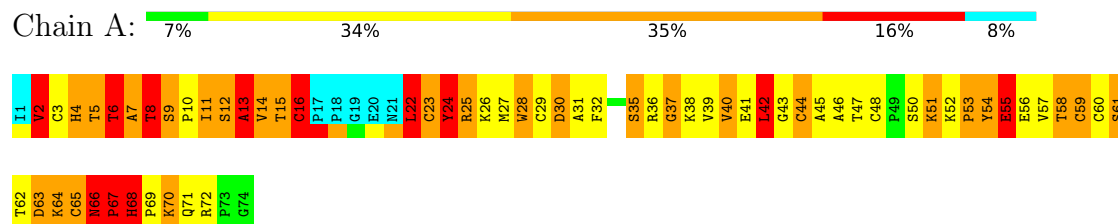
4.2.24 Score per residue for model 24

- Molecule 1: long neurotoxin 1



4.2.25 Score per residue for model 25

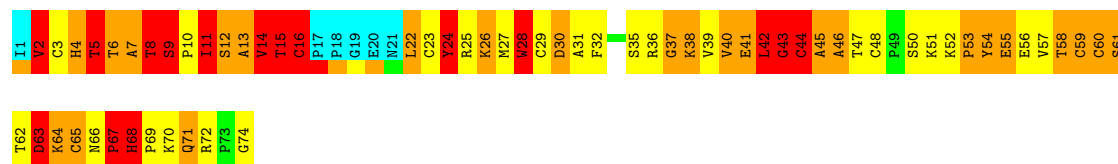
- Molecule 1: long neurotoxin 1



4.2.26 Score per residue for model 26

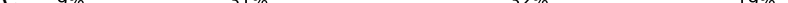
- Molecule 1: long neurotoxin 1

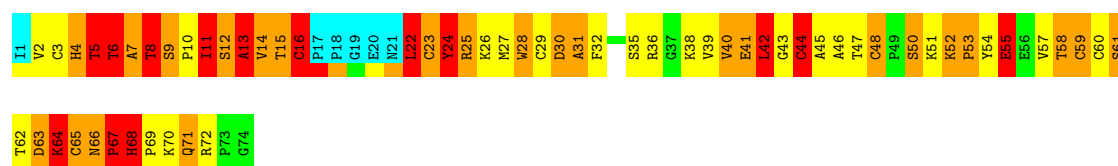
Chain A: 5% 32% 32% 22% 8%



4.2.27 Score per residue for model 27

- Molecule 1: long neurotoxin 1

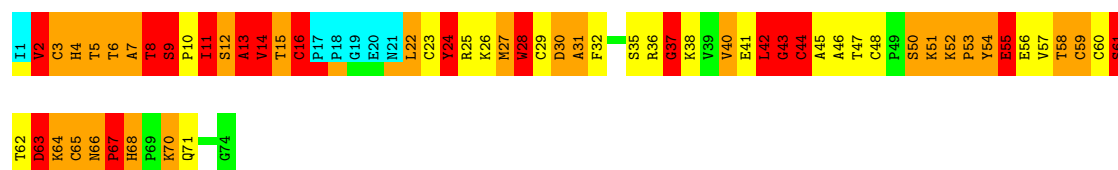
Chain A: 



4.2.28 Score per residue for model 28

- Molecule 1: long neurotoxin 1

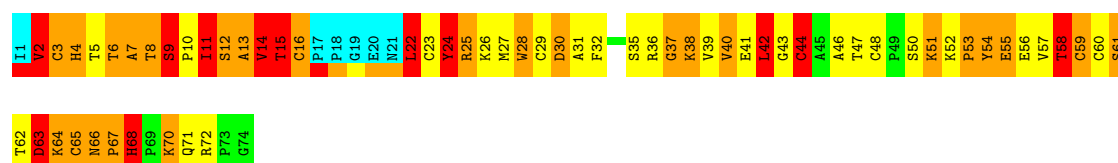
Chain A:



4.2.29 Score per residue for model 29

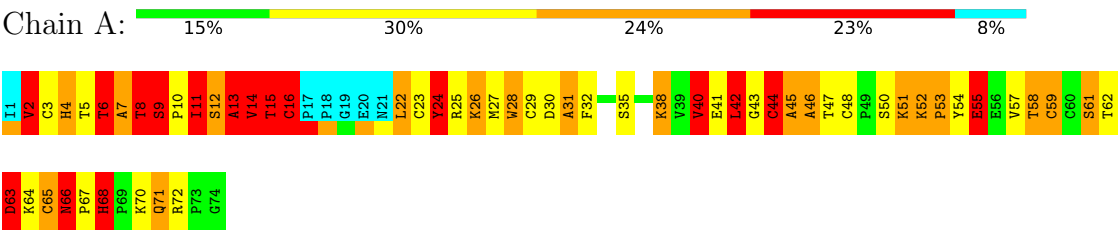
- Molecule 1: long neurotoxin 1

Chain A:



4.2.30 Score per residue for model 30

- Molecule 1: long neurotoxin 1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 30 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
DIANA	structure solution	1.5
Amber	refinement	4.1

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	1.38±0.18	6±3/520 (1.2± 0.6%)	2.43±0.32	31±5/705 (4.5± 0.8%)
All	All	1.40	188/15600 (1.2%)	2.45	942/21150 (4.5%)

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	0.0±0.0	2.9±0.9
All	All	0	86

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	68	HIS	CG-CD2	-22.62	1.10	1.35	15	4
1	A	68	HIS	CD2-NE2	-16.48	1.19	1.37	27	23
1	A	68	HIS	CG-ND1	-15.46	1.21	1.38	15	26
1	A	71	GLN	CD-NE2	-12.93	1.06	1.33	15	1
1	A	68	HIS	CB-CG	11.81	1.66	1.50	15	2
1	A	68	HIS	ND1-CE1	11.70	1.44	1.32	7	15
1	A	68	HIS	CE1-NE2	-11.05	1.21	1.32	24	4
1	A	15	THR	C-O	10.66	1.37	1.24	30	3
1	A	6	THR	C-O	9.27	1.33	1.23	2	2
1	A	5	THR	CB-OG1	-9.26	1.28	1.43	3	9
1	A	71	GLN	CD-OE1	-8.79	1.06	1.23	27	3
1	A	14	VAL	C-O	-8.48	1.14	1.24	28	3
1	A	5	THR	C-N	8.33	1.45	1.33	17	1
1	A	3	CYS	C-O	-8.25	1.13	1.23	20	1
1	A	24	TYR	C-O	-8.14	1.14	1.24	18	3
1	A	15	THR	C-N	-8.12	1.16	1.33	30	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	5	THR	C-O	7.96	1.32	1.24	18	3
1	A	28	TRP	CE2-CZ2	-7.82	1.23	1.39	21	2
1	A	14	VAL	C-N	7.76	1.44	1.33	28	3
1	A	5	THR	CA-C	-7.70	1.44	1.53	17	2
1	A	6	THR	C-N	-7.54	1.23	1.33	21	2
1	A	11	ILE	C-N	-7.29	1.23	1.33	18	3
1	A	6	THR	N-CA	7.15	1.55	1.46	4	9
1	A	2	VAL	N-CA	7.15	1.55	1.46	30	1
1	A	28	TRP	NE1-CE2	-7.07	1.29	1.37	26	10
1	A	64	LYS	CE-NZ	-6.68	1.29	1.49	23	4
1	A	4	HIS	CG-ND1	-6.59	1.31	1.38	16	20
1	A	28	TRP	CD1-NE1	-6.53	1.24	1.37	28	2
1	A	11	ILE	C-O	6.53	1.31	1.24	2	3
1	A	2	VAL	C-O	-6.23	1.16	1.24	20	1
1	A	28	TRP	CD2-CE2	-6.16	1.30	1.41	11	2
1	A	16	CYS	CA-CB	-6.01	1.44	1.53	30	1
1	A	71	GLN	C-N	-5.93	1.21	1.33	20	1
1	A	28	TRP	CG-CD2	-5.91	1.33	1.43	28	2
1	A	3	CYS	C-N	-5.68	1.26	1.33	28	1
1	A	4	HIS	CD2-NE2	-5.64	1.31	1.37	25	1
1	A	63	ASP	C-O	-5.64	1.16	1.24	28	1
1	A	40	VAL	C-O	-5.56	1.17	1.24	20	1
1	A	6	THR	CB-OG1	-5.41	1.35	1.43	21	2
1	A	13	ALA	C-O	-5.35	1.17	1.24	21	1
1	A	58	THR	C-O	-5.31	1.17	1.24	21	1
1	A	42	LEU	C-O	-5.29	1.17	1.24	20	2
1	A	30	ASP	C-O	-5.24	1.17	1.24	28	1
1	A	36	ARG	CA-C	5.22	1.57	1.53	11	1
1	A	40	VAL	C-N	-5.14	1.26	1.33	18	1
1	A	26	LYS	C-O	-5.09	1.17	1.23	21	1
1	A	41	GLU	C-O	-5.08	1.17	1.24	18	1
1	A	66	ASN	CG-OD1	-5.02	1.14	1.23	30	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	68	HIS	CG-CD2-NE2	40.94	148.14	107.20	15	7
1	A	68	HIS	ND1-CG-CD2	-32.38	73.72	106.10	24	15
1	A	68	HIS	CE1-NE2-CD2	-28.79	80.21	109.00	15	14
1	A	5	THR	OG1-CB-CG2	-27.59	54.11	109.30	7	22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	68	HIS	CB-CG-ND1	20.17	152.96	122.70	27	6
1	A	71	GLN	OE1-CD-NE2	-18.28	104.32	122.60	20	11
1	A	5	THR	CA-C-O	-16.28	103.70	120.80	17	6
1	A	66	ASN	N-CA-CB	-13.97	85.50	110.37	20	5
1	A	6	THR	CA-CB-CG2	13.69	133.77	110.50	21	9
1	A	5	THR	CA-CB-CG2	13.28	133.07	110.50	25	9
1	A	5	THR	CA-C-N	12.60	145.61	121.54	18	5
1	A	5	THR	C-N-CA	12.60	145.61	121.54	18	5
1	A	71	GLN	CG-CD-OE1	11.41	143.62	120.80	24	5
1	A	4	HIS	CA-CB-CG	11.15	124.95	113.80	29	7
1	A	5	THR	CA-CB-OG1	10.91	125.96	109.60	27	6
1	A	44	CYS	N-CA-CB	10.36	128.00	110.49	1	8
1	A	51	LYS	CB-CA-C	-10.13	104.88	116.63	30	1
1	A	24	TYR	O-C-N	-10.05	109.23	122.59	25	16
1	A	6	THR	N-CA-C	-9.08	96.41	109.31	2	22
1	A	6	THR	CA-C-O	-9.07	111.20	119.91	21	2
1	A	14	VAL	O-C-N	9.02	133.84	122.57	29	30
1	A	71	GLN	CG-CD-NE2	-8.99	102.91	116.40	24	4
1	A	30	ASP	CA-CB-CG	8.94	121.54	112.60	1	2
1	A	2	VAL	CA-CB-CG1	8.86	125.45	110.40	25	9
1	A	16	CYS	N-CA-CB	-8.81	94.68	110.37	17	17
1	A	24	TYR	CA-C-N	-8.66	111.26	122.77	18	15
1	A	24	TYR	C-N-CA	-8.66	111.26	122.77	18	15
1	A	68	HIS	CG-ND1-CE1	8.57	123.87	109.30	24	8
1	A	2	VAL	CG1-CB-CG2	8.53	129.56	110.80	10	9
1	A	68	HIS	ND1-CE1-NE2	8.47	116.87	108.40	22	13
1	A	16	CYS	CA-CB-SG	8.37	133.64	114.40	30	4
1	A	68	HIS	CA-CB-CG	-8.32	105.48	113.80	15	5
1	A	6	THR	CB-CA-C	-8.29	104.03	114.40	21	1
1	A	40	VAL	CG1-CB-CG2	-8.24	92.68	110.80	9	29
1	A	5	THR	N-CA-CB	8.19	124.33	110.49	25	6
1	A	15	THR	CA-CB-CG2	-8.11	96.72	110.50	30	3
1	A	67	PRO	CB-CA-C	8.04	124.82	111.56	27	25
1	A	64	LYS	CB-CG-CD	-8.00	92.90	111.30	27	10
1	A	5	THR	O-C-N	7.99	136.39	121.70	19	15
1	A	6	THR	CA-CB-OG1	7.91	121.47	109.60	27	26
1	A	42	LEU	CD1-CG-CD2	-7.82	93.61	110.80	18	16
1	A	14	VAL	CA-C-O	-7.76	111.08	120.78	9	21
1	A	44	CYS	CB-CA-C	-7.75	95.01	110.42	1	3
1	A	25	ARG	CB-CA-C	7.67	122.34	109.84	25	22
1	A	66	ASN	OD1-CG-ND2	-7.66	114.94	122.60	30	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	3	CYS	CA-CB-SG	7.60	131.88	114.40	29	1
1	A	37	GLY	O-C-N	7.51	132.46	122.70	10	20
1	A	11	ILE	CA-CB-CG2	7.36	123.01	110.50	11	27
1	A	63	ASP	CA-CB-CG	7.34	119.94	112.60	1	26
1	A	51	LYS	CG-CD-CE	-7.22	94.70	111.30	28	1
1	A	15	THR	CA-CB-OG1	7.20	120.40	109.60	14	5
1	A	40	VAL	CB-CA-C	7.15	123.02	111.29	30	1
1	A	26	LYS	CG-CD-CE	7.03	127.46	111.30	6	18
1	A	4	HIS	CB-CG-CD2	-6.98	122.12	131.20	21	3
1	A	24	TYR	CA-C-O	6.97	128.33	120.80	9	5
1	A	13	ALA	CA-C-O	-6.91	110.64	120.51	17	16
1	A	43	GLY	O-C-N	6.90	131.67	122.70	24	6
1	A	61	SER	CA-CB-OG	6.88	124.87	111.10	9	17
1	A	3	CYS	N-CA-CB	-6.88	100.26	110.17	13	2
1	A	66	ASN	CA-CB-CG	6.87	119.47	112.60	20	3
1	A	26	LYS	CA-C-O	-6.82	113.46	121.44	30	13
1	A	64	LYS	CD-CE-NZ	6.81	133.70	111.90	23	8
1	A	66	ASN	CB-CG-OD1	-6.64	107.51	120.80	30	12
1	A	9	SER	CA-C-N	6.64	126.23	119.19	5	1
1	A	9	SER	C-N-CA	6.64	126.23	119.19	5	1
1	A	44	CYS	CA-CB-SG	-6.63	99.16	114.40	22	14
1	A	51	LYS	CA-CB-CG	6.62	127.34	114.10	30	1
1	A	71	GLN	CA-C-N	6.58	137.87	121.80	20	1
1	A	71	GLN	C-N-CA	6.58	137.87	121.80	20	1
1	A	16	CYS	CA-C-O	-6.57	111.17	120.16	30	2
1	A	66	ASN	CB-CG-ND2	6.54	126.22	116.40	20	11
1	A	63	ASP	CA-C-O	-6.46	111.28	120.51	11	5
1	A	60	CYS	CA-C-O	-6.43	113.96	120.77	22	4
1	A	4	HIS	CG-CD2-NE2	6.43	113.63	107.20	25	1
1	A	23	CYS	N-CA-C	6.42	117.96	107.23	1	3
1	A	68	HIS	CB-CG-CD2	-6.42	122.86	131.20	18	7
1	A	7	ALA	N-CA-CB	6.42	121.33	110.49	16	5
1	A	13	ALA	N-CA-CB	6.29	121.11	110.49	2	23
1	A	24	TYR	CG-CD1-CE1	6.27	130.60	121.20	11	4
1	A	71	GLN	CB-CG-CD	-6.25	101.98	112.60	27	3
1	A	6	THR	N-CA-CB	6.21	120.98	110.49	18	2
1	A	5	THR	CB-CA-C	-6.20	98.98	114.11	19	10
1	A	27	MET	CA-CB-CG	-6.15	101.79	114.10	28	3
1	A	28	TRP	NE1-CE2-CD2	-6.14	99.42	107.40	21	2
1	A	24	TYR	CB-CA-C	6.12	118.56	110.06	28	2
1	A	58	THR	CA-CB-CG2	6.10	120.87	110.50	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	6	THR	O-C-N	-5.89	114.75	122.59	17	5
1	A	38	LYS	CA-C-O	5.88	125.62	119.51	30	4
1	A	36	ARG	CD-NE-CZ	5.86	132.61	124.40	17	1
1	A	67	PRO	N-CA-CB	5.83	109.37	103.25	27	4
1	A	67	PRO	O-C-N	5.81	130.49	122.64	27	1
1	A	63	ASP	N-CA-CB	5.80	120.29	110.49	29	1
1	A	64	LYS	CG-CD-CE	-5.78	98.02	111.30	27	8
1	A	11	ILE	CA-CB-CG1	-5.76	100.61	110.40	19	5
1	A	53	PRO	CA-N-CD	-5.74	103.97	112.00	30	1
1	A	9	SER	O-C-N	-5.71	114.75	121.32	21	2
1	A	53	PRO	N-CD-CG	5.71	111.77	103.20	27	2
1	A	28	TRP	CE2-CD2-CE3	5.71	124.51	118.80	4	3
1	A	64	LYS	O-C-N	5.70	128.54	123.41	11	2
1	A	8	THR	CA-CB-CG2	5.69	120.17	110.50	2	25
1	A	41	GLU	CA-C-O	-5.66	112.41	120.51	26	1
1	A	42	LEU	O-C-N	5.56	129.98	122.59	5	2
1	A	32	PHE	CA-CB-CG	-5.52	108.28	113.80	11	28
1	A	9	SER	CA-CB-OG	5.51	122.12	111.10	23	20
1	A	16	CYS	CB-CA-C	5.50	121.00	110.17	26	2
1	A	22	LEU	CB-CG-CD1	5.38	126.85	110.70	7	5
1	A	26	LYS	CA-CB-CG	-5.38	103.33	114.10	7	8
1	A	37	GLY	CA-C-N	5.35	130.59	122.08	28	3
1	A	37	GLY	C-N-CA	5.35	130.59	122.08	28	3
1	A	64	LYS	CB-CA-C	-5.28	100.95	110.03	11	3
1	A	51	LYS	CB-CG-CD	-5.22	99.29	111.30	29	2
1	A	2	VAL	CA-CB-CG2	5.21	119.26	110.40	19	1
1	A	4	HIS	CB-CG-ND1	5.20	130.50	122.70	21	1
1	A	4	HIS	CE1-NE2-CD2	-5.19	103.81	109.00	25	1
1	A	66	ASN	CB-CA-C	5.18	120.37	110.17	20	3
1	A	41	GLU	O-C-N	5.17	128.44	122.09	20	3
1	A	6	THR	CA-C-N	5.16	131.39	121.54	21	1
1	A	6	THR	C-N-CA	5.16	131.39	121.54	21	1
1	A	13	ALA	O-C-N	5.13	129.41	122.59	27	2
1	A	3	CYS	N-CA-C	-5.11	103.29	110.50	13	2
1	A	67	PRO	CA-N-CD	-5.09	104.87	112.00	21	1
1	A	28	TRP	NE1-CE2-CZ2	5.03	137.64	130.10	21	1

There are no chirality outliers.

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	24	TYR	Sidechain,Mainchain	28
1	A	43	GLY	Mainchain,Peptide	12
1	A	68	HIS	Sidechain	10
1	A	37	GLY	Mainchain	9
1	A	6	THR	Mainchain	7
1	A	54	TYR	Sidechain	3
1	A	2	VAL	Mainchain	3
1	A	44	CYS	Mainchain	3
1	A	42	LEU	Mainchain	3
1	A	71	GLN	Mainchain	1
1	A	67	PRO	Mainchain	1
1	A	15	THR	Mainchain	1
1	A	58	THR	Mainchain	1
1	A	66	ASN	Sidechain	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	508	135	489	180±21
All	All	15240	4050	14691	5405

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 181.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:HIS:HD2	1:A:71:GLN:NE2	1.14	1.37	24	11
1:A:6:THR:HB	1:A:42:LEU:HD21	1.11	1.14	24	29
1:A:42:LEU:HD23	1:A:66:ASN:HB3	1.11	1.14	30	3
1:A:23:CYS:HA	1:A:44:CYS:SG	1.10	1.87	1	10
1:A:3:CYS:HB2	1:A:66:ASN:HD21	1.09	1.04	9	22
1:A:5:THR:HG21	1:A:67:PRO:HA	1.08	1.21	18	27
1:A:26:LYS:HE3	1:A:57:VAL:HG13	1.08	1.17	24	4
1:A:22:LEU:HG	1:A:61:SER:HB3	1.07	1.19	30	23
1:A:68:HIS:CD2	1:A:71:GLN:NE2	1.07	2.22	24	14
1:A:22:LEU:HD23	1:A:23:CYS:H	1.06	1.07	27	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:CYS:HB2	1:A:66:ASN:ND2	1.04	1.67	11	24
1:A:2:VAL:N	1:A:15:THR:HG21	1.04	1.67	30	10
1:A:50:SER:HA	1:A:59:CYS:SG	1.04	1.92	27	4
1:A:2:VAL:HG21	1:A:16:CYS:SG	1.04	1.93	17	3
1:A:38:LYS:HA	1:A:68:HIS:CE1	1.03	1.87	22	20
1:A:5:THR:CB	1:A:64:LYS:HZ3	1.03	1.67	25	2
1:A:9:SER:HB3	1:A:10:PRO:HD2	1.02	1.31	25	28
1:A:24:TYR:CE2	1:A:51:LYS:HE3	1.01	1.89	28	1
1:A:3:CYS:HA	1:A:64:LYS:HA	1.00	1.32	25	30
1:A:36:ARG:HA	1:A:70:LYS:HZ3	1.00	1.11	25	4
1:A:51:LYS:HE3	1:A:53:PRO:HG2	0.99	1.34	27	2
1:A:27:MET:HG3	1:A:41:GLU:HG2	0.98	1.29	21	26
1:A:16:CYS:SG	1:A:23:CYS:SG	0.98	2.61	30	6
1:A:5:THR:HG22	1:A:6:THR:H	0.98	1.16	14	6
1:A:4:HIS:HD2	1:A:13:ALA:HB1	0.96	1.11	25	27
1:A:5:THR:HG21	1:A:67:PRO:CA	0.96	1.90	24	26
1:A:2:VAL:H	1:A:15:THR:HB	0.96	1.21	29	17
1:A:6:THR:HB	1:A:42:LEU:CD2	0.96	1.90	24	30
1:A:6:THR:HG23	1:A:9:SER:O	0.96	1.60	30	28
1:A:42:LEU:HB2	1:A:66:ASN:HD22	0.95	1.19	20	3
1:A:5:THR:CG2	1:A:67:PRO:HA	0.95	1.91	24	27
1:A:38:LYS:HZ3	1:A:72:ARG:HE	0.94	1.00	24	4
1:A:38:LYS:HD2	1:A:71:GLN:HA	0.94	1.34	27	8
1:A:4:HIS:H	1:A:64:LYS:HG3	0.94	1.19	24	21
1:A:14:VAL:O	1:A:15:THR:HB	0.93	1.64	16	10
1:A:38:LYS:HA	1:A:68:HIS:NE2	0.93	1.78	28	20
1:A:4:HIS:CD2	1:A:13:ALA:HB1	0.93	1.96	25	29
1:A:24:TYR:CD2	1:A:44:CYS:HA	0.93	1.99	5	2
1:A:2:VAL:HG13	1:A:3:CYS:H	0.92	1.25	30	5
1:A:36:ARG:HA	1:A:70:LYS:NZ	0.92	1.79	25	4
1:A:54:TYR:CE2	1:A:55:GLU:HB2	0.92	1.99	24	26
1:A:25:ARG:HD3	1:A:66:ASN:HA	0.91	1.42	29	28
1:A:42:LEU:O	1:A:42:LEU:HD22	0.91	1.66	24	7
1:A:22:LEU:HG	1:A:61:SER:CB	0.91	1.95	30	20
1:A:2:VAL:HG11	1:A:22:LEU:C	0.90	1.92	30	15
1:A:42:LEU:HD22	1:A:42:LEU:O	0.90	1.67	9	21
1:A:42:LEU:HD23	1:A:66:ASN:CB	0.90	1.96	30	28
1:A:26:LYS:HG3	1:A:57:VAL:HG22	0.90	1.43	9	26
1:A:3:CYS:O	1:A:15:THR:HA	0.89	1.67	29	29
1:A:24:TYR:CE2	1:A:51:LYS:HD2	0.89	2.02	29	24
1:A:22:LEU:HA	1:A:61:SER:HA	0.89	1.44	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:LEU:HD21	1:A:48:CYS:HB2	0.89	1.43	25	3
1:A:27:MET:HB3	1:A:40:VAL:HA	0.89	1.44	30	6
1:A:4:HIS:H	1:A:64:LYS:HG2	0.89	1.28	11	7
1:A:42:LEU:HB2	1:A:66:ASN:ND2	0.88	1.82	20	3
1:A:26:LYS:NZ	1:A:51:LYS:HE2	0.88	1.84	27	1
1:A:5:THR:HB	1:A:64:LYS:NZ	0.88	1.84	17	2
1:A:2:VAL:HG11	1:A:61:SER:HA	0.88	1.40	29	1
1:A:24:TYR:H	1:A:44:CYS:HB2	0.88	1.29	26	17
1:A:11:ILE:HG22	1:A:12:SER:H	0.87	1.30	25	28
1:A:28:TRP:HA	1:A:40:VAL:HG22	0.87	1.47	13	27
1:A:24:TYR:CD2	1:A:26:LYS:HE3	0.87	2.02	30	1
1:A:26:LYS:HD2	1:A:51:LYS:HD3	0.87	1.46	28	4
1:A:23:CYS:HA	1:A:44:CYS:HB2	0.87	1.43	25	20
1:A:24:TYR:HA	1:A:48:CYS:SG	0.86	2.09	27	22
1:A:42:LEU:HB2	1:A:66:ASN:HB2	0.86	1.46	27	27
1:A:2:VAL:HG23	1:A:3:CYS:H	0.86	1.31	17	3
1:A:24:TYR:O	1:A:42:LEU:HA	0.86	1.71	27	30
1:A:25:ARG:HG3	1:A:42:LEU:HB3	0.86	1.45	24	28
1:A:6:THR:C	1:A:11:ILE:HG13	0.85	1.95	1	6
1:A:5:THR:CB	1:A:64:LYS:NZ	0.85	2.38	25	2
1:A:4:HIS:N	1:A:64:LYS:HG2	0.85	1.86	15	7
1:A:26:LYS:HD3	1:A:51:LYS:HZ3	0.84	1.31	10	11
1:A:52:LYS:N	1:A:57:VAL:HG11	0.84	1.87	28	3
1:A:26:LYS:HD3	1:A:51:LYS:NZ	0.84	1.86	10	20
1:A:22:LEU:CA	1:A:61:SER:HA	0.83	2.02	25	3
1:A:36:ARG:HG2	1:A:37:GLY:H	0.83	1.30	14	3
1:A:7:ALA:HA	1:A:43:GLY:HA2	0.83	1.50	23	30
1:A:24:TYR:O	1:A:24:TYR:CD1	0.83	2.31	25	21
1:A:15:THR:HG22	1:A:15:THR:O	0.83	1.72	24	3
1:A:6:THR:HG22	1:A:7:ALA:H	0.83	1.32	24	28
1:A:9:SER:HB3	1:A:10:PRO:CD	0.83	2.04	24	28
1:A:15:THR:O	1:A:15:THR:HG22	0.82	1.71	22	7
1:A:7:ALA:HA	1:A:42:LEU:O	0.82	1.74	20	30
1:A:38:LYS:NZ	1:A:72:ARG:HB2	0.82	1.90	13	4
1:A:38:LYS:NZ	1:A:72:ARG:HE	0.82	1.73	23	4
1:A:68:HIS:HB3	1:A:71:GLN:NE2	0.81	1.91	3	18
1:A:25:ARG:HB3	1:A:58:THR:CG2	0.81	2.05	21	28
1:A:26:LYS:HZ1	1:A:51:LYS:HB2	0.81	1.36	30	1
1:A:5:THR:HG22	1:A:68:HIS:CE1	0.81	2.11	27	5
1:A:36:ARG:HH11	1:A:70:LYS:NZ	0.80	1.74	17	1
1:A:15:THR:O	1:A:16:CYS:HB2	0.80	1.75	29	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LYS:HE3	1:A:71:GLN:OE1	0.80	1.77	12	25
1:A:23:CYS:SG	1:A:66:ASN:OD1	0.80	2.40	30	5
1:A:42:LEU:CD2	1:A:66:ASN:HB3	0.80	2.05	30	3
1:A:27:MET:HG3	1:A:41:GLU:CG	0.80	2.06	28	26
1:A:2:VAL:HG23	1:A:15:THR:HG23	0.80	1.53	28	2
1:A:25:ARG:HB2	1:A:66:ASN:ND2	0.80	1.92	21	3
1:A:3:CYS:HA	1:A:64:LYS:CA	0.80	2.07	25	16
1:A:24:TYR:N	1:A:44:CYS:HB2	0.80	1.91	26	17
1:A:3:CYS:HB2	1:A:66:ASN:OD1	0.79	1.76	18	3
1:A:6:THR:CB	1:A:42:LEU:HD21	0.79	2.08	9	28
1:A:40:VAL:HG22	1:A:42:LEU:HD12	0.79	1.51	30	1
1:A:22:LEU:HD23	1:A:23:CYS:N	0.79	1.92	27	10
1:A:68:HIS:HB3	1:A:71:GLN:HE21	0.79	1.38	11	12
1:A:2:VAL:HG11	1:A:22:LEU:O	0.79	1.76	20	18
1:A:7:ALA:CB	1:A:43:GLY:HA2	0.78	2.08	9	30
1:A:26:LYS:NZ	1:A:51:LYS:HB2	0.78	1.94	30	1
1:A:68:HIS:HD2	1:A:71:GLN:HE22	0.78	1.19	24	3
1:A:42:LEU:HD23	1:A:66:ASN:HD22	0.78	1.37	18	3
1:A:5:THR:HB	1:A:66:ASN:ND2	0.78	1.94	16	4
1:A:38:LYS:HZ3	1:A:72:ARG:NE	0.77	1.78	24	2
1:A:22:LEU:HG	1:A:60:CYS:O	0.77	1.80	23	10
1:A:29:CYS:HB3	1:A:55:GLU:CD	0.77	2.04	24	23
1:A:40:VAL:HG12	1:A:42:LEU:HD12	0.77	1.53	20	27
1:A:2:VAL:HG23	1:A:3:CYS:N	0.77	1.94	17	3
1:A:24:TYR:CD2	1:A:51:LYS:HD2	0.77	2.14	24	24
1:A:27:MET:SD	1:A:41:GLU:HG2	0.76	2.21	27	1
1:A:55:GLU:OE2	1:A:56:GLU:HG2	0.75	1.81	21	18
1:A:36:ARG:HD2	1:A:70:LYS:HZ3	0.75	1.42	11	3
1:A:42:LEU:HD23	1:A:66:ASN:ND2	0.75	1.97	18	3
1:A:25:ARG:C	1:A:26:LYS:HD2	0.74	2.07	24	4
1:A:2:VAL:HG21	1:A:22:LEU:CA	0.74	2.12	7	18
1:A:36:ARG:HG2	1:A:37:GLY:N	0.74	1.94	14	3
1:A:24:TYR:CD1	1:A:24:TYR:O	0.74	2.41	9	9
1:A:27:MET:O	1:A:40:VAL:HG13	0.74	1.83	9	27
1:A:25:ARG:CD	1:A:66:ASN:HA	0.73	2.12	30	29
1:A:24:TYR:CD2	1:A:51:LYS:HE3	0.73	2.18	28	1
1:A:38:LYS:HZ1	1:A:71:GLN:NE2	0.73	1.81	20	1
1:A:2:VAL:H	1:A:15:THR:CG2	0.73	1.96	20	16
1:A:63:ASP:O	1:A:64:LYS:HG3	0.73	1.83	28	7
1:A:5:THR:CG2	1:A:6:THR:H	0.73	1.94	17	6
1:A:23:CYS:CA	1:A:44:CYS:HB2	0.73	2.13	24	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LYS:HG3	1:A:71:GLN:OE1	0.73	1.82	30	1
1:A:2:VAL:HG13	1:A:15:THR:HG23	0.73	1.59	14	6
1:A:68:HIS:CE1	1:A:71:GLN:HE22	0.73	2.01	30	2
1:A:24:TYR:HE2	1:A:51:LYS:HE3	0.72	1.40	28	1
1:A:15:THR:O	1:A:16:CYS:SG	0.72	2.47	24	24
1:A:23:CYS:HA	1:A:44:CYS:CB	0.72	2.14	24	17
1:A:4:HIS:H	1:A:64:LYS:CG	0.71	1.98	25	21
1:A:2:VAL:HG22	1:A:3:CYS:N	0.71	1.99	7	17
1:A:7:ALA:CA	1:A:43:GLY:HA2	0.71	2.16	24	30
1:A:16:CYS:HB3	1:A:43:GLY:O	0.71	1.85	22	2
1:A:64:LYS:HZ1	1:A:66:ASN:HD22	0.71	1.28	17	2
1:A:38:LYS:HE2	1:A:72:ARG:HG2	0.71	1.60	30	2
1:A:16:CYS:SG	1:A:44:CYS:N	0.70	2.63	30	3
1:A:40:VAL:HG12	1:A:41:GLU:H	0.70	1.46	9	25
1:A:36:ARG:HB3	1:A:70:LYS:HZ2	0.70	1.45	27	4
1:A:5:THR:OG1	1:A:67:PRO:HA	0.70	1.86	3	15
1:A:42:LEU:HD23	1:A:66:ASN:HB2	0.70	1.61	9	25
1:A:23:CYS:SG	1:A:44:CYS:SG	0.70	2.89	17	7
1:A:52:LYS:O	1:A:57:VAL:HG21	0.70	1.87	23	25
1:A:22:LEU:HG	1:A:61:SER:HB2	0.70	1.61	24	4
1:A:2:VAL:N	1:A:15:THR:CG2	0.70	2.52	30	10
1:A:23:CYS:CA	1:A:44:CYS:SG	0.70	2.77	1	8
1:A:36:ARG:CZ	1:A:70:LYS:NZ	0.70	2.55	7	5
1:A:38:LYS:CD	1:A:71:GLN:HA	0.70	2.14	27	9
1:A:6:THR:CG2	1:A:42:LEU:HD11	0.69	2.16	20	25
1:A:38:LYS:HD2	1:A:71:GLN:CA	0.69	2.16	27	7
1:A:68:HIS:CD2	1:A:71:GLN:HE22	0.69	2.05	9	5
1:A:6:THR:CB	1:A:42:LEU:HD11	0.69	2.18	20	2
1:A:2:VAL:HG13	1:A:3:CYS:N	0.69	2.03	30	5
1:A:5:THR:O	1:A:11:ILE:HB	0.69	1.87	24	21
1:A:5:THR:HG22	1:A:6:THR:N	0.69	1.97	16	26
1:A:8:THR:O	1:A:9:SER:HB2	0.69	1.85	24	28
1:A:36:ARG:CZ	1:A:70:LYS:HZ1	0.69	2.00	23	5
1:A:25:ARG:HG3	1:A:42:LEU:CB	0.69	2.17	21	25
1:A:64:LYS:HZ1	1:A:66:ASN:ND2	0.69	1.86	25	2
1:A:22:LEU:O	1:A:23:CYS:HB2	0.69	1.86	25	3
1:A:23:CYS:HA	1:A:44:CYS:HB3	0.69	1.64	22	1
1:A:36:ARG:HG3	1:A:70:LYS:HZ2	0.68	1.47	14	1
1:A:22:LEU:CD2	1:A:48:CYS:HB2	0.68	2.17	17	8
1:A:52:LYS:H	1:A:57:VAL:HG11	0.68	1.48	30	3
1:A:36:ARG:C	1:A:70:LYS:HZ2	0.68	1.96	21	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ARG:O	1:A:26:LYS:HD2	0.68	1.87	24	4
1:A:24:TYR:H	1:A:44:CYS:HB3	0.68	1.49	5	1
1:A:36:ARG:CB	1:A:70:LYS:HZ2	0.68	2.01	27	2
1:A:26:LYS:HZ3	1:A:51:LYS:HD3	0.68	1.48	30	1
1:A:3:CYS:CB	1:A:66:ASN:HD21	0.68	1.98	27	3
1:A:24:TYR:CD1	1:A:51:LYS:HE2	0.67	2.24	1	2
1:A:22:LEU:HD22	1:A:48:CYS:HB2	0.67	1.65	22	4
1:A:2:VAL:HB	1:A:22:LEU:H	0.67	1.49	7	10
1:A:3:CYS:CA	1:A:64:LYS:HA	0.67	2.17	25	4
1:A:25:ARG:HB3	1:A:58:THR:HG22	0.67	1.64	5	3
1:A:2:VAL:HG21	1:A:22:LEU:HA	0.67	1.66	24	12
1:A:38:LYS:NZ	1:A:71:GLN:NE2	0.67	2.43	20	1
1:A:27:MET:C	1:A:40:VAL:HG13	0.67	2.15	28	26
1:A:64:LYS:NZ	1:A:66:ASN:ND2	0.67	2.43	17	2
1:A:25:ARG:NE	1:A:58:THR:HG21	0.67	2.04	9	25
1:A:4:HIS:N	1:A:64:LYS:HG3	0.67	2.02	17	12
1:A:11:ILE:HD12	1:A:11:ILE:N	0.66	2.04	19	19
1:A:28:TRP:HB3	1:A:56:GLU:HG3	0.66	1.68	20	6
1:A:64:LYS:HG2	1:A:65:CYS:N	0.66	2.03	25	5
1:A:30:ASP:OD1	1:A:39:VAL:HB	0.66	1.90	20	15
1:A:27:MET:HB2	1:A:40:VAL:HA	0.66	1.67	21	25
1:A:40:VAL:CG1	1:A:42:LEU:HD12	0.66	2.19	20	23
1:A:38:LYS:HZ2	1:A:72:ARG:HG3	0.66	1.49	7	9
1:A:6:THR:HB	1:A:42:LEU:HD11	0.66	1.67	20	1
1:A:26:LYS:HD2	1:A:57:VAL:HG22	0.66	1.68	22	1
1:A:38:LYS:CE	1:A:71:GLN:HA	0.66	2.20	24	18
1:A:42:LEU:HD23	1:A:66:ASN:CG	0.66	2.16	25	26
1:A:11:ILE:CG2	1:A:12:SER:H	0.66	2.03	24	28
1:A:24:TYR:OH	1:A:41:GLU:HB3	0.66	1.91	28	27
1:A:2:VAL:HG12	1:A:3:CYS:N	0.66	2.06	9	9
1:A:36:ARG:CD	1:A:70:LYS:HZ3	0.66	2.04	11	3
1:A:36:ARG:HH11	1:A:70:LYS:HZ3	0.66	1.31	17	1
1:A:40:VAL:HG22	1:A:42:LEU:CD1	0.66	2.21	30	1
1:A:4:HIS:HA	1:A:13:ALA:O	0.66	1.90	29	15
1:A:50:SER:CA	1:A:59:CYS:SG	0.66	2.79	27	3
1:A:38:LYS:HE3	1:A:71:GLN:HA	0.65	1.67	24	17
1:A:27:MET:CB	1:A:40:VAL:HA	0.65	2.20	30	28
1:A:16:CYS:HB3	1:A:23:CYS:SG	0.65	2.31	3	8
1:A:25:ARG:HE	1:A:58:THR:HG21	0.65	1.52	3	23
1:A:25:ARG:HD3	1:A:65:CYS:O	0.65	1.91	21	24
1:A:54:TYR:CD2	1:A:55:GLU:HB2	0.65	2.27	24	24

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:THR:HB	1:A:64:LYS:HZ2	0.65	1.49	17	1
1:A:4:HIS:H	1:A:64:LYS:HB2	0.65	1.51	5	2
1:A:2:VAL:HG21	1:A:22:LEU:C	0.65	2.16	21	7
1:A:5:THR:OG1	1:A:64:LYS:NZ	0.65	2.27	10	19
1:A:11:ILE:N	1:A:11:ILE:HD12	0.65	2.05	17	2
1:A:22:LEU:N	1:A:61:SER:HA	0.65	2.06	25	3
1:A:27:MET:SD	1:A:54:TYR:CE2	0.65	2.90	28	2
1:A:22:LEU:CD2	1:A:23:CYS:H	0.65	1.96	27	3
1:A:4:HIS:HA	1:A:13:ALA:HA	0.65	1.68	21	28
1:A:24:TYR:CD2	1:A:44:CYS:CA	0.65	2.80	1	2
1:A:51:LYS:C	1:A:53:PRO:HD2	0.65	2.17	30	2
1:A:3:CYS:SG	1:A:15:THR:HA	0.64	2.32	24	11
1:A:24:TYR:CD1	1:A:24:TYR:C	0.64	2.75	9	30
1:A:2:VAL:HG11	1:A:16:CYS:SG	0.64	2.33	25	1
1:A:2:VAL:HG11	1:A:22:LEU:CA	0.64	2.23	9	10
1:A:51:LYS:CE	1:A:53:PRO:HG2	0.64	2.17	27	2
1:A:26:LYS:HZ1	1:A:51:LYS:HE2	0.64	1.51	27	1
1:A:26:LYS:NZ	1:A:51:LYS:HD3	0.64	2.08	30	1
1:A:24:TYR:CG	1:A:51:LYS:HE2	0.64	2.28	5	2
1:A:7:ALA:O	1:A:8:THR:HB	0.63	1.92	9	28
1:A:2:VAL:CG1	1:A:15:THR:HG23	0.63	2.23	16	3
1:A:22:LEU:HD21	1:A:48:CYS:CB	0.63	2.22	25	3
1:A:67:PRO:O	1:A:68:HIS:HB2	0.63	1.93	3	20
1:A:27:MET:HE3	1:A:27:MET:HA	0.63	1.70	5	2
1:A:38:LYS:HZ1	1:A:72:ARG:N	0.63	1.92	7	17
1:A:26:LYS:CG	1:A:57:VAL:HG22	0.63	2.22	24	9
1:A:38:LYS:HG3	1:A:68:HIS:CE1	0.63	2.29	25	8
1:A:2:VAL:HG13	1:A:23:CYS:SG	0.63	2.33	5	11
1:A:54:TYR:CD2	1:A:55:GLU:N	0.63	2.66	24	27
1:A:2:VAL:CG2	1:A:22:LEU:H	0.63	2.07	20	13
1:A:5:THR:CG2	1:A:6:THR:N	0.63	2.62	25	19
1:A:54:TYR:CG	1:A:55:GLU:N	0.62	2.66	24	29
1:A:64:LYS:O	1:A:65:CYS:HB2	0.62	1.94	9	28
1:A:2:VAL:N	1:A:15:THR:HB	0.62	2.04	29	15
1:A:4:HIS:CA	1:A:13:ALA:HA	0.62	2.25	20	30
1:A:2:VAL:CG2	1:A:3:CYS:H	0.62	2.08	25	3
1:A:36:ARG:NH1	1:A:70:LYS:NZ	0.62	2.46	17	1
1:A:2:VAL:HB	1:A:23:CYS:SG	0.62	2.35	9	6
1:A:24:TYR:CA	1:A:48:CYS:SG	0.62	2.87	27	3
1:A:36:ARG:CA	1:A:70:LYS:NZ	0.61	2.61	19	4
1:A:7:ALA:C	1:A:11:ILE:HD11	0.61	2.21	9	21

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:VAL:HB	1:A:22:LEU:C	0.61	2.20	25	3
1:A:26:LYS:HG2	1:A:51:LYS:HD3	0.61	1.72	21	4
1:A:6:THR:HG21	1:A:40:VAL:HG23	0.61	1.71	5	2
1:A:28:TRP:CA	1:A:40:VAL:HG22	0.61	2.25	21	26
1:A:38:LYS:NZ	1:A:72:ARG:HG2	0.61	2.11	22	8
1:A:68:HIS:CE1	1:A:71:GLN:NE2	0.61	2.69	30	2
1:A:9:SER:CB	1:A:10:PRO:HD2	0.61	2.20	9	25
1:A:24:TYR:CE2	1:A:26:LYS:CE	0.61	2.83	30	1
1:A:2:VAL:HG21	1:A:22:LEU:H	0.61	1.56	3	9
1:A:5:THR:HB	1:A:66:ASN:O	0.61	1.96	29	10
1:A:7:ALA:HA	1:A:43:GLY:CA	0.61	2.26	30	23
1:A:28:TRP:HA	1:A:40:VAL:CG1	0.61	2.25	1	2
1:A:2:VAL:HG11	1:A:22:LEU:N	0.61	2.10	26	15
1:A:42:LEU:CB	1:A:66:ASN:HB2	0.61	2.23	27	27
1:A:5:THR:O	1:A:6:THR:O	0.61	2.18	17	6
1:A:28:TRP:HA	1:A:40:VAL:HG12	0.61	1.73	1	2
1:A:22:LEU:CD1	1:A:61:SER:HB2	0.61	2.26	9	19
1:A:38:LYS:HG2	1:A:38:LYS:O	0.60	1.96	30	8
1:A:5:THR:HG21	1:A:67:PRO:C	0.60	2.21	18	17
1:A:2:VAL:HG23	1:A:15:THR:CG2	0.60	2.24	28	2
1:A:2:VAL:CB	1:A:22:LEU:H	0.60	2.09	3	10
1:A:7:ALA:O	1:A:11:ILE:HD12	0.60	1.96	1	2
1:A:8:THR:C	1:A:11:ILE:HD11	0.60	2.21	19	21
1:A:22:LEU:HA	1:A:61:SER:CA	0.60	2.22	25	3
1:A:5:THR:CG2	1:A:68:HIS:CE1	0.60	2.84	24	5
1:A:25:ARG:HD3	1:A:66:ASN:CA	0.60	2.24	29	3
1:A:24:TYR:CE2	1:A:26:LYS:HE3	0.60	2.31	30	1
1:A:25:ARG:HA	1:A:42:LEU:HA	0.60	1.73	1	26
1:A:40:VAL:HB	1:A:42:LEU:HD22	0.60	1.73	5	2
1:A:38:LYS:HG3	1:A:68:HIS:NE2	0.60	2.12	16	7
1:A:64:LYS:HG2	1:A:65:CYS:H	0.60	1.57	17	3
1:A:24:TYR:HE2	1:A:51:LYS:HD2	0.59	1.51	20	3
1:A:15:THR:O	1:A:15:THR:CG2	0.59	2.51	16	8
1:A:3:CYS:CB	1:A:66:ASN:ND2	0.59	2.62	29	9
1:A:6:THR:C	1:A:11:ILE:HD13	0.59	2.22	18	6
1:A:7:ALA:O	1:A:11:ILE:HD11	0.59	1.97	25	7
1:A:34:SER:O	1:A:35:SER:HB2	0.59	1.98	1	2
1:A:68:HIS:HD2	1:A:71:GLN:CD	0.59	2.05	12	8
1:A:42:LEU:CD2	1:A:66:ASN:HD22	0.59	2.09	14	3
1:A:2:VAL:HG12	1:A:15:THR:HB	0.59	1.72	21	2
1:A:5:THR:OG1	1:A:64:LYS:CE	0.59	2.51	26	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LYS:HD3	1:A:51:LYS:HZ1	0.59	1.58	4	6
1:A:37:GLY:O	1:A:68:HIS:CE1	0.59	2.56	23	12
1:A:36:ARG:NH1	1:A:70:LYS:HZ1	0.59	1.96	23	4
1:A:4:HIS:HB2	1:A:64:LYS:HD3	0.59	1.74	15	3
1:A:36:ARG:HG3	1:A:70:LYS:NZ	0.59	2.12	14	3
1:A:67:PRO:C	1:A:68:HIS:CG	0.58	2.79	27	4
1:A:2:VAL:HG21	1:A:22:LEU:O	0.58	1.97	28	8
1:A:2:VAL:CG2	1:A:3:CYS:N	0.58	2.67	25	13
1:A:2:VAL:CG1	1:A:22:LEU:N	0.58	2.65	9	12
1:A:5:THR:CG2	1:A:68:HIS:ND1	0.58	2.67	24	5
1:A:26:LYS:HD3	1:A:51:LYS:CE	0.58	2.29	22	2
1:A:4:HIS:C	1:A:64:LYS:HE3	0.58	2.23	24	4
1:A:26:LYS:HZ2	1:A:51:LYS:HE2	0.58	1.54	27	1
1:A:3:CYS:SG	1:A:16:CYS:SG	0.58	3.01	29	1
1:A:6:THR:HB	1:A:42:LEU:CD1	0.58	2.28	20	3
1:A:4:HIS:HB2	1:A:64:LYS:CD	0.58	2.28	29	5
1:A:26:LYS:CD	1:A:51:LYS:HZ3	0.58	2.11	23	5
1:A:2:VAL:HG22	1:A:15:THR:O	0.58	1.98	25	3
1:A:52:LYS:N	1:A:53:PRO:HD2	0.58	2.12	27	3
1:A:29:CYS:O	1:A:29:CYS:SG	0.58	2.62	5	2
1:A:28:TRP:HA	1:A:40:VAL:CG2	0.58	2.27	9	26
1:A:36:ARG:CG	1:A:70:LYS:HZ2	0.58	2.11	14	1
1:A:5:THR:O	1:A:11:ILE:HG21	0.58	1.98	17	5
1:A:36:ARG:HB3	1:A:70:LYS:NZ	0.58	2.13	27	2
1:A:68:HIS:ND1	1:A:71:GLN:NE2	0.58	2.52	25	8
1:A:38:LYS:NZ	1:A:72:ARG:NE	0.58	2.47	23	4
1:A:2:VAL:HB	1:A:22:LEU:N	0.58	2.13	17	7
1:A:2:VAL:HG12	1:A:15:THR:CG2	0.58	2.29	30	1
1:A:36:ARG:CD	1:A:70:LYS:NZ	0.57	2.67	11	4
1:A:2:VAL:HG21	1:A:22:LEU:N	0.57	2.14	20	13
1:A:11:ILE:HG22	1:A:12:SER:N	0.57	2.14	9	24
1:A:36:ARG:HG3	1:A:37:GLY:N	0.57	2.14	25	11
1:A:38:LYS:NZ	1:A:72:ARG:HB3	0.57	2.14	21	1
1:A:5:THR:OG1	1:A:64:LYS:HE3	0.57	2.00	16	8
1:A:22:LEU:O	1:A:44:CYS:SG	0.57	2.62	30	1
1:A:4:HIS:HB2	1:A:64:LYS:NZ	0.57	2.14	21	2
1:A:2:VAL:HA	1:A:22:LEU:N	0.57	2.14	25	1
1:A:2:VAL:HG22	1:A:15:THR:C	0.57	2.24	25	2
1:A:22:LEU:CG	1:A:61:SER:HB3	0.57	2.30	29	1
1:A:4:HIS:HB2	1:A:64:LYS:HE3	0.57	1.77	1	2
1:A:14:VAL:O	1:A:15:THR:CB	0.57	2.53	24	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:LEU:CG	1:A:61:SER:HB2	0.57	2.30	24	4
1:A:7:ALA:CA	1:A:42:LEU:O	0.56	2.52	20	28
1:A:38:LYS:CA	1:A:68:HIS:CE1	0.56	2.79	22	4
1:A:25:ARG:HD2	1:A:66:ASN:HA	0.56	1.76	1	19
1:A:67:PRO:C	1:A:68:HIS:CD2	0.56	2.83	21	1
1:A:52:LYS:HB3	1:A:53:PRO:HD2	0.56	1.76	9	24
1:A:55:GLU:CD	1:A:56:GLU:HG2	0.56	2.25	28	4
1:A:5:THR:HB	1:A:64:LYS:HZ3	0.56	1.55	17	1
1:A:6:THR:O	1:A:11:ILE:HG13	0.56	2.01	1	2
1:A:5:THR:CB	1:A:64:LYS:HZ2	0.56	2.08	17	1
1:A:2:VAL:CG1	1:A:15:THR:HB	0.56	2.31	21	2
1:A:27:MET:HB3	1:A:40:VAL:CA	0.56	2.28	30	1
1:A:66:ASN:N	1:A:67:PRO:HD3	0.56	2.16	20	15
1:A:64:LYS:HG3	1:A:65:CYS:N	0.56	2.16	1	2
1:A:2:VAL:CG2	1:A:15:THR:HG23	0.56	2.29	28	2
1:A:38:LYS:CE	1:A:72:ARG:HG2	0.56	2.31	30	1
1:A:22:LEU:HD12	1:A:61:SER:HB2	0.56	1.78	7	9
1:A:5:THR:CB	1:A:64:LYS:HE3	0.56	2.31	27	2
1:A:62:THR:O	1:A:62:THR:HG22	0.56	2.01	24	26
1:A:16:CYS:HB2	1:A:43:GLY:O	0.55	2.02	28	25
1:A:3:CYS:HA	1:A:64:LYS:HG2	0.55	1.78	20	2
1:A:66:ASN:N	1:A:67:PRO:CD	0.55	2.69	20	26
1:A:2:VAL:H	1:A:15:THR:HG21	0.55	1.59	13	18
1:A:24:TYR:CD2	1:A:51:LYS:CE	0.55	2.88	28	1
1:A:16:CYS:SG	1:A:43:GLY:C	0.55	2.89	30	2
1:A:25:ARG:HB3	1:A:58:THR:HG23	0.55	1.79	28	8
1:A:37:GLY:C	1:A:68:HIS:HE1	0.55	2.09	12	7
1:A:25:ARG:HA	1:A:42:LEU:HB3	0.55	1.79	27	4
1:A:68:HIS:CG	1:A:71:GLN:NE2	0.55	2.72	9	2
1:A:26:LYS:HD2	1:A:51:LYS:HD2	0.55	1.79	1	2
1:A:67:PRO:C	1:A:68:HIS:HD2	0.55	2.09	21	1
1:A:62:THR:O	1:A:63:ASP:HB2	0.55	2.02	30	4
1:A:52:LYS:N	1:A:53:PRO:CD	0.55	2.69	28	3
1:A:38:LYS:HD3	1:A:71:GLN:N	0.55	2.17	28	1
1:A:51:LYS:HG3	1:A:53:PRO:HD2	0.54	1.78	27	2
1:A:6:THR:CG2	1:A:7:ALA:H	0.54	2.14	27	19
1:A:6:THR:OG1	1:A:68:HIS:CE1	0.54	2.61	30	2
1:A:2:VAL:HG13	1:A:15:THR:CG2	0.54	2.33	23	4
1:A:57:VAL:HG12	1:A:58:THR:N	0.54	2.16	28	24
1:A:62:THR:O	1:A:63:ASP:CB	0.54	2.55	24	27
1:A:36:ARG:CG	1:A:37:GLY:H	0.54	2.09	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:CYS:HA	1:A:43:GLY:O	0.54	2.02	26	3
1:A:66:ASN:HD22	1:A:66:ASN:N	0.54	2.01	25	3
1:A:3:CYS:N	1:A:15:THR:HG23	0.54	2.17	22	1
1:A:60:CYS:O	1:A:61:SER:HB3	0.54	2.01	9	21
1:A:26:LYS:CD	1:A:51:LYS:NZ	0.54	2.71	7	18
1:A:2:VAL:HG22	1:A:15:THR:HB	0.54	1.78	17	2
1:A:24:TYR:CD2	1:A:26:LYS:CE	0.54	2.85	30	1
1:A:25:ARG:CB	1:A:66:ASN:ND2	0.54	2.69	20	3
1:A:6:THR:OG1	1:A:68:HIS:CG	0.54	2.61	24	1
1:A:25:ARG:HA	1:A:42:LEU:CB	0.54	2.33	30	20
1:A:42:LEU:HD23	1:A:66:ASN:OD1	0.54	2.02	27	21
1:A:38:LYS:HZ2	1:A:72:ARG:CG	0.54	2.15	7	9
1:A:63:ASP:O	1:A:64:LYS:HB2	0.54	2.02	14	18
1:A:25:ARG:NH2	1:A:58:THR:HB	0.53	2.19	29	1
1:A:5:THR:OG1	1:A:64:LYS:HD3	0.53	2.04	5	2
1:A:26:LYS:HG3	1:A:57:VAL:CG2	0.53	2.27	9	19
1:A:4:HIS:ND1	1:A:64:LYS:HE2	0.53	2.18	28	3
1:A:6:THR:H	1:A:42:LEU:HD21	0.53	1.63	20	1
1:A:5:THR:C	1:A:6:THR:O	0.53	2.50	17	10
1:A:2:VAL:HB	1:A:22:LEU:O	0.53	2.03	27	3
1:A:25:ARG:CG	1:A:42:LEU:HB3	0.53	2.27	24	22
1:A:30:ASP:CB	1:A:32:PHE:CZ	0.53	2.92	1	2
1:A:36:ARG:HD3	1:A:70:LYS:NZ	0.53	2.19	2	5
1:A:60:CYS:O	1:A:61:SER:HB2	0.53	2.04	25	7
1:A:5:THR:OG1	1:A:67:PRO:CA	0.53	2.55	27	1
1:A:47:THR:HG22	1:A:47:THR:O	0.53	2.04	24	13
1:A:5:THR:HG22	1:A:68:HIS:ND1	0.53	2.19	15	5
1:A:38:LYS:HD3	1:A:71:GLN:CA	0.53	2.34	28	1
1:A:26:LYS:HE2	1:A:51:LYS:CB	0.53	2.33	30	1
1:A:51:LYS:HB3	1:A:57:VAL:HG11	0.52	1.81	30	1
1:A:42:LEU:CG	1:A:66:ASN:HB2	0.52	2.34	5	2
1:A:25:ARG:HD2	1:A:42:LEU:HD12	0.52	1.82	1	2
1:A:2:VAL:O	1:A:63:ASP:C	0.52	2.52	27	3
1:A:38:LYS:HG2	1:A:68:HIS:NE2	0.52	2.19	28	1
1:A:3:CYS:CB	1:A:66:ASN:OD1	0.52	2.54	16	6
1:A:42:LEU:CD2	1:A:66:ASN:O	0.52	2.58	9	25
1:A:5:THR:CB	1:A:67:PRO:HA	0.52	2.35	5	2
1:A:25:ARG:HA	1:A:42:LEU:CA	0.52	2.35	1	22
1:A:11:ILE:HG22	1:A:14:VAL:CG2	0.52	2.35	1	2
1:A:38:LYS:NZ	1:A:72:ARG:N	0.52	2.58	7	18
1:A:25:ARG:CZ	1:A:58:THR:HG21	0.52	2.35	29	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:THR:O	1:A:48:CYS:C	0.52	2.53	22	28
1:A:26:LYS:HG2	1:A:27:MET:N	0.52	2.20	6	18
1:A:2:VAL:CG2	1:A:22:LEU:N	0.52	2.73	20	4
1:A:6:THR:O	1:A:7:ALA:CB	0.51	2.57	17	26
1:A:2:VAL:H	1:A:15:THR:CB	0.51	2.18	20	13
1:A:7:ALA:HB1	1:A:43:GLY:HA2	0.51	1.82	24	11
1:A:6:THR:OG1	1:A:68:HIS:CD2	0.51	2.64	9	1
1:A:26:LYS:CD	1:A:51:LYS:HD3	0.51	2.36	24	2
1:A:25:ARG:NH2	1:A:58:THR:CB	0.51	2.74	29	1
1:A:10:PRO:C	1:A:11:ILE:HG12	0.51	2.29	1	2
1:A:26:LYS:HZ3	1:A:51:LYS:CD	0.51	2.17	30	1
1:A:6:THR:HG22	1:A:9:SER:O	0.51	2.06	1	2
1:A:24:TYR:CD2	1:A:44:CYS:C	0.51	2.89	1	1
1:A:38:LYS:HZ1	1:A:72:ARG:HG2	0.51	1.66	11	6
1:A:38:LYS:NZ	1:A:72:ARG:CG	0.51	2.74	24	10
1:A:24:TYR:HD1	1:A:44:CYS:H	0.51	1.48	17	20
1:A:38:LYS:NZ	1:A:72:ARG:CB	0.51	2.73	2	7
1:A:6:THR:HG21	1:A:42:LEU:HD11	0.51	1.83	21	7
1:A:8:THR:O	1:A:9:SER:CB	0.50	2.59	24	13
1:A:37:GLY:C	1:A:68:HIS:CE1	0.50	2.90	12	7
1:A:2:VAL:HG13	1:A:23:CYS:HB2	0.50	1.82	30	1
1:A:26:LYS:CE	1:A:51:LYS:HB2	0.50	2.36	30	1
1:A:5:THR:OG1	1:A:66:ASN:CB	0.50	2.59	30	3
1:A:6:THR:N	1:A:42:LEU:HD21	0.50	2.21	20	1
1:A:16:CYS:HB2	1:A:43:GLY:C	0.50	2.30	26	5
1:A:66:ASN:HD22	1:A:66:ASN:H	0.50	1.47	25	3
1:A:5:THR:HG23	1:A:64:LYS:HZ1	0.50	1.67	27	1
1:A:66:ASN:ND2	1:A:66:ASN:N	0.50	2.59	23	22
1:A:24:TYR:CD1	1:A:51:LYS:CE	0.50	2.93	1	2
1:A:64:LYS:HZ1	1:A:66:ASN:H	0.50	1.47	17	1
1:A:69:PRO:O	1:A:71:GLN:HG2	0.50	2.07	10	11
1:A:37:GLY:O	1:A:68:HIS:HE1	0.50	1.88	8	6
1:A:4:HIS:C	1:A:13:ALA:HA	0.50	2.32	29	7
1:A:24:TYR:CD2	1:A:26:LYS:HD3	0.49	2.42	20	2
1:A:62:THR:HG22	1:A:62:THR:O	0.49	2.06	27	2
1:A:7:ALA:N	1:A:11:ILE:HG13	0.49	2.22	1	2
1:A:42:LEU:CD2	1:A:66:ASN:HB2	0.49	2.37	29	18
1:A:6:THR:CA	1:A:42:LEU:HD21	0.49	2.37	20	1
1:A:6:THR:CB	1:A:42:LEU:CD2	0.49	2.90	21	1
1:A:2:VAL:C	1:A:22:LEU:O	0.49	2.55	25	1
1:A:72:ARG:O	1:A:72:ARG:HG3	0.49	2.06	15	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:THR:O	1:A:59:CYS:SG	0.49	2.70	24	8
1:A:15:THR:O	1:A:16:CYS:CB	0.49	2.60	30	8
1:A:6:THR:HG1	1:A:68:HIS:CG	0.49	2.25	24	1
1:A:2:VAL:O	1:A:15:THR:HG22	0.49	2.07	29	1
1:A:27:MET:CG	1:A:41:GLU:HG2	0.49	2.20	21	4
1:A:16:CYS:HB3	1:A:43:GLY:C	0.49	2.32	22	1
1:A:36:ARG:CG	1:A:37:GLY:N	0.49	2.73	14	2
1:A:68:HIS:CD2	1:A:68:HIS:N	0.49	2.80	21	1
1:A:47:THR:O	1:A:47:THR:HG22	0.49	2.07	25	14
1:A:11:ILE:CG2	1:A:12:SER:N	0.49	2.75	24	25
1:A:24:TYR:HD1	1:A:51:LYS:HZ3	0.49	1.50	1	2
1:A:5:THR:HG1	1:A:67:PRO:HA	0.49	1.66	26	7
1:A:27:MET:O	1:A:28:TRP:HB2	0.49	2.08	9	27
1:A:60:CYS:HB2	1:A:65:CYS:HB3	0.49	1.75	18	14
1:A:24:TYR:HE1	1:A:43:GLY:H	0.49	1.48	20	9
1:A:4:HIS:O	1:A:64:LYS:HD2	0.49	2.08	17	2
1:A:67:PRO:O	1:A:68:HIS:CG	0.49	2.66	24	2
1:A:26:LYS:NZ	1:A:51:LYS:CB	0.49	2.74	30	1
1:A:40:VAL:HG12	1:A:41:GLU:N	0.49	2.21	24	4
1:A:38:LYS:NZ	1:A:71:GLN:CD	0.49	2.71	20	1
1:A:27:MET:HG3	1:A:39:VAL:O	0.48	2.08	1	2
1:A:42:LEU:HD23	1:A:66:ASN:O	0.48	2.08	25	25
1:A:4:HIS:C	1:A:64:LYS:HD2	0.48	2.33	19	9
1:A:29:CYS:H	1:A:55:GLU:CD	0.48	2.15	21	1
1:A:41:GLU:C	1:A:42:LEU:HD13	0.48	2.34	20	1
1:A:6:THR:OG1	1:A:42:LEU:HD21	0.48	2.07	21	2
1:A:68:HIS:HD2	1:A:71:GLN:HE21	0.48	1.41	27	1
1:A:5:THR:HG22	1:A:68:HIS:CD2	0.48	2.43	1	1
1:A:22:LEU:CG	1:A:60:CYS:O	0.48	2.60	22	5
1:A:26:LYS:CD	1:A:51:LYS:HD2	0.48	2.38	1	2
1:A:4:HIS:HB3	1:A:13:ALA:CB	0.48	2.38	30	7
1:A:67:PRO:C	1:A:68:HIS:ND1	0.48	2.72	27	2
1:A:27:MET:C	1:A:40:VAL:HG12	0.48	2.34	5	2
1:A:25:ARG:HB2	1:A:66:ASN:HB3	0.48	1.84	16	19
1:A:51:LYS:HG3	1:A:52:LYS:H	0.48	1.69	25	1
1:A:6:THR:HG21	1:A:40:VAL:CG2	0.48	2.37	1	2
1:A:68:HIS:HB2	1:A:71:GLN:NE2	0.48	2.24	7	1
1:A:26:LYS:CE	1:A:51:LYS:CB	0.48	2.92	30	1
1:A:24:TYR:CE2	1:A:44:CYS:C	0.48	2.92	1	1
1:A:28:TRP:CA	1:A:40:VAL:HG12	0.48	2.38	1	2
1:A:12:SER:O	1:A:13:ALA:HB3	0.48	2.09	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:TYR:CG	1:A:44:CYS:HA	0.48	2.42	5	2
1:A:7:ALA:O	1:A:8:THR:CB	0.48	2.62	26	28
1:A:42:LEU:CD1	1:A:42:LEU:N	0.48	2.76	9	23
1:A:24:TYR:CE1	1:A:43:GLY:N	0.48	2.82	19	6
1:A:4:HIS:HA	1:A:13:ALA:CA	0.48	2.38	21	7
1:A:38:LYS:HZ2	1:A:72:ARG:HB2	0.48	1.68	9	1
1:A:27:MET:HB3	1:A:41:GLU:N	0.47	2.24	1	2
1:A:15:THR:O	1:A:16:CYS:C	0.47	2.57	27	3
1:A:3:CYS:HB3	1:A:22:LEU:O	0.47	2.09	27	1
1:A:3:CYS:HB2	1:A:66:ASN:CG	0.47	2.33	29	1
1:A:36:ARG:CG	1:A:70:LYS:HZ1	0.47	2.22	17	1
1:A:36:ARG:HB2	1:A:70:LYS:NZ	0.47	2.24	22	2
1:A:36:ARG:NH2	1:A:70:LYS:HZ3	0.47	2.07	7	1
1:A:6:THR:O	1:A:11:ILE:HG21	0.47	2.09	21	8
1:A:27:MET:HB2	1:A:40:VAL:CA	0.47	2.39	21	2
1:A:7:ALA:HB3	1:A:11:ILE:HG12	0.47	1.86	28	7
1:A:26:LYS:NZ	1:A:48:CYS:SG	0.47	2.87	26	2
1:A:24:TYR:CB	1:A:48:CYS:SG	0.47	3.01	30	1
1:A:9:SER:CB	1:A:10:PRO:CD	0.47	2.90	27	9
1:A:26:LYS:HD2	1:A:51:LYS:CD	0.47	2.32	28	1
1:A:57:VAL:O	1:A:58:THR:HB	0.47	2.08	1	5
1:A:68:HIS:HB2	1:A:71:GLN:HE21	0.47	1.70	7	1
1:A:6:THR:CA	1:A:11:ILE:HD13	0.47	2.40	19	5
1:A:2:VAL:CG1	1:A:3:CYS:H	0.47	2.20	20	2
1:A:32:PHE:CD1	1:A:32:PHE:N	0.47	2.83	1	2
1:A:11:ILE:N	1:A:11:ILE:CD1	0.47	2.78	7	21
1:A:4:HIS:C	1:A:64:LYS:HD3	0.47	2.35	30	2
1:A:12:SER:O	1:A:13:ALA:CB	0.47	2.62	25	2
1:A:24:TYR:CD1	1:A:51:LYS:NZ	0.46	2.82	1	2
1:A:2:VAL:O	1:A:63:ASP:O	0.46	2.33	9	18
1:A:48:CYS:C	1:A:50:SER:H	0.46	2.18	17	8
1:A:38:LYS:NZ	1:A:71:GLN:C	0.46	2.73	24	2
1:A:2:VAL:CB	1:A:22:LEU:N	0.46	2.79	15	8
1:A:2:VAL:CG1	1:A:3:CYS:N	0.46	2.70	9	7
1:A:27:MET:HB2	1:A:41:GLU:N	0.46	2.25	28	8
1:A:24:TYR:CE2	1:A:51:LYS:NZ	0.46	2.84	17	4
1:A:38:LYS:HG3	1:A:71:GLN:NE2	0.46	2.25	27	2
1:A:71:GLN:OE1	1:A:72:ARG:N	0.46	2.48	20	1
1:A:43:GLY:C	1:A:44:CYS:O	0.46	2.55	30	5
1:A:29:CYS:O	1:A:30:ASP:C	0.46	2.58	1	7
1:A:26:LYS:CE	1:A:54:TYR:CE1	0.46	2.99	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LYS:CG	1:A:68:HIS:CE1	0.46	2.98	25	4
1:A:57:VAL:CG1	1:A:58:THR:N	0.46	2.78	28	11
1:A:6:THR:HA	1:A:11:ILE:HG12	0.46	1.88	5	2
1:A:25:ARG:HB2	1:A:66:ASN:CB	0.46	2.41	25	2
1:A:24:TYR:HB2	1:A:48:CYS:SG	0.46	2.51	29	2
1:A:38:LYS:CD	1:A:72:ARG:HG2	0.46	2.41	30	1
1:A:36:ARG:CG	1:A:70:LYS:NZ	0.46	2.79	11	5
1:A:25:ARG:CB	1:A:66:ASN:HD22	0.46	2.24	30	2
1:A:36:ARG:HG3	1:A:70:LYS:CD	0.45	2.42	11	3
1:A:38:LYS:HZ2	1:A:72:ARG:CB	0.45	2.24	21	1
1:A:36:ARG:CZ	1:A:70:LYS:HZ3	0.45	2.23	7	1
1:A:36:ARG:CB	1:A:70:LYS:NZ	0.45	2.76	27	1
1:A:27:MET:CG	1:A:40:VAL:HA	0.45	2.41	30	1
1:A:66:ASN:N	1:A:66:ASN:HD22	0.45	2.09	5	4
1:A:8:THR:O	1:A:8:THR:HG22	0.45	2.11	24	4
1:A:2:VAL:CG1	1:A:22:LEU:H	0.45	2.25	28	2
1:A:5:THR:CB	1:A:66:ASN:O	0.45	2.65	19	14
1:A:38:LYS:HZ3	1:A:71:GLN:CD	0.45	2.20	20	1
1:A:26:LYS:HE2	1:A:50:SER:O	0.45	2.11	24	1
1:A:2:VAL:CG2	1:A:16:CYS:SG	0.45	2.92	25	1
1:A:24:TYR:CE2	1:A:51:LYS:CD	0.45	2.94	7	12
1:A:51:LYS:HG3	1:A:52:LYS:N	0.45	2.26	25	1
1:A:11:ILE:HD13	1:A:11:ILE:N	0.45	2.26	1	2
1:A:29:CYS:HB3	1:A:55:GLU:OE2	0.45	2.11	28	3
1:A:30:ASP:OD1	1:A:39:VAL:CB	0.45	2.65	25	10
1:A:58:THR:HG23	1:A:59:CYS:N	0.45	2.26	1	3
1:A:41:GLU:N	1:A:42:LEU:HD12	0.45	2.27	14	13
1:A:13:ALA:O	1:A:14:VAL:C	0.45	2.60	24	5
1:A:25:ARG:HE	1:A:58:THR:CG2	0.45	2.25	27	1
1:A:54:TYR:O	1:A:55:GLU:C	0.45	2.60	24	7
1:A:62:THR:O	1:A:62:THR:CG2	0.45	2.65	24	3
1:A:43:GLY:O	1:A:44:CYS:O	0.45	2.35	24	3
1:A:26:LYS:CG	1:A:51:LYS:HD3	0.45	2.42	24	1
1:A:51:LYS:CG	1:A:52:LYS:H	0.45	2.25	25	1
1:A:26:LYS:HE3	1:A:54:TYR:CD1	0.44	2.48	1	2
1:A:68:HIS:ND1	1:A:71:GLN:CD	0.44	2.75	25	2
1:A:2:VAL:CG1	1:A:15:THR:CG2	0.44	2.95	30	3
1:A:44:CYS:O	1:A:45:ALA:HB2	0.44	2.12	30	4
1:A:55:GLU:OE1	1:A:56:GLU:HG2	0.44	2.13	17	4
1:A:16:CYS:HB2	1:A:44:CYS:CA	0.44	2.41	23	3
1:A:72:ARG:NE	1:A:74:GLY:OXT	0.44	2.51	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ARG:NE	1:A:70:LYS:NZ	0.44	2.65	27	1
1:A:4:HIS:O	1:A:64:LYS:HD3	0.44	2.11	30	1
1:A:51:LYS:HG3	1:A:53:PRO:CD	0.44	2.42	30	1
1:A:3:CYS:O	1:A:15:THR:HG22	0.44	2.11	25	2
1:A:2:VAL:CG2	1:A:15:THR:O	0.44	2.66	17	2
1:A:2:VAL:CG2	1:A:15:THR:C	0.44	2.90	25	1
1:A:51:LYS:C	1:A:52:LYS:HD2	0.44	2.38	30	1
1:A:4:HIS:HB2	1:A:64:LYS:CE	0.44	2.42	21	4
1:A:6:THR:CG2	1:A:7:ALA:N	0.44	2.80	24	2
1:A:37:GLY:O	1:A:68:HIS:NE2	0.44	2.50	10	4
1:A:6:THR:O	1:A:11:ILE:HG12	0.44	2.13	17	1
1:A:3:CYS:CA	1:A:64:LYS:HG2	0.44	2.41	20	2
1:A:3:CYS:HB3	1:A:23:CYS:HB2	0.44	1.63	3	12
1:A:26:LYS:O	1:A:40:VAL:HG12	0.44	2.12	28	6
1:A:3:CYS:O	1:A:15:THR:CA	0.44	2.55	29	4
1:A:42:LEU:CD2	1:A:66:ASN:ND2	0.43	2.78	16	1
1:A:41:GLU:O	1:A:42:LEU:C	0.43	2.61	24	4
1:A:23:CYS:HB3	1:A:66:ASN:OD1	0.43	2.12	20	1
1:A:25:ARG:CB	1:A:58:THR:HG22	0.43	2.38	1	2
1:A:25:ARG:NE	1:A:58:THR:CG2	0.43	2.82	27	1
1:A:2:VAL:O	1:A:4:HIS:CE1	0.43	2.71	24	9
1:A:3:CYS:N	1:A:23:CYS:SG	0.43	2.89	24	1
1:A:42:LEU:HB2	1:A:66:ASN:CG	0.43	2.37	30	1
1:A:29:CYS:O	1:A:31:ALA:N	0.43	2.51	24	8
1:A:6:THR:OG1	1:A:68:HIS:NE2	0.43	2.51	21	1
1:A:14:VAL:O	1:A:15:THR:HG23	0.43	2.14	5	12
1:A:26:LYS:HG3	1:A:57:VAL:HG13	0.43	1.89	1	2
1:A:24:TYR:CD1	1:A:44:CYS:HA	0.43	2.48	20	4
1:A:26:LYS:HD2	1:A:51:LYS:HG2	0.43	1.90	27	1
1:A:6:THR:CA	1:A:11:ILE:HG13	0.43	2.43	1	1
1:A:26:LYS:HA	1:A:57:VAL:HA	0.43	1.89	25	5
1:A:6:THR:HA	1:A:11:ILE:CG1	0.43	2.44	5	2
1:A:11:ILE:HG22	1:A:13:ALA:H	0.43	1.74	9	8
1:A:38:LYS:HE3	1:A:71:GLN:CD	0.43	2.37	7	1
1:A:68:HIS:CD2	1:A:71:GLN:CD	0.43	2.96	7	1
1:A:5:THR:OG1	1:A:66:ASN:HB2	0.43	2.13	21	2
1:A:26:LYS:HD2	1:A:57:VAL:CG2	0.43	2.39	22	1
1:A:24:TYR:HE1	1:A:43:GLY:N	0.42	2.10	19	1
1:A:30:ASP:CG	1:A:31:ALA:H	0.42	2.22	24	3
1:A:2:VAL:CB	1:A:22:LEU:O	0.42	2.67	17	3
1:A:24:TYR:O	1:A:24:TYR:CE1	0.42	2.70	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:TYR:CZ	1:A:55:GLU:HB2	0.42	2.50	1	2
1:A:5:THR:HG22	1:A:68:HIS:HE1	0.42	1.63	27	1
1:A:24:TYR:CG	1:A:51:LYS:CE	0.42	3.01	1	1
1:A:42:LEU:HB2	1:A:66:ASN:CB	0.42	2.38	1	3
1:A:53:PRO:C	1:A:54:TYR:O	0.42	2.63	24	4
1:A:40:VAL:CG1	1:A:41:GLU:H	0.42	2.23	9	2
1:A:51:LYS:HB2	1:A:57:VAL:CG1	0.42	2.44	28	1
1:A:26:LYS:O	1:A:40:VAL:HG23	0.42	2.14	30	1
1:A:36:ARG:CD	1:A:70:LYS:HZ1	0.42	2.27	17	1
1:A:6:THR:CG2	1:A:9:SER:O	0.42	2.58	20	1
1:A:16:CYS:SG	1:A:23:CYS:CB	0.42	3.07	22	1
1:A:42:LEU:CD2	1:A:42:LEU:N	0.42	2.82	1	2
1:A:16:CYS:CB	1:A:43:GLY:O	0.42	2.66	30	2
1:A:24:TYR:CD1	1:A:44:CYS:N	0.42	2.88	29	6
1:A:42:LEU:N	1:A:42:LEU:CD1	0.42	2.82	19	3
1:A:38:LYS:HZ3	1:A:72:ARG:HG2	0.42	1.74	22	1
1:A:53:PRO:O	1:A:54:TYR:CD1	0.42	2.73	1	1
1:A:26:LYS:O	1:A:41:GLU:HB2	0.42	2.14	24	3
1:A:42:LEU:HD12	1:A:42:LEU:N	0.42	2.29	9	1
1:A:4:HIS:ND1	1:A:63:ASP:O	0.42	2.52	26	3
1:A:5:THR:CG2	1:A:68:HIS:CD2	0.42	3.03	1	1
1:A:24:TYR:HE2	1:A:45:ALA:HB2	0.42	1.73	1	2
1:A:26:LYS:NZ	1:A:58:THR:O	0.42	2.49	20	2
1:A:38:LYS:HG3	1:A:68:HIS:CD2	0.42	2.49	23	1
1:A:54:TYR:CE2	1:A:55:GLU:HB3	0.42	2.50	27	2
1:A:9:SER:HB2	1:A:10:PRO:HD2	0.41	1.91	5	2
1:A:30:ASP:HB3	1:A:32:PHE:CZ	0.41	2.49	1	1
1:A:2:VAL:CA	1:A:22:LEU:N	0.41	2.82	25	1
1:A:42:LEU:O	1:A:42:LEU:CD2	0.41	2.60	20	1
1:A:26:LYS:O	1:A:27:MET:HB2	0.41	2.15	27	1
1:A:36:ARG:HG3	1:A:70:LYS:HD2	0.41	1.91	11	1
1:A:7:ALA:O	1:A:11:ILE:CD1	0.41	2.68	25	2
1:A:6:THR:HG22	1:A:7:ALA:N	0.41	2.21	17	3
1:A:3:CYS:SG	1:A:66:ASN:OD1	0.41	2.78	25	1
1:A:24:TYR:CB	1:A:48:CYS:HA	0.41	2.46	24	1
1:A:35:SER:O	1:A:36:ARG:CG	0.41	2.69	25	1
1:A:11:ILE:HG23	1:A:14:VAL:HB	0.41	1.92	29	2
1:A:30:ASP:O	1:A:54:TYR:OH	0.41	2.39	27	1
1:A:7:ALA:HB1	1:A:16:CYS:HA	0.41	1.92	30	1
1:A:41:GLU:C	1:A:42:LEU:CD1	0.41	2.94	30	1
1:A:51:LYS:CG	1:A:53:PRO:HD2	0.41	2.45	30	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:CYS:CB	1:A:44:CYS:SG	0.41	3.08	20	1
1:A:26:LYS:HD3	1:A:51:LYS:CD	0.41	2.45	22	1
1:A:51:LYS:O	1:A:52:LYS:HB2	0.41	2.16	30	1
1:A:2:VAL:HG13	1:A:22:LEU:H	0.41	1.76	9	1
1:A:64:LYS:CG	1:A:65:CYS:N	0.41	2.84	9	1
1:A:36:ARG:HD3	1:A:70:LYS:HZ2	0.41	1.75	24	1
1:A:40:VAL:HG13	1:A:42:LEU:HD11	0.41	1.93	30	1
1:A:54:TYR:O	1:A:55:GLU:O	0.41	2.38	25	2
1:A:24:TYR:HD1	1:A:44:CYS:N	0.41	2.14	17	2
1:A:27:MET:O	1:A:40:VAL:HG23	0.41	2.14	30	1
1:A:51:LYS:C	1:A:53:PRO:CD	0.41	2.93	30	1
1:A:26:LYS:HE2	1:A:51:LYS:HD3	0.41	1.91	20	1
1:A:16:CYS:CB	1:A:43:GLY:C	0.41	2.94	24	2
1:A:28:TRP:HB3	1:A:56:GLU:CG	0.40	2.42	20	1
1:A:55:GLU:CD	1:A:56:GLU:N	0.40	2.79	21	1
1:A:2:VAL:O	1:A:3:CYS:C	0.40	2.62	29	1
1:A:51:LYS:CA	1:A:53:PRO:HD2	0.40	2.45	30	1
1:A:56:GLU:O	1:A:57:VAL:HG23	0.40	2.16	24	1
1:A:13:ALA:O	1:A:15:THR:N	0.40	2.54	27	1
1:A:39:VAL:O	1:A:39:VAL:HG12	0.40	2.15	27	1
1:A:5:THR:OG1	1:A:66:ASN:HB3	0.40	2.15	20	1
1:A:5:THR:O	1:A:11:ILE:CG2	0.40	2.69	25	1
1:A:4:HIS:N	1:A:64:LYS:CG	0.40	2.81	20	1
1:A:26:LYS:NZ	1:A:51:LYS:CD	0.40	2.82	30	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	67/74 (91%)	13±1 (19±2%)	25±2 (38±3%)	29±2 (43±3%)	0	0
All	All	2010/2220 (91%)	390 (19%)	757 (38%)	863 (43%)	0	0

All 39 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	7	ALA	30
1	A	9	SER	30
1	A	11	ILE	30
1	A	12	SER	30
1	A	13	ALA	30
1	A	14	VAL	30
1	A	15	THR	30
1	A	16	CYS	30
1	A	28	TRP	30
1	A	30	ASP	30
1	A	31	ALA	30
1	A	35	SER	30
1	A	42	LEU	30
1	A	44	CYS	30
1	A	46	ALA	30
1	A	55	GLU	30
1	A	58	THR	30
1	A	59	CYS	30
1	A	61	SER	30
1	A	63	ASP	30
1	A	65	CYS	30
1	A	8	THR	29
1	A	2	VAL	28
1	A	53	PRO	27
1	A	54	TYR	27
1	A	67	PRO	27
1	A	70	LYS	27
1	A	22	LEU	15
1	A	68	HIS	11
1	A	45	ALA	11
1	A	6	THR	7
1	A	51	LYS	6
1	A	64	LYS	5
1	A	23	CYS	3
1	A	24	TYR	3
1	A	52	LYS	3
1	A	50	SER	2
1	A	33	CYS	1
1	A	48	CYS	1

6.3.2 Protein sidechains ⓘ

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	60/65 (92%)	52±4 (87±7%)	8±4 (13±7%)	6	47
All	All	1800/1950 (92%)	1570 (87%)	230 (13%)	6	47

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	22	LEU	30
1	A	24	TYR	30
1	A	42	LEU	30
1	A	44	CYS	20
1	A	5	THR	19
1	A	55	GLU	18
1	A	16	CYS	17
1	A	2	VAL	15
1	A	68	HIS	8
1	A	6	THR	4
1	A	15	THR	3
1	A	66	ASN	3
1	A	11	ILE	2
1	A	12	SER	2
1	A	30	ASP	2
1	A	32	PHE	2
1	A	35	SER	2
1	A	39	VAL	2
1	A	41	GLU	2
1	A	51	LYS	2
1	A	54	TYR	2
1	A	57	VAL	2
1	A	58	THR	2
1	A	60	CYS	2
1	A	62	THR	2
1	A	64	LYS	2
1	A	70	LYS	2
1	A	52	LYS	1
1	A	72	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	40	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	30-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
30	A	15:THR	C	16:CYS	N	1.16

7 Chemical shift validation

No chemical shift data were provided