



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 03:49 AM UTC

PDB ID : 2JMV / pdb_00002jmv
Title : Solution structure of scytovirin refined against residual dipolar couplings
Authors : McFeeters, R.L.; Byrd, R.A.
Deposited on : 2006-12-07

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

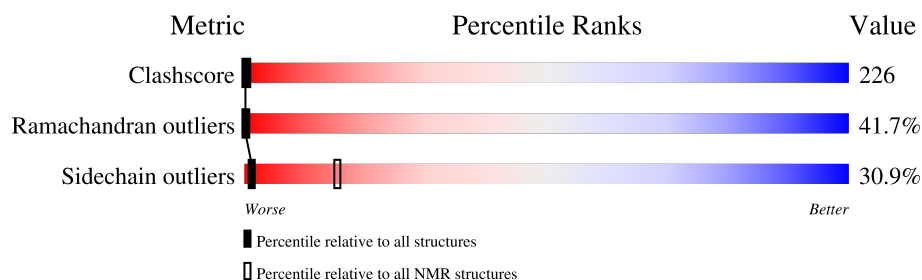
1 Overall quality at a glance

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	95	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:1-A:60, A:65-A:80, A:85-A:94 (86)	0.41	3

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 6 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1258 atoms, of which 590 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Scytovirin.

Mol	Chain	Residues	Atoms						Trace
1	A	94	Total	C	H	N	O	S	0
			1258	389	590	131	138	10	

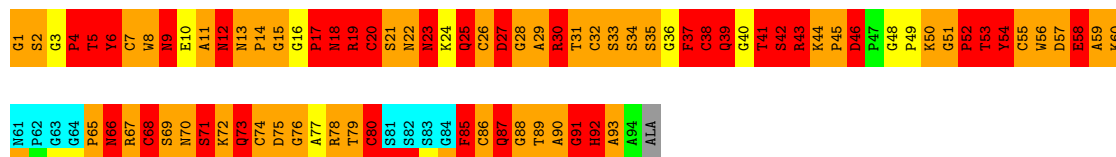
4 Residue-property plots [i](#)

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: Scytovirin

Chain A: 



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: Scytovirin

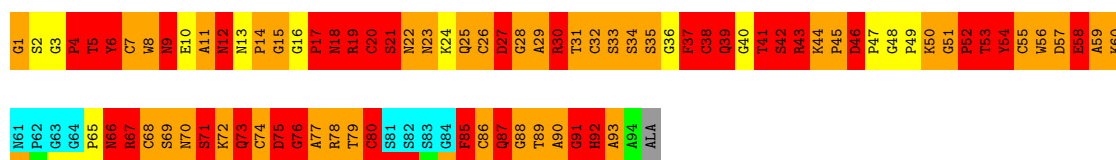
Chain A: 



4.2.2 Score per residue for model 2

- Molecule 1: Scytovirin

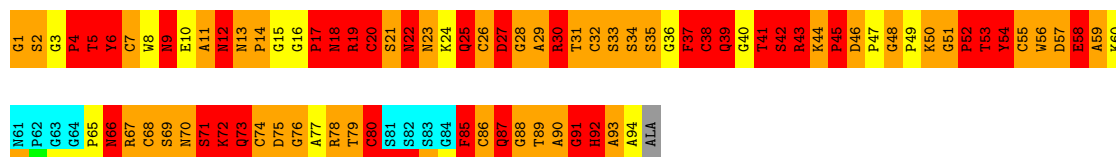
Chain A: 



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Scytovirin

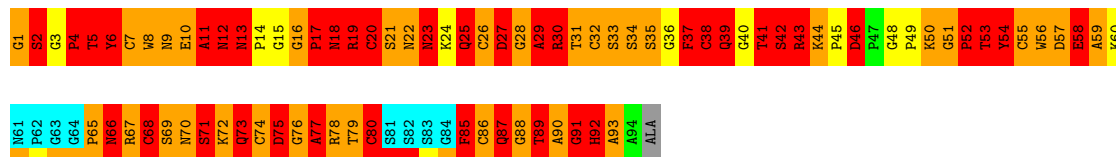
Chain A: 15% 41% 35% 8%



4.2.4 Score per residue for model 4

- Molecule 1: Scytovirin

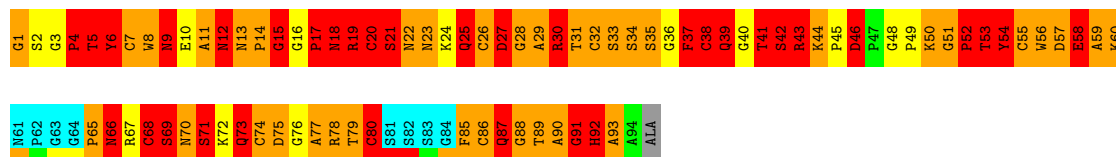
Chain A: 11% 37% 41% 8%



4.2.5 Score per residue for model 5

- Molecule 1: Scytovirin

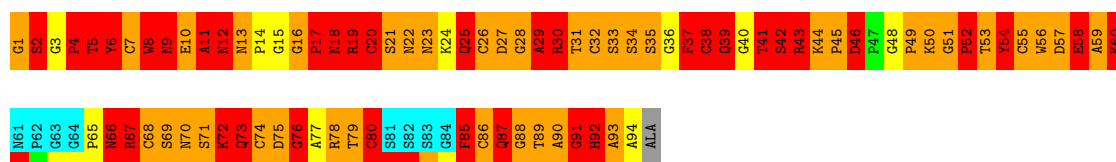
Chain A: 14% 39% 36% 8%



4.2.6 Score per residue for model 6

- Molecule 1: Scytovirin

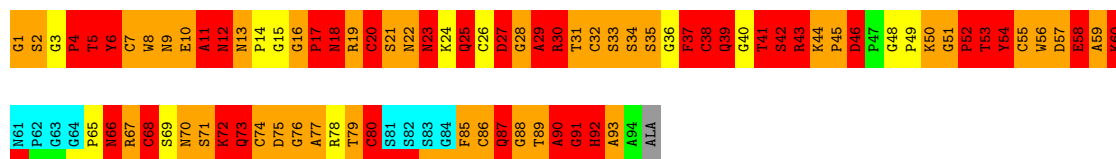
Chain A: 11% 41% 38% 8%



4.2.7 Score per residue for model 7

- Molecule 1: Scytovirin

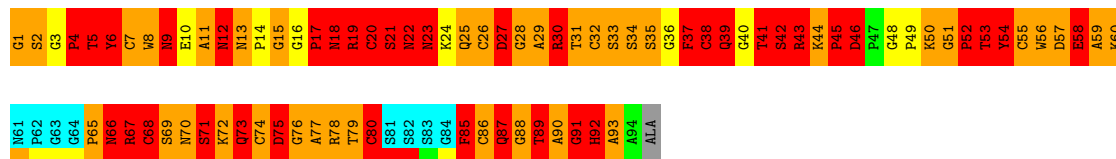
Chain A: . 13% 40% 36% 8% .



4.2.8 Score per residue for model 8

- Molecule 1: Scytovirin

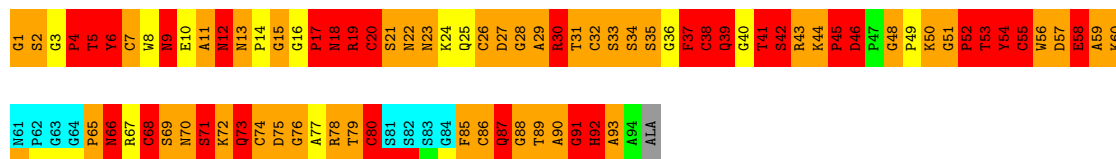
Chain A: . 9% 39% 40% 8% .



4.2.9 Score per residue for model 9

- Molecule 1: Scytovirin

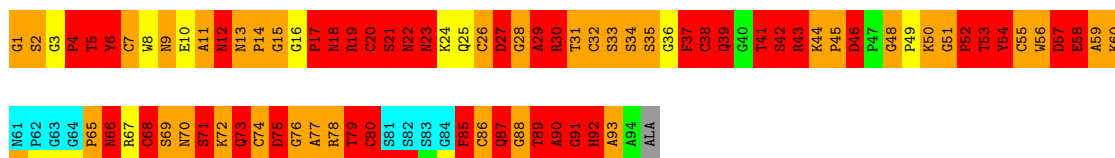
Chain A: . 13% 44% 32% 8% .



4.2.10 Score per residue for model 10

- Molecule 1: Scytovirin

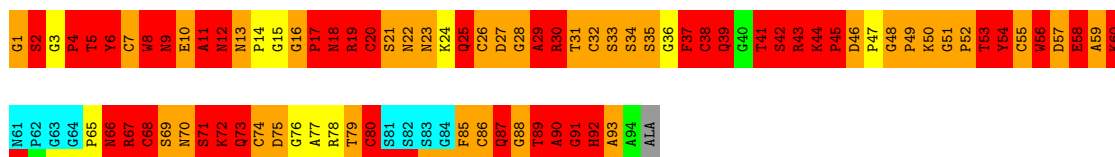
Chain A: . 9% 37% 41% 8% .



4.2.11 Score per residue for model 11

- Molecule 1: Scytovirin

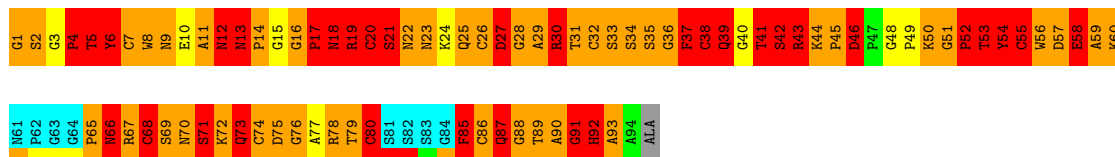
Chain A: . 11% 36% 42% 8% .



4.2.12 Score per residue for model 12

- Molecule 1: Scytovirin

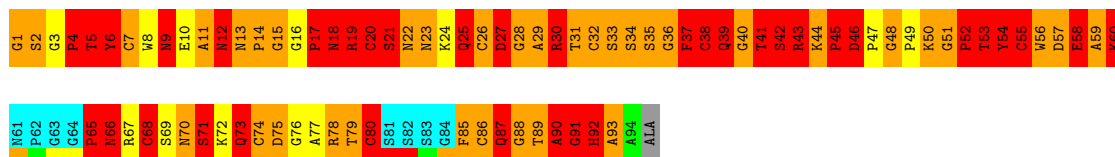
Chain A: . 8% 45% 35% 8% .



4.2.13 Score per residue for model 13

- Molecule 1: Scytovirin

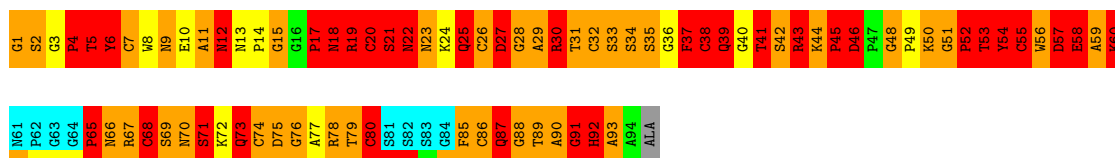
Chain A: . 13% 38% 39% 8% .



4.2.14 Score per residue for model 14

- Molecule 1: Scytovirin

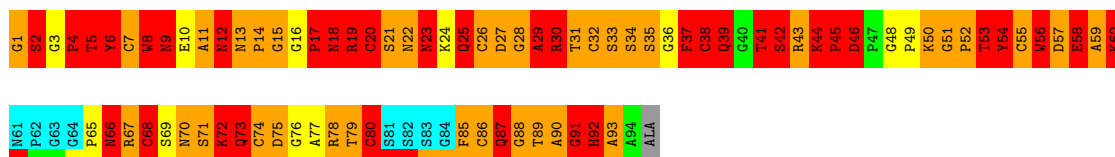
Chain A: . 12% 39% 37% 8% .



4.2.15 Score per residue for model 15

- Molecule 1: Scytovirin

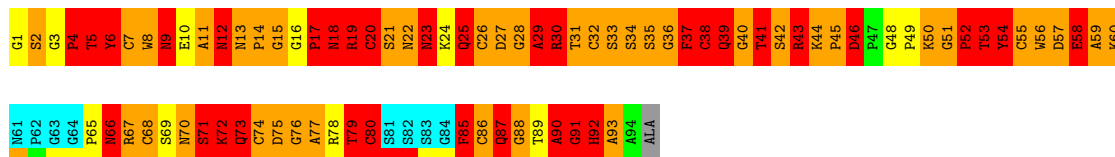
Chain A: . 12% 38% 38% 8% .



4.2.16 Score per residue for model 16

- Molecule 1: Scytovirin

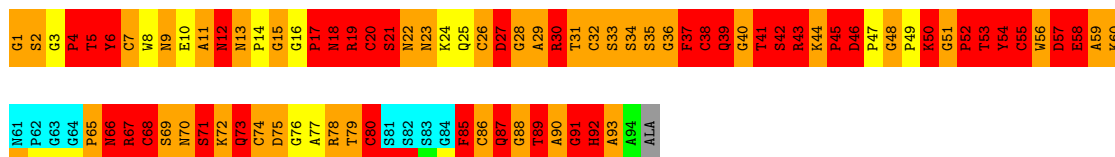
Chain A: . 12% 41% 36% 8% .



4.2.17 Score per residue for model 17

- Molecule 1: Scytovirin

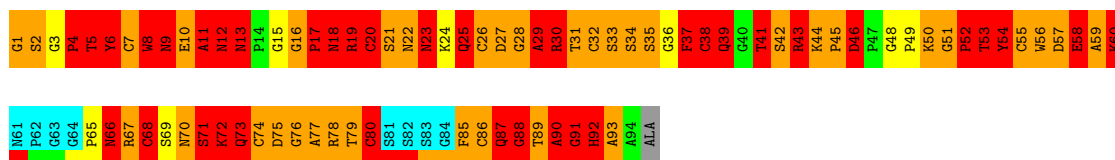
Chain A: . 12% 39% 39% 8% .



4.2.18 Score per residue for model 18

- Molecule 1: Scytovirin

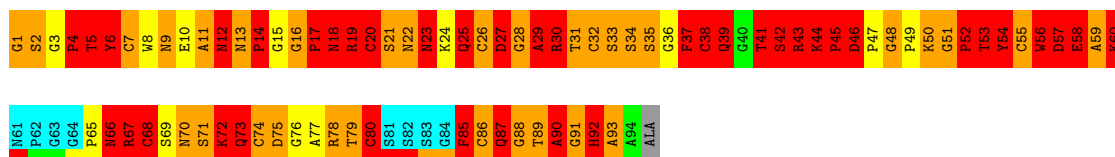
Chain A: . 8% 38% 40% 8% .



4.2.19 Score per residue for model 19

- Molecule 1: Scytovirin

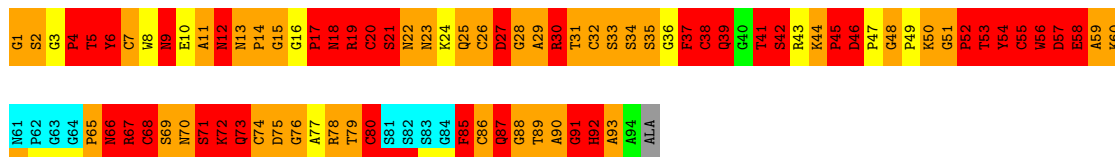
Chain A: • 13% 34% 42% 8% •



4.2.20 Score per residue for model 20

- Molecule 1: Scytovirin

Chain A: • 11% 39% 39% 8% •



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 200 calculated structures, 20 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
X-PLOR NIH	structure solution	2.10
X-PLOR NIH	refinement	2.10
X-PLOR NIH	structure solution	2.14
X-PLOR NIH	refinement	2.14

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	4.37±0.05	127±6/639 (19.9± 0.9%)	1.65±0.03	7±1/863 (0.8± 0.1%)
All	All	4.37	2548/12780 (19.9%)	1.65	135/17260 (0.8%)

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	6	TYR	CA-C	-21.95	1.23	1.52	10	20
1	A	74	CYS	N-CA	19.22	1.71	1.46	7	20
1	A	19	ARG	C-N	18.09	1.59	1.33	17	20
1	A	91	GLY	CA-C	18.07	1.77	1.51	2	20
1	A	26	CYS	CA-C	18.03	1.63	1.53	16	19
1	A	19	ARG	CA-C	-17.28	1.29	1.52	13	20
1	A	31	THR	C-O	-17.18	1.04	1.23	16	20
1	A	42	SER	CA-C	-15.96	1.35	1.53	18	20
1	A	92	HIS	N-CA	15.05	1.65	1.46	2	20
1	A	72	LYS	C-N	-14.88	1.12	1.33	2	20
1	A	44	LYS	CA-C	-14.50	1.34	1.52	9	20
1	A	85	PHE	N-CA	-13.82	1.28	1.46	20	20
1	A	1	GLY	C-N	13.66	1.50	1.33	9	19
1	A	34	SER	C-N	13.56	1.52	1.33	16	20
1	A	37	PHE	C-N	13.52	1.52	1.33	9	20
1	A	32	CYS	N-CA	13.49	1.61	1.46	19	20
1	A	5	THR	C-N	13.46	1.52	1.33	5	20
1	A	60	LYS	CA-C	-13.45	1.35	1.53	2	17
1	A	86	CYS	N-CA	13.06	1.62	1.46	17	20
1	A	75	ASP	N-CA	13.03	1.63	1.45	2	20
1	A	56	TRP	N-CA	-12.96	1.35	1.46	8	17
1	A	85	PHE	C-O	-12.59	1.08	1.24	17	20
1	A	7	CYS	N-CA	-12.51	1.28	1.46	2	20
1	A	6	TYR	CB-CG	12.44	1.79	1.51	5	20
1	A	19	ARG	N-CA	-12.40	1.30	1.46	20	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	41	THR	CA-C	12.39	1.68	1.52	8	20
1	A	4	PRO	CA-C	-12.38	1.34	1.52	10	20
1	A	30	ARG	CA-CB	12.29	1.74	1.53	1	17
1	A	51	GLY	N-CA	-12.16	1.28	1.44	7	20
1	A	79	THR	CA-C	-12.02	1.39	1.53	2	20
1	A	59	ALA	C-O	-11.96	1.10	1.24	18	12
1	A	28	GLY	CA-C	11.75	1.68	1.51	15	20
1	A	46	ASP	CA-CB	11.71	1.69	1.53	9	19
1	A	11	ALA	N-CA	-11.60	1.32	1.46	2	20
1	A	76	GLY	C-O	-11.58	1.14	1.24	4	6
1	A	91	GLY	N-CA	11.57	1.62	1.45	17	20
1	A	68	CYS	CA-C	-11.56	1.37	1.52	17	20
1	A	1	GLY	N-CA	-11.49	1.27	1.45	13	19
1	A	12	ASN	CA-C	11.40	1.68	1.52	19	20
1	A	30	ARG	CA-C	11.35	1.68	1.52	17	20
1	A	39	GLN	C-O	-11.27	1.09	1.23	16	20
1	A	73	GLN	C-O	-11.25	1.09	1.24	15	20
1	A	56	TRP	C-N	11.24	1.49	1.33	14	20
1	A	73	GLN	CA-CB	11.21	1.72	1.53	7	20
1	A	37	PHE	N-CA	-11.13	1.31	1.46	16	20
1	A	22	ASN	CA-C	-11.12	1.39	1.52	18	20
1	A	34	SER	CA-C	11.12	1.66	1.52	5	20
1	A	51	GLY	C-O	-11.12	1.08	1.24	13	20
1	A	74	CYS	C-N	11.10	1.48	1.34	2	20
1	A	54	TYR	C-N	11.04	1.49	1.33	6	17
1	A	31	THR	CA-C	-10.92	1.39	1.52	5	19
1	A	70	ASN	CA-C	-10.84	1.39	1.52	7	20
1	A	27	ASP	CA-C	-10.80	1.39	1.52	18	19
1	A	26	CYS	N-CA	10.75	1.52	1.46	10	14
1	A	34	SER	N-CA	-10.64	1.33	1.46	16	19
1	A	87	GLN	N-CA	-10.62	1.32	1.46	19	7
1	A	33	SER	C-N	-10.58	1.19	1.33	16	20
1	A	21	SER	N-CA	10.46	1.57	1.46	18	20
1	A	79	THR	C-O	-10.30	1.11	1.23	19	8
1	A	55	CYS	N-CA	10.23	1.60	1.46	8	20
1	A	17	PRO	C-N	10.21	1.48	1.33	8	17
1	A	9	ASN	C-N	-10.14	1.20	1.33	16	18
1	A	15	GLY	C-N	-10.11	1.18	1.33	1	19
1	A	80	CYS	C-N	-10.03	1.20	1.33	1	15
1	A	32	CYS	CA-CB	9.96	1.67	1.53	13	20
1	A	71	SER	CA-C	9.91	1.66	1.52	13	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	15	GLY	C-O	-9.90	1.10	1.23	14	1
1	A	43	ARG	CA-C	-9.90	1.39	1.52	7	17
1	A	17	PRO	CA-C	-9.79	1.38	1.52	20	20
1	A	54	TYR	N-CA	9.71	1.58	1.46	19	11
1	A	53	THR	C-N	-9.63	1.20	1.33	7	20
1	A	26	CYS	C-N	-9.53	1.19	1.33	18	4
1	A	86	CYS	CA-CB	-9.41	1.39	1.53	3	15
1	A	75	ASP	CG-OD1	-9.29	1.07	1.25	3	12
1	A	11	ALA	C-N	-9.28	1.20	1.33	5	16
1	A	45	PRO	C-N	-9.28	1.20	1.33	19	3
1	A	30	ARG	C-N	-9.26	1.21	1.33	5	11
1	A	59	ALA	C-N	9.18	1.46	1.33	3	14
1	A	45	PRO	CA-C	-9.17	1.39	1.52	19	12
1	A	79	THR	C-N	9.17	1.46	1.33	15	13
1	A	31	THR	N-CA	-9.14	1.34	1.46	11	14
1	A	68	CYS	C-N	-9.05	1.21	1.33	10	20
1	A	18	ASN	C-N	8.98	1.46	1.33	11	13
1	A	44	LYS	C-O	-8.96	1.12	1.24	9	15
1	A	59	ALA	CA-CB	-8.85	1.40	1.53	4	18
1	A	35	SER	CA-C	-8.84	1.41	1.52	6	20
1	A	86	CYS	C-N	8.82	1.46	1.33	5	14
1	A	80	CYS	CA-C	-8.79	1.41	1.52	3	20
1	A	5	THR	C-O	-8.77	1.12	1.24	6	20
1	A	50	LYS	CA-CB	8.77	1.66	1.53	7	19
1	A	35	SER	N-CA	-8.77	1.34	1.46	17	20
1	A	72	LYS	CA-C	-8.71	1.40	1.52	10	13
1	A	15	GLY	N-CA	8.59	1.57	1.45	19	8
1	A	93	ALA	CA-CB	8.56	1.64	1.53	4	12
1	A	73	GLN	C-N	-8.54	1.25	1.33	13	7
1	A	53	THR	CB-OG1	-8.51	1.30	1.43	12	13
1	A	10	GLU	C-N	-8.43	1.21	1.33	11	5
1	A	28	GLY	C-O	-8.40	1.12	1.23	16	20
1	A	58	GLU	CA-C	-8.40	1.41	1.52	3	20
1	A	5	THR	N-CA	-8.33	1.35	1.46	6	20
1	A	93	ALA	N-CA	8.32	1.57	1.46	13	20
1	A	23	ASN	N-CA	-8.29	1.35	1.46	16	3
1	A	59	ALA	CA-C	8.27	1.63	1.52	14	13
1	A	42	SER	CA-CB	8.26	1.67	1.53	7	11
1	A	71	SER	N-CA	8.23	1.56	1.46	2	6
1	A	7	CYS	CA-C	-8.19	1.43	1.53	20	14
1	A	72	LYS	N-CA	8.19	1.56	1.46	20	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	8	TRP	CA-C	-8.18	1.41	1.52	11	4
1	A	80	CYS	CA-CB	8.11	1.67	1.53	15	5
1	A	6	TYR	C-N	-8.09	1.23	1.33	5	20
1	A	75	ASP	CA-CB	8.06	1.63	1.54	10	5
1	A	38	CYS	C-N	-8.03	1.23	1.33	8	20
1	A	5	THR	CA-C	-7.97	1.42	1.52	4	20
1	A	32	CYS	C-N	-7.96	1.21	1.33	10	20
1	A	16	GLY	CA-C	-7.96	1.40	1.51	12	8
1	A	51	GLY	CA-C	-7.89	1.40	1.51	7	20
1	A	41	THR	C-N	-7.87	1.23	1.33	16	1
1	A	33	SER	CA-C	-7.86	1.41	1.52	16	14
1	A	9	ASN	CA-C	-7.79	1.42	1.52	11	13
1	A	74	CYS	CA-C	-7.74	1.42	1.52	11	7
1	A	2	SER	CA-C	-7.72	1.46	1.52	9	10
1	A	4	PRO	C-N	-7.72	1.22	1.33	4	18
1	A	78	ARG	CA-C	-7.71	1.43	1.52	6	11
1	A	8	TRP	N-CA	7.71	1.56	1.46	11	4
1	A	25	GLN	C-O	-7.57	1.14	1.24	7	11
1	A	55	CYS	C-N	-7.53	1.25	1.32	8	1
1	A	75	ASP	C-N	-7.49	1.22	1.33	18	7
1	A	60	LYS	N-CA	-7.45	1.37	1.46	1	16
1	A	80	CYS	CB-SG	7.39	2.05	1.81	13	14
1	A	91	GLY	C-N	7.37	1.44	1.33	5	13
1	A	30	ARG	NE-CZ	7.36	1.41	1.33	9	6
1	A	22	ASN	C-O	-7.33	1.15	1.23	9	2
1	A	27	ASP	N-CA	-7.33	1.36	1.46	19	8
1	A	52	PRO	C-N	-7.33	1.24	1.33	13	12
1	A	14	PRO	CA-C	7.32	1.60	1.52	8	5
1	A	15	GLY	CA-C	-7.29	1.41	1.51	14	2
1	A	21	SER	C-N	-7.27	1.24	1.33	15	6
1	A	2	SER	C-N	-7.24	1.22	1.33	7	17
1	A	59	ALA	N-CA	7.17	1.52	1.46	19	1
1	A	41	THR	N-CA	7.10	1.54	1.46	8	14
1	A	47	PRO	CA-CB	7.09	1.58	1.53	2	1
1	A	52	PRO	C-O	-6.93	1.15	1.24	7	13
1	A	68	CYS	CA-CB	6.92	1.65	1.53	15	16
1	A	26	CYS	C-O	-6.91	1.15	1.23	11	8
1	A	33	SER	CA-CB	-6.82	1.41	1.53	15	20
1	A	29	ALA	N-CA	6.82	1.54	1.46	15	8
1	A	10	GLU	CA-C	-6.76	1.43	1.52	4	3
1	A	92	HIS	CA-CB	6.76	1.64	1.53	6	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	66	ASN	N-CA	6.74	1.54	1.46	1	10
1	A	71	SER	C-N	6.72	1.43	1.33	16	3
1	A	32	CYS	CA-C	-6.72	1.44	1.53	10	5
1	A	25	GLN	CA-C	-6.69	1.43	1.52	18	8
1	A	19	ARG	C-O	-6.67	1.15	1.24	11	2
1	A	30	ARG	N-CA	6.67	1.54	1.46	11	13
1	A	65	PRO	C-N	-6.65	1.24	1.33	14	8
1	A	67	ARG	C-N	-6.64	1.24	1.33	6	5
1	A	14	PRO	N-CD	-6.63	1.38	1.47	9	8
1	A	30	ARG	CZ-NH1	-6.61	1.23	1.32	14	1
1	A	28	GLY	N-CA	-6.60	1.35	1.45	7	5
1	A	60	LYS	C-O	-6.59	1.16	1.24	13	4
1	A	77	ALA	CA-CB	-6.58	1.44	1.53	2	2
1	A	37	PHE	CA-CB	6.56	1.64	1.53	15	14
1	A	18	ASN	CA-CB	6.55	1.64	1.53	15	7
1	A	20	CYS	CA-CB	6.53	1.64	1.53	20	5
1	A	72	LYS	CA-CB	6.52	1.65	1.53	10	11
1	A	17	PRO	N-CD	-6.52	1.38	1.47	15	4
1	A	33	SER	N-CA	6.50	1.54	1.46	4	12
1	A	42	SER	N-CA	6.49	1.55	1.46	4	7
1	A	38	CYS	CA-C	-6.46	1.44	1.52	9	8
1	A	68	CYS	N-CA	-6.45	1.37	1.46	15	7
1	A	11	ALA	CA-C	-6.43	1.44	1.52	14	2
1	A	89	THR	CA-CB	6.41	1.61	1.53	4	4
1	A	22	ASN	N-CA	6.39	1.53	1.46	7	3
1	A	79	THR	CA-CB	-6.37	1.42	1.52	19	2
1	A	7	CYS	C-N	-6.36	1.24	1.33	19	8
1	A	77	ALA	CA-C	-6.35	1.45	1.53	2	1
1	A	90	ALA	C-N	-6.31	1.24	1.33	18	7
1	A	29	ALA	CA-C	-6.31	1.44	1.52	16	2
1	A	78	ARG	N-CA	-6.29	1.38	1.45	6	4
1	A	53	THR	CA-CB	-6.29	1.42	1.53	6	1
1	A	86	CYS	CB-SG	6.26	2.01	1.81	13	8
1	A	76	GLY	C-N	-6.24	1.24	1.33	2	1
1	A	58	GLU	N-CA	-6.22	1.38	1.46	16	6
1	A	76	GLY	N-CA	6.20	1.54	1.45	6	2
1	A	60	LYS	CA-CB	6.18	1.63	1.53	13	6
1	A	23	ASN	C-N	-6.17	1.25	1.33	16	3
1	A	78	ARG	CA-CB	-6.17	1.44	1.53	8	12
1	A	53	THR	CA-C	-6.14	1.45	1.52	16	4
1	A	41	THR	C-O	-6.11	1.16	1.23	18	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	54	TYR	CA-CB	6.06	1.63	1.53	7	6
1	A	67	ARG	NE-CZ	6.03	1.39	1.33	17	6
1	A	20	CYS	N-CA	6.01	1.53	1.46	15	4
1	A	74	CYS	CB-SG	5.99	2.01	1.81	13	3
1	A	46	ASP	N-CA	-5.96	1.37	1.45	17	6
1	A	65	PRO	N-CD	-5.90	1.39	1.47	4	9
1	A	13	ASN	CA-C	5.85	1.60	1.52	4	3
1	A	75	ASP	CA-C	-5.84	1.48	1.52	10	1
1	A	86	CYS	CA-C	-5.75	1.46	1.52	15	1
1	A	23	ASN	C-O	-5.74	1.16	1.23	7	1
1	A	43	ARG	C-N	5.72	1.45	1.33	19	2
1	A	89	THR	C-N	-5.64	1.25	1.33	19	2
1	A	43	ARG	CB-CG	5.61	1.69	1.52	18	4
1	A	79	THR	N-CA	-5.57	1.37	1.46	1	4
1	A	75	ASP	CG-OD2	-5.49	1.15	1.25	7	3
1	A	67	ARG	CD-NE	5.44	1.53	1.46	17	1
1	A	76	GLY	CA-C	-5.41	1.44	1.51	18	1
1	A	38	CYS	N-CA	5.41	1.53	1.46	6	2
1	A	36	GLY	CA-C	-5.40	1.44	1.51	13	3
1	A	23	ASN	CA-CB	5.39	1.61	1.53	7	2
1	A	11	ALA	CA-CB	-5.39	1.44	1.53	10	2
1	A	69	SER	CA-C	-5.36	1.45	1.52	11	2
1	A	8	TRP	CG-CD2	5.35	1.53	1.43	5	4
1	A	56	TRP	CG-CD2	5.35	1.53	1.43	8	3
1	A	35	SER	CA-CB	-5.33	1.44	1.53	16	5
1	A	8	TRP	CA-CB	-5.33	1.44	1.53	16	1
1	A	20	CYS	CB-SG	5.32	1.98	1.81	17	2
1	A	40	GLY	C-N	5.32	1.40	1.33	16	4
1	A	12	ASN	N-CA	5.29	1.53	1.46	6	1
1	A	23	ASN	CA-C	5.27	1.59	1.52	8	1
1	A	7	CYS	CA-CB	-5.26	1.45	1.53	9	2
1	A	52	PRO	N-CA	5.24	1.54	1.47	19	1
1	A	36	GLY	N-CA	-5.23	1.37	1.45	16	1
1	A	39	GLN	N-CA	-5.23	1.39	1.46	1	1
1	A	46	ASP	CA-C	5.23	1.59	1.52	4	1
1	A	55	CYS	CA-C	5.21	1.58	1.52	19	1
1	A	57	ASP	N-CA	-5.19	1.39	1.46	1	3
1	A	20	CYS	C-N	-5.19	1.25	1.34	14	1
1	A	53	THR	C-O	-5.18	1.17	1.23	19	1
1	A	56	TRP	CA-C	5.13	1.56	1.53	13	1
1	A	10	GLU	N-CA	-5.13	1.39	1.46	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	28	GLY	C-N	5.12	1.40	1.33	6	1
1	A	88	GLY	CA-C	5.09	1.59	1.51	18	1
1	A	57	ASP	CA-C	5.02	1.59	1.52	10	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	86	CYS	N-CA-C	8.49	122.26	108.41	1	20
1	A	56	TRP	N-CA-CB	-7.94	104.20	111.59	14	1
1	A	56	TRP	CB-CA-C	-6.65	106.83	116.54	14	5
1	A	30	ARG	CB-CA-C	-6.49	97.51	110.42	16	1
1	A	34	SER	N-CA-C	-6.45	103.85	112.94	16	16
1	A	20	CYS	N-CA-C	-6.32	97.33	110.80	17	20
1	A	80	CYS	N-CA-CB	6.20	120.96	110.49	15	5
1	A	31	THR	N-CA-CB	-6.02	100.36	111.13	4	18
1	A	6	TYR	CA-CB-CG	-5.97	103.15	113.90	13	20
1	A	6	TYR	N-CA-CB	5.65	120.03	110.49	5	19
1	A	72	LYS	N-CA-C	5.43	119.14	112.03	13	3
1	A	25	GLN	CA-C-N	-5.34	117.42	123.13	4	1
1	A	25	GLN	C-N-CA	-5.34	117.42	123.13	4	1
1	A	41	THR	N-CA-C	5.25	117.06	108.55	16	1
1	A	15	GLY	N-CA-C	-5.21	108.62	114.40	12	1
1	A	74	CYS	CA-C-O	-5.07	115.04	119.91	8	1
1	A	72	LYS	N-CA-CB	-5.05	102.59	111.42	13	1
1	A	68	CYS	N-CA-C	-5.04	100.06	110.80	11	1

There are no chirality outliers.

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	623	553	551	266±9

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	12460	11060	11027	5310

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 226.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:TYR:CB	1:A:6:TYR:CG	1.66	1.75	13	18
1:A:91:GLY:C	1:A:91:GLY:CA	1.59	1.75	13	15
1:A:74:CYS:N	1:A:74:CYS:CA	1.51	1.70	18	5
1:A:80:CYS:CB	1:A:80:CYS:SG	1.47	2.03	16	9
1:A:86:CYS:SG	1:A:86:CYS:CB	1.46	2.01	13	1
1:A:44:LYS:O	1:A:46:ASP:N	1.07	1.86	9	20
1:A:76:GLY:O	1:A:78:ARG:N	1.01	1.94	7	7
1:A:51:GLY:O	1:A:53:THR:N	1.00	1.94	19	20
1:A:17:PRO:C	1:A:19:ARG:H	0.98	1.65	17	20
1:A:17:PRO:O	1:A:19:ARG:N	0.94	2.01	20	20
1:A:30:ARG:NE	1:A:42:SER:N	0.93	2.17	18	3
1:A:6:TYR:CG	1:A:6:TYR:CA	0.93	2.52	9	18
1:A:59:ALA:O	1:A:68:CYS:N	0.91	2.04	6	20
1:A:17:PRO:C	1:A:19:ARG:N	0.90	2.29	18	20
1:A:80:CYS:SG	1:A:86:CYS:N	0.90	2.44	15	20
1:A:80:CYS:H	1:A:85:PHE:H	0.90	1.04	18	20
1:A:31:THR:O	1:A:39:GLN:O	0.89	1.90	16	20
1:A:1:GLY:H2	1:A:27:ASP:CG	0.88	1.76	9	20
1:A:80:CYS:CA	1:A:86:CYS:H	0.85	1.84	7	20
1:A:73:GLN:C	1:A:74:CYS:CA	0.84	2.50	11	5
1:A:20:CYS:SG	1:A:25:GLN:C	0.83	2.61	7	20
1:A:1:GLY:H1	1:A:27:ASP:HA	0.82	1.32	9	20
1:A:80:CYS:N	1:A:85:PHE:H	0.82	1.72	11	19
1:A:1:GLY:N	1:A:27:ASP:HA	0.81	1.89	11	18
1:A:32:CYS:HA	1:A:38:CYS:N	0.80	1.91	16	20
1:A:2:SER:N	1:A:29:ALA:H	0.80	1.74	2	20
1:A:31:THR:OG1	1:A:39:GLN:O	0.80	2.00	14	20
1:A:21:SER:N	1:A:25:GLN:O	0.79	2.16	7	20
1:A:30:ARG:HE	1:A:42:SER:N	0.79	1.76	19	2
1:A:80:CYS:H	1:A:85:PHE:N	0.78	1.76	18	14
1:A:74:CYS:SG	1:A:85:PHE:HB3	0.78	2.18	6	15
1:A:23:ASN:HA	1:A:38:CYS:HA	0.78	1.53	9	20
1:A:53:THR:C	1:A:92:HIS:H	0.78	1.87	19	20
1:A:2:SER:H	1:A:29:ALA:N	0.77	1.76	20	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:GLY:C	1:A:29:ALA:H	0.77	1.88	4	12
1:A:31:THR:O	1:A:39:GLN:N	0.77	2.17	5	20
1:A:14:PRO:C	1:A:16:GLY:H	0.77	1.88	20	8
1:A:53:THR:OG1	1:A:76:GLY:O	0.76	2.04	1	13
1:A:7:CYS:O	1:A:8:TRP:C	0.76	2.29	6	20
1:A:22:ASN:N	1:A:25:GLN:HA	0.75	1.97	17	20
1:A:31:THR:HG1	1:A:39:GLN:C	0.75	1.88	14	2
1:A:10:GLU:H	1:A:18:ASN:HD21	0.75	1.20	18	15
1:A:2:SER:H	1:A:29:ALA:H	0.75	1.24	14	9
1:A:2:SER:N	1:A:29:ALA:N	0.75	2.34	8	20
1:A:51:GLY:C	1:A:53:THR:H	0.75	1.88	15	20
1:A:1:GLY:N	1:A:23:ASN:CG	0.75	2.45	14	20
1:A:8:TRP:HB2	1:A:27:ASP:CB	0.74	2.12	11	20
1:A:6:TYR:CD2	1:A:27:ASP:CG	0.74	2.66	2	20
1:A:31:THR:C	1:A:38:CYS:H	0.73	1.91	9	20
1:A:51:GLY:O	1:A:53:THR:O	0.73	2.05	13	20
1:A:53:THR:O	1:A:92:HIS:N	0.73	2.18	19	15
1:A:19:ARG:O	1:A:20:CYS:O	0.72	2.06	16	20
1:A:52:PRO:O	1:A:93:ALA:N	0.72	2.22	16	20
1:A:23:ASN:OD1	1:A:26:CYS:O	0.72	2.08	7	20
1:A:19:ARG:O	1:A:20:CYS:C	0.72	2.33	11	20
1:A:30:ARG:NE	1:A:42:SER:CB	0.72	2.53	19	1
1:A:55:CYS:H	1:A:75:ASP:CG	0.71	1.93	12	18
1:A:5:THR:O	1:A:7:CYS:N	0.71	2.23	7	20
1:A:10:GLU:N	1:A:18:ASN:HD21	0.70	1.84	18	10
1:A:22:ASN:ND2	1:A:23:ASN:HD21	0.70	1.84	20	3
1:A:86:CYS:SG	1:A:86:CYS:CA	0.70	2.78	13	1
1:A:55:CYS:N	1:A:75:ASP:OD1	0.70	2.24	20	16
1:A:30:ARG:N	1:A:41:THR:O	0.70	2.25	19	20
1:A:31:THR:N	1:A:39:GLN:O	0.69	2.24	16	20
1:A:59:ALA:HB3	1:A:68:CYS:SG	0.69	2.28	13	12
1:A:80:CYS:CA	1:A:86:CYS:N	0.69	2.56	6	20
1:A:80:CYS:HA	1:A:86:CYS:O	0.69	1.87	2	18
1:A:1:GLY:N	1:A:23:ASN:CB	0.69	2.55	17	19
1:A:32:CYS:CA	1:A:38:CYS:N	0.69	2.55	14	20
1:A:30:ARG:HG3	1:A:41:THR:C	0.69	2.13	5	18
1:A:32:CYS:N	1:A:37:PHE:N	0.69	2.40	12	20
1:A:43:ARG:HH21	1:A:54:TYR:H	0.68	1.32	4	2
1:A:30:ARG:HE	1:A:42:SER:CB	0.68	2.00	19	1
1:A:44:LYS:C	1:A:46:ASP:N	0.68	2.51	19	20
1:A:53:THR:N	1:A:92:HIS:N	0.68	2.42	13	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:LYS:H	1:A:38:CYS:HA	0.67	1.49	5	11
1:A:1:GLY:H3	1:A:23:ASN:CB	0.67	2.02	2	10
1:A:10:GLU:C	1:A:17:PRO:HB3	0.67	2.13	1	20
1:A:23:ASN:O	1:A:30:ARG:NE	0.67	2.28	17	16
1:A:80:CYS:CB	1:A:86:CYS:H	0.67	2.02	3	20
1:A:30:ARG:NH1	1:A:42:SER:OG	0.67	2.27	14	8
1:A:30:ARG:HA	1:A:41:THR:H	0.67	1.50	16	2
1:A:80:CYS:HA	1:A:86:CYS:N	0.67	2.05	15	20
1:A:74:CYS:N	1:A:74:CYS:C	0.67	2.48	15	5
1:A:32:CYS:SG	1:A:33:SER:N	0.66	2.68	18	20
1:A:5:THR:C	1:A:7:CYS:N	0.66	2.53	19	20
1:A:22:ASN:O	1:A:26:CYS:N	0.66	2.27	16	20
1:A:1:GLY:N	1:A:27:ASP:CG	0.66	2.53	18	20
1:A:89:THR:HG22	1:A:90:ALA:N	0.66	2.05	7	15
1:A:6:TYR:CD2	1:A:6:TYR:O	0.66	2.48	8	20
1:A:59:ALA:CB	1:A:73:GLN:O	0.66	2.44	6	20
1:A:79:THR:O	1:A:87:GLN:HB3	0.66	1.90	19	5
1:A:80:CYS:HA	1:A:86:CYS:H	0.66	1.51	15	6
1:A:4:PRO:O	1:A:5:THR:HG22	0.66	1.91	13	20
1:A:30:ARG:CZ	1:A:42:SER:OG	0.65	2.44	11	13
1:A:80:CYS:N	1:A:86:CYS:N	0.65	2.44	2	20
1:A:80:CYS:H	1:A:86:CYS:N	0.65	1.88	2	15
1:A:46:ASP:O	1:A:48:GLY:N	0.65	2.29	11	8
1:A:1:GLY:H1	1:A:23:ASN:CG	0.65	1.99	1	15
1:A:32:CYS:H	1:A:37:PHE:N	0.65	1.89	16	20
1:A:32:CYS:HA	1:A:38:CYS:H	0.65	1.50	14	20
1:A:75:ASP:OD1	1:A:76:GLY:N	0.65	2.30	2	10
1:A:65:PRO:O	1:A:67:ARG:N	0.65	2.30	6	20
1:A:92:HIS:O	1:A:92:HIS:CG	0.65	2.50	6	20
1:A:1:GLY:H1	1:A:23:ASN:CB	0.65	2.04	8	13
1:A:23:ASN:HA	1:A:37:PHE:C	0.65	2.15	3	19
1:A:78:ARG:HB2	1:A:85:PHE:O	0.65	1.91	17	18
1:A:15:GLY:O	1:A:19:ARG:CD	0.65	2.45	14	3
1:A:1:GLY:N	1:A:23:ASN:ND2	0.64	2.45	18	8
1:A:31:THR:O	1:A:39:GLN:HG3	0.64	1.92	16	20
1:A:21:SER:O	1:A:22:ASN:ND2	0.64	2.30	4	8
1:A:32:CYS:CB	1:A:37:PHE:H	0.64	2.05	16	20
1:A:32:CYS:H	1:A:35:SER:C	0.64	2.00	18	20
1:A:1:GLY:H3	1:A:23:ASN:ND2	0.64	1.91	12	4
1:A:1:GLY:N	1:A:27:ASP:OD1	0.64	2.31	18	15
1:A:8:TRP:O	1:A:9:ASN:C	0.64	2.39	6	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:GLN:NE2	1:A:40:GLY:N	0.64	2.45	14	13
1:A:71:SER:HA	1:A:85:PHE:HB2	0.64	1.69	1	5
1:A:20:CYS:C	1:A:25:GLN:O	0.64	2.41	7	20
1:A:23:ASN:N	1:A:23:ASN:ND2	0.64	2.46	5	6
1:A:4:PRO:C	1:A:5:THR:HG22	0.64	2.18	19	20
1:A:15:GLY:O	1:A:19:ARG:NE	0.64	2.30	14	1
1:A:51:GLY:N	1:A:77:ALA:HB1	0.63	2.08	12	19
1:A:80:CYS:H	1:A:85:PHE:C	0.63	2.01	13	14
1:A:15:GLY:O	1:A:19:ARG:HD3	0.63	1.93	15	9
1:A:53:THR:O	1:A:54:TYR:CB	0.63	2.46	19	20
1:A:89:THR:CG2	1:A:90:ALA:N	0.63	2.61	18	12
1:A:22:ASN:CG	1:A:23:ASN:ND2	0.63	2.56	3	9
1:A:24:LYS:HB2	1:A:30:ARG:HE	0.63	1.52	14	1
1:A:66:ASN:ND2	1:A:73:GLN:NE2	0.63	2.46	11	3
1:A:59:ALA:O	1:A:68:CYS:SG	0.63	2.57	7	10
1:A:22:ASN:C	1:A:23:ASN:OD1	0.63	2.42	4	11
1:A:43:ARG:NE	1:A:53:THR:OG1	0.62	2.32	8	11
1:A:23:ASN:ND2	1:A:23:ASN:N	0.62	2.47	3	3
1:A:6:TYR:CG	1:A:6:TYR:O	0.62	2.52	4	19
1:A:77:ALA:HB3	1:A:90:ALA:H	0.62	1.55	2	18
1:A:51:GLY:O	1:A:92:HIS:N	0.62	2.33	5	20
1:A:72:LYS:N	1:A:85:PHE:CD2	0.62	2.67	11	8
1:A:32:CYS:HB2	1:A:37:PHE:H	0.62	1.54	5	20
1:A:10:GLU:H	1:A:18:ASN:ND2	0.62	1.90	11	3
1:A:5:THR:O	1:A:7:CYS:HB2	0.62	1.95	20	20
1:A:1:GLY:N	1:A:23:ASN:OD1	0.62	2.33	13	9
1:A:28:GLY:O	1:A:43:ARG:N	0.62	2.33	7	20
1:A:70:ASN:C	1:A:80:CYS:SG	0.62	2.83	6	11
1:A:7:CYS:C	1:A:55:CYS:SG	0.61	2.83	2	20
1:A:34:SER:C	1:A:36:GLY:H	0.61	2.03	6	20
1:A:71:SER:HA	1:A:85:PHE:CB	0.61	2.24	1	6
1:A:53:THR:OG1	1:A:77:ALA:N	0.61	2.32	5	7
1:A:56:TRP:NE1	1:A:58:GLU:O	0.61	2.34	3	7
1:A:43:ARG:O	1:A:44:LYS:C	0.61	2.43	19	20
1:A:6:TYR:CB	1:A:6:TYR:CD1	0.61	2.74	18	17
1:A:55:CYS:N	1:A:75:ASP:OD2	0.61	2.33	4	3
1:A:80:CYS:HA	1:A:86:CYS:C	0.61	2.20	2	20
1:A:56:TRP:N	1:A:75:ASP:OD1	0.61	2.34	7	4
1:A:1:GLY:H3	1:A:23:ASN:CG	0.61	2.04	2	12
1:A:1:GLY:CA	1:A:30:ARG:N	0.61	2.64	18	19
1:A:2:SER:N	1:A:27:ASP:OD1	0.60	2.33	11	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:THR:OG1	1:A:76:GLY:C	0.60	2.44	3	13
1:A:24:LYS:O	1:A:25:GLN:HB2	0.60	1.95	3	20
1:A:3:GLY:O	1:A:5:THR:N	0.60	2.35	7	20
1:A:43:ARG:NE	1:A:76:GLY:O	0.60	2.34	19	9
1:A:87:GLN:OE1	1:A:88:GLY:N	0.60	2.35	17	15
1:A:6:TYR:O	1:A:6:TYR:CG	0.60	2.53	7	1
1:A:23:ASN:HB2	1:A:30:ARG:HB2	0.60	1.73	18	7
1:A:22:ASN:O	1:A:25:GLN:C	0.60	2.44	9	20
1:A:43:ARG:HE	1:A:53:THR:CB	0.60	2.09	8	5
1:A:51:GLY:N	1:A:77:ALA:CB	0.60	2.65	16	19
1:A:56:TRP:CD1	1:A:58:GLU:H	0.60	2.14	4	20
1:A:75:ASP:CG	1:A:76:GLY:N	0.60	2.60	8	4
1:A:8:TRP:O	1:A:55:CYS:SG	0.60	2.59	2	16
1:A:32:CYS:CA	1:A:38:CYS:H	0.59	2.09	14	20
1:A:56:TRP:N	1:A:75:ASP:OD2	0.59	2.35	15	12
1:A:80:CYS:SG	1:A:80:CYS:CA	0.59	2.89	16	9
1:A:87:GLN:CD	1:A:88:GLY:N	0.59	2.59	15	20
1:A:68:CYS:O	1:A:69:SER:CB	0.59	2.50	3	20
1:A:6:TYR:CG	1:A:6:TYR:C	0.59	2.80	12	18
1:A:22:ASN:O	1:A:25:GLN:N	0.59	2.35	1	12
1:A:51:GLY:O	1:A:91:GLY:N	0.59	2.35	19	20
1:A:1:GLY:HA3	1:A:30:ARG:N	0.59	2.12	20	19
1:A:4:PRO:O	1:A:5:THR:CB	0.59	2.51	4	20
1:A:7:CYS:O	1:A:7:CYS:SG	0.59	2.61	1	20
1:A:10:GLU:O	1:A:17:PRO:HB3	0.59	1.97	15	4
1:A:65:PRO:C	1:A:67:ARG:N	0.59	2.59	6	20
1:A:56:TRP:NE1	1:A:59:ALA:HB2	0.59	2.13	15	5
1:A:30:ARG:HH11	1:A:30:ARG:CG	0.59	2.11	2	1
1:A:28:GLY:O	1:A:43:ARG:HB3	0.59	1.98	16	4
1:A:59:ALA:C	1:A:68:CYS:SG	0.59	2.85	19	7
1:A:91:GLY:O	1:A:92:HIS:ND1	0.59	2.36	10	20
1:A:30:ARG:HH11	1:A:42:SER:CB	0.59	2.11	14	1
1:A:20:CYS:SG	1:A:25:GLN:CB	0.58	2.92	14	20
1:A:56:TRP:CG	1:A:57:ASP:H	0.58	2.16	8	18
1:A:51:GLY:O	1:A:91:GLY:CA	0.58	2.51	1	20
1:A:66:ASN:CG	1:A:73:GLN:NE2	0.58	2.61	14	2
1:A:8:TRP:HB2	1:A:27:ASP:N	0.58	2.14	18	19
1:A:22:ASN:C	1:A:23:ASN:CG	0.58	2.71	5	19
1:A:30:ARG:NE	1:A:42:SER:OG	0.58	2.36	19	3
1:A:71:SER:N	1:A:80:CYS:SG	0.58	2.76	3	10
1:A:55:CYS:N	1:A:75:ASP:CG	0.58	2.62	3	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:ARG:CB	1:A:85:PHE:O	0.58	2.52	17	20
1:A:30:ARG:HE	1:A:42:SER:CA	0.58	2.12	19	1
1:A:30:ARG:HD2	1:A:42:SER:CA	0.58	2.29	15	15
1:A:12:ASN:O	1:A:12:ASN:CG	0.58	2.47	3	20
1:A:58:GLU:O	1:A:58:GLU:HG3	0.58	1.98	18	20
1:A:59:ALA:HB3	1:A:73:GLN:O	0.58	1.99	18	8
1:A:8:TRP:NE1	1:A:21:SER:H	0.58	1.96	7	10
1:A:23:ASN:HA	1:A:38:CYS:CA	0.57	2.29	9	19
1:A:37:PHE:O	1:A:37:PHE:CD2	0.57	2.57	1	12
1:A:29:ALA:O	1:A:30:ARG:O	0.57	2.22	16	14
1:A:52:PRO:O	1:A:93:ALA:HB2	0.57	1.99	11	4
1:A:22:ASN:ND2	1:A:23:ASN:ND2	0.57	2.53	20	3
1:A:1:GLY:O	1:A:29:ALA:C	0.57	2.48	4	8
1:A:6:TYR:CG	1:A:27:ASP:CG	0.57	2.83	9	19
1:A:11:ALA:O	1:A:12:ASN:CB	0.57	2.53	4	20
1:A:51:GLY:C	1:A:91:GLY:CA	0.57	2.78	18	20
1:A:54:TYR:HA	1:A:75:ASP:OD1	0.57	2.00	3	9
1:A:79:THR:N	1:A:87:GLN:OE1	0.57	2.38	17	13
1:A:11:ALA:N	1:A:18:ASN:OD1	0.57	2.36	19	18
1:A:74:CYS:N	1:A:74:CYS:CB	0.57	2.61	15	5
1:A:6:TYR:CD2	1:A:27:ASP:OD2	0.56	2.58	9	16
1:A:53:THR:HG1	1:A:76:GLY:C	0.56	2.06	2	2
1:A:5:THR:HG21	1:A:93:ALA:O	0.56	1.99	4	3
1:A:56:TRP:H	1:A:75:ASP:CG	0.56	2.07	11	11
1:A:49:PRO:CB	1:A:53:THR:HG23	0.56	2.29	6	1
1:A:7:CYS:O	1:A:9:ASN:N	0.56	2.39	16	20
1:A:80:CYS:N	1:A:86:CYS:H	0.56	1.99	7	4
1:A:13:ASN:O	1:A:16:GLY:O	0.56	2.23	12	18
1:A:29:ALA:HB3	1:A:43:ARG:H	0.56	1.61	7	7
1:A:43:ARG:O	1:A:45:PRO:N	0.56	2.39	19	16
1:A:56:TRP:C	1:A:75:ASP:OD2	0.56	2.49	6	12
1:A:24:LYS:N	1:A:38:CYS:HA	0.56	2.15	19	15
1:A:30:ARG:HE	1:A:41:THR:C	0.56	2.07	18	1
1:A:8:TRP:CH2	1:A:22:ASN:ND2	0.56	2.73	18	4
1:A:44:LYS:O	1:A:46:ASP:CA	0.56	2.54	17	5
1:A:65:PRO:C	1:A:67:ARG:H	0.56	2.09	6	18
1:A:89:THR:O	1:A:90:ALA:HB3	0.56	2.00	9	20
1:A:28:GLY:O	1:A:29:ALA:CB	0.56	2.53	16	20
1:A:31:THR:O	1:A:39:GLN:C	0.56	2.48	16	20
1:A:56:TRP:CZ2	1:A:66:ASN:OD1	0.56	2.59	3	17
1:A:6:TYR:CG	1:A:27:ASP:OD1	0.56	2.58	8	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:SER:O	1:A:71:SER:OG	0.56	2.22	10	6
1:A:71:SER:O	1:A:72:LYS:HB3	0.56	1.99	11	9
1:A:59:ALA:CB	1:A:68:CYS:SG	0.56	2.93	13	7
1:A:42:SER:O	1:A:43:ARG:C	0.56	2.49	17	20
1:A:56:TRP:CZ2	1:A:66:ASN:CG	0.56	2.84	2	6
1:A:70:ASN:O	1:A:71:SER:CB	0.55	2.54	17	20
1:A:92:HIS:O	1:A:92:HIS:CD2	0.55	2.59	14	17
1:A:2:SER:C	1:A:29:ALA:HA	0.55	2.26	18	19
1:A:8:TRP:O	1:A:10:GLU:N	0.55	2.39	1	16
1:A:22:ASN:O	1:A:23:ASN:C	0.55	2.48	9	20
1:A:71:SER:OG	1:A:71:SER:O	0.55	2.23	14	5
1:A:1:GLY:O	1:A:30:ARG:O	0.55	2.25	1	10
1:A:54:TYR:CD2	1:A:75:ASP:OD2	0.55	2.60	10	8
1:A:23:ASN:O	1:A:26:CYS:N	0.55	2.36	8	4
1:A:66:ASN:ND2	1:A:73:GLN:HE22	0.55	1.99	11	1
1:A:53:THR:C	1:A:92:HIS:N	0.55	2.63	6	19
1:A:56:TRP:CG	1:A:57:ASP:N	0.55	2.73	8	17
1:A:7:CYS:O	1:A:55:CYS:SG	0.55	2.65	11	20
1:A:51:GLY:HA2	1:A:91:GLY:N	0.55	2.17	15	19
1:A:30:ARG:CG	1:A:30:ARG:NH1	0.55	2.70	2	4
1:A:8:TRP:CG	1:A:26:CYS:O	0.55	2.60	7	1
1:A:22:ASN:O	1:A:23:ASN:OD1	0.55	2.24	9	6
1:A:54:TYR:O	1:A:54:TYR:CD1	0.55	2.60	13	20
1:A:20:CYS:C	1:A:25:GLN:HB3	0.55	2.26	2	19
1:A:20:CYS:CA	1:A:25:GLN:O	0.55	2.55	14	20
1:A:68:CYS:SG	1:A:69:SER:N	0.55	2.78	12	11
1:A:87:GLN:C	1:A:87:GLN:CD	0.55	2.74	8	7
1:A:78:ARG:NH1	1:A:88:GLY:C	0.55	2.64	20	1
1:A:19:ARG:C	1:A:20:CYS:O	0.54	2.49	15	20
1:A:42:SER:O	1:A:44:LYS:N	0.54	2.40	11	2
1:A:6:TYR:CB	1:A:27:ASP:OD1	0.54	2.55	1	20
1:A:71:SER:HA	1:A:80:CYS:SG	0.54	2.42	2	2
1:A:30:ARG:HD2	1:A:42:SER:CB	0.54	2.32	7	14
1:A:1:GLY:C	1:A:29:ALA:N	0.54	2.63	4	8
1:A:32:CYS:O	1:A:35:SER:N	0.54	2.33	7	19
1:A:10:GLU:N	1:A:18:ASN:ND2	0.54	2.54	11	2
1:A:20:CYS:SG	1:A:25:GLN:O	0.54	2.65	18	20
1:A:23:ASN:ND2	1:A:27:ASP:OD2	0.54	2.41	7	2
1:A:1:GLY:H1	1:A:23:ASN:HB2	0.54	1.63	8	1
1:A:72:LYS:O	1:A:73:GLN:CB	0.54	2.56	11	17
1:A:4:PRO:C	1:A:5:THR:CG2	0.54	2.81	19	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:SER:C	1:A:86:CYS:SG	0.54	2.91	10	7
1:A:54:TYR:CD2	1:A:75:ASP:OD1	0.54	2.61	19	7
1:A:42:SER:O	1:A:43:ARG:NH1	0.54	2.41	19	2
1:A:4:PRO:O	1:A:5:THR:CG2	0.54	2.56	13	20
1:A:76:GLY:C	1:A:78:ARG:N	0.54	2.65	7	6
1:A:77:ALA:HB3	1:A:90:ALA:N	0.53	2.17	6	15
1:A:2:SER:O	1:A:29:ALA:HA	0.53	2.03	4	19
1:A:54:TYR:CA	1:A:75:ASP:OD1	0.53	2.56	6	6
1:A:23:ASN:HB2	1:A:26:CYS:O	0.53	2.02	18	3
1:A:30:ARG:NE	1:A:41:THR:C	0.53	2.67	18	1
1:A:34:SER:C	1:A:36:GLY:N	0.53	2.66	7	20
1:A:89:THR:O	1:A:90:ALA:CB	0.53	2.56	10	20
1:A:32:CYS:C	1:A:35:SER:H	0.53	2.11	8	20
1:A:30:ARG:NE	1:A:42:SER:H	0.53	1.98	18	1
1:A:23:ASN:C	1:A:25:GLN:N	0.53	2.65	16	5
1:A:5:THR:C	1:A:7:CYS:H	0.53	2.12	6	19
1:A:60:LYS:O	1:A:69:SER:CB	0.53	2.57	13	9
1:A:87:GLN:CD	1:A:87:GLN:C	0.52	2.76	4	13
1:A:15:GLY:O	1:A:19:ARG:CG	0.52	2.57	14	1
1:A:56:TRP:NE1	1:A:66:ASN:HB2	0.52	2.20	10	11
1:A:20:CYS:SG	1:A:26:CYS:N	0.52	2.83	7	12
1:A:30:ARG:HD2	1:A:42:SER:N	0.52	2.19	12	6
1:A:12:ASN:O	1:A:12:ASN:ND2	0.52	2.42	10	4
1:A:56:TRP:CD1	1:A:59:ALA:HB2	0.52	2.39	19	5
1:A:17:PRO:O	1:A:18:ASN:C	0.52	2.53	3	17
1:A:23:ASN:CB	1:A:30:ARG:HB2	0.52	2.34	13	8
1:A:24:LYS:HB2	1:A:30:ARG:NH1	0.52	2.20	19	1
1:A:23:ASN:HD22	1:A:37:PHE:HB2	0.52	1.65	12	3
1:A:68:CYS:SG	1:A:73:GLN:O	0.52	2.67	18	4
1:A:21:SER:O	1:A:22:ASN:OD1	0.52	2.28	11	2
1:A:23:ASN:CA	1:A:38:CYS:HA	0.52	2.35	15	19
1:A:28:GLY:O	1:A:43:ARG:CB	0.52	2.58	7	13
1:A:32:CYS:N	1:A:35:SER:C	0.52	2.68	18	18
1:A:10:GLU:O	1:A:73:GLN:NE2	0.52	2.42	14	1
1:A:74:CYS:SG	1:A:86:CYS:HB3	0.52	2.44	1	6
1:A:80:CYS:SG	1:A:85:PHE:HB2	0.52	2.44	5	5
1:A:59:ALA:O	1:A:67:ARG:CA	0.52	2.58	7	5
1:A:11:ALA:O	1:A:18:ASN:OD1	0.51	2.29	18	5
1:A:23:ASN:HB3	1:A:30:ARG:HB3	0.51	1.82	16	1
1:A:30:ARG:CD	1:A:42:SER:N	0.51	2.73	18	1
1:A:71:SER:HA	1:A:85:PHE:CG	0.51	2.40	13	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ASN:O	1:A:25:GLN:CA	0.51	2.57	9	4
1:A:22:ASN:H	1:A:25:GLN:HA	0.51	1.66	17	7
1:A:10:GLU:O	1:A:11:ALA:HB2	0.51	2.06	4	5
1:A:56:TRP:CE2	1:A:66:ASN:HB2	0.51	2.41	8	13
1:A:30:ARG:CG	1:A:30:ARG:HH11	0.51	2.18	9	3
1:A:44:LYS:C	1:A:46:ASP:H	0.51	2.06	19	1
1:A:26:CYS:HB2	1:A:30:ARG:NE	0.51	2.20	8	12
1:A:1:GLY:H3	1:A:23:ASN:HB3	0.51	1.66	9	3
1:A:54:TYR:HB3	1:A:92:HIS:N	0.51	2.21	15	14
1:A:14:PRO:O	1:A:16:GLY:N	0.51	2.39	10	5
1:A:23:ASN:CB	1:A:30:ARG:CB	0.51	2.89	16	1
1:A:22:ASN:OD1	1:A:23:ASN:ND2	0.50	2.44	3	2
1:A:14:PRO:C	1:A:16:GLY:N	0.50	2.68	12	7
1:A:80:CYS:HA	1:A:86:CYS:CA	0.50	2.37	17	20
1:A:1:GLY:CA	1:A:29:ALA:H	0.50	2.19	7	11
1:A:56:TRP:CD1	1:A:57:ASP:H	0.50	2.25	4	4
1:A:23:ASN:OD1	1:A:27:ASP:CB	0.50	2.60	16	1
1:A:32:CYS:C	1:A:34:SER:H	0.50	2.13	7	17
1:A:44:LYS:O	1:A:46:ASP:CB	0.50	2.60	13	6
1:A:8:TRP:HE1	1:A:21:SER:H	0.49	1.49	7	3
1:A:73:GLN:O	1:A:73:GLN:OE1	0.49	2.30	14	1
1:A:11:ALA:C	1:A:18:ASN:OD1	0.49	2.55	15	18
1:A:53:THR:N	1:A:92:HIS:H	0.49	2.06	13	14
1:A:23:ASN:HA	1:A:38:CYS:N	0.49	2.22	14	13
1:A:51:GLY:C	1:A:53:THR:N	0.49	2.65	8	10
1:A:74:CYS:SG	1:A:86:CYS:SG	0.49	3.10	1	6
1:A:24:LYS:O	1:A:25:GLN:CB	0.49	2.60	19	8
1:A:52:PRO:O	1:A:93:ALA:CB	0.49	2.59	15	4
1:A:43:ARG:HH21	1:A:54:TYR:N	0.49	2.04	4	1
1:A:31:THR:C	1:A:39:GLN:O	0.49	2.54	16	1
1:A:79:THR:H	1:A:88:GLY:H	0.49	1.50	16	3
1:A:20:CYS:SG	1:A:25:GLN:HB3	0.49	2.48	5	19
1:A:31:THR:O	1:A:39:GLN:CA	0.49	2.61	1	20
1:A:52:PRO:C	1:A:92:HIS:C	0.49	2.80	8	16
1:A:36:GLY:C	1:A:37:PHE:CD2	0.49	2.90	5	5
1:A:53:THR:CA	1:A:92:HIS:HA	0.49	2.37	13	17
1:A:22:ASN:H	1:A:25:GLN:C	0.49	2.16	14	9
1:A:54:TYR:CD1	1:A:54:TYR:C	0.49	2.91	15	8
1:A:26:CYS:O	1:A:27:ASP:HB2	0.49	2.06	7	4
1:A:79:THR:O	1:A:87:GLN:CB	0.49	2.60	7	4
1:A:1:GLY:CA	1:A:27:ASP:OD1	0.49	2.60	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ASN:OD1	1:A:26:CYS:C	0.48	2.56	9	6
1:A:71:SER:O	1:A:72:LYS:CB	0.48	2.59	20	8
1:A:56:TRP:HE1	1:A:58:GLU:C	0.48	2.16	10	3
1:A:23:ASN:O	1:A:30:ARG:CD	0.48	2.60	7	9
1:A:24:LYS:CB	1:A:30:ARG:HE	0.48	2.21	14	1
1:A:20:CYS:CB	1:A:25:GLN:HB3	0.48	2.38	1	18
1:A:43:ARG:CD	1:A:76:GLY:O	0.48	2.62	13	3
1:A:5:THR:O	1:A:7:CYS:CB	0.48	2.61	13	13
1:A:22:ASN:C	1:A:25:GLN:H	0.48	2.17	7	11
1:A:80:CYS:SG	1:A:85:PHE:CB	0.48	3.01	15	8
1:A:54:TYR:CD2	1:A:75:ASP:CG	0.48	2.91	15	3
1:A:28:GLY:O	1:A:43:ARG:CG	0.48	2.61	19	7
1:A:1:GLY:HA3	1:A:30:ARG:CB	0.48	2.37	16	1
1:A:21:SER:C	1:A:22:ASN:HD22	0.48	2.16	17	1
1:A:9:ASN:O	1:A:10:GLU:C	0.48	2.56	11	15
1:A:8:TRP:HB2	1:A:27:ASP:HB2	0.48	1.86	11	2
1:A:18:ASN:OD1	1:A:18:ASN:N	0.48	2.41	10	1
1:A:93:ALA:O	1:A:94:ALA:C	0.48	2.57	6	2
1:A:77:ALA:HB3	1:A:90:ALA:CA	0.47	2.39	6	14
1:A:56:TRP:O	1:A:75:ASP:OD2	0.47	2.31	20	8
1:A:32:CYS:H	1:A:36:GLY:C	0.47	2.17	16	8
1:A:22:ASN:C	1:A:23:ASN:ND2	0.47	2.72	5	1
1:A:6:TYR:CB	1:A:6:TYR:CD2	0.47	2.78	15	3
1:A:43:ARG:O	1:A:43:ARG:CD	0.47	2.62	16	5
1:A:39:GLN:C	1:A:39:GLN:CD	0.47	2.82	5	19
1:A:56:TRP:O	1:A:57:ASP:CB	0.47	2.63	3	16
1:A:51:GLY:CA	1:A:91:GLY:N	0.47	2.78	19	3
1:A:67:ARG:O	1:A:73:GLN:CB	0.47	2.62	5	5
1:A:53:THR:OG1	1:A:77:ALA:CA	0.47	2.63	6	1
1:A:78:ARG:HB3	1:A:85:PHE:O	0.47	2.09	7	2
1:A:21:SER:C	1:A:22:ASN:ND2	0.47	2.72	17	1
1:A:65:PRO:O	1:A:66:ASN:C	0.47	2.57	2	20
1:A:78:ARG:NH1	1:A:89:THR:CA	0.47	2.78	4	2
1:A:18:ASN:O	1:A:19:ARG:HB2	0.47	2.10	10	9
1:A:1:GLY:CA	1:A:30:ARG:HB2	0.47	2.39	16	1
1:A:5:THR:O	1:A:6:TYR:C	0.47	2.57	2	18
1:A:22:ASN:CG	1:A:23:ASN:HD21	0.47	2.15	14	2
1:A:43:ARG:CD	1:A:43:ARG:O	0.47	2.63	8	3
1:A:73:GLN:O	1:A:74:CYS:CA	0.47	2.61	11	5
1:A:58:GLU:O	1:A:65:PRO:HB3	0.47	2.09	15	9
1:A:78:ARG:NH1	1:A:89:THR:C	0.47	2.73	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:GLY:C	1:A:17:PRO:O	0.47	2.56	18	9
1:A:22:ASN:O	1:A:23:ASN:O	0.47	2.33	10	4
1:A:56:TRP:H	1:A:75:ASP:HA	0.47	1.69	15	6
1:A:35:SER:O	1:A:36:GLY:C	0.47	2.58	7	18
1:A:59:ALA:O	1:A:67:ARG:HA	0.47	2.10	11	5
1:A:71:SER:C	1:A:85:PHE:CG	0.47	2.93	13	1
1:A:8:TRP:CZ2	1:A:22:ASN:ND2	0.46	2.83	17	1
1:A:22:ASN:CB	1:A:23:ASN:ND2	0.46	2.79	5	8
1:A:13:ASN:CB	1:A:17:PRO:O	0.46	2.63	4	11
1:A:23:ASN:OD1	1:A:27:ASP:CG	0.46	2.58	5	5
1:A:76:GLY:C	1:A:78:ARG:H	0.46	2.13	7	1
1:A:89:THR:HG22	1:A:90:ALA:C	0.46	2.36	14	9
1:A:58:GLU:O	1:A:58:GLU:CG	0.46	2.62	1	13
1:A:1:GLY:CA	1:A:27:ASP:HA	0.46	2.41	4	4
1:A:78:ARG:HH11	1:A:89:THR:C	0.46	2.19	4	1
1:A:23:ASN:C	1:A:30:ARG:HG2	0.46	2.35	16	1
1:A:16:GLY:O	1:A:17:PRO:O	0.46	2.33	18	6
1:A:59:ALA:HA	1:A:65:PRO:HB2	0.46	1.88	5	8
1:A:71:SER:CA	1:A:80:CYS:SG	0.46	3.04	6	2
1:A:31:THR:CA	1:A:39:GLN:O	0.46	2.63	16	1
1:A:1:GLY:C	1:A:29:ALA:C	0.46	2.84	7	6
1:A:8:TRP:CA	1:A:27:ASP:HB3	0.46	2.40	7	6
1:A:45:PRO:HB3	1:A:77:ALA:HA	0.46	1.86	8	1
1:A:78:ARG:NH1	1:A:88:GLY:O	0.46	2.49	20	1
1:A:77:ALA:HB3	1:A:90:ALA:HA	0.46	1.87	17	10
1:A:30:ARG:NH1	1:A:30:ARG:HG2	0.46	2.26	2	2
1:A:51:GLY:N	1:A:77:ALA:HB2	0.46	2.25	4	7
1:A:56:TRP:HE1	1:A:59:ALA:HB2	0.46	1.70	7	5
1:A:42:SER:C	1:A:44:LYS:N	0.46	2.74	11	1
1:A:32:CYS:HB2	1:A:37:PHE:C	0.46	2.36	16	1
1:A:30:ARG:CD	1:A:41:THR:C	0.46	2.89	18	1
1:A:23:ASN:HA	1:A:37:PHE:O	0.46	2.10	9	3
1:A:51:GLY:O	1:A:91:GLY:C	0.46	2.59	10	18
1:A:1:GLY:HA2	1:A:29:ALA:H	0.46	1.70	8	5
1:A:31:THR:C	1:A:38:CYS:N	0.45	2.70	9	5
1:A:32:CYS:N	1:A:38:CYS:H	0.45	2.08	9	13
1:A:51:GLY:C	1:A:91:GLY:HA3	0.45	2.36	18	17
1:A:8:TRP:CB	1:A:27:ASP:CB	0.45	2.92	7	10
1:A:32:CYS:HA	1:A:38:CYS:CA	0.45	2.41	16	9
1:A:31:THR:OG1	1:A:39:GLN:OE1	0.45	2.35	19	9
1:A:86:CYS:O	1:A:87:GLN:CB	0.45	2.64	14	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ASN:CB	1:A:23:ASN:OD1	0.45	2.64	12	4
1:A:46:ASP:C	1:A:46:ASP:OD1	0.45	2.59	14	3
1:A:49:PRO:HB2	1:A:53:THR:HG23	0.45	1.88	6	1
1:A:53:THR:HG1	1:A:77:ALA:HA	0.45	1.72	6	1
1:A:75:ASP:OD1	1:A:90:ALA:HB2	0.45	2.11	8	2
1:A:67:ARG:HG3	1:A:67:ARG:HH11	0.45	1.72	11	1
1:A:74:CYS:SG	1:A:86:CYS:CB	0.45	3.04	1	4
1:A:55:CYS:H	1:A:75:ASP:C	0.45	2.19	18	7
1:A:74:CYS:HB2	1:A:85:PHE:CA	0.45	2.42	11	4
1:A:53:THR:OG1	1:A:77:ALA:HB2	0.45	2.11	6	1
1:A:4:PRO:O	1:A:52:PRO:O	0.45	2.35	18	3
1:A:24:LYS:O	1:A:30:ARG:NH2	0.45	2.48	10	1
1:A:31:THR:OG1	1:A:39:GLN:C	0.45	2.60	18	8
1:A:56:TRP:CB	1:A:74:CYS:O	0.45	2.64	18	3
1:A:46:ASP:OD1	1:A:46:ASP:C	0.45	2.60	15	8
1:A:32:CYS:N	1:A:37:PHE:CA	0.45	2.80	13	10
1:A:32:CYS:H	1:A:36:GLY:N	0.45	2.10	15	14
1:A:23:ASN:CA	1:A:37:PHE:O	0.45	2.66	5	4
1:A:39:GLN:CD	1:A:39:GLN:C	0.45	2.86	9	1
1:A:42:SER:C	1:A:43:ARG:HG3	0.45	2.37	19	1
1:A:1:GLY:HA2	1:A:28:GLY:H	0.44	1.71	16	1
1:A:4:PRO:CB	1:A:53:THR:HG22	0.44	2.43	6	1
1:A:32:CYS:C	1:A:34:SER:N	0.44	2.75	6	7
1:A:56:TRP:O	1:A:57:ASP:OD1	0.44	2.36	9	3
1:A:51:GLY:H	1:A:77:ALA:HB2	0.44	1.72	10	1
1:A:22:ASN:ND2	1:A:37:PHE:CD1	0.44	2.84	20	1
1:A:68:CYS:O	1:A:69:SER:OG	0.44	2.33	6	8
1:A:69:SER:CA	1:A:86:CYS:SG	0.44	3.05	4	2
1:A:8:TRP:HE1	1:A:21:SER:N	0.44	2.11	7	1
1:A:78:ARG:NH1	1:A:89:THR:O	0.44	2.50	8	1
1:A:71:SER:CA	1:A:85:PHE:CD2	0.44	3.01	9	2
1:A:15:GLY:O	1:A:19:ARG:CZ	0.44	2.65	14	1
1:A:6:TYR:O	1:A:7:CYS:C	0.44	2.58	19	17
1:A:75:ASP:OD1	1:A:90:ALA:CB	0.44	2.66	10	2
1:A:14:PRO:O	1:A:15:GLY:C	0.44	2.60	2	1
1:A:19:ARG:O	1:A:21:SER:HB2	0.44	2.12	11	2
1:A:79:THR:CA	1:A:87:GLN:OE1	0.44	2.66	17	2
1:A:12:ASN:O	1:A:12:ASN:OD1	0.44	2.35	13	2
1:A:22:ASN:O	1:A:26:CYS:O	0.44	2.36	16	1
1:A:5:THR:HB	1:A:93:ALA:H	0.43	1.72	10	10
1:A:56:TRP:O	1:A:57:ASP:CG	0.43	2.61	10	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:SER:OG	1:A:70:ASN:OD1	0.43	2.36	7	5
1:A:53:THR:H	1:A:92:HIS:N	0.43	2.11	13	2
1:A:59:ALA:O	1:A:67:ARG:C	0.43	2.61	18	3
1:A:23:ASN:O	1:A:24:LYS:C	0.43	2.61	16	2
1:A:22:ASN:H	1:A:25:GLN:CA	0.43	2.26	14	2
1:A:71:SER:CA	1:A:85:PHE:CD1	0.43	3.01	5	2
1:A:23:ASN:CB	1:A:26:CYS:O	0.43	2.66	18	1
1:A:8:TRP:NE1	1:A:18:ASN:HD22	0.43	2.11	16	2
1:A:8:TRP:HB2	1:A:27:ASP:CA	0.43	2.42	18	9
1:A:60:LYS:HB3	1:A:86:CYS:SG	0.43	2.53	2	1
1:A:4:PRO:HA	1:A:43:ARG:CB	0.43	2.43	6	4
1:A:53:THR:HG1	1:A:77:ALA:N	0.43	2.11	10	1
1:A:13:ASN:C	1:A:16:GLY:O	0.43	2.61	12	1
1:A:30:ARG:HH11	1:A:42:SER:N	0.43	2.11	4	2
1:A:29:ALA:O	1:A:30:ARG:C	0.43	2.61	10	5
1:A:66:ASN:O	1:A:67:ARG:HB2	0.43	2.14	14	5
1:A:20:CYS:HA	1:A:25:GLN:O	0.43	2.13	17	5
1:A:41:THR:O	1:A:41:THR:CG2	0.43	2.67	16	1
1:A:21:SER:O	1:A:21:SER:OG	0.43	2.36	18	5
1:A:73:GLN:OE1	1:A:73:GLN:C	0.43	2.62	14	1
1:A:23:ASN:HB3	1:A:30:ARG:CB	0.43	2.43	16	1
1:A:5:THR:O	1:A:5:THR:OG1	0.43	2.37	19	10
1:A:3:GLY:O	1:A:6:TYR:N	0.43	2.46	5	3
1:A:30:ARG:HG3	1:A:41:THR:N	0.43	2.29	18	2
1:A:70:ASN:O	1:A:80:CYS:CB	0.43	2.67	15	3
1:A:56:TRP:CH2	1:A:66:ASN:OD1	0.42	2.72	3	2
1:A:23:ASN:O	1:A:30:ARG:CG	0.42	2.66	3	1
1:A:30:ARG:NH2	1:A:42:SER:OG	0.42	2.52	19	1
1:A:23:ASN:ND2	1:A:37:PHE:HB2	0.42	2.29	14	4
1:A:66:ASN:OD1	1:A:73:GLN:NE2	0.42	2.51	14	1
1:A:8:TRP:C	1:A:10:GLU:N	0.42	2.76	1	4
1:A:11:ALA:N	1:A:17:PRO:HB3	0.42	2.30	4	1
1:A:32:CYS:N	1:A:38:CYS:N	0.42	2.67	9	2
1:A:30:ARG:C	1:A:31:THR:HG23	0.42	2.39	4	2
1:A:23:ASN:N	1:A:23:ASN:HD22	0.42	2.13	5	1
1:A:73:GLN:CA	1:A:73:GLN:OE1	0.42	2.67	5	1
1:A:23:ASN:O	1:A:25:GLN:N	0.42	2.52	16	2
1:A:1:GLY:HA3	1:A:30:ARG:CA	0.42	2.45	14	1
1:A:10:GLU:OE1	1:A:85:PHE:CE1	0.42	2.72	20	2
1:A:33:SER:N	1:A:38:CYS:SG	0.42	2.92	18	1
1:A:50:LYS:NZ	1:A:77:ALA:O	0.42	2.49	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:GLY:C	1:A:27:ASP:OD1	0.42	2.62	13	1
1:A:73:GLN:OE1	1:A:73:GLN:CA	0.42	2.68	14	1
1:A:8:TRP:HB2	1:A:27:ASP:H	0.42	1.72	15	4
1:A:23:ASN:CG	1:A:26:CYS:O	0.42	2.61	9	2
1:A:53:THR:N	1:A:92:HIS:CA	0.42	2.83	4	2
1:A:56:TRP:HB2	1:A:74:CYS:O	0.42	2.15	7	3
1:A:24:LYS:HB2	1:A:30:ARG:NE	0.41	2.30	20	1
1:A:24:LYS:CB	1:A:30:ARG:NH1	0.41	2.84	16	1
1:A:48:GLY:O	1:A:49:PRO:C	0.41	2.62	11	1
1:A:37:PHE:CD1	1:A:37:PHE:O	0.41	2.74	20	1
1:A:43:ARG:O	1:A:43:ARG:HD2	0.41	2.15	13	1
1:A:56:TRP:CE2	1:A:66:ASN:OD1	0.41	2.73	10	1
1:A:23:ASN:N	1:A:37:PHE:O	0.41	2.54	14	1
1:A:89:THR:HG23	1:A:90:ALA:N	0.41	2.30	18	2
1:A:65:PRO:O	1:A:67:ARG:HG2	0.41	2.15	2	1
1:A:52:PRO:C	1:A:93:ALA:N	0.41	2.78	4	1
1:A:67:ARG:HG3	1:A:67:ARG:NH1	0.41	2.31	4	2
1:A:23:ASN:ND2	1:A:27:ASP:CG	0.41	2.78	1	1
1:A:31:THR:OG1	1:A:39:GLN:HG3	0.41	2.15	4	4
1:A:74:CYS:HB2	1:A:85:PHE:CB	0.41	2.46	19	1
1:A:38:CYS:O	1:A:38:CYS:SG	0.41	2.79	7	2
1:A:1:GLY:H2	1:A:27:ASP:HA	0.41	1.68	8	1
1:A:46:ASP:OD1	1:A:48:GLY:N	0.41	2.54	14	1
1:A:89:THR:HG22	1:A:90:ALA:O	0.41	2.15	14	1
1:A:23:ASN:C	1:A:25:GLN:H	0.41	2.23	16	1
1:A:22:ASN:N	1:A:25:GLN:CA	0.41	2.82	20	1
1:A:56:TRP:N	1:A:75:ASP:CG	0.41	2.78	20	1
1:A:80:CYS:SG	1:A:85:PHE:HB3	0.41	2.56	3	2
1:A:6:TYR:O	1:A:7:CYS:HB3	0.41	2.15	4	1
1:A:54:TYR:CA	1:A:76:GLY:HA3	0.41	2.45	20	1
1:A:43:ARG:HE	1:A:53:THR:HB	0.40	1.76	18	1
1:A:51:GLY:C	1:A:91:GLY:N	0.40	2.80	19	1
1:A:8:TRP:HB2	1:A:27:ASP:HB3	0.40	1.92	1	1
1:A:43:ARG:NE	1:A:53:THR:CB	0.40	2.83	8	1
1:A:11:ALA:N	1:A:18:ASN:H	0.40	2.14	11	1
1:A:72:LYS:HA	1:A:85:PHE:CE2	0.40	2.52	11	1
1:A:30:ARG:HE	1:A:41:THR:CA	0.40	2.29	16	1
1:A:16:GLY:N	1:A:19:ARG:HD3	0.40	2.31	2	1
1:A:71:SER:C	1:A:85:PHE:CD2	0.40	3.00	12	1
1:A:91:GLY:O	1:A:92:HIS:CG	0.40	2.75	14	1
1:A:32:CYS:O	1:A:39:GLN:CG	0.40	2.69	19	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	84/95 (88%)	24±2 (29±2%)	25±2 (29±3%)	35±2 (42±2%)	0	0
All	All	1680/1900 (88%)	488 (29%)	491 (29%)	701 (42%)	0	0

All 47 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	4	PRO	20
1	A	5	THR	20
1	A	6	TYR	20
1	A	12	ASN	20
1	A	17	PRO	20
1	A	18	ASN	20
1	A	20	CYS	20
1	A	29	ALA	20
1	A	30	ARG	20
1	A	37	PHE	20
1	A	38	CYS	20
1	A	45	PRO	20
1	A	48	GLY	20
1	A	49	PRO	20
1	A	52	PRO	20
1	A	54	TYR	20
1	A	57	ASP	20
1	A	58	GLU	20
1	A	71	SER	20
1	A	73	GLN	20
1	A	80	CYS	20
1	A	87	GLN	20
1	A	88	GLY	20
1	A	90	ALA	20
1	A	92	HIS	20
1	A	91	GLY	19
1	A	19	ARG	16

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Mol	Chain	Res	Type	Models (Total)
1	A	66	ASN	16
1	A	67	ARG	15
1	A	27	ASP	14
1	A	9	ASN	13
1	A	14	PRO	13
1	A	69	SER	13
1	A	43	ARG	13
1	A	68	CYS	11
1	A	72	LYS	9
1	A	76	GLY	8
1	A	25	GLN	8
1	A	77	ALA	7
1	A	8	TRP	6
1	A	47	PRO	6
1	A	11	ALA	5
1	A	44	LYS	3
1	A	23	ASN	2
1	A	65	PRO	2
1	A	15	GLY	1
1	A	85	PHE	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	67/72 (93%)	46±2 (69±3%)	21±2 (31±3%)	1	15
All	All	1340/1440 (93%)	926 (69%)	414 (31%)	1	15

All 33 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	5	THR	20
1	A	13	ASN	20
1	A	18	ASN	20
1	A	23	ASN	20
1	A	39	GLN	20

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Mol	Chain	Res	Type	Models (Total)
1	A	41	THR	20
1	A	50	LYS	20
1	A	54	TYR	20
1	A	66	ASN	20
1	A	30	ARG	19
1	A	53	THR	19
1	A	46	ASP	18
1	A	89	THR	18
1	A	42	SER	17
1	A	80	CYS	15
1	A	87	GLN	14
1	A	43	ARG	13
1	A	12	ASN	11
1	A	19	ARG	11
1	A	25	GLN	10
1	A	85	PHE	10
1	A	60	LYS	10
1	A	21	SER	9
1	A	73	GLN	6
1	A	55	CYS	6
1	A	56	TRP	5
1	A	68	CYS	5
1	A	75	ASP	4
1	A	22	ASN	4
1	A	2	SER	4
1	A	79	THR	2
1	A	57	ASP	2
1	A	72	LYS	2

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](#)

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	12-A	4
1	1-A	3
1	3-A	3
1	4-A	3
1	7-A	3
1	10-A	3
1	14-A	3
1	16-A	3
1	18-A	3
1	13-A	2
1	20-A	2
1	2-A	2
1	6-A	2
1	17-A	2
1	11-A	1
1	15-A	1
1	19-A	1
1	5-A	1
1	8-A	1
1	9-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	80:CYS	C	81:SER	N	1.20
3	A	9:ASN	C	10:GLU	N	1.20
4	A	33:SER	C	34:SER	N	1.20
7	A	53:THR	C	54:TYR	N	1.20
7	A	72:LYS	C	73:GLN	N	1.20
10	A	9:ASN	C	10:GLU	N	1.20

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
12	A	9:ASN	C	10:GLU	N	1.20
12	A	15:GLY	C	16:GLY	N	1.20
13	A	33:SER	C	34:SER	N	1.20
14	A	33:SER	C	34:SER	N	1.20
14	A	80:CYS	C	81:SER	N	1.20
16	A	9:ASN	C	10:GLU	N	1.20
18	A	72:LYS	C	73:GLN	N	1.20
20	A	9:ASN	C	10:GLU	N	1.20
2	A	15:GLY	C	16:GLY	N	1.19
4	A	15:GLY	C	16:GLY	N	1.19
6	A	15:GLY	C	16:GLY	N	1.19
7	A	15:GLY	C	16:GLY	N	1.19
10	A	33:SER	C	34:SER	N	1.19
11	A	15:GLY	C	16:GLY	N	1.19
12	A	33:SER	C	34:SER	N	1.19
15	A	72:LYS	C	73:GLN	N	1.19
16	A	33:SER	C	34:SER	N	1.19
17	A	33:SER	C	34:SER	N	1.19
18	A	26:CYS	C	27:ASP	N	1.19
19	A	72:LYS	C	73:GLN	N	1.19
1	A	15:GLY	C	16:GLY	N	1.18
3	A	15:GLY	C	16:GLY	N	1.18
6	A	72:LYS	C	73:GLN	N	1.18
18	A	15:GLY	C	16:GLY	N	1.18
3	A	72:LYS	C	73:GLN	N	1.15
14	A	72:LYS	C	73:GLN	N	1.15
4	A	72:LYS	C	73:GLN	N	1.14
10	A	72:LYS	C	73:GLN	N	1.14
16	A	72:LYS	C	73:GLN	N	1.14
17	A	72:LYS	C	73:GLN	N	1.14
20	A	72:LYS	C	73:GLN	N	1.14
1	A	72:LYS	C	73:GLN	N	1.13
5	A	72:LYS	C	73:GLN	N	1.13
8	A	72:LYS	C	73:GLN	N	1.13
9	A	72:LYS	C	73:GLN	N	1.13
12	A	72:LYS	C	73:GLN	N	1.13
13	A	72:LYS	C	73:GLN	N	1.13
2	A	72:LYS	C	73:GLN	N	1.12

7 Chemical shift validation

No chemical shift data were provided