



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 02:44 PM UTC

PDB ID : 1PXE / pdb_00001pxe
Title : Solution Structure of a CCHHC Domain of Neural Zinc Finger Factor-1
Authors : Berkovits-Cymet, H.J.; Amann, B.T.; Berg, J.M.
Deposited on : 2003-07-03

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

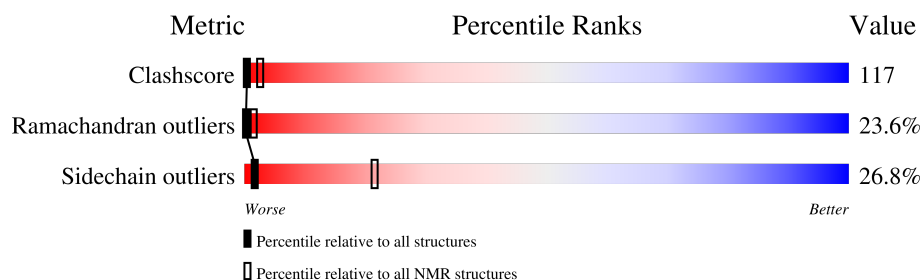
1 Overall quality at a glance

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	63	

2 Ensemble composition and analysis

This entry contains 21 models. Model 1 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:19-A:55 (37)	0.71	1

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 5 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 10, 13, 16, 18, 20
2	7, 9, 14
3	8, 11
4	12, 15
5	5, 6
Single-model clusters	17; 19; 21

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 723 atoms, of which 355 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called neural zinc finger transcription factor 1.

Mol	Chain	Residues	Atoms						Trace
1	A	48	Total	C	H	N	O	S	0
			722	225	355	71	67	4	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P70475
A	32	THR	ASN	SEE REMARK 999	UNP P70475

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

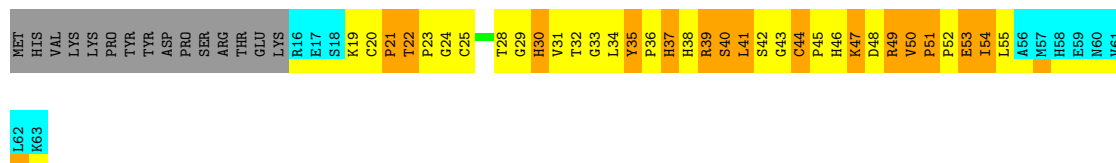
4 Residue-property plots [i](#)

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: neural zinc finger transcription factor 1

Chain A: 32% 24% 17% 24%



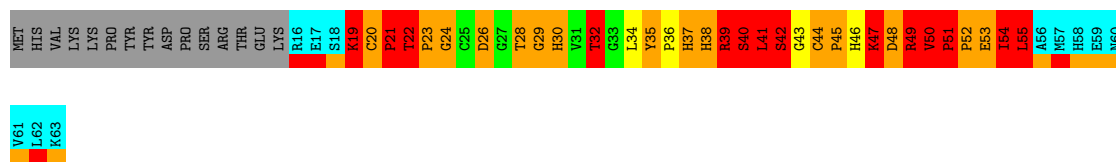
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: neural zinc finger transcription factor 1

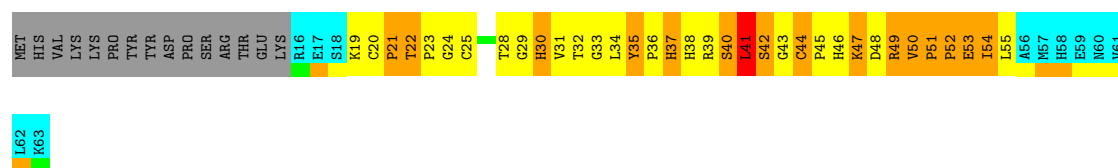
Chain A: 6% 6% 24% 22% 17% 24%



4.2.2 Score per residue for model 2

- Molecule 1: neural zinc finger transcription factor 1

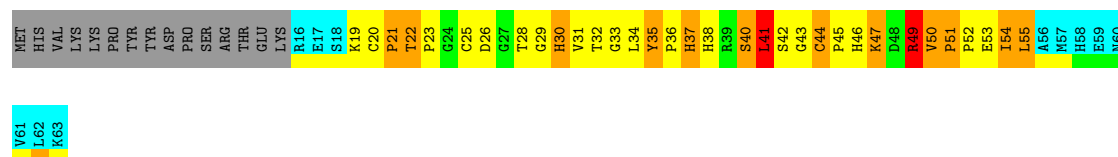
Chain A: 30% 24% 17% 24%



4.2.3 Score per residue for model 3

- Molecule 1: neural zinc finger transcription factor 1

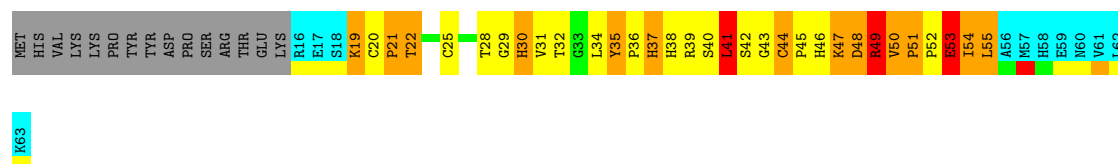
Chain A: 6% 30% 19% 17% 24%



4.2.4 Score per residue for model 4

- Molecule 1: neural zinc finger transcription factor 1

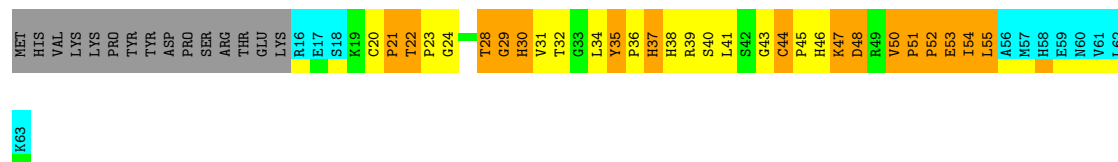
Chain A: 8% 25% 21% 5% 17% 24%



4.2.5 Score per residue for model 5

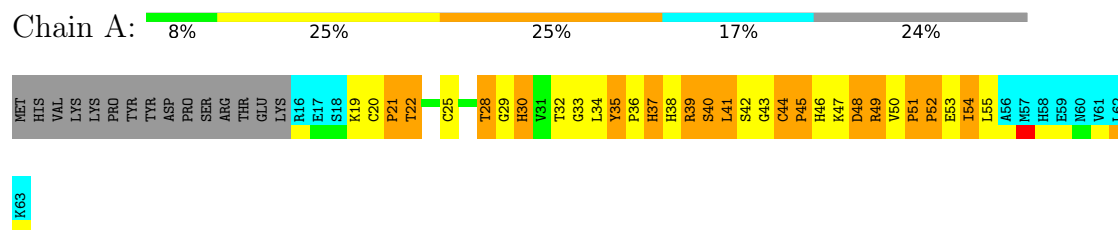
- Molecule 1: neural zinc finger transcription factor 1

Chain A: 11% 22% 25% 17% 24%



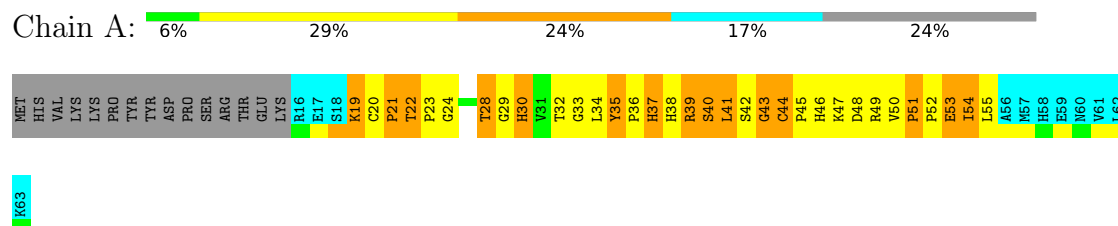
4.2.6 Score per residue for model 6

- Molecule 1: neural zinc finger transcription factor 1



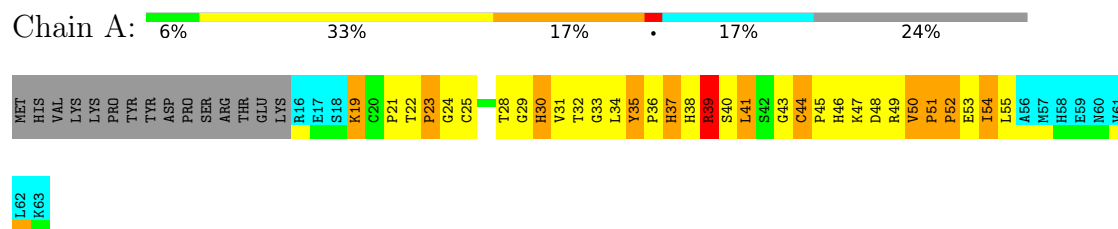
4.2.7 Score per residue for model 7

- Molecule 1: neural zinc finger transcription factor 1



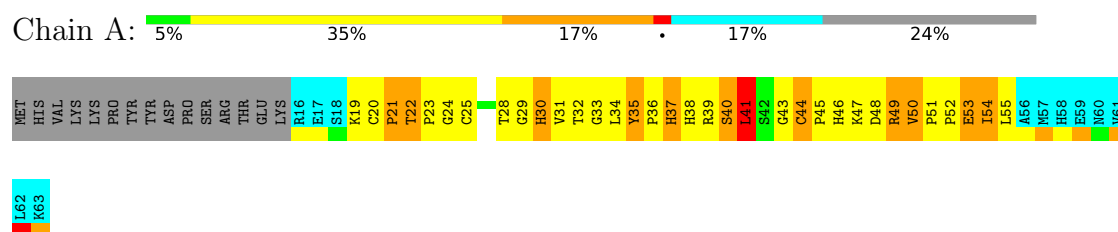
4.2.8 Score per residue for model 8

- Molecule 1: neural zinc finger transcription factor 1



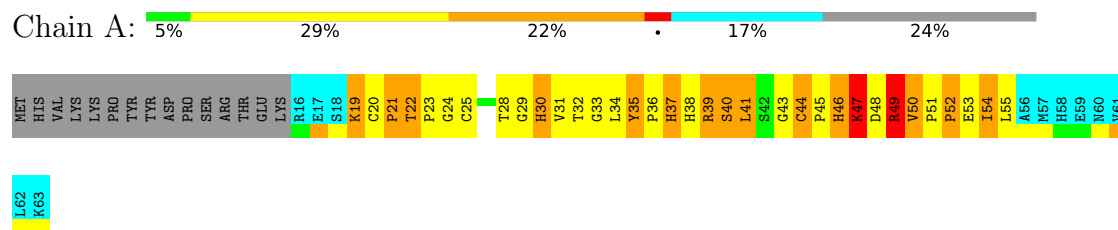
4.2.9 Score per residue for model 9

- Molecule 1: neural zinc finger transcription factor 1



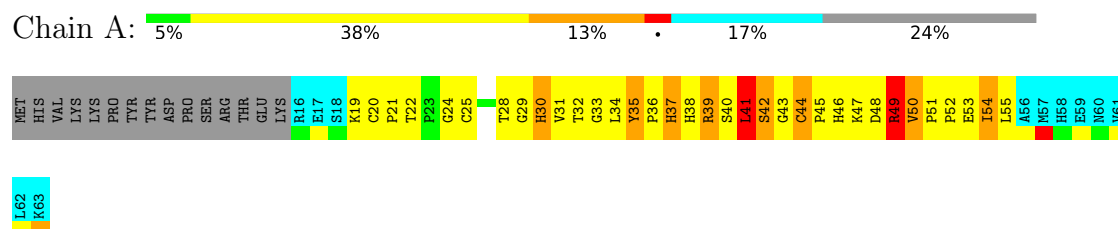
4.2.10 Score per residue for model 10

- Molecule 1: neural zinc finger transcription factor 1



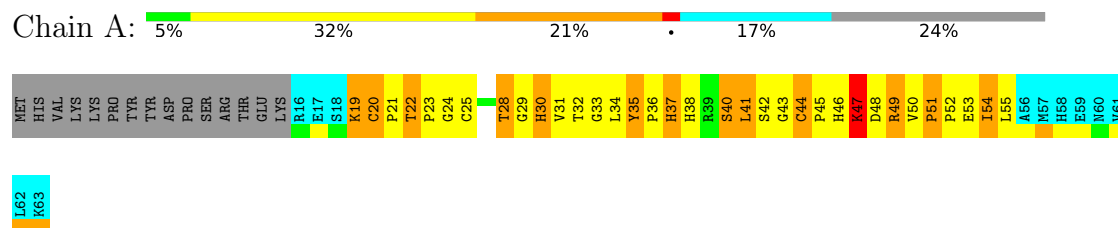
4.2.11 Score per residue for model 11

- Molecule 1: neural zinc finger transcription factor 1



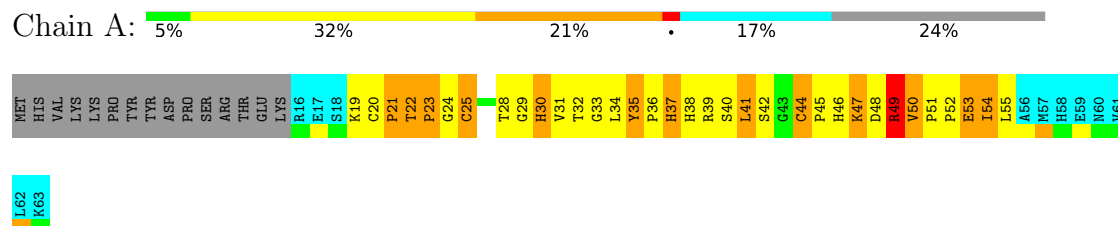
4.2.12 Score per residue for model 12

- Molecule 1: neural zinc finger transcription factor 1



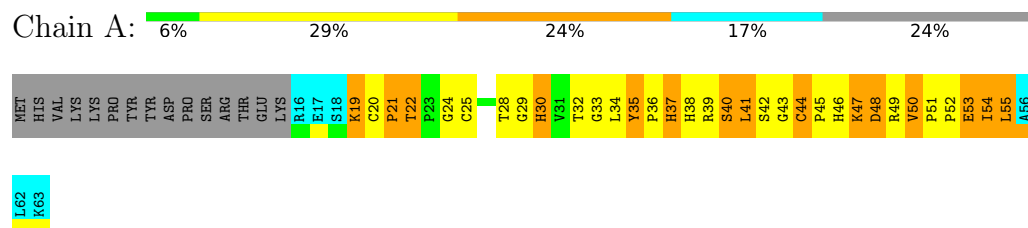
4.2.13 Score per residue for model 13

- Molecule 1: neural zinc finger transcription factor 1



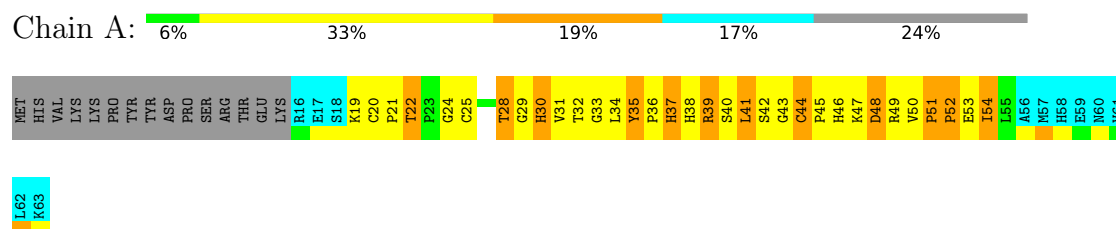
4.2.14 Score per residue for model 14

- Molecule 1: neural zinc finger transcription factor 1



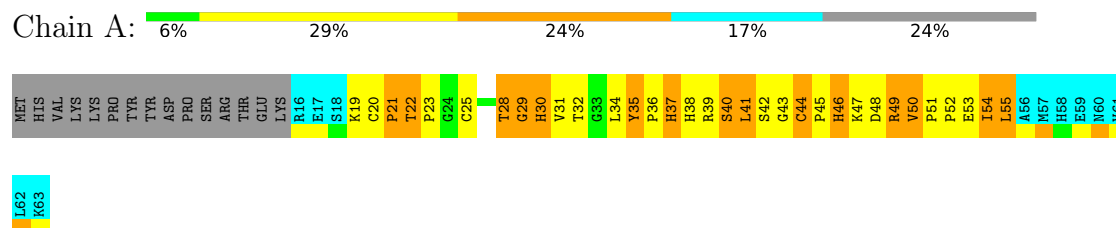
4.2.15 Score per residue for model 15

- Molecule 1: neural zinc finger transcription factor 1



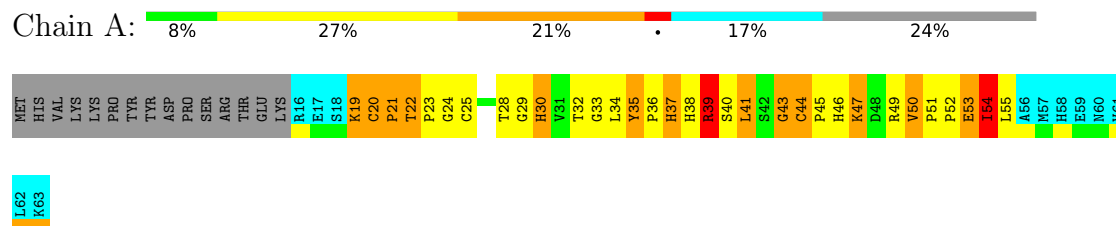
4.2.16 Score per residue for model 16

- Molecule 1: neural zinc finger transcription factor 1



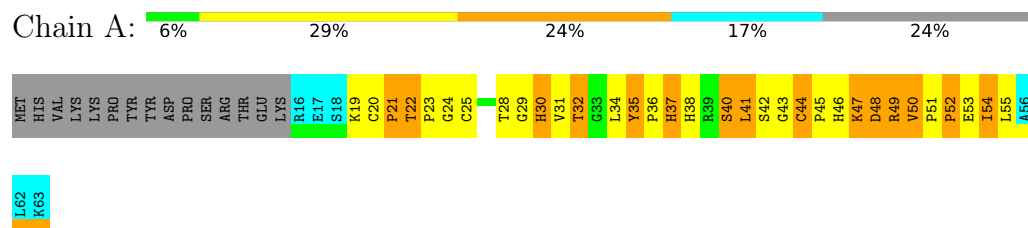
4.2.17 Score per residue for model 17

- Molecule 1: neural zinc finger transcription factor 1



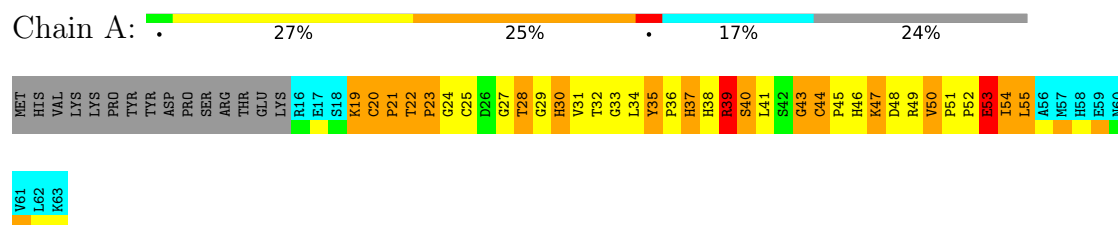
4.2.18 Score per residue for model 18

- Molecule 1: neural zinc finger transcription factor 1



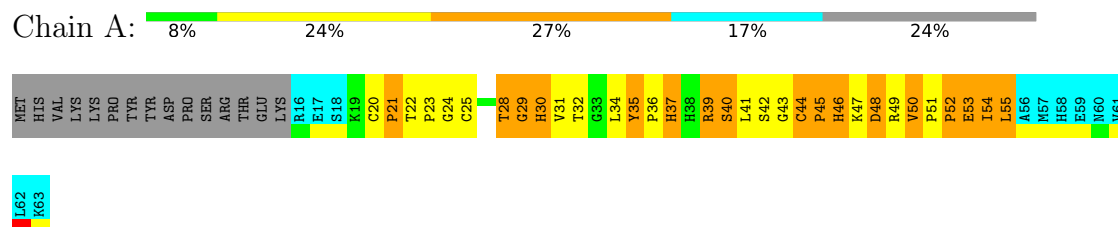
4.2.19 Score per residue for model 19

- Molecule 1: neural zinc finger transcription factor 1



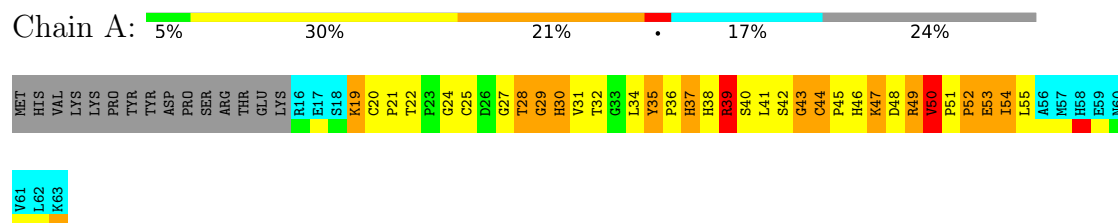
4.2.20 Score per residue for model 20

- Molecule 1: neural zinc finger transcription factor 1



4.2.21 Score per residue for model 21

- Molecule 1: neural zinc finger transcription factor 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Torsion angle dynamics Simulated annealing*.

Of the 30 calculated structures, 21 were deposited, based on the following criterion: *The submitted conformer models are those with the lowest energies..*

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1.35±3.39	6±25/287 (2.0± 8.8%)	1.34±1.63	4±16/393 (0.9± 4.1%)
All	All	3.64	119/6027 (2.0%)	2.11	76/8253 (0.9%)

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±0.4	0.0±0.0
All	All	2	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	49	ARG	CZ-NH2	-66.43	0.47	1.33	1	1
1	A	49	ARG	CD-NE	-65.47	0.54	1.46	1	1
1	A	22	THR	CB-OG1	-55.15	0.55	1.43	1	1
1	A	38	HIS	C-N	-54.21	0.57	1.33	1	1
1	A	49	ARG	CZ-NH1	-54.00	0.57	1.32	1	1
1	A	49	ARG	NE-CZ	-52.48	0.75	1.33	1	1
1	A	39	ARG	CZ-NH1	-51.83	0.60	1.32	1	1
1	A	39	ARG	CZ-NH2	-51.11	0.67	1.33	1	1
1	A	39	ARG	CD-NE	-49.67	0.76	1.46	1	1
1	A	50	VAL	C-N	-48.94	0.75	1.33	1	1
1	A	53	GLU	CD-OE1	-48.19	0.33	1.25	1	1
1	A	19	LYS	CA-CB	-44.85	0.88	1.53	1	1
1	A	49	ARG	C-O	-44.17	0.68	1.24	1	1
1	A	48	ASP	CG-OD2	-42.77	0.44	1.25	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	19	LYS	N-CA	-41.28	0.86	1.46	1	1
1	A	40	SER	CB-OG	-40.73	0.60	1.42	1	1
1	A	38	HIS	C-O	-40.61	0.63	1.24	1	1
1	A	19	LYS	CE-NZ	-39.91	0.29	1.49	1	1
1	A	39	ARG	NE-CZ	-39.12	0.90	1.33	1	1
1	A	42	SER	CB-OG	-35.98	0.70	1.42	1	1
1	A	48	ASP	CG-OD1	-35.24	0.58	1.25	1	1
1	A	19	LYS	CG-CD	-34.61	0.48	1.52	1	1
1	A	26	ASP	CG-OD2	-34.17	0.60	1.25	1	1
1	A	49	ARG	C-N	-34.13	0.94	1.33	1	1
1	A	53	GLU	CD-OE2	-34.05	0.60	1.25	1	1
1	A	51	PRO	CA-CB	-32.71	1.09	1.54	1	1
1	A	26	ASP	CG-OD1	-32.27	0.64	1.25	1	1
1	A	41	LEU	C-O	-31.95	0.83	1.24	1	1
1	A	51	PRO	N-CD	-31.43	1.03	1.47	1	1
1	A	53	GLU	CG-CD	-30.42	0.76	1.52	1	1
1	A	55	LEU	C-N	-29.76	0.89	1.33	1	1
1	A	47	LYS	CD-CE	-28.80	0.66	1.52	1	1
1	A	55	LEU	CG-CD1	-27.03	0.63	1.52	1	1
1	A	47	LYS	CB-CG	-26.99	0.71	1.52	1	1
1	A	50	VAL	C-O	-26.03	0.91	1.24	1	1
1	A	32	THR	CB-OG1	-24.95	1.03	1.43	1	1
1	A	41	LEU	C-N	-24.68	0.99	1.33	1	1
1	A	39	ARG	CB-CG	-24.57	0.78	1.52	1	1
1	A	49	ARG	CB-CG	-24.00	0.80	1.52	1	1
1	A	55	LEU	CG-CD2	-23.99	0.73	1.52	1	1
1	A	22	THR	CB-CG2	-22.96	0.76	1.52	1	1
1	A	21	PRO	N-CD	-22.51	1.16	1.47	1	1
1	A	47	LYS	CE-NZ	-20.80	0.86	1.49	1	1
1	A	39	ARG	CG-CD	-20.42	0.91	1.52	1	1
1	A	21	PRO	CA-CB	-20.11	1.25	1.53	1	1
1	A	48	ASP	C-N	-19.78	1.05	1.33	1	1
1	A	50	VAL	CB-CG2	-18.71	0.90	1.52	1	1
1	A	49	ARG	CG-CD	-18.66	0.96	1.52	1	1
1	A	55	LEU	CB-CG	-18.60	1.16	1.53	1	1
1	A	20	CYS	C-O	-18.42	1.00	1.24	1	1
1	A	19	LYS	CD-CE	-18.42	0.97	1.52	1	1
1	A	48	ASP	N-CA	-17.19	1.27	1.46	1	1
1	A	50	VAL	CA-CB	-15.95	1.33	1.54	1	1
1	A	47	LYS	CA-CB	-15.50	1.27	1.53	1	1
1	A	47	LYS	CA-C	-15.47	1.32	1.52	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	51	PRO	CA-C	-15.15	1.38	1.52	1	1
1	A	48	ASP	CA-CB	-15.12	1.21	1.53	1	1
1	A	28	THR	C-O	-14.67	1.05	1.23	1	1
1	A	20	CYS	C-N	-14.28	1.00	1.33	1	1
1	A	51	PRO	C-O	-14.14	1.08	1.24	1	1
1	A	40	SER	CA-CB	-13.80	1.30	1.53	1	1
1	A	39	ARG	CA-CB	-13.65	1.30	1.53	1	1
1	A	22	THR	CA-CB	-13.19	1.33	1.53	1	1
1	A	52	PRO	N-CD	-13.10	1.29	1.47	1	1
1	A	55	LEU	CA-CB	-13.05	1.31	1.53	1	1
1	A	55	LEU	CA-C	-12.85	1.35	1.52	1	1
1	A	48	ASP	CB-CG	-12.69	1.20	1.52	1	1
1	A	52	PRO	N-CA	-12.00	1.31	1.47	1	1
1	A	23	PRO	C-O	-11.63	1.08	1.24	1	1
1	A	21	PRO	C-N	-11.55	1.14	1.33	1	1
1	A	28	THR	C-N	-11.52	1.16	1.33	1	1
1	A	22	THR	N-CA	-11.40	1.32	1.46	1	1
1	A	41	LEU	CB-CG	-11.40	1.30	1.53	1	1
1	A	49	ARG	CA-CB	-11.32	1.34	1.53	1	1
1	A	24	GLY	C-O	-11.26	1.08	1.23	1	1
1	A	39	ARG	CA-C	-11.21	1.37	1.52	1	1
1	A	52	PRO	CA-CB	-11.01	1.38	1.53	1	1
1	A	23	PRO	C-N	-10.94	1.17	1.33	1	1
1	A	50	VAL	CA-C	-10.87	1.41	1.52	1	1
1	A	40	SER	N-CA	-10.83	1.32	1.46	1	1
1	A	48	ASP	C-O	-10.77	1.09	1.24	1	1
1	A	51	PRO	CG-CD	-10.73	1.14	1.50	1	1
1	A	47	LYS	CG-CD	-10.46	1.21	1.52	1	1
1	A	19	LYS	CB-CG	-10.46	1.21	1.52	1	1
1	A	50	VAL	CB-CG1	-10.07	1.19	1.52	1	1
1	A	55	LEU	C-O	-9.63	1.11	1.24	1	1
1	A	24	GLY	C-N	-9.57	1.20	1.33	1	1
1	A	21	PRO	CA-C	-9.46	1.39	1.52	1	1
1	A	53	GLU	CB-CG	-9.09	1.25	1.52	1	1
1	A	21	PRO	C-O	-8.96	1.12	1.24	1	1
1	A	45	PRO	C-N	-8.95	1.21	1.33	1	1
1	A	32	THR	CB-CG2	-8.80	1.23	1.52	1	1
1	A	51	PRO	C-N	-8.77	1.13	1.33	1	1
1	A	41	LEU	CA-CB	-8.69	1.38	1.53	1	1
1	A	41	LEU	CG-CD2	-8.55	1.24	1.52	1	1
1	A	40	SER	C-O	-7.09	1.15	1.24	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	49	ARG	CA-C	-7.01	1.43	1.52	1	1
1	A	47	LYS	C-O	-7.00	1.15	1.24	1	1
1	A	41	LEU	CG-CD1	-6.95	1.29	1.52	1	1
1	A	54	ILE	C-O	-6.93	1.14	1.23	1	1
1	A	52	PRO	CG-CD	-6.85	1.27	1.50	1	1
1	A	41	LEU	CA-C	-6.83	1.43	1.52	1	1
1	A	51	PRO	N-CA	-6.50	1.33	1.46	1	1
1	A	21	PRO	CG-CD	-6.28	1.29	1.50	1	1
1	A	42	SER	C-O	-6.27	1.16	1.24	1	1
1	A	23	PRO	CA-CB	-6.12	1.45	1.53	1	1
1	A	42	SER	CA-CB	-6.09	1.43	1.53	1	1
1	A	23	PRO	N-CD	-5.98	1.39	1.47	1	1
1	A	19	LYS	C-O	-5.82	1.16	1.23	1	1
1	A	24	GLY	N-CA	-5.72	1.37	1.45	1	1
1	A	29	GLY	C-O	-5.71	1.16	1.23	1	1
1	A	42	SER	C-N	-5.65	1.25	1.33	1	1
1	A	42	SER	N-CA	-5.59	1.39	1.46	1	1
1	A	50	VAL	N-CA	-5.43	1.39	1.46	1	1
1	A	23	PRO	CA-C	-5.32	1.44	1.52	1	1
1	A	29	GLY	C-N	-5.29	1.26	1.33	1	1
1	A	49	ARG	N-CA	-5.06	1.39	1.46	1	1
1	A	46	HIS	CA-C	5.05	1.54	1.52	10	1
1	A	45	PRO	C-O	-5.05	1.17	1.24	1	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	38	HIS	O-C-N	-82.72	8.93	122.26	1	1
1	A	38	HIS	CA-C-O	49.13	176.77	119.78	1	1
1	A	26	ASP	OD1-CG-OD2	-35.73	37.16	122.90	1	1
1	A	48	ASP	OD1-CG-OD2	-32.38	45.18	122.90	1	1
1	A	38	HIS	CA-C-N	28.07	175.15	121.54	1	1
1	A	38	HIS	C-N-CA	28.07	175.15	121.54	1	1
1	A	22	THR	CA-CB-CG2	26.20	155.05	110.50	1	1
1	A	53	GLU	CB-CG-CD	25.64	156.18	112.60	1	1
1	A	50	VAL	O-C-N	-24.62	93.03	121.10	1	1
1	A	49	ARG	NH1-CZ-NH2	-24.43	87.54	119.30	1	1
1	A	49	ARG	O-C-N	-24.05	90.61	122.59	1	1
1	A	55	LEU	CD1-CG-CD2	-23.69	58.68	110.80	1	1
1	A	47	LYS	CA-CB-CG	23.57	161.25	114.10	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	47	LYS	CG-CD-CE	23.23	164.74	111.30	1	1
1	A	22	THR	OG1-CB-CG2	-22.94	63.42	109.30	1	1
1	A	39	ARG	NH1-CZ-NH2	-22.91	89.52	119.30	1	1
1	A	47	LYS	CB-CG-CD	22.54	163.15	111.30	1	1
1	A	39	ARG	NE-CZ-NH2	21.19	138.28	119.20	1	1
1	A	49	ARG	NE-CZ-NH1	20.08	141.58	121.50	1	1
1	A	49	ARG	CB-CG-CD	19.28	155.64	111.30	1	1
1	A	26	ASP	CB-CG-OD1	18.95	162.00	118.40	1	1
1	A	26	ASP	CB-CG-OD2	18.45	160.85	118.40	1	1
1	A	48	ASP	CB-CG-OD1	18.38	160.66	118.40	1	1
1	A	39	ARG	CB-CG-CD	17.80	152.25	111.30	1	1
1	A	47	LYS	CD-CE-NZ	17.18	166.88	111.90	1	1
1	A	51	PRO	CA-N-CD	16.92	135.69	112.00	1	1
1	A	22	THR	CA-CB-OG1	16.55	134.43	109.60	1	1
1	A	41	LEU	O-C-N	-16.41	100.76	122.59	1	1
1	A	50	VAL	CA-C-O	16.34	141.84	119.95	1	1
1	A	49	ARG	CA-CB-CG	16.16	146.43	114.10	1	1
1	A	51	PRO	N-CD-CG	-15.67	79.70	103.20	1	1
1	A	48	ASP	CB-CG-OD2	15.54	154.15	118.40	1	1
1	A	19	LYS	N-CA-CB	-15.44	86.82	111.22	1	1
1	A	19	LYS	N-CA-C	14.64	129.98	109.18	1	1
1	A	20	CYS	O-C-N	-13.97	105.25	121.32	1	1
1	A	42	SER	CA-CB-OG	13.24	137.58	111.10	1	1
1	A	51	PRO	N-CA-C	13.23	126.84	110.70	1	1
1	A	49	ARG	NE-CZ-NH2	12.97	130.88	119.20	1	1
1	A	19	LYS	CD-CE-NZ	12.91	153.23	111.90	1	1
1	A	39	ARG	CD-NE-CZ	12.68	142.15	124.40	1	1
1	A	53	GLU	CG-CD-OE2	12.49	147.13	118.40	1	1
1	A	50	VAL	CA-CB-CG1	12.45	131.57	110.40	1	1
1	A	49	ARG	CA-C-N	11.97	144.27	122.13	1	1
1	A	49	ARG	C-N-CA	11.97	144.27	122.13	1	1
1	A	39	ARG	CA-CB-CG	11.71	137.52	114.10	1	1
1	A	21	PRO	N-CD-CG	-11.60	85.80	103.20	1	1
1	A	55	LEU	CA-C-O	11.24	136.58	120.51	1	1
1	A	55	LEU	CB-CG-CD1	10.73	142.90	110.70	1	1
1	A	39	ARG	NE-CZ-NH1	10.70	132.20	121.50	1	1
1	A	49	ARG	CG-CD-NE	10.46	135.02	112.00	1	1
1	A	48	ASP	CA-C-O	10.16	129.55	119.08	1	1
1	A	39	ARG	CG-CD-NE	9.09	132.00	112.00	1	1
1	A	55	LEU	CB-CG-CD2	8.90	137.39	110.70	1	1
1	A	49	ARG	CD-NE-CZ	8.64	136.50	124.40	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	32	THR	CA-CB-CG2	8.62	125.15	110.50	1	1
1	A	21	PRO	CA-N-CD	8.40	123.76	112.00	1	1
1	A	51	PRO	CB-CG-CD	7.85	131.21	106.10	1	1
1	A	21	PRO	CB-CG-CD	7.83	131.14	106.10	1	1
1	A	20	CYS	CA-C-O	7.79	130.83	120.16	1	1
1	A	55	LEU	CA-C-N	-7.75	109.76	122.08	1	1
1	A	55	LEU	C-N-CA	-7.75	109.76	122.08	1	1
1	A	19	LYS	CB-CA-C	7.62	127.11	111.11	1	1
1	A	28	THR	O-C-N	-7.53	113.31	123.24	1	1
1	A	41	LEU	CA-C-N	6.81	134.55	121.54	1	1
1	A	41	LEU	C-N-CA	6.81	134.55	121.54	1	1
1	A	50	VAL	C-N-CD	-6.56	98.11	125.00	1	1
1	A	53	GLU	OE1-CD-OE2	-6.46	107.40	122.90	1	1
1	A	19	LYS	CB-CG-CD	6.39	125.99	111.30	1	1
1	A	51	PRO	N-CA-CB	-6.24	97.03	103.08	1	1
1	A	49	ARG	CA-C-O	6.18	129.35	120.51	1	1
1	A	48	ASP	O-C-N	-5.74	114.29	122.04	1	1
1	A	50	VAL	CA-C-N	5.65	126.20	120.38	1	1
1	A	50	VAL	C-N-CA	5.65	126.20	120.38	1	1
1	A	24	GLY	O-C-N	-5.64	115.37	122.70	1	1
1	A	53	GLU	CG-CD-OE1	-5.62	105.47	118.40	1	1
1	A	21	PRO	CA-CB-CG	-5.19	94.64	104.50	1	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	19	LYS	CA	1
1	A	22	THR	CB	1

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	276	265	265	63±23

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	5817	5565	5557	1326

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 117.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:LEU:CD2	1:A:55:LEU:CB	1.56	1.77	1	1
1:A:47:LYS:CE	1:A:47:LYS:CG	1.55	1.85	1	1
1:A:47:LYS:CB	1:A:47:LYS:CD	1.46	1.90	1	1
1:A:39:ARG:CG	1:A:39:ARG:CA	1.44	1.95	1	1
1:A:47:LYS:CG	1:A:47:LYS:CA	1.44	1.95	1	1
1:A:40:SER:OG	1:A:40:SER:CA	1.41	1.63	1	1
1:A:53:GLU:CD	1:A:53:GLU:CB	1.36	1.96	1	1
1:A:22:THR:CG2	1:A:22:THR:CA	1.34	2.05	1	1
1:A:48:ASP:OD1	1:A:48:ASP:CB	1.34	1.76	1	1
1:A:22:THR:CA	1:A:22:THR:OG1	1.33	1.76	1	1
1:A:38:HIS:C	1:A:39:ARG:CA	1.33	2.01	1	1
1:A:49:ARG:O	1:A:50:VAL:HG23	1.31	1.11	1	3
1:A:51:PRO:HB2	1:A:52:PRO:CD	1.28	1.46	1	3
1:A:51:PRO:CB	1:A:52:PRO:CD	1.16	2.07	1	7
1:A:38:HIS:CA	1:A:39:ARG:N	1.15	2.08	1	1
1:A:49:ARG:C	1:A:50:VAL:HG23	1.13	1.69	1	4
1:A:42:SER:OG	1:A:42:SER:CA	1.09	2.00	1	1
1:A:42:SER:OG	1:A:42:SER:HB2	1.08	1.31	1	1
1:A:20:CYS:N	1:A:21:PRO:HD2	1.07	1.55	1	11
1:A:20:CYS:N	1:A:21:PRO:CD	1.05	2.06	1	17
1:A:42:SER:OG	1:A:42:SER:HB3	1.05	1.31	1	1
1:A:22:THR:OG1	1:A:22:THR:HB	1.04	1.49	1	1
1:A:40:SER:OG	1:A:40:SER:HB2	1.04	1.30	1	1
1:A:55:LEU:CD2	1:A:55:LEU:HD12	1.03	1.64	1	1
1:A:40:SER:OG	1:A:40:SER:HB3	1.03	1.30	1	1
1:A:55:LEU:CD2	1:A:55:LEU:HG	1.02	1.61	1	1
1:A:22:THR:CG2	1:A:22:THR:HB	1.01	1.58	1	1
1:A:22:THR:CG2	1:A:22:THR:OG1	1.01	0.71	1	1
1:A:26:ASP:OD2	1:A:26:ASP:CB	1.01	2.07	1	1
1:A:29:GLY:O	1:A:30:HIS:O	1.01	1.76	1	19
1:A:22:THR:OG1	1:A:22:THR:HG23	1.01	1.28	1	1
1:A:42:SER:OG	1:A:42:SER:CB	1.00	0.70	1	1
1:A:26:ASP:CB	1:A:26:ASP:OD1	0.96	2.11	1	1
1:A:49:ARG:O	1:A:50:VAL:CG2	0.96	1.80	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:VAL:HA	1:A:44:CYS:O	0.96	1.59	19	3
1:A:51:PRO:CB	1:A:52:PRO:HD2	0.95	1.72	1	4
1:A:40:SER:O	1:A:41:LEU:HD12	0.95	1.60	1	12
1:A:19:LYS:C	1:A:21:PRO:HD2	0.93	1.89	1	3
1:A:40:SER:OG	1:A:40:SER:CB	0.90	0.60	1	1
1:A:41:LEU:HD23	1:A:54:ILE:HG22	0.89	1.43	12	7
1:A:22:THR:CB	1:A:22:THR:HG22	0.88	1.42	1	1
1:A:26:ASP:OD1	1:A:26:ASP:CG	0.88	0.64	1	1
1:A:22:THR:CB	1:A:22:THR:HG21	0.87	1.42	1	1
1:A:22:THR:HG23	1:A:22:THR:CB	0.87	1.42	1	1
1:A:38:HIS:CE1	1:A:44:CYS:HA	0.86	2.05	19	18
1:A:40:SER:C	1:A:41:LEU:HG	0.86	1.93	1	5
1:A:51:PRO:HB2	1:A:52:PRO:HD2	0.85	0.87	1	3
1:A:22:THR:OG1	1:A:22:THR:CB	0.85	0.55	1	1
1:A:30:HIS:HB2	1:A:35:TYR:HB2	0.84	1.48	15	19
1:A:39:ARG:CG	1:A:39:ARG:HB3	0.84	1.37	1	1
1:A:55:LEU:CG	1:A:55:LEU:HD23	0.84	1.39	1	1
1:A:26:ASP:OD2	1:A:26:ASP:CG	0.83	0.60	1	1
1:A:39:ARG:CG	1:A:39:ARG:HB2	0.83	1.37	1	1
1:A:50:VAL:HB	1:A:51:PRO:HD3	0.82	1.52	11	9
1:A:22:THR:OG1	1:A:22:THR:HG21	0.81	1.04	1	1
1:A:51:PRO:CB	1:A:52:PRO:HD3	0.81	2.05	1	2
1:A:53:GLU:CD	1:A:53:GLU:HG3	0.81	1.30	1	1
1:A:53:GLU:CD	1:A:53:GLU:HG2	0.80	1.30	1	1
1:A:44:CYS:SG	1:A:54:ILE:HG23	0.80	2.15	20	19
1:A:55:LEU:CD2	1:A:55:LEU:HB3	0.80	2.03	1	1
1:A:40:SER:O	1:A:41:LEU:CD1	0.79	2.29	1	1
1:A:32:THR:CG2	1:A:34:LEU:HD12	0.79	2.07	2	8
1:A:30:HIS:CB	1:A:35:TYR:HB2	0.79	2.08	15	21
1:A:55:LEU:HD23	1:A:55:LEU:O	0.79	1.76	6	1
1:A:47:LYS:CG	1:A:47:LYS:C	0.78	2.55	1	1
1:A:50:VAL:HG13	1:A:51:PRO:HD3	0.78	1.56	5	1
1:A:39:ARG:CG	1:A:39:ARG:CB	0.77	0.78	1	1
1:A:39:ARG:CB	1:A:39:ARG:HG2	0.77	1.33	1	1
1:A:48:ASP:OD1	1:A:48:ASP:CG	0.77	0.58	1	1
1:A:22:THR:CG2	1:A:22:THR:CB	0.76	0.76	1	1
1:A:40:SER:OG	1:A:40:SER:C	0.76	2.29	1	1
1:A:31:VAL:HG13	1:A:32:THR:HG23	0.76	1.56	3	11
1:A:53:GLU:CD	1:A:53:GLU:CG	0.76	0.76	1	1
1:A:51:PRO:HD3	1:A:55:LEU:HD23	0.76	1.58	7	1
1:A:20:CYS:N	1:A:21:PRO:HD3	0.75	1.96	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:GLY:O	1:A:33:GLY:N	0.75	2.19	15	11
1:A:47:LYS:O	1:A:47:LYS:HG2	0.75	1.81	1	1
1:A:46:HIS:CB	1:A:53:GLU:HA	0.75	2.11	6	21
1:A:40:SER:O	1:A:41:LEU:CG	0.74	2.35	1	1
1:A:28:THR:O	1:A:28:THR:HG23	0.74	1.82	20	3
1:A:47:LYS:CG	1:A:47:LYS:O	0.73	2.36	1	1
1:A:39:ARG:CB	1:A:39:ARG:HG3	0.73	1.33	1	1
1:A:28:THR:HG22	1:A:28:THR:O	0.73	1.83	21	2
1:A:47:LYS:CE	1:A:47:LYS:HZ2	0.73	1.43	1	1
1:A:50:VAL:HG12	1:A:51:PRO:HD2	0.73	1.61	9	2
1:A:50:VAL:HG23	1:A:53:GLU:CD	0.73	2.09	14	2
1:A:51:PRO:O	1:A:53:GLU:N	0.72	2.22	5	7
1:A:39:ARG:O	1:A:40:SER:OG	0.72	2.07	19	1
1:A:29:GLY:O	1:A:33:GLY:CA	0.72	2.37	10	5
1:A:48:ASP:O	1:A:49:ARG:HG2	0.72	1.84	9	2
1:A:55:LEU:CD2	1:A:55:LEU:CG	0.72	0.73	1	1
1:A:47:LYS:CG	1:A:47:LYS:HB3	0.72	1.26	1	1
1:A:20:CYS:O	1:A:22:THR:N	0.72	2.23	20	15
1:A:47:LYS:HB3	1:A:54:ILE:HD11	0.72	1.61	11	6
1:A:32:THR:HG21	1:A:34:LEU:HD12	0.72	1.62	9	9
1:A:47:LYS:CG	1:A:47:LYS:HB2	0.71	1.26	1	1
1:A:47:LYS:CB	1:A:47:LYS:HG2	0.71	1.25	1	1
1:A:40:SER:C	1:A:41:LEU:CG	0.71	2.59	1	1
1:A:47:LYS:CB	1:A:47:LYS:HG3	0.71	1.25	1	1
1:A:47:LYS:CE	1:A:47:LYS:HZ1	0.71	1.43	1	1
1:A:25:CYS:SG	1:A:53:GLU:O	0.71	2.48	17	8
1:A:47:LYS:CE	1:A:47:LYS:NZ	0.71	0.87	1	1
1:A:55:LEU:HD13	1:A:55:LEU:O	0.71	1.86	5	1
1:A:50:VAL:HA	1:A:55:LEU:HD22	0.70	1.60	2	2
1:A:47:LYS:CE	1:A:47:LYS:HZ3	0.70	1.43	1	1
1:A:46:HIS:O	1:A:47:LYS:HG2	0.70	1.87	9	3
1:A:24:GLY:C	1:A:52:PRO:HA	0.70	2.12	1	11
1:A:48:ASP:HB3	1:A:53:GLU:OE1	0.70	1.87	1	1
1:A:51:PRO:HB3	1:A:52:PRO:CD	0.70	2.15	1	1
1:A:46:HIS:HB3	1:A:53:GLU:CD	0.70	2.10	15	5
1:A:46:HIS:HB3	1:A:53:GLU:HG3	0.69	1.65	2	11
1:A:49:ARG:O	1:A:50:VAL:HG22	0.69	1.85	1	1
1:A:47:LYS:CE	1:A:47:LYS:HD2	0.68	1.21	1	1
1:A:46:HIS:HB3	1:A:53:GLU:HA	0.68	1.66	6	2
1:A:50:VAL:HG13	1:A:51:PRO:CD	0.68	2.18	5	1
1:A:50:VAL:HB	1:A:51:PRO:CD	0.67	2.19	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:THR:CG2	1:A:55:LEU:HD22	0.67	2.19	19	1
1:A:44:CYS:CB	1:A:54:ILE:HG23	0.67	2.19	19	1
1:A:47:LYS:CE	1:A:47:LYS:HD3	0.67	1.21	1	1
1:A:47:LYS:N	1:A:53:GLU:HG3	0.67	2.05	21	1
1:A:28:THR:O	1:A:28:THR:CG2	0.67	2.42	5	5
1:A:46:HIS:CG	1:A:53:GLU:HA	0.66	2.25	21	17
1:A:47:LYS:CD	1:A:47:LYS:HE2	0.66	1.21	1	1
1:A:29:GLY:O	1:A:45:PRO:HG3	0.66	1.90	18	5
1:A:41:LEU:O	1:A:43:GLY:N	0.66	2.25	1	4
1:A:22:THR:OG1	1:A:22:THR:N	0.66	2.29	1	1
1:A:47:LYS:CD	1:A:47:LYS:HE3	0.65	1.21	1	1
1:A:41:LEU:HD23	1:A:54:ILE:CG2	0.65	2.20	12	5
1:A:32:THR:OG1	1:A:34:LEU:HD12	0.65	1.91	19	12
1:A:48:ASP:HB3	1:A:53:GLU:CD	0.65	2.16	1	5
1:A:47:LYS:NZ	1:A:47:LYS:HE3	0.65	1.34	1	1
1:A:50:VAL:HG23	1:A:53:GLU:OE1	0.65	1.92	14	1
1:A:22:THR:CG2	1:A:22:THR:HG1	0.64	1.37	1	1
1:A:29:GLY:O	1:A:33:GLY:HA2	0.64	1.91	10	8
1:A:55:LEU:CD2	1:A:55:LEU:CD1	0.64	0.67	1	1
1:A:22:THR:HB	1:A:23:PRO:HD2	0.63	1.68	20	3
1:A:32:THR:OG1	1:A:34:LEU:CD1	0.63	2.46	1	9
1:A:19:LYS:HA	1:A:40:SER:HA	0.63	1.68	9	7
1:A:22:THR:HG22	1:A:55:LEU:HD22	0.63	1.70	19	1
1:A:47:LYS:NZ	1:A:47:LYS:HE2	0.63	1.34	1	1
1:A:30:HIS:CG	1:A:43:GLY:HA3	0.63	2.28	7	15
1:A:51:PRO:HB3	1:A:52:PRO:HD3	0.62	1.71	1	1
1:A:30:HIS:O	1:A:45:PRO:HB3	0.62	1.94	1	15
1:A:47:LYS:CB	1:A:54:ILE:HD11	0.62	2.24	11	5
1:A:47:LYS:CG	1:A:47:LYS:CB	0.62	0.71	1	1
1:A:47:LYS:O	1:A:48:ASP:HB2	0.62	1.93	5	2
1:A:40:SER:O	1:A:41:LEU:HD23	0.61	1.95	11	3
1:A:19:LYS:O	1:A:41:LEU:HD11	0.61	1.95	8	2
1:A:50:VAL:CB	1:A:51:PRO:CD	0.61	2.79	3	5
1:A:40:SER:O	1:A:41:LEU:CB	0.61	2.48	1	15
1:A:43:GLY:O	1:A:44:CYS:O	0.61	2.19	18	13
1:A:46:HIS:O	1:A:47:LYS:HB3	0.61	1.93	1	1
1:A:44:CYS:SG	1:A:54:ILE:HG12	0.61	2.36	13	9
1:A:30:HIS:O	1:A:45:PRO:CD	0.60	2.49	6	16
1:A:29:GLY:O	1:A:30:HIS:C	0.60	2.40	1	13
1:A:47:LYS:O	1:A:48:ASP:CB	0.60	2.50	5	1
1:A:53:GLU:CD	1:A:54:ILE:H	0.60	2.05	21	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:GLY:O	1:A:53:GLU:N	0.60	2.34	20	1
1:A:19:LYS:HB2	1:A:39:ARG:O	0.59	1.97	11	1
1:A:51:PRO:HB2	1:A:52:PRO:HD3	0.59	1.73	14	5
1:A:19:LYS:HB2	1:A:21:PRO:HD2	0.59	1.74	7	1
1:A:22:THR:HG23	1:A:25:CYS:H	0.59	1.56	15	1
1:A:48:ASP:CB	1:A:53:GLU:HG3	0.59	2.28	18	2
1:A:32:THR:HG23	1:A:34:LEU:HD12	0.59	1.75	15	6
1:A:50:VAL:HB	1:A:51:PRO:HD2	0.58	1.73	3	4
1:A:30:HIS:O	1:A:45:PRO:CB	0.58	2.51	2	14
1:A:30:HIS:CE1	1:A:35:TYR:CD2	0.58	2.91	5	19
1:A:36:PRO:O	1:A:37:HIS:CG	0.58	2.56	17	21
1:A:30:HIS:O	1:A:45:PRO:CG	0.58	2.52	6	9
1:A:30:HIS:O	1:A:45:PRO:N	0.58	2.36	3	10
1:A:22:THR:HG22	1:A:23:PRO:HD2	0.58	1.75	1	2
1:A:25:CYS:HA	1:A:52:PRO:HA	0.58	1.74	17	1
1:A:30:HIS:C	1:A:45:PRO:HD3	0.58	2.24	5	2
1:A:53:GLU:CG	1:A:54:ILE:N	0.58	2.67	21	1
1:A:19:LYS:HB3	1:A:39:ARG:O	0.57	1.99	1	1
1:A:22:THR:OG1	1:A:23:PRO:HD2	0.57	1.99	17	6
1:A:46:HIS:O	1:A:47:LYS:HG3	0.57	1.99	4	2
1:A:48:ASP:HB3	1:A:50:VAL:HG22	0.57	1.77	15	1
1:A:35:TYR:CD1	1:A:35:TYR:N	0.57	2.73	6	20
1:A:48:ASP:O	1:A:49:ARG:O	0.57	2.22	13	3
1:A:30:HIS:CG	1:A:35:TYR:HB2	0.57	2.34	15	21
1:A:38:HIS:C	1:A:39:ARG:N	0.57	0.57	1	1
1:A:20:CYS:O	1:A:22:THR:HG23	0.57	2.00	20	1
1:A:20:CYS:N	1:A:40:SER:HA	0.56	2.14	11	2
1:A:22:THR:HG21	1:A:55:LEU:HD13	0.56	1.75	19	1
1:A:35:TYR:HB3	1:A:36:PRO:HD2	0.56	1.78	10	2
1:A:49:ARG:O	1:A:49:ARG:HG3	0.56	2.00	4	1
1:A:55:LEU:HD23	1:A:55:LEU:C	0.55	2.26	11	1
1:A:22:THR:HG23	1:A:24:GLY:H	0.55	1.59	17	1
1:A:21:PRO:HD3	1:A:40:SER:HA	0.55	1.78	19	1
1:A:20:CYS:H	1:A:40:SER:HA	0.55	1.61	19	2
1:A:46:HIS:O	1:A:47:LYS:CG	0.55	2.55	13	5
1:A:48:ASP:OD1	1:A:48:ASP:CA	0.55	2.44	1	1
1:A:24:GLY:CA	1:A:55:LEU:HD21	0.55	2.32	20	1
1:A:48:ASP:HB3	1:A:53:GLU:HG3	0.55	1.79	12	3
1:A:39:ARG:O	1:A:40:SER:CB	0.55	2.54	19	2
1:A:31:VAL:C	1:A:45:PRO:HG3	0.55	2.26	21	2
1:A:42:SER:CB	1:A:42:SER:HG	0.55	1.26	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:ASP:CB	1:A:53:GLU:HG2	0.55	2.31	1	3
1:A:46:HIS:HB3	1:A:53:GLU:CG	0.55	2.31	20	11
1:A:47:LYS:HA	1:A:54:ILE:HG13	0.55	1.78	13	7
1:A:46:HIS:CB	1:A:53:GLU:CA	0.55	2.85	18	6
1:A:48:ASP:CB	1:A:53:GLU:CD	0.54	2.80	1	3
1:A:50:VAL:N	1:A:51:PRO:HD2	0.54	2.18	5	1
1:A:55:LEU:C	1:A:55:LEU:HD13	0.54	2.27	8	1
1:A:25:CYS:HB2	1:A:53:GLU:O	0.54	2.03	16	8
1:A:46:HIS:CD2	1:A:53:GLU:HA	0.54	2.37	21	2
1:A:41:LEU:CD2	1:A:54:ILE:HG22	0.54	2.33	5	2
1:A:24:GLY:HA3	1:A:55:LEU:HD21	0.54	1.80	20	1
1:A:36:PRO:C	1:A:37:HIS:CG	0.53	2.86	19	21
1:A:55:LEU:CD2	1:A:55:LEU:HD11	0.53	0.92	1	1
1:A:38:HIS:ND1	1:A:44:CYS:HA	0.53	2.18	10	8
1:A:31:VAL:C	1:A:45:PRO:HB3	0.53	2.28	20	3
1:A:53:GLU:CG	1:A:54:ILE:H	0.53	2.15	21	1
1:A:30:HIS:O	1:A:45:PRO:CA	0.53	2.57	10	2
1:A:30:HIS:CG	1:A:35:TYR:CG	0.53	2.97	5	11
1:A:50:VAL:CB	1:A:51:PRO:HD3	0.52	2.34	2	1
1:A:35:TYR:N	1:A:35:TYR:CD1	0.52	2.77	1	1
1:A:30:HIS:CD2	1:A:38:HIS:HB3	0.52	2.40	4	13
1:A:48:ASP:O	1:A:50:VAL:HG23	0.52	2.05	7	2
1:A:48:ASP:CB	1:A:53:GLU:OE1	0.52	2.57	1	1
1:A:47:LYS:HG3	1:A:54:ILE:HD12	0.52	1.82	17	1
1:A:36:PRO:O	1:A:37:HIS:CB	0.51	2.57	17	20
1:A:47:LYS:CA	1:A:54:ILE:HD11	0.51	2.35	9	4
1:A:49:ARG:C	1:A:51:PRO:HD2	0.51	2.30	18	2
1:A:38:HIS:CE1	1:A:45:PRO:HD3	0.51	2.41	10	2
1:A:50:VAL:O	1:A:53:GLU:HG3	0.51	2.06	19	1
1:A:49:ARG:O	1:A:53:GLU:OE1	0.51	2.29	2	2
1:A:41:LEU:C	1:A:43:GLY:H	0.51	2.14	3	3
1:A:48:ASP:HB2	1:A:53:GLU:OE1	0.51	2.06	12	1
1:A:39:ARG:O	1:A:40:SER:HB3	0.50	2.05	1	3
1:A:19:LYS:HA	1:A:40:SER:HB2	0.50	1.82	7	1
1:A:20:CYS:H	1:A:21:PRO:HD3	0.50	1.65	1	1
1:A:40:SER:OG	1:A:40:SER:N	0.50	2.35	1	1
1:A:51:PRO:HD2	1:A:53:GLU:OE1	0.50	2.06	13	2
1:A:32:THR:HG1	1:A:34:LEU:HD12	0.50	1.66	21	2
1:A:39:ARG:CA	1:A:39:ARG:HG3	0.50	1.96	1	1
1:A:19:LYS:C	1:A:21:PRO:CD	0.50	2.85	12	1
1:A:50:VAL:N	1:A:55:LEU:HB2	0.50	2.22	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:CYS:HB2	1:A:41:LEU:HG	0.50	1.82	13	1
1:A:21:PRO:HD3	1:A:39:ARG:HA	0.50	1.82	13	1
1:A:32:THR:O	1:A:34:LEU:HG	0.50	2.07	12	1
1:A:24:GLY:HA3	1:A:52:PRO:HA	0.50	1.83	19	1
1:A:38:HIS:CD2	1:A:39:ARG:N	0.50	2.79	21	5
1:A:27:GLY:HA2	1:A:38:HIS:CE1	0.50	2.42	19	1
1:A:47:LYS:CE	1:A:47:LYS:CD	0.49	0.66	1	1
1:A:31:VAL:HA	1:A:45:PRO:HB3	0.49	1.84	21	2
1:A:47:LYS:N	1:A:53:GLU:CG	0.49	2.75	21	1
1:A:20:CYS:SG	1:A:21:PRO:HD2	0.49	2.47	17	1
1:A:21:PRO:CG	1:A:54:ILE:HA	0.49	2.37	17	1
1:A:55:LEU:HD22	1:A:55:LEU:HD13	0.49	0.50	1	1
1:A:50:VAL:HG23	1:A:51:PRO:CD	0.49	2.37	21	1
1:A:20:CYS:O	1:A:55:LEU:HD21	0.49	2.08	19	1
1:A:50:VAL:HG23	1:A:51:PRO:HD2	0.49	1.82	21	1
1:A:22:THR:HG22	1:A:24:GLY:H	0.49	1.67	21	1
1:A:19:LYS:CA	1:A:40:SER:HA	0.49	2.37	11	2
1:A:50:VAL:HA	1:A:55:LEU:HD12	0.49	1.84	10	1
1:A:22:THR:HB	1:A:25:CYS:HB2	0.48	1.85	8	1
1:A:19:LYS:HB3	1:A:40:SER:OG	0.48	2.09	19	1
1:A:19:LYS:CB	1:A:21:PRO:HD2	0.48	2.38	16	2
1:A:22:THR:HB	1:A:55:LEU:HD13	0.48	1.84	6	1
1:A:47:LYS:CG	1:A:54:ILE:HD11	0.48	2.37	14	1
1:A:40:SER:CB	1:A:40:SER:HG	0.48	1.19	1	1
1:A:49:ARG:O	1:A:50:VAL:CB	0.48	2.61	4	4
1:A:30:HIS:O	1:A:45:PRO:HG3	0.48	2.07	5	2
1:A:47:LYS:O	1:A:47:LYS:CG	0.48	2.60	11	4
1:A:20:CYS:SG	1:A:41:LEU:HD23	0.48	2.48	5	3
1:A:40:SER:C	1:A:41:LEU:HD23	0.48	2.34	19	1
1:A:20:CYS:H	1:A:21:PRO:CD	0.48	2.10	1	2
1:A:50:VAL:H	1:A:55:LEU:HD13	0.48	1.68	13	2
1:A:22:THR:HB	1:A:25:CYS:CB	0.48	2.37	8	1
1:A:22:THR:OG1	1:A:23:PRO:CD	0.48	2.61	17	2
1:A:52:PRO:O	1:A:53:GLU:HG3	0.48	2.09	9	4
1:A:44:CYS:SG	1:A:53:GLU:O	0.48	2.72	19	2
1:A:29:GLY:O	1:A:45:PRO:HB3	0.48	2.09	19	2
1:A:50:VAL:C	1:A:52:PRO:HD2	0.48	2.34	12	2
1:A:46:HIS:CD2	1:A:53:GLU:O	0.48	2.67	6	3
1:A:46:HIS:HB2	1:A:53:GLU:HG2	0.48	1.84	21	1
1:A:48:ASP:H	1:A:53:GLU:CD	0.48	2.17	21	1
1:A:30:HIS:CE1	1:A:42:SER:O	0.48	2.67	21	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:VAL:HB	1:A:43:GLY:O	0.48	2.09	3	1
1:A:50:VAL:HG23	1:A:52:PRO:HD2	0.48	1.85	12	2
1:A:49:ARG:O	1:A:51:PRO:CD	0.47	2.61	13	4
1:A:38:HIS:CG	1:A:44:CYS:H	0.47	2.27	2	6
1:A:50:VAL:N	1:A:53:GLU:OE2	0.47	2.46	19	1
1:A:46:HIS:HB3	1:A:53:GLU:OE1	0.47	2.09	20	2
1:A:28:THR:O	1:A:45:PRO:HG3	0.47	2.09	19	1
1:A:51:PRO:N	1:A:55:LEU:HD13	0.47	2.25	14	1
1:A:22:THR:HG21	1:A:22:THR:HG1	0.47	1.09	1	1
1:A:38:HIS:C	1:A:39:ARG:CB	0.47	2.77	1	1
1:A:48:ASP:HB2	1:A:53:GLU:HG2	0.47	1.87	1	2
1:A:39:ARG:O	1:A:40:SER:HB2	0.47	2.09	7	2
1:A:49:ARG:O	1:A:51:PRO:HD3	0.47	2.09	11	2
1:A:43:GLY:O	1:A:44:CYS:C	0.47	2.57	21	2
1:A:47:LYS:H	1:A:54:ILE:CG1	0.47	2.23	15	3
1:A:24:GLY:C	1:A:52:PRO:HB3	0.47	2.35	11	1
1:A:53:GLU:HG2	1:A:54:ILE:HG13	0.47	1.87	21	1
1:A:51:PRO:O	1:A:53:GLU:CD	0.46	2.58	4	1
1:A:28:THR:HA	1:A:37:HIS:CD2	0.46	2.45	16	3
1:A:28:THR:HA	1:A:37:HIS:CG	0.46	2.45	16	1
1:A:50:VAL:O	1:A:51:PRO:C	0.46	2.58	7	6
1:A:40:SER:C	1:A:41:LEU:HD12	0.46	2.36	12	1
1:A:41:LEU:O	1:A:42:SER:C	0.46	2.58	12	6
1:A:52:PRO:O	1:A:53:GLU:CG	0.46	2.64	9	4
1:A:19:LYS:C	1:A:21:PRO:HD3	0.46	2.35	15	3
1:A:46:HIS:HD2	1:A:53:GLU:O	0.46	1.94	19	2
1:A:30:HIS:ND1	1:A:35:TYR:CG	0.46	2.82	10	8
1:A:40:SER:C	1:A:40:SER:HG	0.46	2.14	1	1
1:A:49:ARG:O	1:A:51:PRO:HD2	0.46	2.11	16	3
1:A:30:HIS:HD2	1:A:37:HIS:O	0.46	1.93	16	6
1:A:31:VAL:HA	1:A:45:PRO:CB	0.46	2.40	21	2
1:A:50:VAL:HA	1:A:55:LEU:HA	0.46	1.87	5	1
1:A:51:PRO:HD2	1:A:53:GLU:HG2	0.46	1.86	20	1
1:A:46:HIS:HB2	1:A:53:GLU:HA	0.46	1.87	2	2
1:A:50:VAL:HG12	1:A:51:PRO:HD3	0.46	1.87	3	1
1:A:30:HIS:CE1	1:A:35:TYR:CE2	0.46	3.04	5	1
1:A:47:LYS:O	1:A:47:LYS:HG3	0.46	2.11	9	2
1:A:49:ARG:C	1:A:50:VAL:HG22	0.46	2.36	21	1
1:A:30:HIS:O	1:A:45:PRO:HD3	0.46	2.11	5	3
1:A:50:VAL:CG1	1:A:51:PRO:CD	0.46	2.92	5	1
1:A:22:THR:O	1:A:24:GLY:N	0.45	2.49	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:THR:HA	1:A:37:HIS:HB3	0.45	1.87	19	1
1:A:31:VAL:HA	1:A:44:CYS:C	0.45	2.36	16	4
1:A:28:THR:OG1	1:A:37:HIS:CD2	0.45	2.69	16	8
1:A:48:ASP:O	1:A:49:ARG:CG	0.45	2.64	7	1
1:A:20:CYS:HB2	1:A:40:SER:C	0.45	2.35	11	1
1:A:35:TYR:HB3	1:A:36:PRO:CD	0.45	2.42	12	1
1:A:32:THR:OG1	1:A:34:LEU:HG	0.45	2.12	1	1
1:A:30:HIS:ND1	1:A:35:TYR:CD1	0.45	2.85	5	2
1:A:32:THR:OG1	1:A:34:LEU:CG	0.45	2.64	5	9
1:A:49:ARG:O	1:A:50:VAL:C	0.45	2.59	6	2
1:A:50:VAL:CG1	1:A:51:PRO:HD3	0.45	2.41	2	2
1:A:49:ARG:CG	1:A:50:VAL:N	0.45	2.77	8	1
1:A:19:LYS:HA	1:A:39:ARG:O	0.45	2.10	14	1
1:A:41:LEU:C	1:A:43:GLY:N	0.45	2.75	3	6
1:A:31:VAL:HB	1:A:43:GLY:HA2	0.45	1.88	19	3
1:A:19:LYS:N	1:A:19:LYS:CD	0.45	2.80	8	1
1:A:31:VAL:HA	1:A:45:PRO:CG	0.45	2.42	21	2
1:A:48:ASP:N	1:A:53:GLU:OE1	0.45	2.50	10	1
1:A:50:VAL:O	1:A:53:GLU:OE1	0.45	2.35	14	3
1:A:38:HIS:O	1:A:40:SER:N	0.45	2.49	8	3
1:A:40:SER:HB2	1:A:40:SER:HG	0.44	1.29	1	1
1:A:52:PRO:O	1:A:53:GLU:CD	0.44	2.60	14	2
1:A:46:HIS:CB	1:A:53:GLU:CG	0.44	2.95	21	1
1:A:31:VAL:N	1:A:43:GLY:C	0.44	2.75	10	4
1:A:30:HIS:CE1	1:A:43:GLY:CA	0.44	3.00	4	2
1:A:49:ARG:O	1:A:50:VAL:HB	0.44	2.12	4	1
1:A:50:VAL:HG12	1:A:52:PRO:HD2	0.44	1.87	7	1
1:A:19:LYS:HB2	1:A:40:SER:HA	0.44	1.88	13	3
1:A:38:HIS:CG	1:A:39:ARG:N	0.44	2.85	11	1
1:A:22:THR:CB	1:A:22:THR:HG1	0.44	1.15	1	1
1:A:22:THR:CG2	1:A:23:PRO:HD2	0.44	2.42	8	2
1:A:48:ASP:O	1:A:49:ARG:C	0.44	2.50	1	2
1:A:21:PRO:HD3	1:A:40:SER:CA	0.44	2.43	19	1
1:A:47:LYS:HE2	1:A:54:ILE:HD12	0.44	1.90	17	1
1:A:19:LYS:HA	1:A:40:SER:CB	0.44	2.43	7	1
1:A:49:ARG:HD2	1:A:50:VAL:HG23	0.44	1.88	13	1
1:A:30:HIS:CG	1:A:35:TYR:CB	0.44	3.01	15	1
1:A:29:GLY:C	1:A:30:HIS:O	0.43	2.53	1	8
1:A:55:LEU:CD1	1:A:55:LEU:HD21	0.43	0.97	1	1
1:A:50:VAL:HG13	1:A:55:LEU:CD1	0.43	2.43	6	1
1:A:50:VAL:C	1:A:52:PRO:CD	0.43	2.91	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:THR:CB	1:A:23:PRO:HD2	0.43	2.43	16	3
1:A:52:PRO:C	1:A:53:GLU:HG2	0.43	2.38	15	2
1:A:38:HIS:O	1:A:39:ARG:C	0.43	2.61	4	2
1:A:49:ARG:HG3	1:A:50:VAL:HG23	0.43	1.90	8	1
1:A:29:GLY:O	1:A:45:PRO:CG	0.43	2.63	18	1
1:A:42:SER:HG	1:A:42:SER:N	0.43	2.11	1	1
1:A:46:HIS:CB	1:A:53:GLU:CB	0.43	2.96	4	1
1:A:48:ASP:H	1:A:53:GLU:CG	0.43	2.26	21	1
1:A:32:THR:CG2	1:A:34:LEU:CD1	0.43	2.92	7	2
1:A:25:CYS:N	1:A:51:PRO:O	0.43	2.51	17	1
1:A:52:PRO:C	1:A:53:GLU:CD	0.43	2.87	20	1
1:A:55:LEU:CD2	1:A:55:LEU:HB2	0.43	2.17	1	1
1:A:20:CYS:SG	1:A:54:ILE:HG23	0.43	2.53	15	2
1:A:35:TYR:C	1:A:37:HIS:H	0.43	2.20	10	1
1:A:50:VAL:N	1:A:55:LEU:HD13	0.43	2.29	13	1
1:A:48:ASP:O	1:A:49:ARG:HG3	0.43	2.14	7	1
1:A:29:GLY:O	1:A:45:PRO:HD3	0.43	2.14	16	1
1:A:38:HIS:C	1:A:40:SER:N	0.43	2.77	8	7
1:A:46:HIS:HB2	1:A:53:GLU:CA	0.42	2.44	19	2
1:A:48:ASP:HB3	1:A:53:GLU:OE2	0.42	2.14	14	1
1:A:38:HIS:O	1:A:41:LEU:HG	0.42	2.14	19	1
1:A:48:ASP:HA	1:A:54:ILE:CG1	0.42	2.44	5	1
1:A:29:GLY:C	1:A:33:GLY:HA2	0.42	2.39	11	1
1:A:20:CYS:CB	1:A:40:SER:HA	0.42	2.43	20	1
1:A:46:HIS:HB2	1:A:53:GLU:CG	0.42	2.45	21	1
1:A:22:THR:C	1:A:24:GLY:N	0.42	2.77	20	4
1:A:25:CYS:CB	1:A:53:GLU:O	0.42	2.68	16	1
1:A:20:CYS:O	1:A:21:PRO:C	0.42	2.62	17	1
1:A:21:PRO:CD	1:A:40:SER:HA	0.42	2.43	19	1
1:A:47:LYS:HG3	1:A:54:ILE:CD1	0.42	2.44	19	1
1:A:51:PRO:C	1:A:53:GLU:OE1	0.42	2.62	3	1
1:A:45:PRO:O	1:A:46:HIS:C	0.42	2.63	5	1
1:A:22:THR:HG21	1:A:55:LEU:HD22	0.42	1.90	6	1
1:A:24:GLY:HA3	1:A:51:PRO:C	0.42	2.40	14	1
1:A:27:GLY:O	1:A:37:HIS:HB3	0.42	2.14	21	1
1:A:47:LYS:HZ1	1:A:47:LYS:HE3	0.42	1.26	1	1
1:A:49:ARG:HA	1:A:55:LEU:HB3	0.42	1.92	20	1
1:A:47:LYS:HG3	1:A:47:LYS:O	0.42	2.15	4	1
1:A:22:THR:HG23	1:A:23:PRO:HD2	0.42	1.91	8	1
1:A:30:HIS:CD2	1:A:37:HIS:O	0.42	2.73	16	2
1:A:48:ASP:O	1:A:49:ARG:CB	0.41	2.45	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:PRO:CD	1:A:55:LEU:HD23	0.41	2.37	7	1
1:A:47:LYS:CG	1:A:54:ILE:CD1	0.41	2.99	14	2
1:A:25:CYS:SG	1:A:26:ASP:N	0.41	2.93	3	1
1:A:41:LEU:HD12	1:A:42:SER:N	0.41	2.30	4	2
1:A:49:ARG:HA	1:A:55:LEU:HA	0.41	1.92	10	1
1:A:47:LYS:HB2	1:A:54:ILE:HD11	0.41	1.92	1	1
1:A:50:VAL:O	1:A:51:PRO:O	0.41	2.38	6	1
1:A:25:CYS:N	1:A:52:PRO:HA	0.41	2.30	21	2
1:A:47:LYS:HA	1:A:54:ILE:CD1	0.41	2.46	15	1
1:A:50:VAL:HG12	1:A:51:PRO:CD	0.41	2.45	3	1
1:A:51:PRO:C	1:A:53:GLU:OE2	0.41	2.63	20	1
1:A:48:ASP:N	1:A:53:GLU:HG3	0.41	2.31	21	1
1:A:52:PRO:O	1:A:53:GLU:OE1	0.41	2.39	6	1
1:A:25:CYS:HA	1:A:52:PRO:C	0.41	2.41	20	1
1:A:24:GLY:N	1:A:51:PRO:O	0.41	2.53	12	1
1:A:49:ARG:C	1:A:49:ARG:HG3	0.41	2.30	1	1
1:A:24:GLY:O	1:A:52:PRO:HB3	0.41	2.16	10	1
1:A:50:VAL:HA	1:A:55:LEU:HD13	0.41	1.92	3	1
1:A:50:VAL:N	1:A:51:PRO:CD	0.41	2.84	6	1
1:A:25:CYS:SG	1:A:46:HIS:CD2	0.41	3.14	15	2
1:A:47:LYS:N	1:A:54:ILE:HD11	0.40	2.31	8	1
1:A:46:HIS:O	1:A:47:LYS:CB	0.40	2.69	12	1
1:A:50:VAL:HA	1:A:55:LEU:HD23	0.40	1.92	5	1
1:A:24:GLY:C	1:A:52:PRO:CB	0.40	2.95	11	1
1:A:30:HIS:CD2	1:A:43:GLY:HA3	0.40	2.51	15	1
1:A:35:TYR:N	1:A:35:TYR:HD1	0.40	2.14	2	1
1:A:50:VAL:CG1	1:A:51:PRO:HD2	0.40	2.47	7	1
1:A:44:CYS:SG	1:A:54:ILE:CG2	0.40	3.06	17	1
1:A:55:LEU:CD2	1:A:55:LEU:HD13	0.40	1.07	1	1
1:A:49:ARG:O	1:A:51:PRO:N	0.40	2.54	8	1
1:A:55:LEU:HD22	1:A:55:LEU:O	0.40	2.16	8	1
1:A:53:GLU:OE1	1:A:54:ILE:HG13	0.40	2.16	19	1
1:A:53:GLU:HG2	1:A:54:ILE:CG1	0.40	2.47	21	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	37/63 (59%)	15±2 (42±7%)	13±3 (35±7%)	9±2 (24±4%)	0	1
All	All	777/1323 (59%)	324 (42%)	270 (35%)	183 (24%)	0	1

All 25 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	30	HIS	21
1	A	44	CYS	21
1	A	37	HIS	20
1	A	21	PRO	16
1	A	40	SER	13
1	A	50	VAL	12
1	A	51	PRO	10
1	A	52	PRO	10
1	A	39	ARG	8
1	A	49	ARG	8
1	A	53	GLU	8
1	A	41	LEU	6
1	A	55	LEU	4
1	A	29	GLY	4
1	A	43	GLY	4
1	A	47	LYS	3
1	A	23	PRO	3
1	A	42	SER	2
1	A	48	ASP	2
1	A	20	CYS	2
1	A	46	HIS	2
1	A	19	LYS	1
1	A	45	PRO	1
1	A	25	CYS	1
1	A	54	ILE	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	32/57 (56%)	23±2 (73±5%)	9±2 (27±5%)	2	21
All	All	672/1197 (56%)	492 (73%)	180 (27%)	2	21

All 19 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	28	THR	21
1	A	35	TYR	21
1	A	54	ILE	21
1	A	22	THR	17
1	A	41	LEU	17
1	A	47	LYS	14
1	A	19	LYS	12
1	A	49	ARG	11
1	A	39	ARG	10
1	A	50	VAL	7
1	A	48	ASP	7
1	A	42	SER	6
1	A	55	LEU	5
1	A	53	GLU	5
1	A	32	THR	2
1	A	40	SER	1
1	A	20	CYS	1
1	A	37	HIS	1
1	A	45	PRO	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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	1-A	22

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	24:GLY	C	25:CYS	N	1.20
1	A	61:VAL	C	62:LEU	N	1.20
1	A	23:PRO	C	24:GLY	N	1.17
1	A	28:THR	C	29:GLY	N	1.16
1	A	21:PRO	C	22:THR	N	1.14
1	A	51:PRO	C	52:PRO	N	1.13
1	A	48:ASP	C	49:ARG	N	1.06
1	A	20:CYS	C	21:PRO	N	1.00
1	A	41:LEU	C	42:SER	N	0.99
1	A	57:MET	C	58:HIS	N	0.97
1	A	17:GLU	C	18:SER	N	0.95
1	A	49:ARG	C	50:VAL	N	0.94
1	A	55:LEU	C	56:ALA	N	0.89
1	A	60:ASN	C	61:VAL	N	0.76
1	A	50:VAL	C	51:PRO	N	0.75
1	A	16:ARG	C	17:GLU	N	0.74
1	A	62:LEU	C	63:LYS	N	0.72
1	A	59:GLU	C	60:ASN	N	0.70
1	A	18:SER	C	19:LYS	N	0.66
1	A	56:ALA	C	57:MET	N	0.65
1	A	38:HIS	C	39:ARG	N	0.57
1	A	58:HIS	C	59:GLU	N	0.55

7 Chemical shift validation

No chemical shift data were provided