



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 04:18 PM UTC

PDB ID : 8K31 / pdb_00008k31
BMRB ID : 50583
Title : The complex of WRKY33 C terminal DBD and SIB1
Authors : Dong, X.; Gong, Z.; Hu, Y.F.
Deposited on : 2023-07-14

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
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

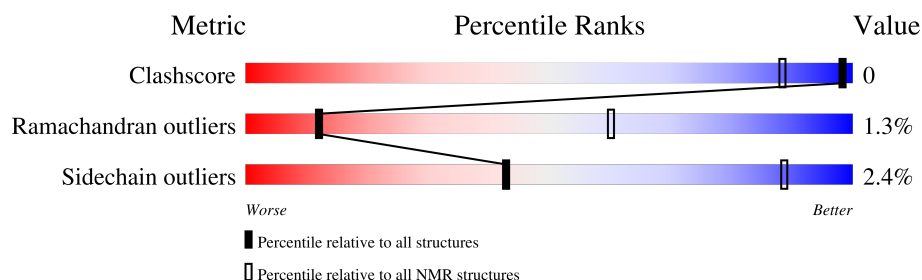
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 1%.

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	98	
2	B	101	

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 20 as representative, based on the following criterion: *lowest energy*.

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:49-A:70, B:346-B:421 (98)	1.14	5

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1820 atoms, of which 904 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sigma factor binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms						Trace
1	A	35	Total	C	H	N	O	S	0
			544	170	269	47	56	2	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	initiating methionine	UNP Q9LDH1
A	101	LEU	-	expression tag	UNP Q9LDH1
A	102	GLU	-	expression tag	UNP Q9LDH1
A	103	HIS	-	expression tag	UNP Q9LDH1
A	104	HIS	-	expression tag	UNP Q9LDH1
A	105	HIS	-	expression tag	UNP Q9LDH1
A	106	HIS	-	expression tag	UNP Q9LDH1
A	107	HIS	-	expression tag	UNP Q9LDH1

- Molecule 2 is a protein called Probable WRKY transcription factor 33.

Mol	Chain	Residues	Atoms						Trace
2	B	79	Total	C	H	N	O	S	0
			1275	397	635	123	115	5	

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	330	MET	-	initiating methionine	UNP Q8S8P5
B	357	CYS	ASP	engineered mutation	UNP Q8S8P5
B	376	CYS	LYS	engineered mutation	UNP Q8S8P5
B	423	LEU	-	expression tag	UNP Q8S8P5
B	424	GLU	-	expression tag	UNP Q8S8P5
B	425	HIS	-	expression tag	UNP Q8S8P5
B	426	HIS	-	expression tag	UNP Q8S8P5
B	427	HIS	-	expression tag	UNP Q8S8P5
B	428	HIS	-	expression tag	UNP Q8S8P5
B	429	HIS	-	expression tag	UNP Q8S8P5
B	430	HIS	-	expression tag	UNP Q8S8P5

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

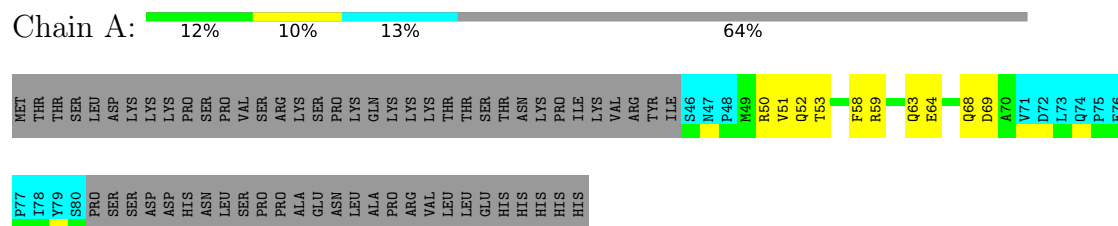
Mol	Chain	Residues	Atoms	
			Total	Zn
3	B	1	1	1

4 Residue-property plots [i](#)

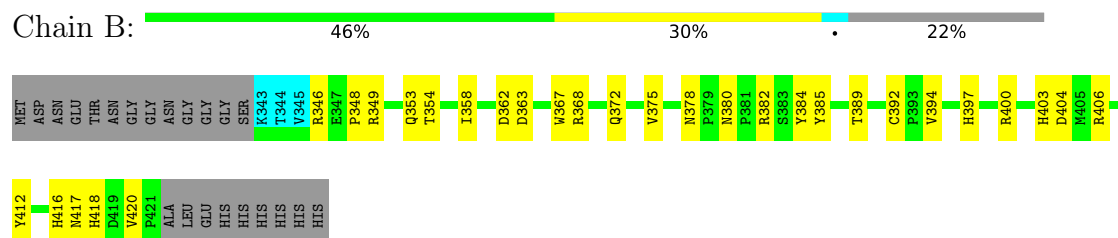
4.1 Average score per residue in the NMR ensemble

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: Sigma factor binding protein 1, chloroplastic



- Molecule 2: Probable WRKY transcription factor 33

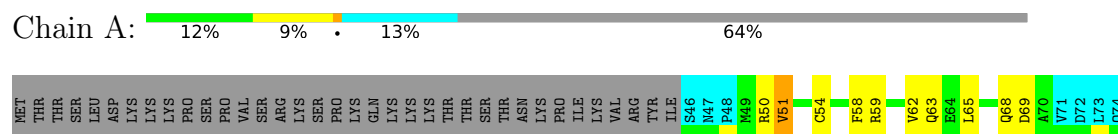


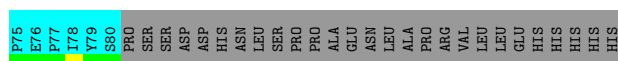
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

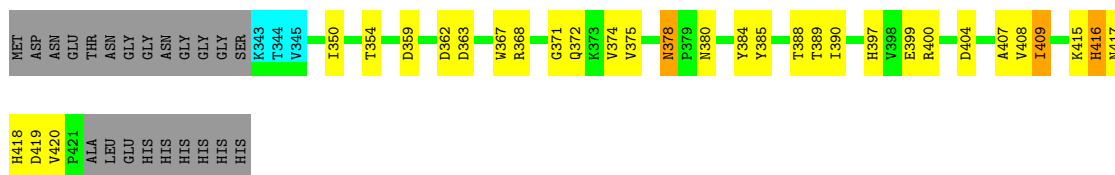
- Molecule 1: Sigma factor binding protein 1, chloroplastic





- Molecule 2: Probable WRKY transcription factor 33

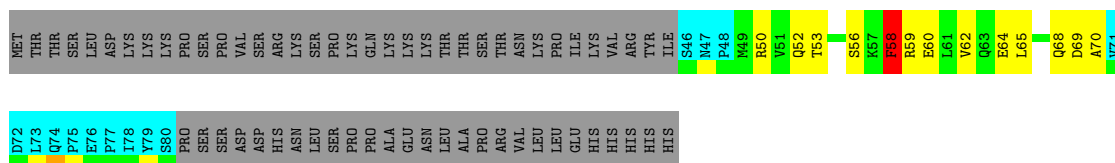
Chain B: 45% 28% 22%



4.2.2 Score per residue for model 2

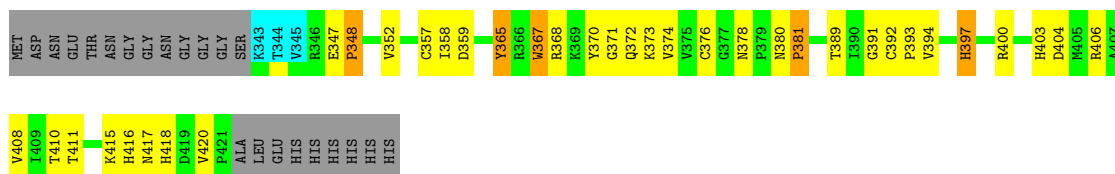
- Molecule 1: Sigma factor binding protein 1, chloroplastic

Chain A: 9% 12% 64%



- Molecule 2: Probable WRKY transcription factor 33

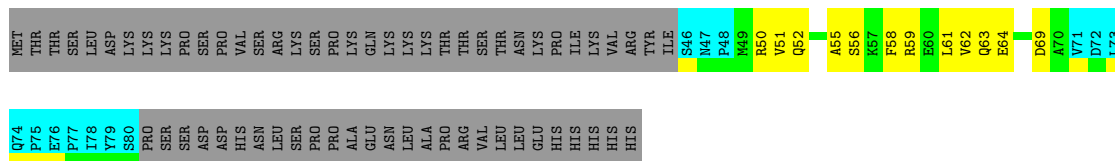
Chain B: 40% 31% 22%



4.2.3 Score per residue for model 3

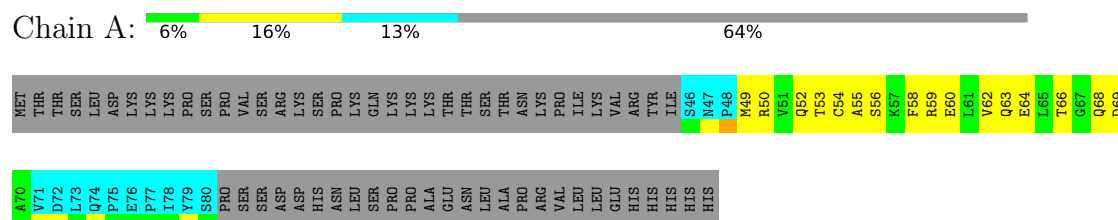
- Molecule 1: Sigma factor binding protein 1, chloroplastic

Chain A: 10% 12% 64%

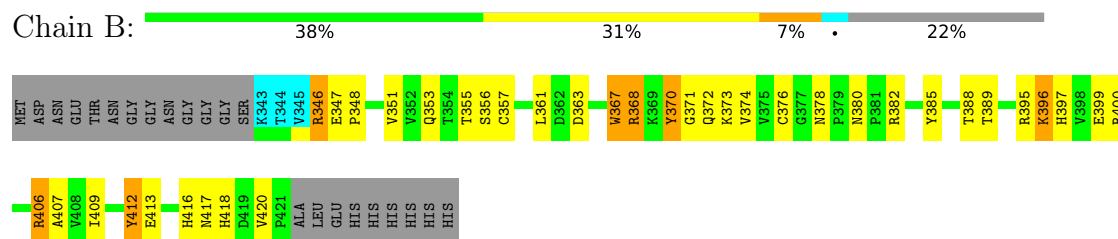


- Molecule 2: Probable WRKY transcription factor 33

- Molecule 1: Sigma factor binding protein 1, chloroplastic

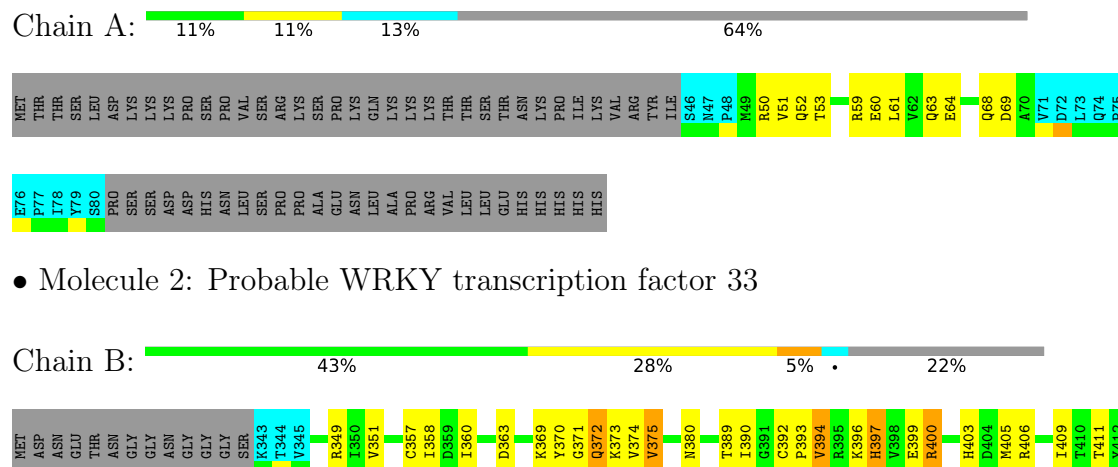


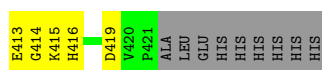
- Molecule 2: Probable WRKY transcription factor 33



4.2.5 Score per residue for model 5 (medoid)

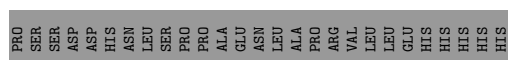
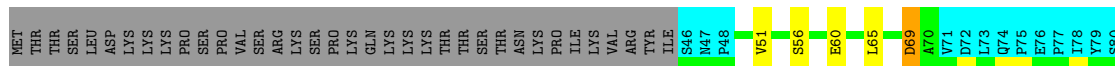
- Molecule 1: Sigma factor binding protein 1, chloroplastic





4.2.6 Score per residue for model 6

- Molecule 1: Sigma factor binding protein 1, chloroplastic

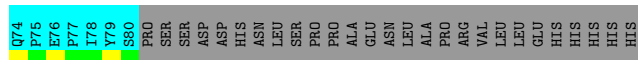
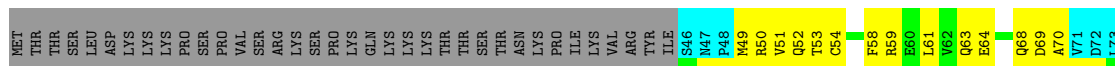


- Molecule 2: Probable WRKY transcription factor 33

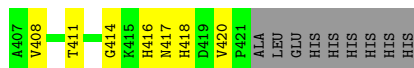


4.2.7 Score per residue for model 7

- Molecule 1: Sigma factor binding protein 1, chloroplastic

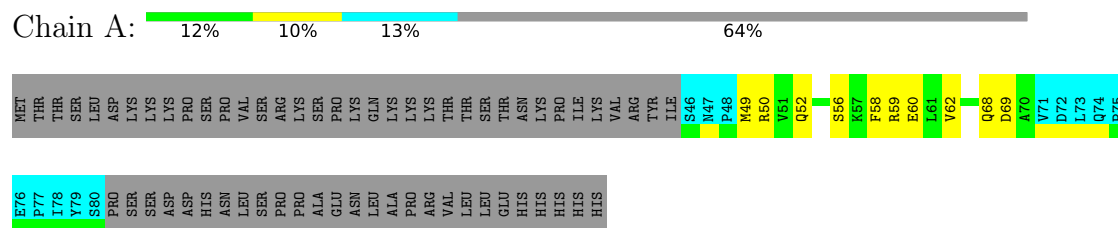


- Molecule 2: Probable WRKY transcription factor 33

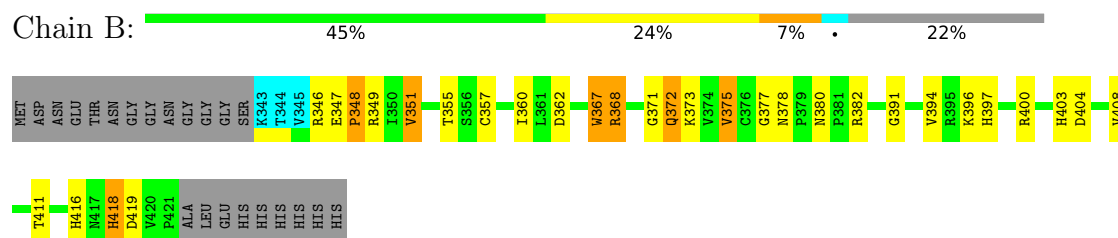


4.2.8 Score per residue for model 8

- Molecule 1: Sigma factor binding protein 1, chloroplastic

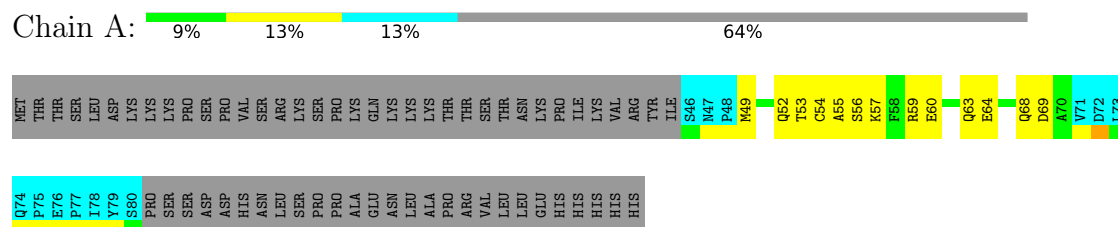


- Molecule 2: Probable WRKY transcription factor 33

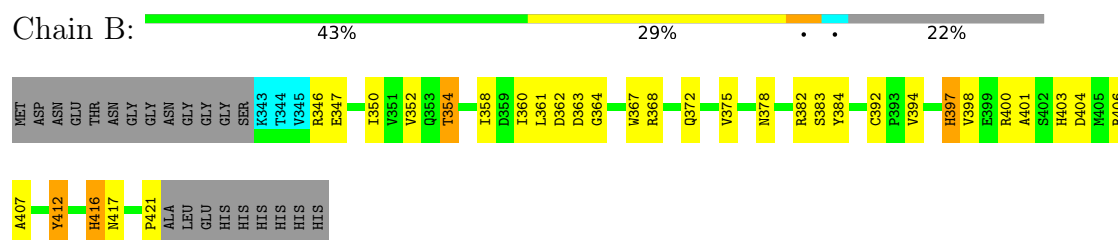


4.2.9 Score per residue for model 9

- Molecule 1: Sigma factor binding protein 1, chloroplastic



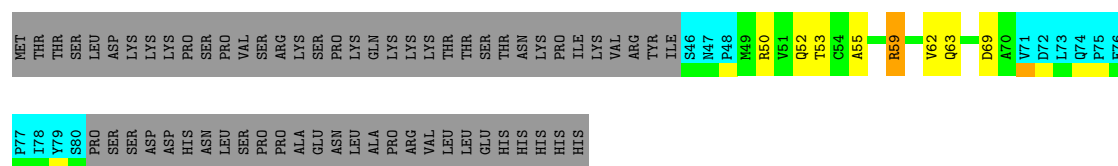
- Molecule 2: Probable WRKY transcription factor 33



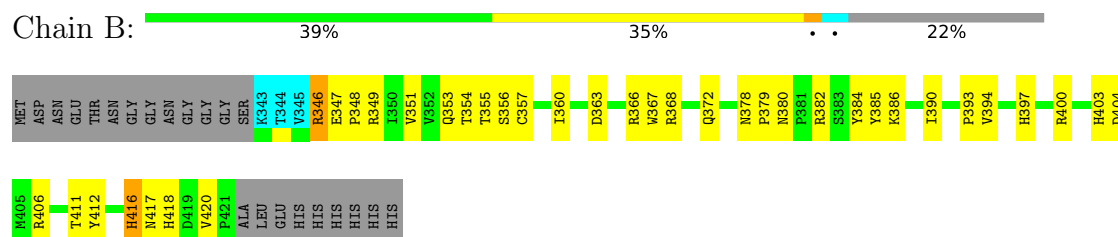
4.2.10 Score per residue for model 10

- Molecule 1: Sigma factor binding protein 1, chloroplastic



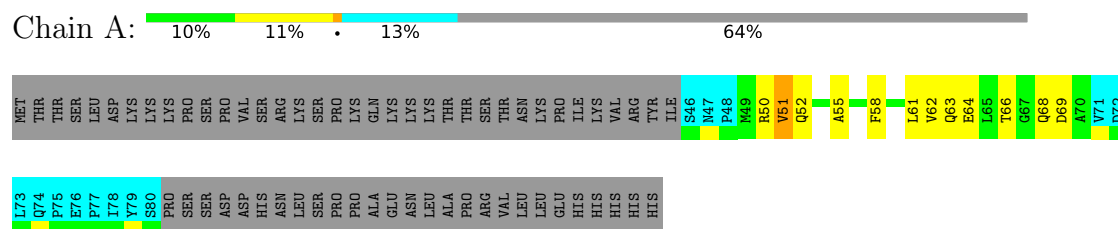


- Molecule 2: Probable WRKY transcription factor 33

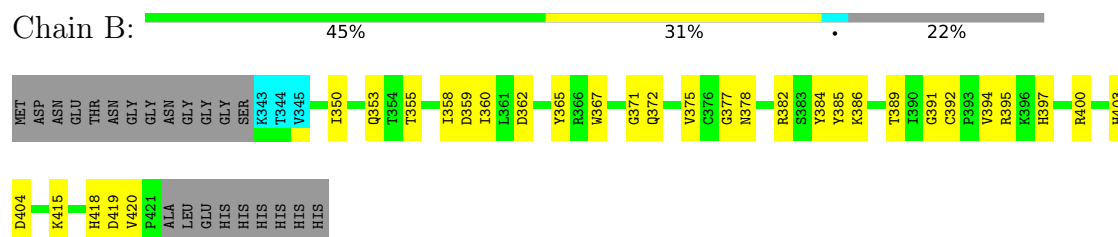


4.2.11 Score per residue for model 11

- Molecule 1: Sigma factor binding protein 1, chloroplastic

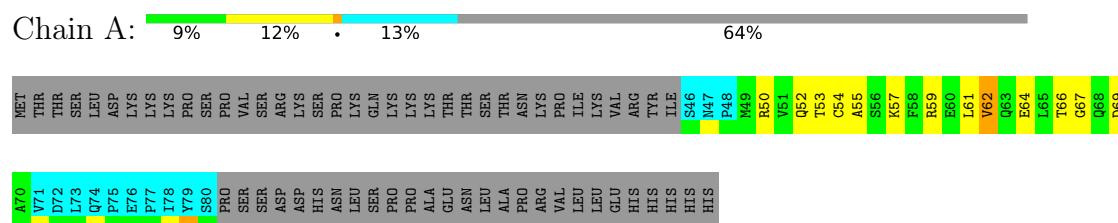


- Molecule 2: Probable WRKY transcription factor 33



4.2.12 Score per residue for model 12

- Molecule 1: Sigma factor binding protein 1, chloroplastic



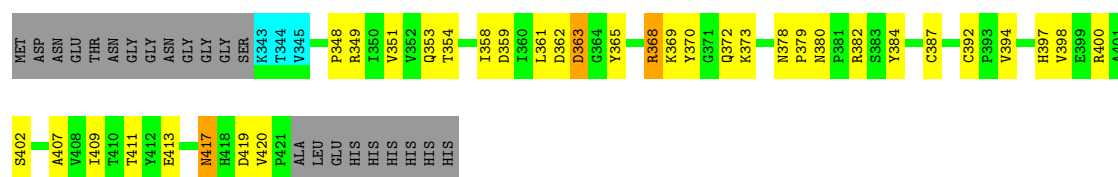
- | | |
|------|------|
| D419 | MET |
| V420 | ASN |
| P421 | ASP |
| ALA | GLU |
| LEU | THR |
| GLU | ASN |
| HIS | GLY |
| HIS | GLY |
| HIS | ASN |
| HIS | GLY |
| HIS | GLY |
| HIS | GLY |
| HIS | SER |
| | K343 |
| | T344 |
| | V345 |
| | R346 |
| | E347 |
| | P348 |
| | R349 |
| | I350 |
| | Q353 |
| | T354 |
| | I360 |
| | L361 |
| | D362 |
| | R368 |
| | Q372 |
| | N378 |
| | P379 |
| | K380 |
| | P381 |
| | H382 |
| | T388 |
| | P393 |
| | V394 |
| | R395 |
| | K396 |
| | H397 |
| | A401 |
| | S402 |
| | H403 |
| | D404 |
| | M405 |
| | R406 |
| | A407 |
| | E413 |
| | G414 |
| | K415 |
| | H416 |
| | N417 |
| | V418 |

E76	P77	I78	Y79	S80	PRO	SER	SER	SER	ASP	ASP	HIS	ASN	LEU	VAL	PRO	PRO	ARG	LYS	SER	PRO	GLN	LYS	ALA	ALA	PRO	ARG	VAL	LEU	GLU	HIS	HIS	HIS	HIS																			
MET	THR	SER	LEU	ASP	LYS	LYS	LYS	PRO	SER	PRO	SER	VAL	ARG	LYS	SER	PRO	GLN	LYS	LYS	THR	SER	THR	ASN	LYS	PRO	ILE	VAL	ARG	TYR	ILE	S46	N47	P48	M49	R50	V51	Q52	T53	C54	A55	S56	K57	F58	R59	E64	D69	A70	V71	D72	L73	O74	G75

- | | | |
|------|------|-----|
| T410 | | MET |
| T411 | | ASP |
| M417 | | ASN |
| H418 | | GLU |
| D419 | | THR |
| V420 | | ASN |
| P421 | | GLY |
| A4A | | GLY |
| ALA | | ASN |
| LEU | | GLY |
| GLU | | GLY |
| HIS | | GLY |
| HIS | | SER |
| HIS | K343 | |
| HIS | T344 | |
| HIS | V345 | |
| HIS | R346 | |
| HIS | E347 | |
| HIS | P348 | |
| HIS | R349 | |
| | I350 | |
| | V351 | |
| | V352 | |
| | | |
| | I358 | |
| | D359 | |
| | I360 | |
| | L361 | |
| | D362 | |
| | D363 | |
| | G364 | |
| | V365 | |
| | R366 | |
| | V367 | |
| | R368 | |
| | R369 | |
| | | |
| | V374 | |
| | | |
| | N378 | |
| | | |
| | S383 | |
| | Y384 | |
| | Y385 | |
| | K386 | |
| | C387 | |
| | | |
| | I390 | |
| | G391 | |
| | C392 | |
| | | |
| | H397 | |
| | V398 | |
| | E399 | |
| | | |
| | S402 | |
| | H403 | |
| | | |
| | V408 | |
| | T409 | |

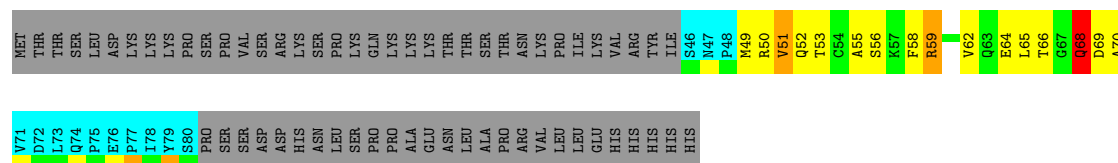
L73	Q74	P75	E76	P77	I78	Y79	S80	PRO	SER	SER	ASP	ASP	HIS	ASN	ASN	LEU	LEU	PRO	PRO	ALA	GLU	ALA	ASN	LEU	LEU	GLU	HIS	HIS	HIS	HIS																				
MET	THR	SER	LEU	ASP	LYS	LYS	LVS	PRO	SER	PRO	VAL	SER	ARG	LVS	LYS	LYS	THR	THR	THR	ASN	LYS	PRO	ILE	LVS	ARG	TYR	ILE	S46	N47	P48	R49	S50	T51	Q52	T53	C54	A55	S56	F58	R59	E60	L61	V62	Q63	L64	Q68	D69	A70	V71	P72

- Chain B:  41% 32% • • 22%

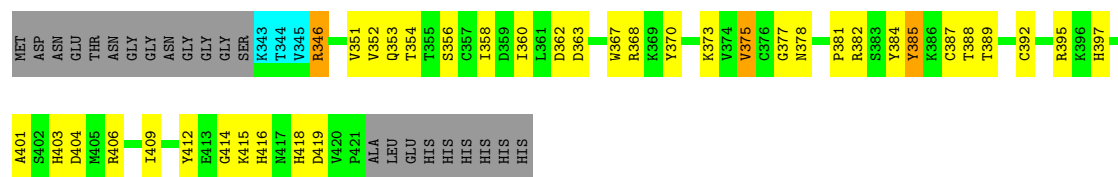


4.2.15 Score per residue for model 15

- Molecule 1: Sigma factor binding protein 1, chloroplastic

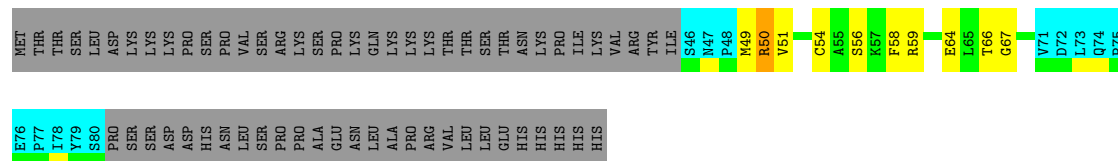


- Molecule 2: Probable WRKY transcription factor 33

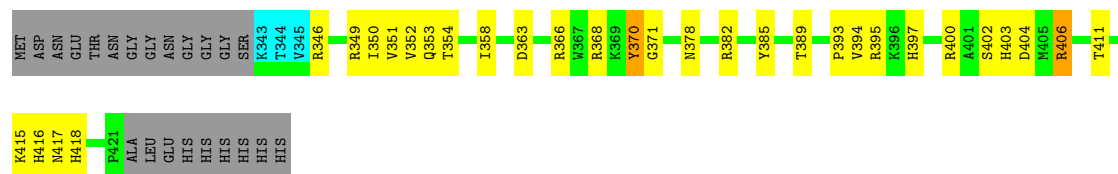


4.2.16 Score per residue for model 16

- Molecule 1: Sigma factor binding protein 1, chloroplastic

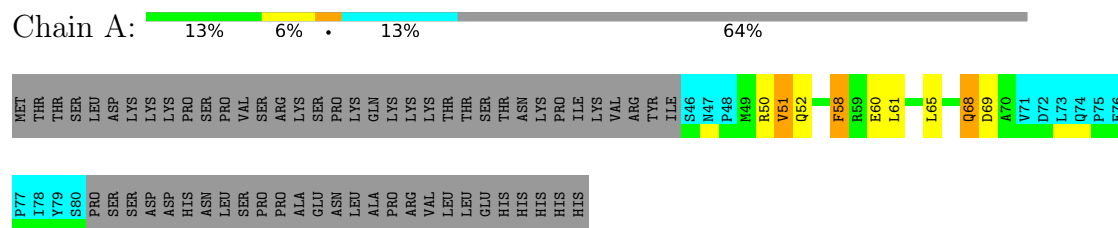


- Molecule 2: Probable WRKY transcription factor 33

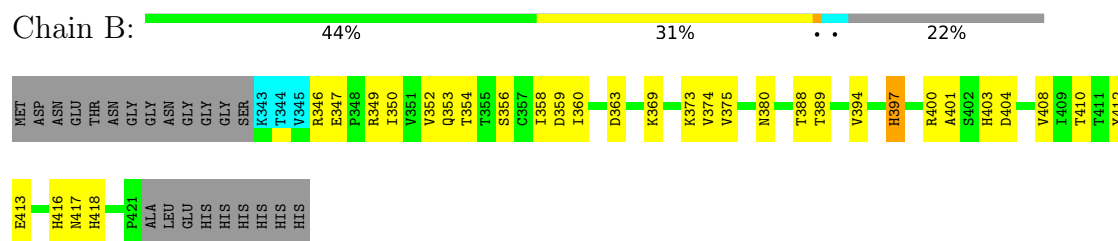


4.2.17 Score per residue for model 17

- Molecule 1: Sigma factor binding protein 1, chloroplastic

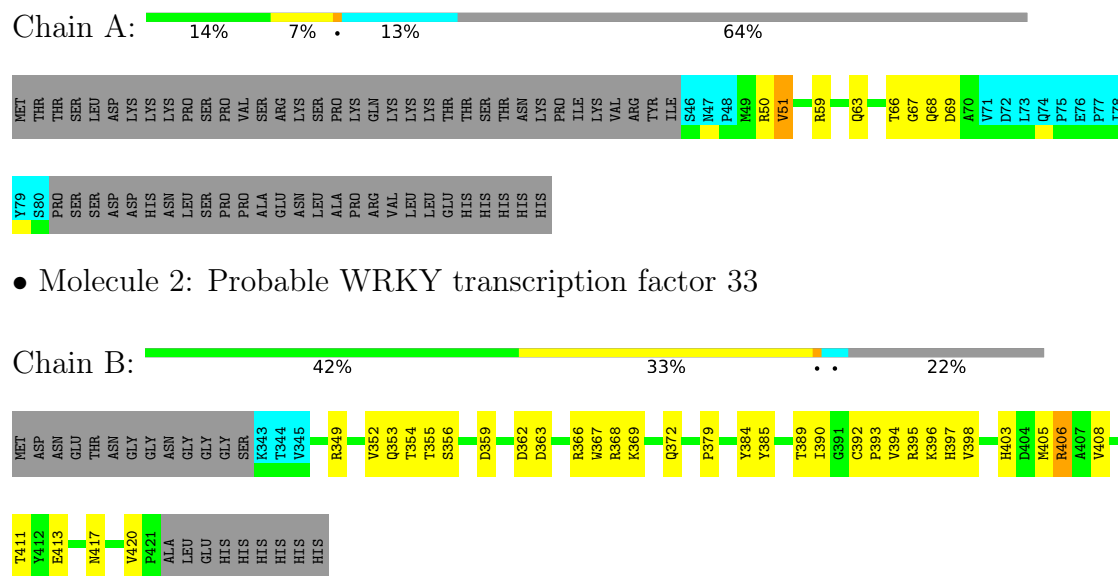


- Molecule 2: Probable WRKY transcription factor 33



4.2.18 Score per residue for model 18

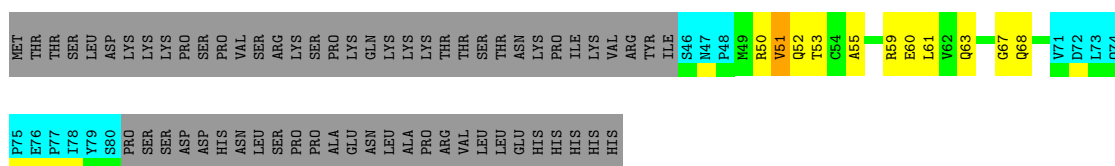
- Molecule 1: Sigma factor binding protein 1, chloroplastic



4.2.19 Score per residue for model 19

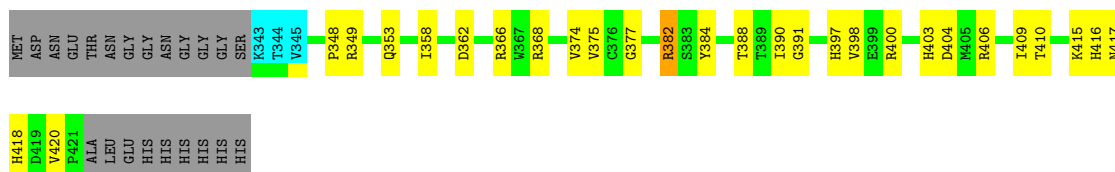
- Molecule 1: Sigma factor binding protein 1, chloroplastic

Chain A: 11% 10% 1% 13% 64%



- Molecule 2: Probable WRKY transcription factor 33

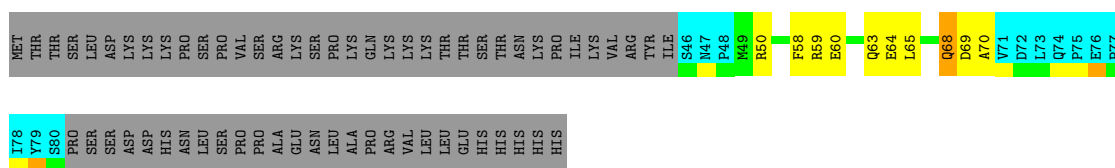
Chain B: 48% 27% 22%



4.2.20 Score per residue for model 20

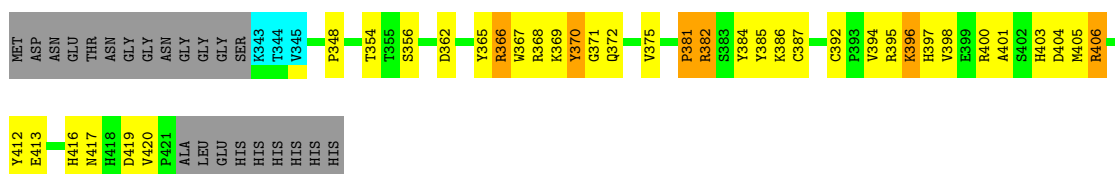
- Molecule 1: Sigma factor binding protein 1, chloroplastic

Chain A: 12% 9% 13% 64%



- Molecule 2: Probable WRKY transcription factor 33

Chain B: 39% 31% 6% 22%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 240 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
Amber	structure calculation	
Amber	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	30
Number of shifts mapped to atoms	30
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

6 Model quality (i)

6.1 Standard geometry (i)

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	2.04±0.12	4±2/174 (2.5± 1.1%)	2.51±0.13	12±3/233 (5.3± 1.5%)
2	B	2.08±0.05	16±3/632 (2.5± 0.5%)	2.36±0.07	34±5/856 (3.9± 0.6%)
All	All	2.07	400/16120 (2.5%)	2.39	922/21780 (4.2%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.3±0.6
2	B	0.0±0.0	3.0±1.8
All	All	0	67

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
2	B	420	VAL	CA-C	11.86	1.66	1.52	19	4
2	B	398	VAL	CA-C	10.36	1.65	1.52	14	3
2	B	368	ARG	N-CA	10.14	1.58	1.46	16	2
2	B	348	PRO	CA-C	9.46	1.61	1.52	14	1
1	A	63	GLN	CA-C	9.45	1.64	1.52	1	3
2	B	390	ILE	CA-CB	9.30	1.63	1.54	18	2
1	A	53	THR	N-CA	9.29	1.57	1.46	2	3
2	B	403	HIS	CE1-NE2	9.27	1.41	1.32	15	2
1	A	50	ARG	N-CA	9.26	1.58	1.46	19	4
2	B	378	ASN	CA-C	9.11	1.63	1.52	10	2
2	B	374	VAL	CA-C	8.63	1.62	1.52	19	3
1	A	67	GLY	N-CA	8.52	1.52	1.44	18	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	347	GLU	CA-C	8.47	1.62	1.52	13	3
2	B	371	GLY	CA-C	8.35	1.61	1.51	11	2
2	B	381	PRO	CA-C	8.27	1.62	1.52	15	1
2	B	418	HIS	CA-C	8.25	1.62	1.52	7	3
2	B	391	GLY	CA-C	8.24	1.63	1.51	3	2
2	B	350	ILE	CA-C	8.01	1.61	1.52	11	3
1	A	61	LEU	CA-C	8.00	1.63	1.52	7	4
2	B	389	THR	N-CA	7.95	1.55	1.46	6	3
2	B	403	HIS	N-CA	7.94	1.55	1.46	11	2
2	B	382	ARG	CZ-NH2	-7.93	1.23	1.33	8	2
1	A	60	GLU	N-CA	7.92	1.56	1.45	17	1
2	B	406	ARG	NE-CZ	-7.89	1.24	1.33	5	1
2	B	375	VAL	CA-C	7.88	1.61	1.52	15	3
1	A	68	GLN	N-CA	7.86	1.55	1.46	7	1
2	B	347	GLU	N-CA	7.80	1.54	1.46	17	1
2	B	418	HIS	ND1-CE1	7.74	1.40	1.32	1	2
1	A	51	VAL	N-CA	7.66	1.55	1.46	19	4
2	B	392	CYS	CA-C	7.66	1.61	1.52	5	3
2	B	359	ASP	C-N	7.63	1.41	1.33	1	1
1	A	58	PHE	N-CA	7.58	1.55	1.46	8	3
2	B	400	ARG	N-CA	7.55	1.55	1.45	17	1
2	B	403	HIS	CD2-NE2	-7.53	1.29	1.37	7	1
1	A	59	ARG	N-CA	7.48	1.55	1.46	5	1
2	B	411	THR	CA-C	-7.47	1.43	1.52	5	1
2	B	358	ILE	C-O	7.44	1.31	1.23	13	1
2	B	418	HIS	CD2-NE2	7.34	1.46	1.37	4	2
2	B	409	ILE	CA-CB	7.33	1.63	1.54	13	1
2	B	394	VAL	CA-C	7.31	1.60	1.52	11	5
2	B	387	CYS	CA-C	7.29	1.62	1.52	15	1
2	B	418	HIS	CE1-NE2	7.29	1.39	1.32	11	1
2	B	397	HIS	CE1-NE2	7.12	1.39	1.32	1	6
2	B	360	ILE	CA-C	7.12	1.60	1.53	12	2
2	B	416	HIS	ND1-CE1	7.06	1.39	1.32	19	3
2	B	348	PRO	CA-CB	-7.05	1.44	1.54	20	2
1	A	68	GLN	CA-C	7.04	1.61	1.53	11	2
2	B	352	VAL	CA-C	7.02	1.60	1.52	2	2
2	B	416	HIS	CE1-NE2	7.01	1.39	1.32	19	3
2	B	397	HIS	ND1-CE1	6.98	1.39	1.32	15	4
2	B	346	ARG	CZ-NH2	-6.96	1.24	1.33	6	2
1	A	55	ALA	CA-C	6.93	1.62	1.52	11	2
2	B	383	SER	N-CA	6.92	1.54	1.46	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	417	ASN	N-CA	6.92	1.53	1.46	19	2
1	A	49	MET	N-CA	6.92	1.55	1.45	7	2
1	A	56	SER	N-CA	6.91	1.54	1.45	15	4
2	B	403	HIS	ND1-CE1	6.91	1.39	1.32	9	5
2	B	408	VAL	CA-C	6.91	1.61	1.52	13	3
2	B	385	TYR	N-CA	6.90	1.54	1.46	7	2
1	A	64	GLU	N-CA	6.88	1.55	1.46	7	2
1	A	51	VAL	CA-CB	6.87	1.61	1.54	5	2
1	A	67	GLY	CA-C	6.83	1.59	1.51	16	1
2	B	409	ILE	N-CA	6.82	1.55	1.46	13	2
2	B	396	LYS	N-CA	6.79	1.53	1.46	7	2
2	B	348	PRO	N-CA	6.78	1.55	1.47	8	1
2	B	362	ASP	N-CA	6.76	1.54	1.46	3	2
2	B	368	ARG	CZ-NH1	-6.76	1.23	1.32	19	3
2	B	360	ILE	CA-CB	6.76	1.61	1.53	9	1
2	B	346	ARG	N-CA	6.75	1.54	1.46	16	1
1	A	54	CYS	N-CA	6.71	1.53	1.46	16	3
2	B	408	VAL	N-CA	6.71	1.54	1.46	17	2
2	B	395	ARG	CA-CB	-6.69	1.43	1.53	4	1
2	B	398	VAL	C-O	-6.68	1.17	1.24	19	1
2	B	402	SER	CA-C	6.65	1.64	1.52	6	3
2	B	371	GLY	N-CA	6.64	1.51	1.45	20	1
1	A	65	LEU	C-N	6.64	1.43	1.33	15	2
2	B	368	ARG	CA-CB	6.61	1.63	1.53	20	1
2	B	379	PRO	N-CA	-6.60	1.38	1.47	6	1
2	B	395	ARG	CZ-NH2	-6.60	1.24	1.33	16	1
2	B	394	VAL	CA-CB	6.57	1.61	1.53	5	1
1	A	61	LEU	N-CA	6.55	1.54	1.46	5	1
2	B	420	VAL	CA-CB	-6.55	1.45	1.54	19	2
1	A	50	ARG	CZ-NH1	-6.55	1.23	1.32	16	1
2	B	372	GLN	N-CA	6.54	1.53	1.46	2	3
2	B	417	ASN	CA-C	6.54	1.61	1.52	2	2
2	B	368	ARG	CA-C	6.52	1.60	1.52	2	2
1	A	58	PHE	CA-C	6.48	1.60	1.52	7	1
2	B	376	CYS	N-CA	6.47	1.54	1.46	4	1
2	B	398	VAL	N-CA	6.47	1.53	1.46	20	2
2	B	358	ILE	CA-C	6.46	1.60	1.52	9	2
2	B	355	THR	CA-C	-6.46	1.45	1.52	7	2
2	B	349	ARG	CD-NE	6.46	1.55	1.46	5	1
2	B	350	ILE	N-CA	6.43	1.53	1.46	12	3
2	B	373	LYS	N-CA	6.39	1.53	1.45	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	410	THR	N-CA	6.37	1.53	1.46	2	1
2	B	407	ALA	N-CA	6.37	1.53	1.46	12	1
2	B	356	SER	CB-OG	6.36	1.54	1.42	18	1
1	A	53	THR	CB-OG1	-6.35	1.33	1.43	2	1
2	B	346	ARG	CZ-NH1	-6.35	1.23	1.32	8	1
1	A	59	ARG	CZ-NH2	-6.33	1.25	1.33	9	2
1	A	57	LYS	N-CA	6.32	1.53	1.45	9	1
2	B	404	ASP	CA-C	6.32	1.60	1.52	3	3
2	B	363	ASP	N-CA	6.29	1.51	1.46	18	2
2	B	413	GLU	N-CA	6.26	1.55	1.46	6	1
2	B	397	HIS	CG-ND1	6.23	1.45	1.38	11	2
2	B	406	ARG	CZ-NH2	-6.22	1.25	1.33	5	2
2	B	346	ARG	CD-NE	6.22	1.54	1.46	12	1
2	B	368	ARG	C-O	-6.21	1.16	1.24	1	2
2	B	356	SER	CA-C	6.21	1.60	1.52	3	1
2	B	389	THR	CB-OG1	-6.19	1.33	1.43	15	1
2	B	414	GLY	CA-C	6.19	1.58	1.52	5	2
2	B	403	HIS	CG-ND1	6.17	1.45	1.38	13	2
2	B	395	ARG	CD-NE	6.17	1.54	1.46	11	1
2	B	357	CYS	C-O	-6.15	1.16	1.24	2	1
2	B	403	HIS	CB-CG	6.13	1.58	1.50	7	1
2	B	416	HIS	CA-C	6.13	1.60	1.52	17	1
2	B	355	THR	CB-OG1	-6.11	1.33	1.43	4	1
2	B	419	ASP	CA-C	6.10	1.60	1.52	15	1
2	B	371	GLY	C-O	6.08	1.30	1.23	20	2
1	A	52	GLN	CA-C	6.08	1.61	1.52	4	3
2	B	356	SER	N-CA	-6.07	1.38	1.46	15	2
2	B	352	VAL	C-N	6.04	1.41	1.33	17	1
2	B	375	VAL	N-CA	6.03	1.53	1.46	8	3
2	B	412	TYR	CA-CB	6.00	1.64	1.53	9	1
2	B	360	ILE	N-CA	5.99	1.54	1.46	15	3
2	B	403	HIS	CA-C	5.97	1.60	1.52	15	2
2	B	406	ARG	CA-CB	5.96	1.61	1.53	10	2
2	B	372	GLN	CA-C	5.95	1.59	1.52	18	2
2	B	400	ARG	CZ-NH2	-5.94	1.25	1.33	7	1
2	B	393	PRO	C-N	5.93	1.41	1.33	18	1
2	B	358	ILE	N-CA	5.89	1.52	1.46	15	3
2	B	397	HIS	CA-C	5.89	1.59	1.52	10	1
1	A	68	GLN	C-O	-5.88	1.15	1.24	5	1
2	B	377	GLY	CA-C	5.84	1.59	1.51	19	1
2	B	400	ARG	CA-CB	5.84	1.63	1.53	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	69	ASP	CA-C	5.83	1.60	1.53	8	2
2	B	388	THR	N-CA	5.82	1.53	1.46	12	1
2	B	420	VAL	N-CA	5.82	1.53	1.46	4	2
2	B	368	ARG	CZ-NH2	-5.81	1.25	1.33	18	2
2	B	406	ARG	CA-C	5.77	1.60	1.52	18	1
2	B	351	VAL	CA-C	-5.76	1.45	1.52	15	2
2	B	354	THR	C-N	5.75	1.41	1.33	17	1
2	B	369	LYS	N-CA	5.72	1.53	1.45	18	2
2	B	384	TYR	N-CA	5.72	1.53	1.46	14	3
2	B	418	HIS	N-CA	5.71	1.52	1.46	8	3
2	B	417	ASN	CA-CB	5.70	1.63	1.53	18	1
2	B	365	TYR	N-CA	5.70	1.52	1.45	14	1
2	B	384	TYR	CA-C	5.68	1.59	1.52	18	1
2	B	374	VAL	CA-CB	5.67	1.60	1.54	17	2
1	A	59	ARG	CD-NE	-5.66	1.38	1.46	15	1
2	B	360	ILE	CB-CG1	5.65	1.64	1.53	3	1
2	B	349	ARG	CA-CB	5.65	1.57	1.53	17	2
2	B	418	HIS	CG-CD2	5.65	1.42	1.35	16	1
2	B	374	VAL	N-CA	5.65	1.52	1.46	1	1
1	A	63	GLN	N-CA	5.65	1.53	1.45	18	1
2	B	361	LEU	CA-C	5.64	1.59	1.52	6	2
2	B	406	ARG	CD-NE	5.63	1.54	1.46	4	2
2	B	416	HIS	N-CA	5.63	1.53	1.46	16	2
2	B	375	VAL	CA-CB	5.62	1.63	1.54	19	1
2	B	349	ARG	CZ-NH2	-5.61	1.26	1.33	3	2
1	A	64	GLU	CA-C	-5.61	1.45	1.52	20	1
2	B	401	ALA	C-O	-5.59	1.17	1.23	9	1
2	B	369	LYS	CA-C	5.59	1.60	1.52	20	1
1	A	59	ARG	NE-CZ	5.59	1.39	1.33	8	1
2	B	367	TRP	CA-C	5.59	1.59	1.52	13	2
2	B	386	LYS	N-CA	5.58	1.52	1.45	6	2
2	B	413	GLU	CA-CB	5.58	1.60	1.53	18	2
1	A	62	VAL	N-CA	5.56	1.53	1.46	8	1
2	B	412	TYR	N-CA	5.52	1.52	1.46	4	1
2	B	354	THR	N-CA	5.52	1.52	1.46	12	1
2	B	381	PRO	N-CA	5.52	1.53	1.47	2	1
2	B	412	TYR	CA-C	5.50	1.59	1.52	15	1
2	B	406	ARG	CZ-NH1	-5.49	1.25	1.32	19	2
1	A	53	THR	CA-C	5.49	1.59	1.52	10	1
2	B	367	TRP	CZ2-CH2	5.48	1.47	1.37	2	1
2	B	362	ASP	CA-C	5.47	1.60	1.52	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	366	ARG	CZ-NH2	-5.47	1.26	1.33	16	1
2	B	415	LYS	CA-C	-5.46	1.46	1.52	16	2
2	B	368	ARG	NE-CZ	-5.46	1.27	1.33	9	2
2	B	391	GLY	N-CA	5.46	1.53	1.45	2	1
1	A	56	SER	CA-C	5.39	1.60	1.53	14	3
2	B	380	ASN	CA-C	5.39	1.59	1.52	6	1
2	B	357	CYS	CA-C	5.38	1.60	1.52	3	1
1	A	58	PHE	C-O	-5.38	1.17	1.23	14	1
2	B	351	VAL	N-CA	-5.38	1.40	1.46	14	1
2	B	390	ILE	N-CA	5.38	1.53	1.46	5	1
2	B	385	TYR	CA-C	5.38	1.59	1.52	15	1
1	A	54	CYS	CA-C	5.37	1.61	1.52	13	3
2	B	365	TYR	CA-C	5.37	1.59	1.52	20	1
2	B	379	PRO	N-CD	-5.36	1.40	1.47	10	1
2	B	411	THR	N-CA	5.36	1.52	1.46	7	1
2	B	397	HIS	CB-CG	5.35	1.57	1.50	8	2
2	B	419	ASP	N-CA	5.34	1.53	1.46	13	2
2	B	415	LYS	N-CA	5.34	1.52	1.45	1	1
2	B	413	GLU	CA-C	5.33	1.58	1.52	12	1
2	B	419	ASP	CA-CB	5.32	1.62	1.53	20	1
1	A	51	VAL	C-O	-5.31	1.18	1.24	5	1
1	A	60	GLU	CA-C	5.30	1.60	1.53	20	2
1	A	62	VAL	CA-CB	5.30	1.62	1.54	3	1
2	B	397	HIS	CG-CD2	-5.30	1.30	1.35	9	2
2	B	419	ASP	C-O	5.30	1.30	1.24	13	1
2	B	388	THR	CA-C	5.29	1.60	1.52	15	1
1	A	51	VAL	C-N	5.29	1.41	1.33	15	1
2	B	354	THR	CA-C	-5.28	1.46	1.52	14	1
2	B	373	LYS	CA-C	5.27	1.59	1.52	15	1
2	B	361	LEU	N-CA	5.26	1.52	1.45	6	1
2	B	399	GLU	CA-C	5.26	1.59	1.52	13	1
2	B	372	GLN	C-N	5.26	1.40	1.33	9	1
2	B	390	ILE	C-O	-5.26	1.18	1.24	13	1
2	B	374	VAL	C-N	5.26	1.40	1.33	17	1
2	B	416	HIS	CG-ND1	5.24	1.44	1.38	7	1
1	A	65	LEU	C-O	-5.24	1.17	1.24	17	1
1	A	53	THR	C-O	-5.24	1.17	1.24	4	1
2	B	363	ASP	CA-C	5.24	1.58	1.52	9	1
1	A	49	MET	CA-C	5.21	1.59	1.52	15	1
2	B	367	TRP	NE1-CE2	-5.20	1.31	1.37	1	1
2	B	416	HIS	CB-CG	5.20	1.57	1.50	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	66	THR	CA-C	5.19	1.60	1.52	15	2
2	B	384	TYR	C-N	5.18	1.40	1.33	15	1
2	B	390	ILE	C-N	5.18	1.40	1.33	5	1
1	A	63	GLN	CA-CB	-5.15	1.44	1.53	1	1
2	B	392	CYS	CA-CB	5.15	1.60	1.53	15	1
2	B	355	THR	CA-CB	-5.15	1.46	1.53	18	1
2	B	404	ASP	CA-CB	5.13	1.60	1.53	20	1
2	B	404	ASP	N-CA	5.13	1.52	1.46	10	2
2	B	352	VAL	C-O	-5.12	1.18	1.24	15	1
1	A	65	LEU	CA-C	5.11	1.61	1.52	17	1
2	B	401	ALA	CA-CB	5.10	1.61	1.53	12	1
2	B	350	ILE	CA-CB	5.10	1.60	1.54	7	1
2	B	353	GLN	N-CA	-5.10	1.39	1.46	6	1
2	B	365	TYR	C-N	5.09	1.40	1.33	2	1
2	B	370	TYR	N-CA	5.09	1.53	1.45	16	1
2	B	359	ASP	CA-C	5.08	1.59	1.52	14	1
2	B	382	ARG	CA-CB	5.08	1.60	1.53	6	1
1	A	53	THR	CA-CB	5.07	1.61	1.53	13	1
2	B	396	LYS	C-O	-5.07	1.17	1.23	5	1
1	A	63	GLN	C-N	-5.06	1.27	1.34	4	1
2	B	364	GLY	CA-C	5.06	1.59	1.51	6	1
2	B	384	TYR	C-O	-5.05	1.17	1.23	6	1
2	B	354	THR	C-O	-5.05	1.17	1.23	9	1
2	B	411	THR	CB-OG1	-5.05	1.35	1.43	13	1
2	B	387	CYS	CA-CB	5.04	1.61	1.53	13	1
2	B	405	MET	CA-C	5.03	1.59	1.52	18	1
2	B	414	GLY	N-CA	5.03	1.50	1.45	15	1
2	B	407	ALA	C-O	5.00	1.30	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
2	B	359	ASP	CA-CB-CG	12.13	124.73	112.60	2	7
2	B	397	HIS	CB-CG-CD2	-11.54	116.20	131.20	19	11
2	B	363	ASP	CA-CB-CG	11.44	124.04	112.60	1	4
2	B	357	CYS	CA-C-N	11.02	132.99	121.97	7	2
2	B	357	CYS	C-N-CA	11.02	132.99	121.97	7	2
1	A	68	GLN	OE1-CD-NE2	-10.57	112.03	122.60	9	6
2	B	418	HIS	CA-CB-CG	10.56	124.36	113.80	13	3
2	B	417	ASN	CA-CB-CG	10.55	123.15	112.60	13	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	414	GLY	CA-C-O	-9.74	114.40	122.29	15	2
1	A	50	ARG	NE-CZ-NH2	9.68	127.91	119.20	8	11
2	B	416	HIS	CB-CG-CD2	-9.63	118.68	131.20	20	12
1	A	68	GLN	CA-C-N	9.47	136.28	122.63	15	3
1	A	68	GLN	C-N-CA	9.47	136.28	122.63	15	3
2	B	372	GLN	OE1-CD-NE2	-9.42	113.18	122.60	1	7
2	B	349	ARG	NH1-CZ-NH2	-9.32	107.19	119.30	18	2
1	A	49	MET	N-CA-C	9.22	123.24	110.24	16	1
2	B	400	ARG	NE-CZ-NH1	9.13	130.63	121.50	10	4
2	B	401	ALA	CA-C-O	-9.04	111.97	121.55	15	1
2	B	419	ASP	CA-C-N	9.03	132.41	123.02	6	2
2	B	419	ASP	C-N-CA	9.03	132.41	123.02	6	2
1	A	69	ASP	O-C-N	-9.01	110.60	122.59	2	7
2	B	397	HIS	ND1-CG-CD2	8.97	115.07	106.10	19	5
2	B	395	ARG	NE-CZ-NH2	8.85	127.17	119.20	18	1
1	A	69	ASP	CA-C-N	8.81	137.55	121.70	1	7
1	A	69	ASP	C-N-CA	8.81	137.55	121.70	1	7
1	A	55	ALA	N-CA-C	8.78	122.99	111.75	9	3
2	B	362	ASP	CA-C-N	8.72	133.60	120.17	12	6
2	B	362	ASP	C-N-CA	8.72	133.60	120.17	12	6
2	B	374	VAL	N-CA-C	8.63	120.09	109.30	13	3
1	A	59	ARG	NE-CZ-NH2	8.56	126.91	119.20	10	8
2	B	400	ARG	NE-CZ-NH2	-8.54	111.51	119.20	14	3
1	A	58	PHE	CA-CB-CG	8.49	122.30	113.80	7	7
2	B	353	GLN	OE1-CD-NE2	-8.48	114.12	122.60	17	11
2	B	365	TYR	O-C-N	-8.48	112.22	122.65	7	1
2	B	368	ARG	NE-CZ-NH1	8.46	129.96	121.50	8	4
1	A	51	VAL	CA-C-N	8.46	131.61	120.28	6	1
1	A	51	VAL	C-N-CA	8.46	131.61	120.28	6	1
2	B	366	ARG	N-CA-C	8.44	122.48	108.73	13	1
2	B	368	ARG	NE-CZ-NH2	-8.39	111.65	119.20	15	5
2	B	378	ASN	CA-C-N	8.36	128.08	119.64	14	4
2	B	378	ASN	C-N-CA	8.36	128.08	119.64	14	4
2	B	417	ASN	OD1-CG-ND2	-8.35	114.25	122.60	7	7
2	B	404	ASP	CA-CB-CG	8.26	120.86	112.60	20	5
2	B	403	HIS	CB-CG-CD2	-8.21	120.53	131.20	18	8
1	A	53	THR	CA-C-N	8.18	132.31	120.38	9	1
1	A	53	THR	C-N-CA	8.18	132.31	120.38	9	1
2	B	346	ARG	NE-CZ-NH1	8.13	129.63	121.50	10	2
2	B	419	ASP	CA-CB-CG	8.06	120.66	112.60	5	5
2	B	380	ASN	OD1-CG-ND2	-8.00	114.60	122.60	17	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	368	ARG	CD-NE-CZ	7.98	135.57	124.40	12	4
1	A	66	THR	O-C-N	-7.97	114.46	122.99	11	1
2	B	373	LYS	CA-C-N	7.94	132.34	120.75	8	3
2	B	373	LYS	C-N-CA	7.94	132.34	120.75	8	3
1	A	51	VAL	CA-CB-CG1	7.94	123.89	110.40	11	1
2	B	404	ASP	CA-C-N	7.90	131.65	120.28	1	5
2	B	404	ASP	C-N-CA	7.90	131.65	120.28	1	5
2	B	354	THR	N-CA-C	7.88	120.88	109.14	3	3
1	A	52	GLN	OE1-CD-NE2	-7.86	114.74	122.60	8	10
2	B	356	SER	O-C-N	-7.85	114.17	123.27	10	2
2	B	382	ARG	NE-CZ-NH1	7.79	129.29	121.50	15	4
2	B	406	ARG	NE-CZ-NH1	-7.77	113.73	121.50	18	4
1	A	50	ARG	N-CA-C	7.77	122.90	112.88	3	3
2	B	371	GLY	O-C-N	-7.76	116.26	123.78	8	3
2	B	385	TYR	N-CA-C	7.72	121.70	109.50	11	1
2	B	388	THR	O-C-N	-7.71	112.91	122.24	1	1
2	B	378	ASN	N-CA-CB	-7.71	98.91	110.32	16	3
2	B	378	ASN	OD1-CG-ND2	-7.69	114.91	122.60	1	3
2	B	389	THR	CA-CB-CG2	7.67	123.54	110.50	5	1
2	B	401	ALA	N-CA-C	7.66	120.19	110.24	20	2
2	B	381	PRO	N-CA-C	7.62	123.15	111.34	7	1
2	B	362	ASP	CA-CB-CG	7.59	120.19	112.60	8	4
2	B	403	HIS	ND1-CG-CD2	7.52	113.62	106.10	7	3
1	A	62	VAL	O-C-N	-7.49	114.74	123.05	2	1
2	B	404	ASP	CA-C-O	7.49	129.28	120.14	16	2
1	A	66	THR	CA-C-N	7.46	130.75	121.06	12	2
1	A	66	THR	C-N-CA	7.46	130.75	121.06	12	2
2	B	378	ASN	N-CA-C	7.45	119.04	109.65	11	2
2	B	404	ASP	N-CA-C	7.45	120.55	108.34	19	3
2	B	371	GLY	N-CA-C	7.41	121.25	110.80	1	3
2	B	406	ARG	CA-C-O	-7.41	112.62	120.55	3	1
1	A	66	THR	CA-CB-CG2	7.39	123.06	110.50	4	1
2	B	417	ASN	CA-C-N	7.38	131.97	121.42	20	3
2	B	417	ASN	C-N-CA	7.38	131.97	121.42	20	3
2	B	370	TYR	CA-C-O	7.36	126.94	118.77	2	1
2	B	407	ALA	CB-CA-C	7.35	121.83	109.48	14	1
1	A	50	ARG	NE-CZ-NH1	-7.33	114.17	121.50	11	5
2	B	390	ILE	N-CA-CB	7.33	118.95	110.82	19	1
2	B	366	ARG	NE-CZ-NH1	7.30	128.80	121.50	10	2
2	B	352	VAL	CA-CB-CG2	7.30	122.81	110.40	6	1
1	A	60	GLU	N-CA-C	7.28	120.14	110.53	19	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	50	ARG	CD-NE-CZ	7.24	134.54	124.40	1	6
2	B	416	HIS	ND1-CE1-NE2	7.23	115.63	108.40	5	4
1	A	51	VAL	N-CA-C	7.23	117.33	110.53	6	1
2	B	349	ARG	NE-CZ-NH1	7.22	128.72	121.50	14	4
1	A	54	CYS	N-CA-C	7.16	122.10	113.23	4	1
2	B	375	VAL	O-C-N	-7.11	115.36	122.97	9	2
1	A	54	CYS	O-C-N	-7.10	114.10	122.20	9	1
2	B	400	ARG	NH1-CZ-NH2	-7.08	110.09	119.30	10	1
2	B	372	GLN	N-CA-C	7.07	118.92	108.60	5	2
2	B	358	ILE	O-C-N	-7.07	115.22	123.00	16	5
2	B	387	CYS	CA-C-O	-7.06	113.43	121.19	20	2
1	A	59	ARG	CD-NE-CZ	7.06	134.28	124.40	1	2
2	B	392	CYS	CA-C-O	7.05	124.54	119.32	2	2
1	A	64	GLU	N-CA-CB	-7.05	98.57	110.41	7	1
2	B	383	SER	CA-C-O	-7.03	112.83	120.92	13	1
1	A	67	GLY	N-CA-C	7.01	121.64	112.25	12	1
2	B	380	ASN	CA-C-N	6.99	126.95	120.03	5	4
2	B	380	ASN	C-N-CA	6.99	126.95	120.03	5	4
2	B	346	ARG	NH1-CZ-NH2	-6.98	110.23	119.30	10	2
1	A	70	ALA	O-C-N	-6.97	111.85	123.00	7	1
2	B	416	HIS	CA-CB-CG	6.97	120.77	113.80	12	2
2	B	365	TYR	CB-CG-CD2	-6.97	110.34	120.80	11	1
2	B	400	ARG	CA-C-O	-6.96	113.36	121.16	20	3
2	B	346	ARG	CD-NE-CZ	6.94	134.12	124.40	15	1
2	B	392	CYS	CA-C-N	6.92	127.07	119.87	15	4
2	B	392	CYS	C-N-CA	6.92	127.07	119.87	15	4
1	A	69	ASP	CB-CA-C	6.85	120.95	111.63	1	2
1	A	49	MET	CB-CA-C	6.85	121.00	109.84	4	1
2	B	397	HIS	CA-CB-CG	6.82	120.62	113.80	19	2
2	B	386	LYS	CA-C-N	6.82	134.57	121.54	3	2
2	B	386	LYS	C-N-CA	6.82	134.57	121.54	3	2
2	B	348	PRO	N-CA-CB	6.82	110.06	103.51	19	2
2	B	416	HIS	ND1-CG-CD2	6.80	112.90	106.10	15	4
2	B	378	ASN	CA-C-O	-6.80	114.22	119.46	15	2
2	B	395	ARG	NE-CZ-NH1	6.74	128.24	121.50	12	2
1	A	63	GLN	OE1-CD-NE2	-6.74	115.86	122.60	10	5
2	B	392	CYS	O-C-N	-6.74	115.15	121.35	2	3
2	B	358	ILE	CA-C-O	-6.73	115.31	120.96	3	3
1	A	59	ARG	N-CA-C	6.71	118.67	111.36	13	3
2	B	387	CYS	N-CA-C	6.70	120.09	110.24	14	1
2	B	409	ILE	CA-C-O	-6.69	113.43	120.39	4	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	69	ASP	CA-CB-CG	6.68	119.28	112.60	4	2
2	B	362	ASP	O-C-N	-6.65	115.12	122.84	12	1
1	A	64	GLU	CA-C-N	6.64	131.80	120.72	7	5
1	A	64	GLU	C-N-CA	6.64	131.80	120.72	7	5
2	B	378	ASN	CB-CA-C	6.63	118.96	109.08	16	3
1	A	53	THR	CA-C-O	-6.62	113.53	120.55	15	2
1	A	53	THR	CA-CB-CG2	6.60	121.72	110.50	14	1
2	B	393	PRO	N-CA-CB	6.59	109.46	103.20	5	3
2	B	381	PRO	N-CD-CG	6.59	113.09	103.20	20	1
2	B	391	GLY	CA-C-N	6.58	130.42	121.74	19	1
2	B	391	GLY	C-N-CA	6.58	130.42	121.74	19	1
2	B	358	ILE	N-CA-CB	-6.57	100.20	112.36	9	2
2	B	354	THR	CA-C-O	-6.56	113.76	121.44	20	2
2	B	407	ALA	N-CA-C	6.56	120.09	109.40	9	2
2	B	347	GLU	N-CA-C	6.54	124.27	109.81	12	1
2	B	360	ILE	O-C-N	-6.53	115.32	122.64	13	1
2	B	405	MET	O-C-N	-6.52	115.20	122.12	5	1
1	A	64	GLU	N-CA-C	6.51	119.20	111.71	4	3
2	B	403	HIS	CA-C-N	6.51	132.13	121.58	9	1
2	B	403	HIS	C-N-CA	6.51	132.13	121.58	9	1
2	B	367	TRP	CG-CD2-CE3	6.51	140.41	133.90	13	1
1	A	65	LEU	CA-C-O	6.50	129.81	120.51	20	1
2	B	378	ASN	CA-CB-CG	6.50	119.10	112.60	12	2
2	B	394	VAL	O-C-N	6.50	130.70	122.57	18	1
2	B	350	ILE	CB-CA-C	6.50	120.59	111.63	16	2
2	B	380	ASN	O-C-N	-6.50	114.16	121.43	5	2
2	B	404	ASP	O-C-N	-6.49	116.02	123.42	16	3
1	A	56	SER	N-CA-C	6.49	118.68	110.24	9	2
2	B	366	ARG	NE-CZ-NH2	6.49	125.04	119.20	18	2
2	B	355	THR	CA-C-O	6.46	127.84	120.54	8	1
1	A	68	GLN	CA-CB-CG	6.46	127.02	114.10	2	1
2	B	397	HIS	CB-CA-C	6.44	122.46	109.38	9	1
2	B	358	ILE	CA-CB-CG2	6.44	121.45	110.50	14	1
2	B	389	THR	CA-C-N	6.44	130.54	121.66	7	3
2	B	389	THR	C-N-CA	6.44	130.54	121.66	7	3
2	B	367	TRP	CA-C-N	6.41	132.86	122.29	4	3
2	B	367	TRP	C-N-CA	6.41	132.86	122.29	4	3
2	B	391	GLY	O-C-N	-6.40	114.84	122.33	8	1
2	B	349	ARG	N-CA-C	6.40	117.96	110.41	14	2
2	B	400	ARG	CD-NE-CZ	6.39	133.35	124.40	17	1
1	A	69	ASP	N-CA-C	6.39	120.41	112.24	5	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	352	VAL	O-C-N	-6.39	116.30	123.20	15	2
2	B	418	HIS	CA-C-O	6.38	127.73	120.84	6	1
2	B	362	ASP	N-CA-C	6.38	118.46	108.96	15	3
2	B	372	GLN	CB-CA-C	6.37	122.70	109.38	10	1
2	B	417	ASN	N-CA-C	6.37	120.15	112.38	20	1
2	B	396	LYS	O-C-N	6.37	130.23	123.42	12	2
2	B	380	ASN	CA-C-O	-6.36	114.85	120.19	2	2
2	B	363	ASP	N-CA-C	-6.34	105.00	114.64	15	1
2	B	418	HIS	CB-CG-CD2	-6.34	122.96	131.20	17	4
2	B	397	HIS	O-C-N	-6.33	115.52	123.17	2	2
1	A	64	GLU	CA-C-O	6.32	127.25	119.79	2	2
2	B	371	GLY	CA-C-O	-6.32	116.05	122.56	5	1
2	B	366	ARG	CD-NE-CZ	6.30	133.23	124.40	19	1
2	B	394	VAL	N-CA-CB	6.29	118.04	110.31	9	2
2	B	347	GLU	O-C-N	-6.28	114.76	120.92	13	2
2	B	414	GLY	O-C-N	6.28	129.90	122.68	7	1
1	A	68	GLN	N-CA-C	6.28	120.80	113.20	8	1
1	A	53	THR	N-CA-C	-6.26	103.74	112.45	7	1
2	B	381	PRO	CA-C-N	6.25	130.74	122.30	15	2
2	B	381	PRO	C-N-CA	6.25	130.74	122.30	15	2
2	B	400	ARG	O-C-N	-6.25	115.72	122.85	14	1
2	B	388	THR	CA-C-O	6.25	126.75	119.32	1	1
2	B	367	TRP	CE2-CD2-CE3	-6.25	112.55	118.80	13	3
2	B	416	HIS	CB-CG-ND1	6.24	132.06	122.70	20	1
2	B	388	THR	N-CA-C	6.24	118.88	111.71	19	2
2	B	350	ILE	CA-C-O	-6.23	113.69	121.11	11	1
1	A	70	ALA	CA-C-N	6.23	131.78	122.75	2	3
1	A	70	ALA	C-N-CA	6.23	131.78	122.75	2	3
2	B	380	ASN	CB-CG-ND2	-6.23	107.05	116.40	4	2
2	B	388	THR	CA-C-N	6.23	129.67	120.95	3	2
2	B	388	THR	C-N-CA	6.23	129.67	120.95	3	2
2	B	415	LYS	N-CA-C	6.16	119.45	109.40	19	2
2	B	405	MET	N-CA-C	-6.16	104.64	111.36	12	2
2	B	369	LYS	N-CA-C	6.16	119.16	110.23	3	1
1	A	61	LEU	CA-C-N	6.16	131.41	123.03	14	2
1	A	61	LEU	C-N-CA	6.16	131.41	123.03	14	2
2	B	363	ASP	CA-C-O	6.15	128.70	119.23	17	2
2	B	368	ARG	O-C-N	6.15	131.02	123.21	1	1
2	B	394	VAL	CA-C-O	-6.15	113.51	120.95	11	3
2	B	368	ARG	NH1-CZ-NH2	-6.12	111.34	119.30	8	4
1	A	50	ARG	CA-CB-CG	-6.12	101.87	114.10	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	346	ARG	CA-C-N	6.11	127.33	120.06	13	2
2	B	346	ARG	C-N-CA	6.11	127.33	120.06	13	2
2	B	410	THR	CB-CA-C	6.11	119.60	109.53	19	1
2	B	394	VAL	N-CA-C	6.10	116.89	108.84	20	2
1	A	60	GLU	O-C-N	-6.09	115.85	122.79	19	1
2	B	365	TYR	CA-C-N	6.09	131.57	123.05	3	1
2	B	365	TYR	C-N-CA	6.09	131.57	123.05	3	1
1	A	50	ARG	CA-C-N	6.09	128.74	120.77	5	3
1	A	50	ARG	C-N-CA	6.09	128.74	120.77	5	3
2	B	351	VAL	CA-CB-CG2	6.08	120.74	110.40	8	1
2	B	403	HIS	CB-CG-ND1	6.08	131.82	122.70	20	3
2	B	412	TYR	CA-C-N	6.08	131.05	122.05	9	2
2	B	412	TYR	C-N-CA	6.08	131.05	122.05	9	2
2	B	366	ARG	CA-C-O	-6.08	114.27	120.71	20	2
2	B	397	HIS	CB-CG-ND1	6.06	131.80	122.70	20	1
2	B	411	THR	CA-C-N	6.06	130.50	121.72	8	2
2	B	411	THR	C-N-CA	6.06	130.50	121.72	8	2
1	A	49	MET	O-C-N	-6.05	115.96	123.04	4	1
2	B	393	PRO	O-C-N	-6.04	112.45	122.36	12	1
2	B	418	HIS	CE1-NE2-CD2	-6.04	102.96	109.00	15	2
2	B	366	ARG	O-C-N	6.03	130.29	122.87	16	1
2	B	347	GLU	CA-C-O	-6.02	112.14	117.98	7	2
2	B	408	VAL	CA-C-O	6.01	126.98	120.43	17	1
2	B	381	PRO	N-CA-CB	6.00	109.68	103.38	20	2
1	A	63	GLN	O-C-N	-6.00	116.22	122.94	9	1
2	B	373	LYS	N-CA-C	6.00	119.49	109.95	17	1
2	B	374	VAL	CA-C-N	6.00	131.21	122.69	3	1
2	B	374	VAL	C-N-CA	6.00	131.21	122.69	3	1
2	B	370	TYR	CA-CB-CG	-5.99	103.12	113.90	15	1
2	B	367	TRP	CA-C-O	-5.97	114.25	120.70	18	1
2	B	364	GLY	CA-C-O	-5.96	113.05	118.95	9	1
2	B	392	CYS	CB-CA-C	5.95	117.95	109.38	13	2
2	B	353	GLN	CB-CG-CD	5.94	122.69	112.60	14	1
1	A	52	GLN	CB-CA-C	5.93	119.61	109.24	11	1
2	B	406	ARG	NH1-CZ-NH2	-5.91	111.62	119.30	10	2
1	A	61	LEU	O-C-N	-5.88	114.58	122.23	14	1
2	B	413	GLU	CA-C-N	5.88	131.51	121.87	3	1
2	B	413	GLU	C-N-CA	5.88	131.51	121.87	3	1
2	B	385	TYR	CA-C-N	5.88	131.99	122.29	18	2
2	B	385	TYR	C-N-CA	5.88	131.99	122.29	18	2
2	B	382	ARG	CA-C-O	-5.87	114.30	120.58	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	409	ILE	CB-CA-C	5.87	117.71	110.73	19	1
1	A	67	GLY	CA-C-N	5.86	132.74	121.54	19	1
1	A	67	GLY	C-N-CA	5.86	132.74	121.54	19	1
2	B	406	ARG	NE-CZ-NH2	-5.86	113.93	119.20	7	1
2	B	415	LYS	CA-C-N	5.85	129.66	121.24	15	1
2	B	415	LYS	C-N-CA	5.85	129.66	121.24	15	1
2	B	352	VAL	CA-CB-CG1	5.85	120.34	110.40	9	1
1	A	59	ARG	NE-CZ-NH1	-5.84	115.66	121.50	2	1
2	B	380	ASN	N-CA-C	5.84	118.19	110.36	6	2
2	B	349	ARG	CA-C-N	5.83	128.39	120.63	8	2
2	B	349	ARG	C-N-CA	5.83	128.39	120.63	8	2
2	B	369	LYS	CA-C-O	-5.83	114.40	121.05	13	1
2	B	357	CYS	CB-CA-C	5.83	121.19	110.11	5	1
2	B	399	GLU	O-C-N	5.83	130.22	123.17	4	1
2	B	353	GLN	CA-C-N	5.82	131.67	122.36	3	1
2	B	353	GLN	C-N-CA	5.82	131.67	122.36	3	1
2	B	352	VAL	CA-C-O	5.81	126.14	120.27	16	2
2	B	414	GLY	N-CA-C	5.80	119.99	112.68	15	1
2	B	420	VAL	CA-C-O	-5.80	112.17	119.95	20	2
2	B	372	GLN	O-C-N	-5.79	116.78	123.33	12	1
2	B	413	GLU	O-C-N	-5.79	115.72	123.14	14	1
2	B	402	SER	CA-C-N	5.79	131.86	121.66	16	1
2	B	402	SER	C-N-CA	5.79	131.86	121.66	16	1
2	B	361	LEU	N-CA-C	5.79	118.99	109.72	4	1
2	B	397	HIS	ND1-CE1-NE2	5.78	114.18	108.40	2	3
2	B	354	THR	CA-CB-CG2	5.78	120.32	110.50	1	2
2	B	418	HIS	CG-CD2-NE2	5.77	112.97	107.20	15	1
2	B	368	ARG	CA-C-N	5.76	129.66	121.42	13	2
2	B	368	ARG	C-N-CA	5.76	129.66	121.42	13	2
2	B	390	ILE	O-C-N	-5.76	116.80	122.67	5	1
2	B	367	TRP	CD2-CE3-CZ3	5.75	126.08	118.60	3	1
2	B	416	HIS	O-C-N	-5.75	116.31	123.04	5	2
2	B	368	ARG	CA-C-O	-5.75	114.61	120.71	16	3
2	B	350	ILE	CA-CB-CG2	-5.74	100.74	110.50	13	1
2	B	417	ASN	O-C-N	-5.74	113.18	122.42	16	2
1	A	69	ASP	CA-C-O	-5.73	113.92	121.08	12	2
2	B	354	THR	CA-CB-OG1	-5.73	101.01	109.60	1	1
2	B	370	TYR	CA-C-N	5.72	131.57	121.32	14	1
2	B	370	TYR	C-N-CA	5.72	131.57	121.32	14	1
2	B	413	GLU	CB-CA-C	5.71	119.97	111.17	17	1
2	B	416	HIS	N-CA-C	5.70	118.04	108.23	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	372	GLN	CA-CB-CG	5.69	125.48	114.10	8	1
1	A	60	GLU	CA-C-O	-5.69	114.93	121.47	4	2
2	B	349	ARG	CD-NE-CZ	5.69	132.36	124.40	19	1
2	B	351	VAL	N-CA-C	5.69	115.86	108.35	10	1
1	A	64	GLU	CB-CG-CD	5.68	122.26	112.60	16	1
2	B	413	GLU	N-CA-C	5.68	120.20	113.16	5	1
2	B	368	ARG	CB-CA-C	-5.68	98.53	109.37	15	2
2	B	379	PRO	N-CA-C	-5.67	106.30	114.18	14	1
2	B	367	TRP	N-CA-C	5.66	118.63	109.40	18	2
2	B	369	LYS	CA-C-N	5.65	130.60	123.03	14	1
2	B	369	LYS	C-N-CA	5.65	130.60	123.03	14	1
1	A	53	THR	O-C-N	-5.64	116.00	122.09	5	1
2	B	364	GLY	CA-C-N	5.64	131.51	121.75	13	1
2	B	364	GLY	C-N-CA	5.64	131.51	121.75	13	1
2	B	415	LYS	O-C-N	-5.64	115.90	123.23	19	1
2	B	411	THR	CA-C-O	-5.63	114.62	120.70	10	1
2	B	418	HIS	ND1-CG-CD2	-5.63	100.47	106.10	15	1
2	B	419	ASP	CA-C-O	5.62	126.09	119.06	14	1
2	B	376	CYS	CA-CB-SG	-5.62	101.48	114.40	2	1
1	A	62	VAL	N-CA-C	5.62	116.21	107.28	1	1
2	B	380	ASN	CA-CB-CG	5.60	118.20	112.60	8	1
2	B	399	GLU	CA-C-O	-5.59	113.89	120.60	5	2
1	A	57	LYS	O-C-N	-5.59	116.95	123.27	13	1
2	B	393	PRO	CB-CA-C	-5.58	103.53	111.68	2	1
1	A	63	GLN	CA-C-O	-5.58	115.64	121.55	19	2
2	B	389	THR	CA-CB-OG1	-5.57	101.25	109.60	5	2
2	B	395	ARG	CA-C-N	5.57	131.68	122.33	11	1
2	B	395	ARG	C-N-CA	5.57	131.68	122.33	11	1
2	B	362	ASP	CA-C-O	5.56	128.45	121.66	9	2
2	B	356	SER	CA-C-O	-5.54	113.89	120.43	17	1
2	B	394	VAL	CA-C-N	5.54	132.12	122.81	12	2
2	B	394	VAL	C-N-CA	5.54	132.12	122.81	12	2
1	A	59	ARG	NH1-CZ-NH2	-5.54	112.10	119.30	9	1
2	B	398	VAL	O-C-N	5.54	129.20	123.05	18	1
2	B	370	TYR	N-CA-CB	-5.53	102.63	110.81	4	1
1	A	57	LYS	CA-C-N	5.53	132.24	121.63	13	2
1	A	57	LYS	C-N-CA	5.53	132.24	121.63	13	2
2	B	417	ASN	CA-C-O	5.52	127.74	119.23	16	1
1	A	63	GLN	CB-CA-C	5.52	118.86	109.53	3	1
2	B	412	TYR	O-C-N	-5.52	116.05	123.23	10	1
1	A	55	ALA	CA-C-N	5.52	128.68	120.90	13	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	55	ALA	C-N-CA	5.52	128.68	120.90	13	4
2	B	348	PRO	N-CA-C	-5.51	108.36	114.92	14	1
2	B	394	VAL	CA-CB-CG1	5.50	119.76	110.40	3	2
2	B	389	THR	N-CA-CB	5.50	118.05	109.85	18	1
2	B	355	THR	CA-CB-OG1	5.50	117.84	109.60	7	1
2	B	416	HIS	CE1-NE2-CD2	-5.48	103.52	109.00	5	2
2	B	376	CYS	N-CA-CB	-5.48	101.96	110.29	3	1
1	A	55	ALA	N-CA-CB	-5.48	102.52	110.47	19	1
2	B	403	HIS	CE1-NE2-CD2	-5.47	103.53	109.00	20	2
2	B	351	VAL	CA-C-N	5.47	130.66	123.11	5	1
2	B	351	VAL	C-N-CA	5.47	130.66	123.11	5	1
2	B	411	THR	N-CA-C	5.46	117.30	108.34	6	1
1	A	58	PHE	CA-C-N	5.46	128.04	120.29	13	2
1	A	58	PHE	C-N-CA	5.46	128.04	120.29	13	2
2	B	390	ILE	CA-CB-CG1	5.45	119.67	110.40	10	1
2	B	395	ARG	CB-CG-CD	5.45	123.83	111.30	11	1
2	B	346	ARG	N-CA-C	5.44	122.39	110.80	4	1
2	B	379	PRO	CA-C-N	5.44	130.76	121.35	18	1
2	B	379	PRO	C-N-CA	5.44	130.76	121.35	18	1
2	B	409	ILE	O-C-N	-5.43	117.44	122.71	14	1
1	A	59	ARG	CA-C-N	5.43	131.28	121.06	1	2
1	A	59	ARG	C-N-CA	5.43	131.28	121.06	1	2
2	B	403	HIS	N-CA-C	5.42	119.95	113.23	16	1
2	B	421	PRO	N-CA-CB	5.42	108.96	103.00	9	1
1	A	59	ARG	CB-CA-C	-5.41	99.33	109.72	20	1
2	B	413	GLU	N-CA-CB	-5.41	103.27	110.57	4	1
2	B	361	LEU	O-C-N	5.40	129.53	123.27	14	1
2	B	393	PRO	CA-C-N	5.39	127.92	120.49	16	1
2	B	393	PRO	C-N-CA	5.39	127.92	120.49	16	1
1	A	62	VAL	CA-C-N	5.38	128.49	120.95	11	1
1	A	62	VAL	C-N-CA	5.38	128.49	120.95	11	1
1	A	56	SER	CA-C-O	-5.38	115.85	121.55	4	2
1	A	68	GLN	O-C-N	-5.38	115.44	122.59	17	1
1	A	55	ALA	O-C-N	-5.38	115.46	122.39	19	1
2	B	397	HIS	CA-C-O	-5.37	115.16	121.44	19	2
2	B	392	CYS	CA-CB-SG	-5.37	102.05	114.40	20	2
1	A	53	THR	CB-CA-C	5.37	119.38	110.90	5	1
1	A	65	LEU	O-C-N	-5.37	115.45	122.59	20	1
2	B	416	HIS	CA-C-N	5.36	131.39	122.54	10	1
2	B	416	HIS	C-N-CA	5.36	131.39	122.54	10	1
2	B	360	ILE	CA-C-N	5.35	131.32	121.85	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	360	ILE	C-N-CA	5.35	131.32	121.85	17	1
1	A	68	GLN	CG-CD-NE2	5.34	124.41	116.40	11	1
2	B	377	GLY	O-C-N	5.33	129.64	122.70	15	1
1	A	56	SER	O-C-N	5.33	129.15	122.86	2	1
2	B	402	SER	N-CA-C	5.33	119.40	113.01	3	1
2	B	359	ASP	CA-C-N	5.32	128.34	122.22	18	1
2	B	359	ASP	C-N-CA	5.32	128.34	122.22	18	1
2	B	394	VAL	CG1-CB-CG2	-5.32	99.11	110.80	3	1
2	B	384	TYR	O-C-N	-5.31	116.46	123.21	1	1
2	B	417	ASN	N-CA-CB	-5.31	102.87	110.57	17	1
1	A	60	GLU	CB-CG-CD	5.31	121.62	112.60	9	2
2	B	413	GLU	CB-CG-CD	-5.30	103.58	112.60	6	1
1	A	62	VAL	CA-C-O	5.30	126.61	120.67	4	1
2	B	407	ALA	O-C-N	-5.30	116.91	123.33	12	1
1	A	66	THR	OG1-CB-CG2	-5.30	98.71	109.30	4	1
2	B	402	SER	CA-C-O	-5.29	115.26	120.82	14	1
1	A	52	GLN	CB-CG-CD	5.29	121.59	112.60	9	1
1	A	52	GLN	CA-C-N	5.29	127.36	120.28	15	2
1	A	52	GLN	C-N-CA	5.29	127.36	120.28	15	2
2	B	356	SER	N-CA-C	5.29	116.32	108.60	3	2
2	B	358	ILE	CB-CG1-CD1	5.27	124.86	113.80	11	1
2	B	375	VAL	CA-CB-CG2	5.27	119.36	110.40	9	1
1	A	50	ARG	NH1-CZ-NH2	-5.26	112.46	119.30	14	1
1	A	51	VAL	CA-C-O	-5.26	115.27	120.85	7	2
2	B	372	GLN	CA-C-O	-5.26	115.82	121.45	14	1
2	B	347	GLU	CA-C-N	5.25	124.87	119.56	10	1
2	B	347	GLU	C-N-CA	5.25	124.87	119.56	10	1
2	B	403	HIS	CA-C-O	5.25	125.38	119.18	15	2
2	B	406	ARG	CD-NE-CZ	5.24	131.74	124.40	20	2
2	B	389	THR	CA-C-O	-5.24	114.67	120.70	17	1
2	B	354	THR	CB-CA-C	5.24	120.33	109.38	9	1
2	B	380	ASN	N-CA-CB	-5.24	103.67	109.74	6	1
2	B	382	ARG	NH1-CZ-NH2	-5.24	112.50	119.30	20	2
2	B	408	VAL	O-C-N	-5.22	117.25	123.05	1	1
1	A	65	LEU	CA-C-N	5.22	129.14	120.94	6	1
1	A	65	LEU	C-N-CA	5.22	129.14	120.94	6	1
2	B	411	THR	OG1-CB-CG2	-5.22	98.87	109.30	2	1
2	B	358	ILE	N-CA-C	5.22	115.88	108.42	16	1
2	B	357	CYS	N-CA-CB	-5.21	101.46	110.32	8	1
2	B	381	PRO	CB-CA-C	-5.21	104.12	110.95	3	1
2	B	386	LYS	N-CA-CB	-5.20	101.90	111.37	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	418	HIS	CB-CG-ND1	5.19	130.48	122.70	15	1
2	B	411	THR	CA-CB-OG1	5.18	117.37	109.60	16	1
2	B	351	VAL	O-C-N	-5.17	117.86	123.14	4	1
2	B	349	ARG	O-C-N	-5.17	116.97	122.30	3	1
2	B	410	THR	CA-CB-CG2	5.17	119.29	110.50	17	1
2	B	366	ARG	NH1-CZ-NH2	-5.17	112.58	119.30	18	1
2	B	376	CYS	CA-C-N	5.17	130.12	120.87	6	1
2	B	376	CYS	C-N-CA	5.17	130.12	120.87	6	1
2	B	355	THR	CA-C-N	5.17	130.82	122.29	11	1
2	B	355	THR	C-N-CA	5.17	130.82	122.29	11	1
1	A	52	GLN	N-CA-C	5.16	116.98	111.36	5	2
2	B	348	PRO	N-CD-CG	5.16	110.94	103.20	4	1
2	B	379	PRO	O-C-N	5.16	128.87	122.22	6	1
2	B	375	VAL	N-CA-C	5.13	116.28	108.80	19	1
2	B	417	ASN	CB-CG-ND2	5.12	124.08	116.40	13	1
2	B	382	ARG	NE-CZ-NH2	5.12	123.81	119.20	16	1
2	B	381	PRO	O-C-N	-5.11	116.52	122.86	12	1
2	B	409	ILE	CA-CB-CG2	-5.11	101.81	110.50	15	1
1	A	56	SER	CB-CA-C	5.11	118.21	109.72	3	1
2	B	403	HIS	CG-CD2-NE2	-5.11	102.09	107.20	7	1
2	B	367	TRP	CZ3-CH2-CZ2	-5.11	114.86	121.50	10	1
2	B	386	LYS	O-C-N	-5.11	117.26	123.29	10	1
2	B	353	GLN	O-C-N	-5.10	117.04	123.27	6	1
2	B	391	GLY	CA-C-O	5.10	126.05	119.68	8	2
2	B	361	LEU	CD1-CG-CD2	-5.10	99.59	110.80	9	1
2	B	392	CYS	N-CA-C	5.10	116.32	109.24	5	1
2	B	369	LYS	O-C-N	5.10	129.15	123.19	17	1
2	B	351	VAL	CA-C-O	5.09	126.09	120.64	16	1
2	B	395	ARG	CA-C-O	-5.08	115.41	121.56	20	1
1	A	49	MET	CA-C-N	5.08	129.41	121.08	8	2
1	A	49	MET	C-N-CA	5.08	129.41	121.08	8	2
2	B	379	PRO	N-CA-CB	5.08	108.18	103.46	12	1
2	B	348	PRO	CA-C-N	5.08	130.89	122.62	20	2
2	B	348	PRO	C-N-CA	5.08	130.89	122.62	20	2
2	B	390	ILE	N-CA-C	5.08	115.95	109.30	6	1
2	B	406	ARG	N-CA-CB	-5.07	103.31	110.81	7	1
1	A	67	GLY	O-C-N	-5.07	117.49	122.86	18	1
2	B	408	VAL	CG1-CB-CG2	-5.07	99.64	110.80	18	1
2	B	409	ILE	CA-CB-CG1	5.07	119.02	110.40	1	1
2	B	420	VAL	CA-CB-CG1	5.07	119.01	110.40	1	1
2	B	410	THR	OG1-CB-CG2	-5.06	99.17	109.30	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	58	PHE	O-C-N	-5.06	117.82	123.48	14	1
2	B	405	MET	CA-CB-CG	5.06	124.21	114.10	18	1
2	B	411	THR	CA-CB-CG2	5.06	119.10	110.50	18	1
2	B	367	TRP	N-CA-CB	-5.05	102.13	111.53	1	1
2	B	373	LYS	CB-CA-C	5.05	118.22	110.14	4	1
2	B	374	VAL	CB-CA-C	-5.05	103.81	111.33	5	1
2	B	349	ARG	NE-CZ-NH2	-5.05	114.66	119.20	14	1
2	B	418	HIS	O-C-N	-5.05	116.80	123.21	1	1
2	B	346	ARG	CB-CA-C	5.05	120.46	110.42	17	1
2	B	412	TYR	N-CA-C	5.04	117.90	110.59	6	1
1	A	49	MET	CA-C-O	5.04	126.44	120.69	4	1
2	B	384	TYR	CA-C-O	5.04	125.87	120.38	11	1
2	B	348	PRO	CB-CA-C	-5.03	104.37	110.00	14	1
1	A	49	MET	N-CA-CB	-5.02	102.24	109.83	9	1
2	B	358	ILE	CA-CB-CG1	5.02	118.94	110.40	11	1
1	A	56	SER	CA-C-N	5.02	129.60	122.08	16	1
1	A	56	SER	C-N-CA	5.02	129.60	122.08	16	1
2	B	420	VAL	N-CA-CB	-5.01	104.17	110.33	2	2
2	B	359	ASP	N-CA-CB	-5.00	102.75	110.46	2	1
2	B	346	ARG	NE-CZ-NH2	5.00	123.70	119.20	6	1
1	A	51	VAL	CA-CB-CG2	5.00	118.91	110.40	13	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
2	B	406	ARG	Sidechain	7
2	B	385	TYR	Sidechain	6
2	B	400	ARG	Sidechain	6
2	B	412	TYR	Sidechain,Peptide	5
2	B	370	TYR	Sidechain	4
2	B	382	ARG	Sidechain	4
2	B	416	HIS	Sidechain	3
2	B	381	PRO	Mainchain,Peptide	3
2	B	397	HIS	Sidechain	3
1	A	59	ARG	Sidechain	3
2	B	384	TYR	Sidechain	3
1	A	58	PHE	Sidechain	2
2	B	367	TRP	Mainchain,Peptide	2
2	B	366	ARG	Sidechain	2

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Mol	Chain	Res	Type	Group	Models (Total)
2	B	368	ARG	Sidechain	2
2	B	396	LYS	Mainchain,Peptide	2
2	B	365	TYR	Sidechain	1
2	B	357	CYS	Mainchain	1
2	B	394	VAL	Peptide	1
2	B	418	HIS	Sidechain	1
2	B	346	ARG	Sidechain	1
2	B	361	LEU	Peptide	1
2	B	348	PRO	Peptide	1
2	B	395	ARG	Sidechain	1
1	A	50	ARG	Sidechain	1
1	A	61	LEU	Mainchain	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	173	174	174	0±0
2	B	617	606	606	0±1
All	All	15820	15600	15600	9

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:PHE:CZ	2:B:415:LYS:HE3	0.57	2.33	2	1
2:B:367:TRP:CD2	2:B:396:LYS:HE2	0.50	2.41	8	3
2:B:347:GLU:N	2:B:348:PRO:CD	0.49	2.75	3	1
2:B:368:ARG:HG2	2:B:388:THR:HG22	0.46	1.86	4	1
2:B:347:GLU:HB3	2:B:348:PRO:HD3	0.43	1.90	2	1
2:B:370:TYR:CE2	2:B:386:LYS:HB3	0.42	2.50	20	1
2:B:367:TRP:CE2	2:B:396:LYS:HE2	0.40	2.51	8	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	22/98 (22%)	19±1 (85±5%)	3±1 (12±6%)	1±1 (4±3%)	4	32
2	B	75/101 (74%)	69±2 (92±2%)	5±2 (7±2%)	0±1 (1±1%)	20	70
All	All	1940/3980 (49%)	1755 (90%)	159 (8%)	26 (1%)	12	60

All 10 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	51	VAL	10
1	A	68	GLN	4
2	B	346	ARG	3
2	B	377	GLY	2
2	B	360	ILE	2
2	B	350	ILE	1
1	A	69	ASP	1
1	A	62	VAL	1
2	B	363	ASP	1
2	B	417	ASN	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	19/93 (20%)	18±1 (97±3%)	1±1 (3±3%)	33	83
2	B	69/88 (78%)	68±1 (98±2%)	1±1 (2±2%)	46	90
All	All	1760/3620 (49%)	1718 (98%)	42 (2%)	43	89

All 24 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)
2	B	375	VAL	5
2	B	372	GLN	4
1	A	68	GLN	4
2	B	409	ILE	3
1	A	62	VAL	3
1	A	58	PHE	2
2	B	397	HIS	2
2	B	354	THR	2
1	A	51	VAL	2
1	A	65	LEU	1
2	B	378	ASN	1
2	B	369	LYS	1
1	A	60	GLU	1
2	B	386	LYS	1
2	B	379	PRO	1
2	B	390	ILE	1
2	B	408	VAL	1
2	B	348	PRO	1
2	B	351	VAL	1
2	B	355	THR	1
2	B	406	ARG	1
2	B	420	VAL	1
2	B	363	ASP	1
2	B	352	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 1% for the well-defined parts and 2% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *wk11_CS*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	30
Number of shifts mapped to atoms	30
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 1%, i.e. 16 atoms were assigned a chemical shift out of a possible 1362. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	16/486 (3%)	8/197 (4%)	0/196 (0%)	8/93 (9%)
Sidechain	0/781 (0%)	0/502 (0%)	0/235 (0%)	0/44 (0%)
Aromatic	0/95 (0%)	0/47 (0%)	0/43 (0%)	0/5 (0%)
Overall	16/1362 (1%)	8/746 (1%)	0/474 (0%)	8/142 (6%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 30 atoms were assigned a chemical shift out of a possible 1574. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	30/560 (5%)	15/226 (7%)	0/228 (0%)	15/106 (14%)
Sidechain	0/910 (0%)	0/586 (0%)	0/277 (0%)	0/47 (0%)
Aromatic	0/104 (0%)	0/51 (0%)	0/48 (0%)	0/5 (0%)
Overall	30/1574 (2%)	15/863 (2%)	0/553 (0%)	15/158 (9%)

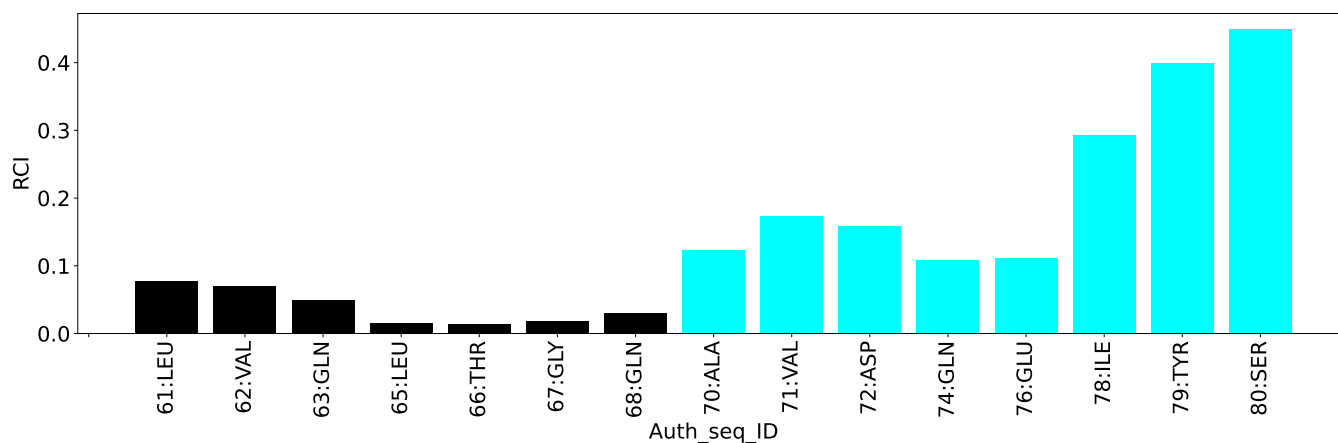
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	17
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	17
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.1
Number of long range restraints per residue ¹	0.0

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.3	0.2
0.2-0.5 (Medium)	0.8	0.5
>0.5 (Large)	4.0	5.61

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis

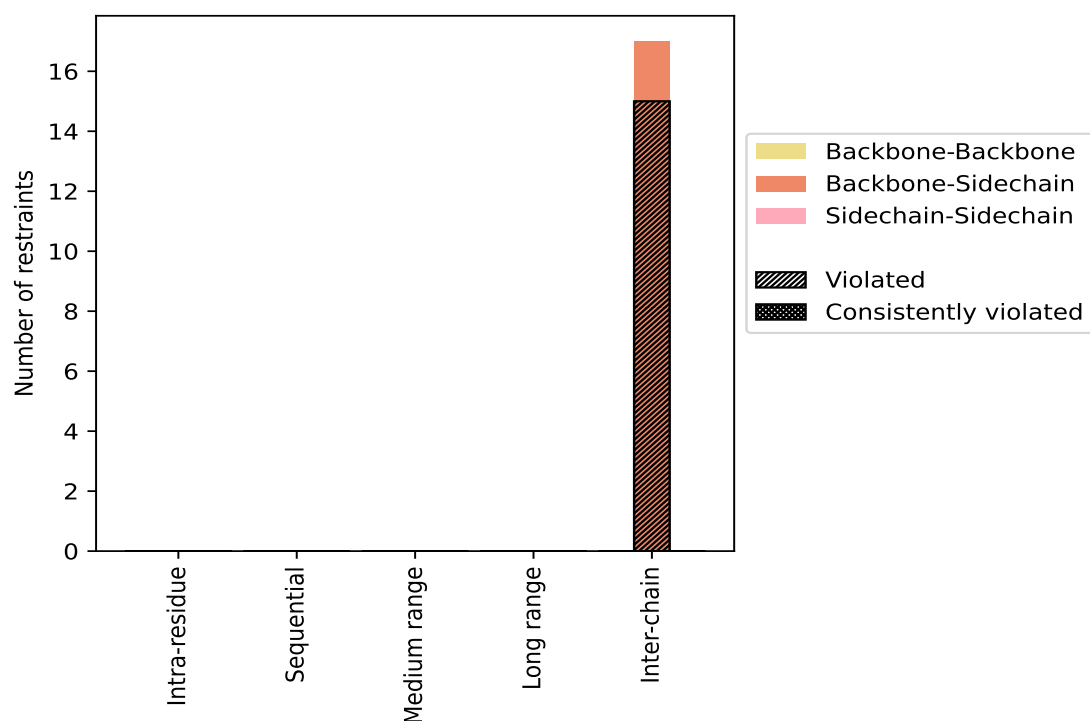
9.1 Summary of distance violations

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($ i-j =0$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($ i-j \geq 5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	17	100.0	15	88.2	88.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	17	100.0	15	88.2	88.2	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	17	100.0	15	88.2	88.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	17	100.0	15	88.2	88.2	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfid bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	0	7	7	1.54	4.31	1.27	1.05
2	0	0	0	0	5	5	1.39	2.84	0.84	1.27
3	0	0	0	0	6	6	0.9	2.89	0.9	0.56
4	0	0	0	0	3	3	0.77	1.36	0.42	0.48
5	0	0	0	0	3	3	0.81	1.57	0.59	0.75
6	0	0	0	0	3	3	0.34	0.54	0.14	0.24
7	0	0	0	0	3	3	0.48	0.67	0.2	0.56
8	0	0	0	0	4	4	1.58	3.18	1.08	1.5
9	0	0	0	0	5	5	0.94	1.97	0.59	0.8
10	0	0	0	0	4	4	0.83	1.54	0.43	0.68

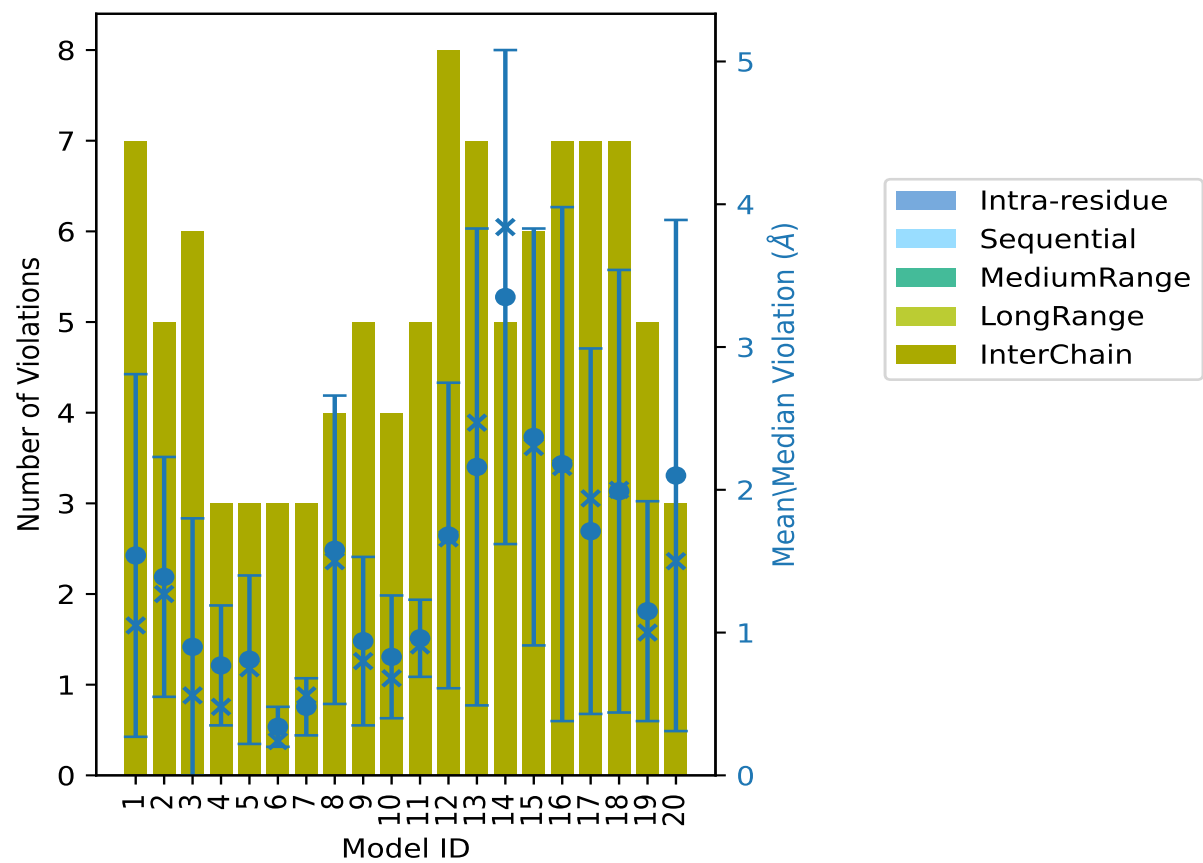
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	0	5	5	0.96	1.3	0.27	0.91
12	0	0	0	0	8	8	1.68	3.68	1.07	1.66
13	0	0	0	0	7	7	2.16	5.1	1.67	2.47
14	0	0	0	0	5	5	3.35	5.25	1.73	3.84
15	0	0	0	0	6	6	2.37	4.89	1.46	2.3
16	0	0	0	0	7	7	2.18	5.61	1.8	2.16
17	0	0	0	0	7	7	1.71	3.77	1.28	1.94
18	0	0	0	0	7	7	1.99	5.27	1.55	2.0
19	0	0	0	0	5	5	1.15	2.58	0.77	1.0
20	0	0	0	0	3	3	2.1	4.52	1.79	1.5

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble

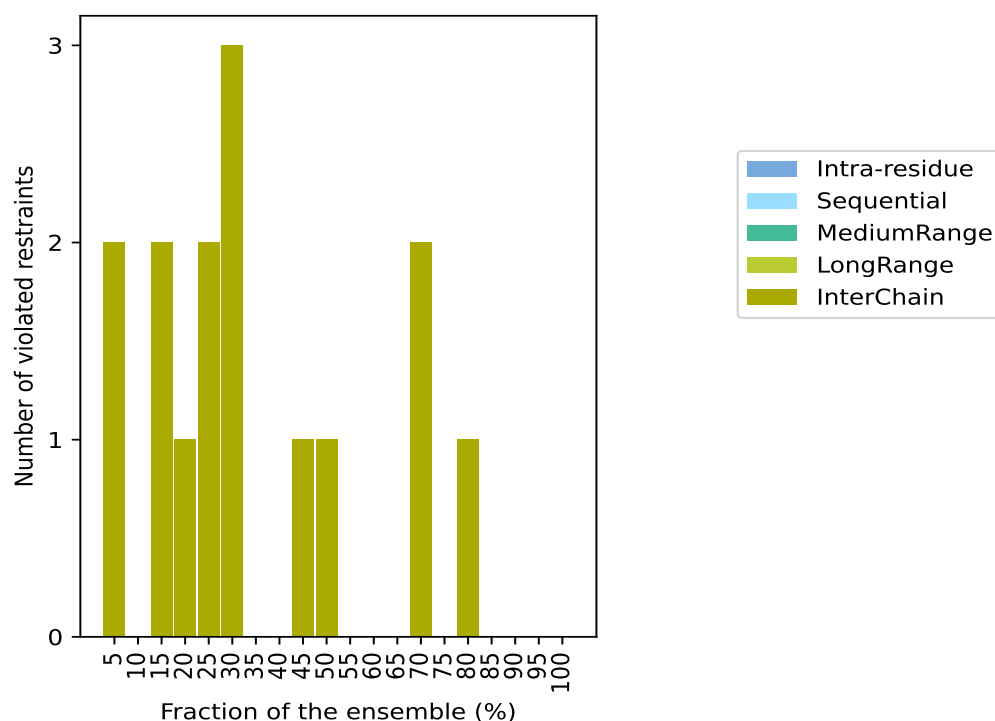
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2(IR:0, SQ:0, MR:0, LR:0, IC:2) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	2	2	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	2	2	3	15.0
0	0	0	0	1	1	4	20.0
0	0	0	0	2	2	5	25.0
0	0	0	0	3	3	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	1	1	9	45.0
0	0	0	0	1	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	2	2	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	1	1	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

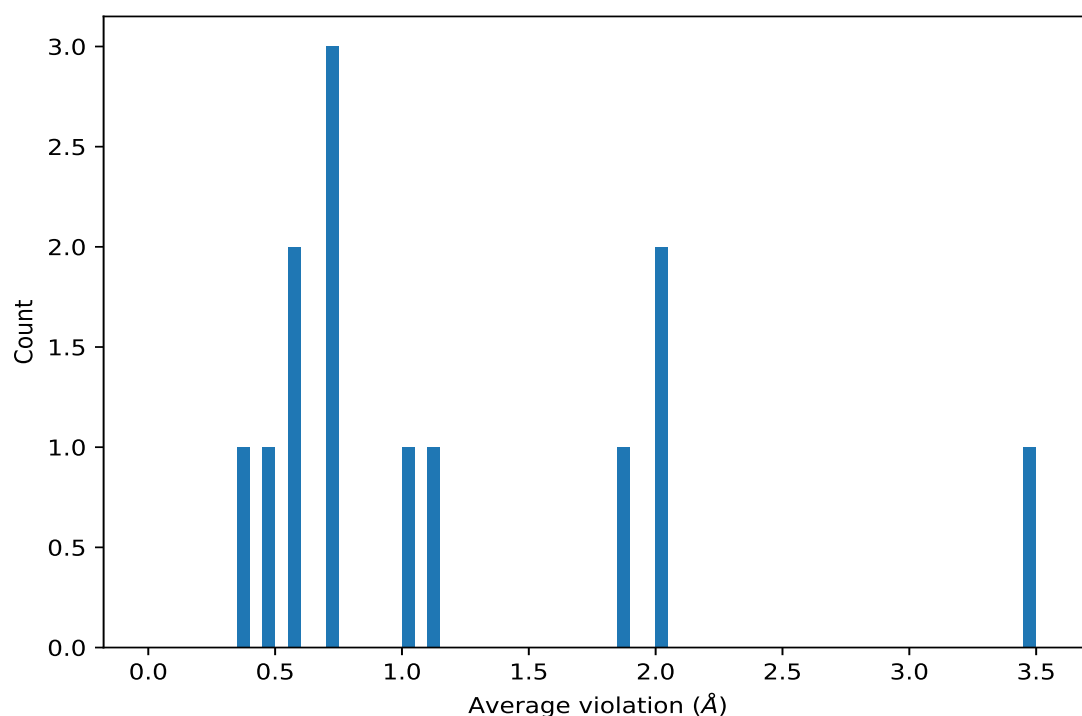
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

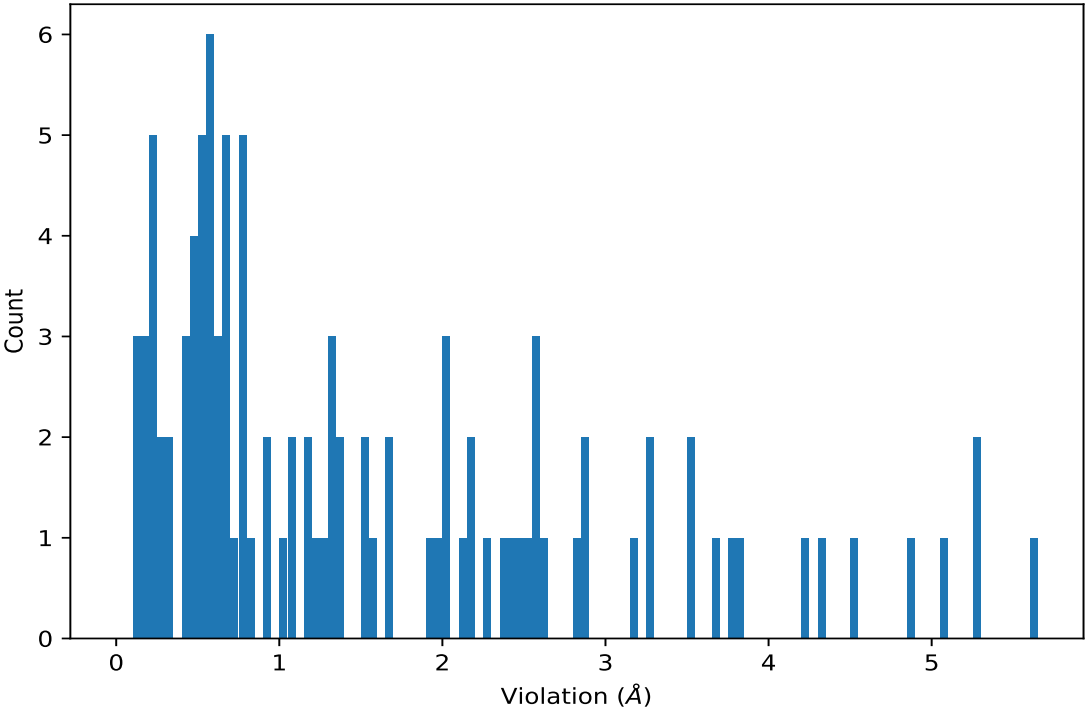
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	16	3.46	1.7	3.72
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	14	2.03	0.96	1.82
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	14	1.87	1.11	1.97
(1,6)	2:376:B:CYS:HG	1:79:A:TYR:H	10	2.0	0.95	2.18
(1,17)	2:357:B:CYS:HG	1:80:A:SER:H	9	0.7	0.39	0.64
(1,14)	2:357:B:CYS:HG	1:76:A:GLU:H	6	0.7	0.41	0.52
(1,15)	2:357:B:CYS:HG	1:78:A:ILE:H	6	0.57	0.25	0.57
(1,13)	2:357:B:CYS:HG	1:71:A:VAL:H	6	0.49	0.32	0.4
(1,12)	2:357:B:CYS:HG	1:70:A:ALA:H	5	0.57	0.29	0.63
(1,8)	2:357:B:CYS:HG	1:63:A:GLN:H	5	0.35	0.19	0.33
(1,16)	2:357:B:CYS:HG	1:79:A:TYR:H	4	1.04	0.43	1.02
(1,1)	2:376:B:CYS:HG	1:67:A:GLY:H	3	1.12	0.63	0.79
(1,3)	2:376:B:CYS:HG	1:71:A:VAL:H	3	0.72	0.09	0.76

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations ⓘ

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	16	5.61
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	18	5.27
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	14	5.25
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	13	5.1
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	15	4.89
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	20	4.52
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	1	4.31
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	14	4.21
(1,6)	2:376:B:CYS:HG	1:79:A:TYR:H	14	3.84
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	17	3.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	12	3.68
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	16	3.54
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	13	3.53
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	14	3.3
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	15	3.29
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	8	3.18
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	3	2.89
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	17	2.88
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	2	2.84
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	12	2.65
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	19	2.58
(1,6)	2:376:B:CYS:HG	1:79:A:TYR:H	13	2.57
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	18	2.56
(1,6)	2:376:B:CYS:HG	1:79:A:TYR:H	16	2.52
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	13	2.47
(1,6)	2:376:B:CYS:HG	1:79:A:TYR:H	15	2.42
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	1	2.36
(1,6)	2:376:B:CYS:HG	1:79:A:TYR:H	17	2.26
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	15	2.18
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	16	2.16
(1,6)	2:376:B:CYS:HG	1:79:A:TYR:H	12	2.1
(1,6)	2:376:B:CYS:HG	1:79:A:TYR:H	18	2.03
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	18	2.0
(1,1)	2:376:B:CYS:HG	1:67:A:GLY:H	12	2.0
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	9	1.97
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	17	1.94
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	8	1.69
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	2	1.68
(1,16)	2:357:B:CYS:HG	1:79:A:TYR:H	5	1.57
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	10	1.54
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	20	1.5
(1,17)	2:357:B:CYS:HG	1:80:A:SER:H	18	1.38
(1,16)	2:357:B:CYS:HG	1:79:A:TYR:H	4	1.36
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	8	1.31
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	12	1.31
(1,14)	2:357:B:CYS:HG	1:76:A:GLU:H	11	1.3
(1,17)	2:357:B:CYS:HG	1:80:A:SER:H	2	1.27
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	11	1.24
(1,14)	2:357:B:CYS:HG	1:76:A:GLU:H	1	1.2
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	19	1.17
(1,13)	2:357:B:CYS:HG	1:71:A:VAL:H	9	1.06
(1,6)	2:376:B:CYS:HG	1:79:A:TYR:H	1	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,12)	2:357:B:CYS:HG	1:70:A:ALA:H	19	1.0
(1,17)	2:357:B:CYS:HG	1:80:A:SER:H	1	0.91
(1,15)	2:357:B:CYS:HG	1:78:A:ILE:H	11	0.91
(1,3)	2:376:B:CYS:HG	1:71:A:VAL:H	9	0.8
(1,15)	2:357:B:CYS:HG	1:78:A:ILE:H	15	0.79
(1,1)	2:376:B:CYS:HG	1:67:A:GLY:H	13	0.79
(1,3)	2:376:B:CYS:HG	1:71:A:VAL:H	10	0.76
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	11	0.75
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	5	0.75
(1,17)	2:357:B:CYS:HG	1:80:A:SER:H	12	0.71
(1,8)	2:357:B:CYS:HG	1:63:A:GLN:H	16	0.7
(1,16)	2:357:B:CYS:HG	1:79:A:TYR:H	9	0.68
(1,13)	2:357:B:CYS:HG	1:71:A:VAL:H	3	0.67
(1,6)	2:376:B:CYS:HG	1:79:A:TYR:H	7	0.67
(1,12)	2:357:B:CYS:HG	1:70:A:ALA:H	2	0.66
(1,17)	2:357:B:CYS:HG	1:80:A:SER:H	15	0.64
(1,12)	2:357:B:CYS:HG	1:70:A:ALA:H	1	0.63
(1,11)	2:357:B:CYS:HG	1:68:A:GLN:H	3	0.62
(1,15)	2:357:B:CYS:HG	1:78:A:ILE:H	10	0.59
(1,3)	2:376:B:CYS:HG	1:71:A:VAL:H	11	0.59
(1,13)	2:357:B:CYS:HG	1:71:A:VAL:H	19	0.57
(1,16)	2:357:B:CYS:HG	1:79:A:TYR:H	7	0.56
(1,1)	2:376:B:CYS:HG	1:67:A:GLY:H	16	0.56
(1,15)	2:357:B:CYS:HG	1:78:A:ILE:H	17	0.55
(1,6)	2:376:B:CYS:HG	1:79:A:TYR:H	6	0.54
(1,14)	2:357:B:CYS:HG	1:76:A:GLU:H	12	0.53
(1,17)	2:357:B:CYS:HG	1:80:A:SER:H	13	0.51
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	3	0.51
(1,14)	2:357:B:CYS:HG	1:76:A:GLU:H	18	0.5
(1,14)	2:357:B:CYS:HG	1:76:A:GLU:H	2	0.49
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	4	0.48
(1,15)	2:357:B:CYS:HG	1:78:A:ILE:H	4	0.46
(1,12)	2:357:B:CYS:HG	1:70:A:ALA:H	12	0.46
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	10	0.43
(1,17)	2:357:B:CYS:HG	1:80:A:SER:H	19	0.42
(1,9)	2:357:B:CYS:HG	1:66:A:THR:H	3	0.41
(1,8)	2:357:B:CYS:HG	1:63:A:GLN:H	1	0.34
(1,8)	2:357:B:CYS:HG	1:63:A:GLN:H	17	0.33
(1,7)	2:376:B:CYS:HG	1:80:A:SER:H	3	0.3
(1,8)	2:357:B:CYS:HG	1:63:A:GLN:H	20	0.27
(1,17)	2:357:B:CYS:HG	1:80:A:SER:H	6	0.24
(1,13)	2:357:B:CYS:HG	1:71:A:VAL:H	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	2:357:B:CYS:HG	1:80:A:SER:H	17	0.22
(1,13)	2:357:B:CYS:HG	1:71:A:VAL:H	18	0.22
(1,4)	2:376:B:CYS:HG	1:76:A:GLU:H	7	0.2
(1,5)	2:376:B:CYS:HG	1:78:A:ILE:H	9	0.18
(1,14)	2:357:B:CYS:HG	1:76:A:GLU:H	16	0.16
(1,13)	2:357:B:CYS:HG	1:71:A:VAL:H	8	0.16
(1,8)	2:357:B:CYS:HG	1:63:A:GLN:H	14	0.13
(1,15)	2:357:B:CYS:HG	1:78:A:ILE:H	5	0.12
(1,12)	2:357:B:CYS:HG	1:70:A:ALA:H	13	0.12

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found