



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 06:06 AM EST

PDB ID : 5Y0U
BMRB ID : 36108
Title : The solution structure of AEBP2 C2H2 zinc fingers
Authors : Sun, A.; Shi, Y.; Wu, J.
Deposited on : 2017-07-18

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 : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

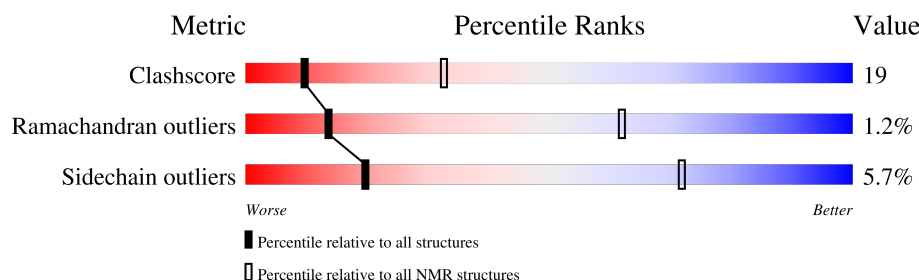
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 77%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	109	

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 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:260-A:353 (94)	0.76	8

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. No single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1633 atoms, of which 778 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc finger protein AEBP2.

Mol	Chain	Residues	Atoms						Trace
1	A	109	Total	C	H	N	O	S	0
			1630	525	778	167	150	10	

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	MET	-	expression tag	UNP Q6ZN18
A	250	GLY	-	expression tag	UNP Q6ZN18
A	251	HIS	-	expression tag	UNP Q6ZN18
A	252	HIS	-	expression tag	UNP Q6ZN18
A	253	HIS	-	expression tag	UNP Q6ZN18
A	254	HIS	-	expression tag	UNP Q6ZN18
A	255	HIS	-	expression tag	UNP Q6ZN18
A	256	HIS	-	expression tag	UNP Q6ZN18
A	257	ASN	-	expression tag	UNP Q6ZN18

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

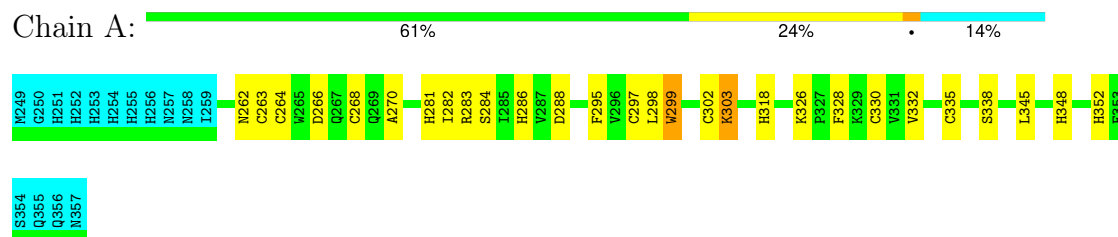
Mol	Chain	Residues	Atoms	
2	A	3	Total	Zn
			3	3

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: Zinc finger protein AEBP2

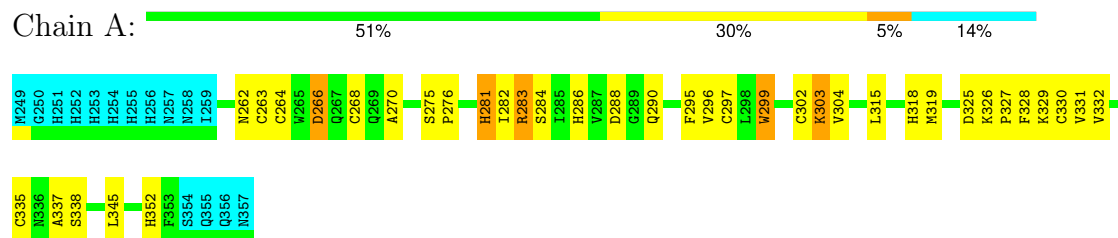


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Zinc finger protein AEBP2



4.2.2 Score per residue for model 2

- Molecule 1: Zinc finger protein AEBP2

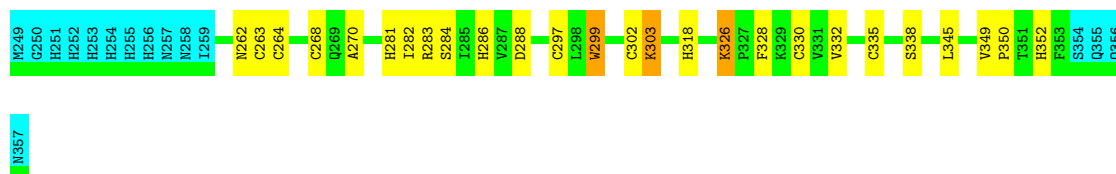




4.2.3 Score per residue for model 3

- Molecule 1: Zinc finger protein AEBP2

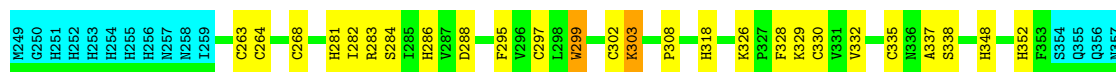
Chain A: 62% 21% 14%



4.2.4 Score per residue for model 4

- Molecule 1: Zinc finger protein AEBP2

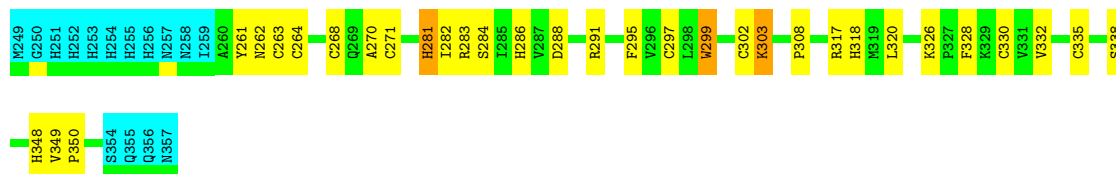
Chain A: 62% 22% 14%



4.2.5 Score per residue for model 5

- Molecule 1: Zinc finger protein AEBP2

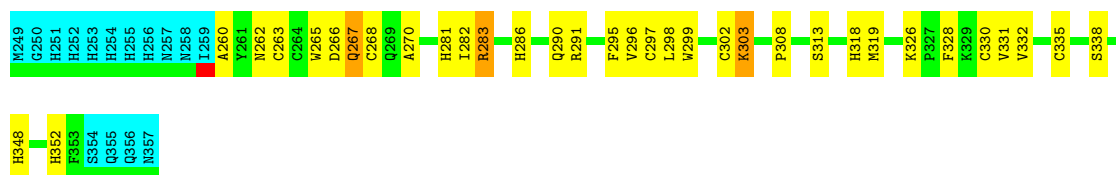
Chain A: 57% 27% 14%



4.2.6 Score per residue for model 6

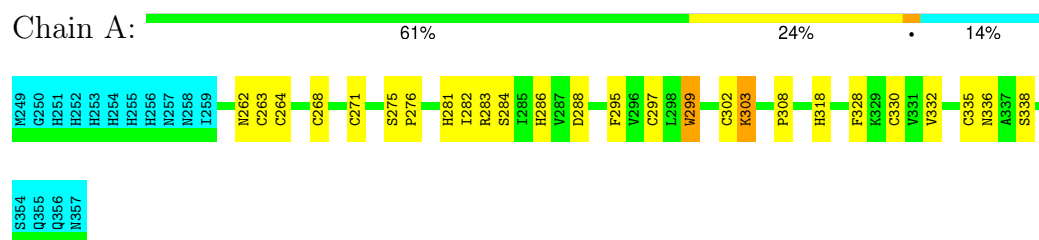
- Molecule 1: Zinc finger protein AEBP2

Chain A: 55% 28% 14%



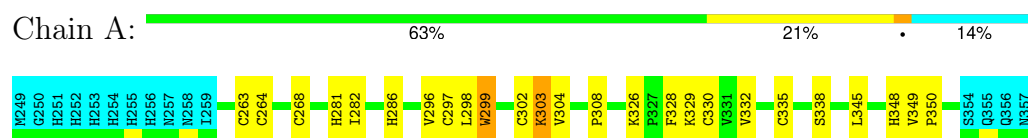
4.2.7 Score per residue for model 7

- Molecule 1: Zinc finger protein AEBP2



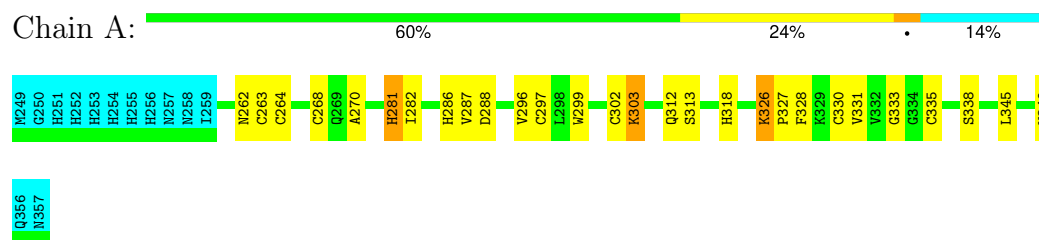
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Zinc finger protein AEBP2



4.2.9 Score per residue for model 9

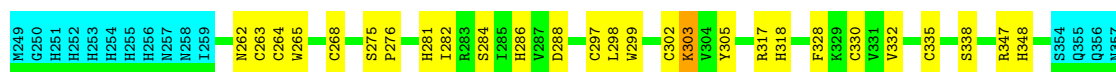
- Molecule 1: Zinc finger protein AEBP2



4.2.10 Score per residue for model 10

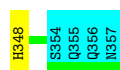
- Molecule 1: Zinc finger protein AEBP2





4.2.11 Score per residue for model 11

- Molecule 1: Zinc finger protein AEBP2



4.2.12 Score per residue for model 12

- Molecule 1: Zinc finger protein AEBP2



4.2.13 Score per residue for model 13

- Molecule 1: Zinc finger protein AEBP2



4.2.14 Score per residue for model 14

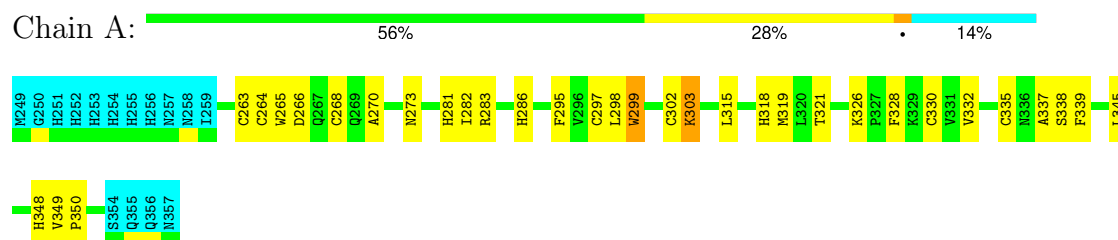
- Molecule 1: Zinc finger protein AEBP2





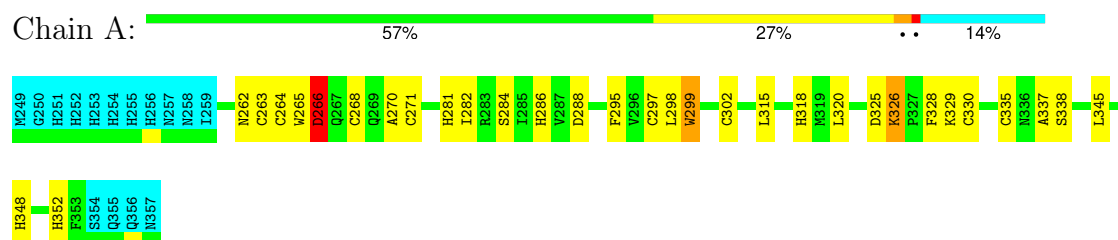
4.2.15 Score per residue for model 15

- Molecule 1: Zinc finger protein AEBP2



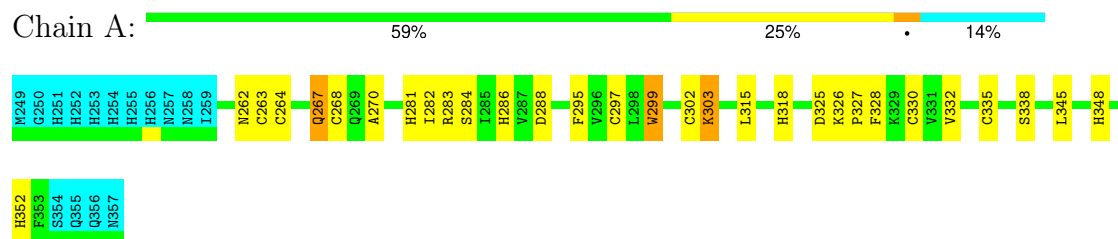
4.2.16 Score per residue for model 16

- Molecule 1: Zinc finger protein AEBP2



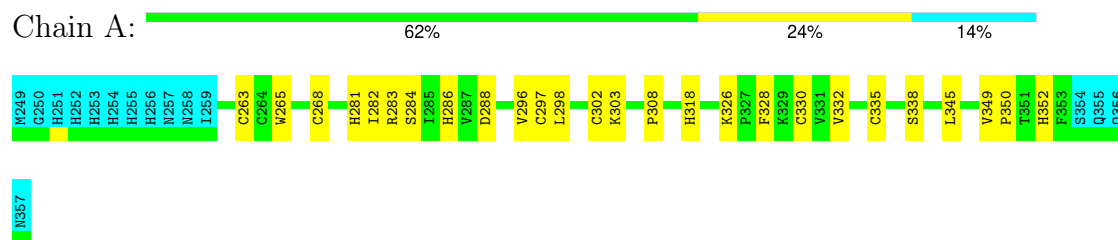
4.2.17 Score per residue for model 17

- Molecule 1: Zinc finger protein AEBP2



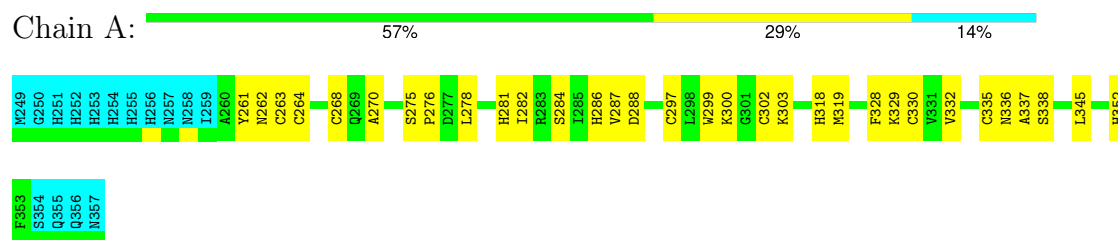
4.2.18 Score per residue for model 18

- Molecule 1: Zinc finger protein AEBP2



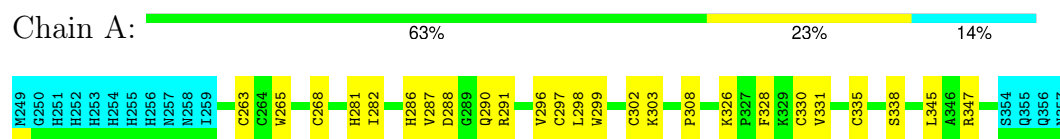
4.2.19 Score per residue for model 19

- Molecule 1: Zinc finger protein AEBP2



4.2.20 Score per residue for model 20

- Molecule 1: Zinc finger protein AEBP2



5 Refinement protocol and experimental data overview

The models were refined using the following method: *na*.

Of the 100 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
CNS	refinement	1.2
CYANA	structure solution	
Sparky	structure solution	

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	1007
Number of shifts mapped to atoms	1007
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

6 Model quality

6.1 Standard geometry

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

There are no covalent bond-length or bond-angle outliers.

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	0.1±0.4
All	All	0	3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	291	ARG	Sidechain	1
1	A	283	ARG	Sidechain	1
1	A	317	ARG	Sidechain	1

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	724	672	678	27±3
2	A	3	0	0	11±1
All	All	14540	13440	13560	546

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:268:CYS:HG	2:A:401:ZN:ZN	0.94	0.72	16	20
1:A:297:CYS:HG	2:A:402:ZN:ZN	0.94	0.71	1	19
1:A:330:CYS:HG	2:A:403:ZN:ZN	0.88	0.60	19	20
1:A:302:CYS:HG	2:A:402:ZN:ZN	0.86	0.58	9	2
1:A:335:CYS:HG	2:A:403:ZN:ZN	0.80	0.85	7	19
1:A:263:CYS:HG	2:A:401:ZN:ZN	0.80	0.56	2	14
1:A:268:CYS:SG	2:A:401:ZN:ZN	0.79	1.72	6	20
1:A:263:CYS:SG	2:A:401:ZN:ZN	0.78	1.73	13	20
1:A:302:CYS:SG	2:A:402:ZN:ZN	0.78	1.73	6	20
1:A:297:CYS:SG	2:A:402:ZN:ZN	0.77	1.74	8	20
1:A:335:CYS:SG	2:A:403:ZN:ZN	0.77	1.74	7	20
1:A:330:CYS:SG	2:A:403:ZN:ZN	0.76	1.74	7	20
1:A:330:CYS:HG	1:A:335:CYS:HG	0.65	1.34	4	16
1:A:328:PHE:O	1:A:338:SER:HA	0.59	1.97	10	20
1:A:265:TRP:CD1	1:A:298:LEU:HB2	0.59	2.32	12	10
1:A:267:GLN:HE21	1:A:267:GLN:N	0.59	1.95	6	1
1:A:264:CYS:O	1:A:299:TRP:HA	0.58	1.98	13	16
1:A:262:ASN:HA	1:A:270:ALA:O	0.57	2.00	14	12
1:A:303:LYS:HD3	1:A:303:LYS:H	0.56	1.60	3	12
1:A:284:SER:O	1:A:288:ASP:HB3	0.54	2.02	12	15
1:A:330:CYS:SG	1:A:335:CYS:SG	0.53	3.06	19	20
1:A:263:CYS:SG	1:A:270:ALA:HB3	0.53	2.44	12	3
1:A:288:ASP:O	1:A:291:ARG:HG2	0.52	2.04	20	2
1:A:287:VAL:HG21	1:A:319:MET:SD	0.52	2.45	19	2
1:A:283:ARG:O	1:A:288:ASP:HB2	0.52	2.05	12	2
1:A:332:VAL:HB	1:A:335:CYS:HB3	0.52	1.82	3	11
1:A:297:CYS:SG	1:A:299:TRP:HB2	0.52	2.44	5	4
1:A:329:LYS:HA	1:A:337:ALA:O	0.52	2.05	16	5
1:A:295:PHE:O	1:A:308:PRO:HA	0.52	2.04	5	3
1:A:287:VAL:HG12	1:A:331:VAL:HG23	0.51	1.81	20	1
1:A:268:CYS:SG	1:A:281:HIS:NE2	0.51	2.84	12	15
1:A:325:ASP:OD1	1:A:327:PRO:HD2	0.51	2.06	17	1
1:A:262:ASN:HB3	1:A:271:CYS:SG	0.50	2.47	7	2
1:A:337:ALA:HB1	1:A:339:PHE:CZ	0.50	2.42	15	1
1:A:282:ILE:O	1:A:286:HIS:HB2	0.50	2.07	14	19
1:A:332:VAL:HG21	1:A:352:HIS:CG	0.50	2.40	3	9
1:A:261:TYR:O	1:A:271:CYS:HA	0.50	2.06	5	2
1:A:279:ALA:HB1	1:A:325:ASP:HB2	0.49	1.83	14	1
1:A:296:VAL:HG22	1:A:308:PRO:HB3	0.49	1.83	6	4
1:A:297:CYS:SG	1:A:302:CYS:SG	0.49	3.11	4	19
1:A:316:GLN:O	1:A:319:MET:HG2	0.49	2.08	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:320:LEU:HA	1:A:325:ASP:OD2	0.49	2.08	16	1
1:A:299:TRP:CZ3	1:A:322:HIS:HB3	0.48	2.43	2	1
1:A:263:CYS:SG	1:A:281:HIS:CE1	0.48	3.06	5	2
1:A:287:VAL:HG12	1:A:331:VAL:HG13	0.48	1.86	9	1
1:A:335:CYS:HG	1:A:352:HIS:CE1	0.47	2.27	16	2
1:A:267:GLN:NE2	1:A:267:GLN:HA	0.47	2.24	17	1
1:A:302:CYS:SG	1:A:318:HIS:NE2	0.46	2.88	17	17
1:A:290:GLN:HB3	1:A:295:PHE:CD2	0.46	2.45	6	1
1:A:295:PHE:CB	1:A:315:LEU:HG	0.46	2.40	16	5
1:A:261:TYR:HB3	1:A:278:LEU:HD22	0.46	1.88	14	2
1:A:335:CYS:SG	1:A:348:HIS:NE2	0.45	2.90	5	14
1:A:290:GLN:HG2	1:A:296:VAL:H	0.45	1.71	20	2
1:A:332:VAL:HB	1:A:335:CYS:CB	0.45	2.42	14	2
1:A:295:PHE:HB3	1:A:315:LEU:HD22	0.45	1.89	11	1
1:A:263:CYS:SG	1:A:268:CYS:SG	0.45	3.14	7	7
1:A:263:CYS:HG	1:A:268:CYS:HG	0.45	1.52	13	1
1:A:325:ASP:OD2	1:A:327:PRO:HD2	0.44	2.12	1	1
1:A:295:PHE:HB3	1:A:315:LEU:HG	0.44	1.89	17	2
1:A:329:LYS:HG2	1:A:338:SER:OG	0.44	2.13	8	2
1:A:312:GLN:HG2	1:A:349:VAL:HG11	0.44	1.89	9	1
1:A:303:LYS:HD2	1:A:304:VAL:HG13	0.43	1.91	8	3
1:A:263:CYS:SG	1:A:281:HIS:NE2	0.43	2.92	9	2
1:A:297:CYS:SG	1:A:318:HIS:NE2	0.43	2.91	5	2
1:A:283:ARG:NH1	1:A:331:VAL:HA	0.43	2.29	6	2
1:A:275:SER:N	1:A:276:PRO:HD2	0.43	2.29	2	7
1:A:318:HIS:O	1:A:321:THR:HG22	0.43	2.14	15	1
1:A:342:GLN:OE1	1:A:345:LEU:HD22	0.42	2.14	2	1
1:A:281:HIS:HA	1:A:284:SER:OG	0.42	2.14	1	1
1:A:317:ARG:O	1:A:320:LEU:HB3	0.42	2.14	2	2
1:A:302:CYS:SG	1:A:322:HIS:NE2	0.42	2.93	2	2
1:A:349:VAL:N	1:A:350:PRO:HD2	0.41	2.30	14	8
1:A:266:ASP:OD2	1:A:298:LEU:HB3	0.41	2.15	16	1
1:A:326:LYS:H	1:A:327:PRO:HD2	0.41	1.76	9	1
1:A:299:TRP:HB3	1:A:302:CYS:SG	0.40	2.56	4	1
1:A:342:GLN:OE1	1:A:342:GLN:HA	0.40	2.17	2	1
1:A:297:CYS:O	1:A:305:TYR:HB2	0.40	2.16	10	1
1:A:288:ASP:HB2	1:A:331:VAL:O	0.40	2.17	9	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	94/109 (86%)	86±2 (91±2%)	7±2 (8±3%)	1±1 (1±1%)	14	62
All	All	1880/2180 (86%)	1711 (91%)	146 (8%)	23 (1%)	14	62

All 6 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	326	LYS	15
1	A	266	ASP	4
1	A	327	PRO	1
1	A	291	ARG	1
1	A	333	GLY	1
1	A	267	GLN	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	79/93 (85%)	74±2 (94±2%)	4±2 (6±2%)	20	72
All	All	1580/1860 (85%)	1490 (94%)	90 (6%)	20	72

All 19 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	303	LYS	19
1	A	299	TRP	14
1	A	345	LEU	14
1	A	283	ARG	10

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Mol	Chain	Res	Type	Models (Total)
1	A	266	ASP	6
1	A	281	HIS	3
1	A	319	MET	3
1	A	262	ASN	3
1	A	277	ASP	3
1	A	326	LYS	2
1	A	267	GLN	2
1	A	313	SER	2
1	A	336	ASN	2
1	A	347	ARG	2
1	A	298	LEU	1
1	A	296	VAL	1
1	A	290	GLN	1
1	A	273	ASN	1
1	A	300	LYS	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 3 ligands modelled in this entry, 3 are 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 72% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `showstar.txt`

7.1.1 Bookkeeping [i](#)

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	1007
Number of shifts mapped to atoms	1007
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	103	-0.41 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	94	0.42 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	96	-0.03 ± 0.28	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 77%, i.e. 929 atoms were assigned a chemical shift out of a possible 1203. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	369/471 (78%)	188/193 (97%)	93/188 (49%)	88/90 (98%)
Sidechain	509/586 (87%)	348/381 (91%)	152/179 (85%)	9/26 (35%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	51/146 (35%)	48/75 (64%)	0/62 (0%)	3/9 (33%)
Overall	929/1203 (77%)	584/649 (90%)	245/429 (57%)	100/125 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 1007 atoms were assigned a chemical shift out of a possible 1406. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	404/547 (74%)	205/224 (92%)	103/218 (47%)	96/105 (91%)
Sidechain	551/671 (82%)	374/435 (86%)	166/205 (81%)	11/31 (35%)
Aromatic	52/188 (28%)	49/99 (49%)	0/74 (0%)	3/15 (20%)
Overall	1007/1406 (72%)	628/758 (83%)	269/497 (54%)	110/151 (73%)

7.1.4 Statistically unusual chemical shifts [i](#)

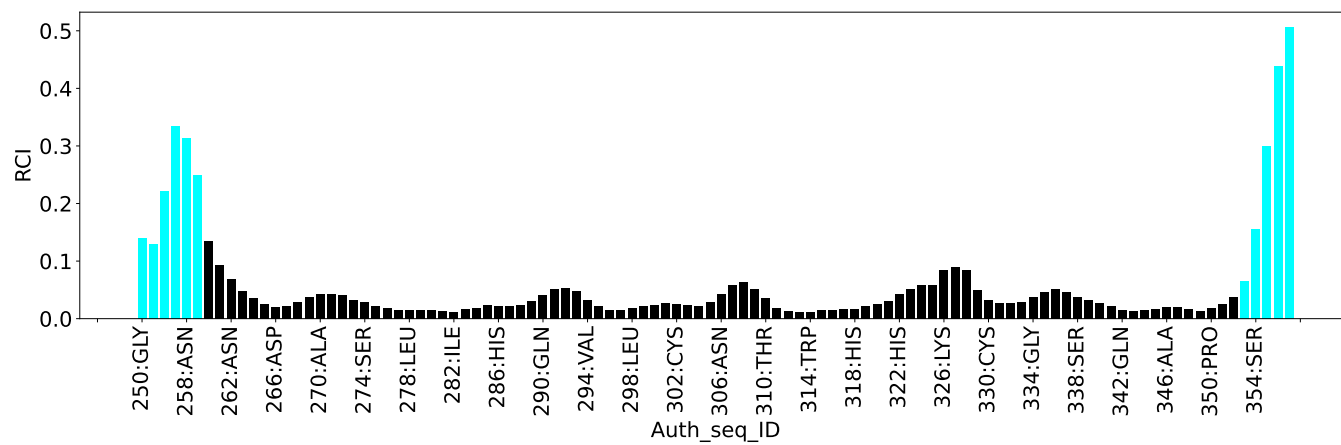
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	264	CYS	HB3	0.03	0.69 – 5.10	-6.5
1	A	286	HIS	HB3	0.68	1.18 – 4.91	-6.3
1	A	322	HIS	HB3	1.05	1.18 – 4.91	-5.3

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	1664
Intra-residue ($ i-j =0$)	360
Sequential ($ i-j =1$)	472
Medium range ($ i-j >1$ and $ i-j <5$)	375
Long range ($ i-j \geq 5$)	429
Inter-chain	0
Hydrogen bond restraints	19
Disulfide bond restraints	3
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	14.9
Number of long range restraints per residue ¹	3.9

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)	12.7	0.2
0.2-0.5 (Medium)	2.1	0.33
>0.5 (Large)	None	None

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 ⓘ

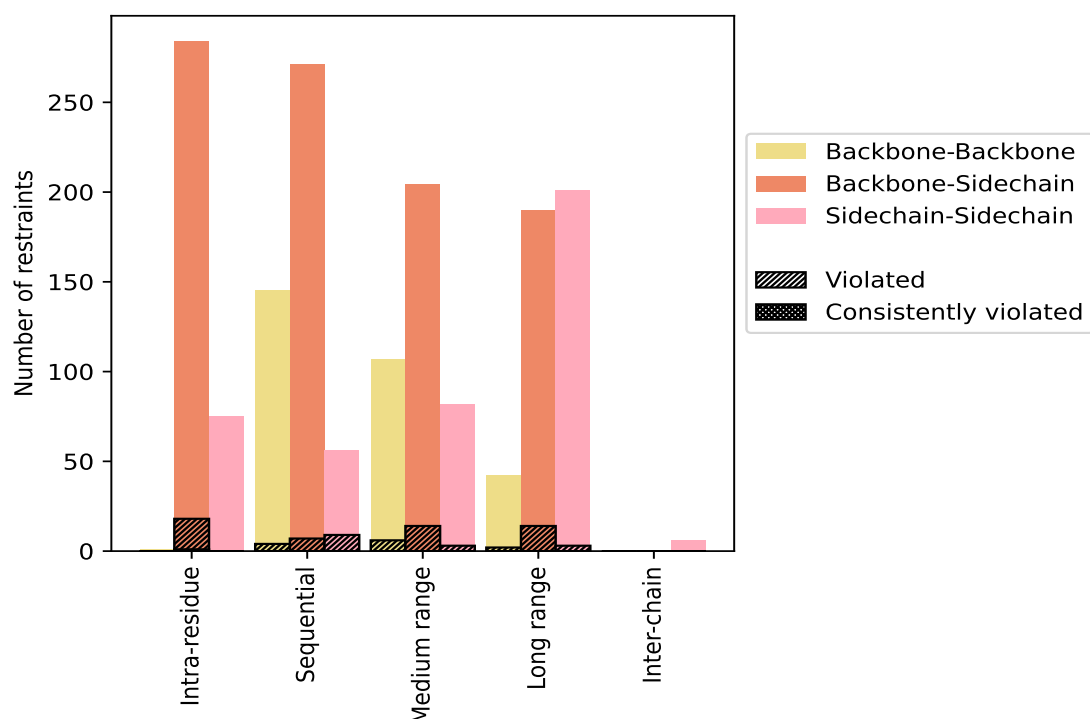
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	360	21.6	18	5.0	1.1	1	0.3	0.1
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	284	17.1	18	6.3	1.1	1	0.4	0.1
Sidechain-Sidechain	75	4.5	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	472	28.4	20	4.2	1.2	0	0.0	0.0
Backbone-Backbone	145	8.7	4	2.8	0.2	0	0.0	0.0
Backbone-Sidechain	271	16.3	7	2.6	0.4	0	0.0	0.0
Sidechain-Sidechain	56	3.4	9	16.1	0.5	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	375	22.5	23	6.1	1.4	0	0.0	0.0
Backbone-Backbone	107	6.4	6	5.6	0.4	0	0.0	0.0
Backbone-Sidechain	188	11.3	14	7.4	0.8	0	0.0	0.0
Sidechain-Sidechain	80	4.8	3	3.8	0.2	0	0.0	0.0
Long range ($i-j \geq 5$)	429	25.8	19	4.4	1.1	0	0.0	0.0
Backbone-Backbone	42	2.5	2	4.8	0.1	0	0.0	0.0
Backbone-Sidechain	190	11.4	14	7.4	0.8	0	0.0	0.0
Sidechain-Sidechain	197	11.8	3	1.5	0.2	0	0.0	0.0
Inter-chain	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
Hydrogen bond	19	1.1	0	0.0	0.0	0	0.0	0.0
Disulfide bond	3	0.2	0	0.0	0.0	0	0.0	0.0
Total	1664	100.0	80	4.8	4.8	1	0.1	0.1
Backbone-Backbone	295	17.7	12	4.1	0.7	0	0.0	0.0
Backbone-Sidechain	949	57.0	53	5.6	3.2	1	0.1	0.1
Sidechain-Sidechain	420	25.2	15	3.6	0.9	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 disulfied 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	3	7	5	4	0	19	0.15	0.29	0.05	0.14
2	5	2	4	3	0	14	0.15	0.26	0.05	0.14
3	5	8	3	1	0	17	0.14	0.23	0.04	0.12
4	2	3	8	2	0	15	0.14	0.24	0.04	0.13
5	5	4	5	0	0	14	0.15	0.22	0.04	0.14
6	2	3	4	2	0	11	0.17	0.25	0.05	0.16
7	4	4	5	3	0	16	0.13	0.24	0.04	0.12
8	4	4	6	4	0	18	0.15	0.26	0.05	0.14
9	5	3	6	2	0	16	0.15	0.32	0.06	0.12
10	3	4	6	2	0	15	0.14	0.24	0.04	0.12

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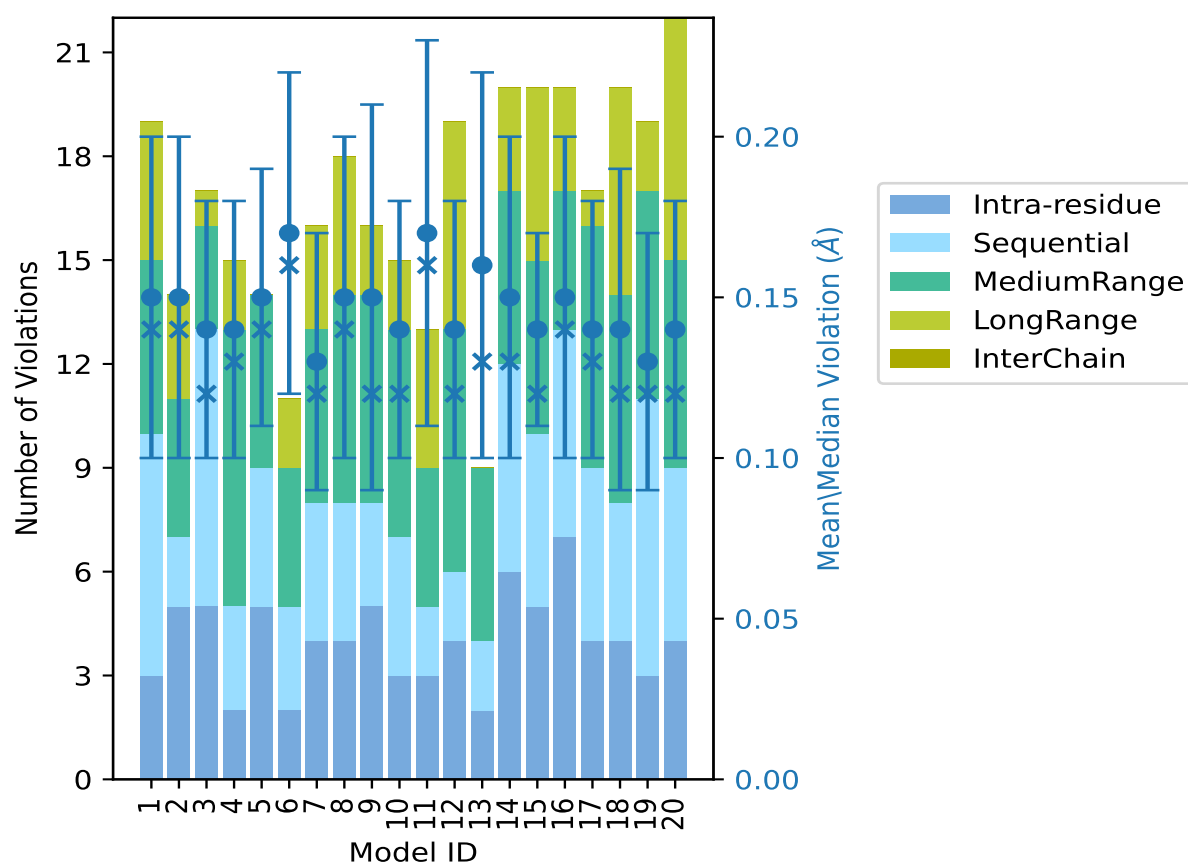
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	3	2	4	4	0	13	0.17	0.27	0.06	0.16
12	4	2	7	6	0	19	0.14	0.25	0.04	0.12
13	2	2	5	0	0	9	0.16	0.27	0.06	0.13
14	6	6	5	3	0	20	0.15	0.33	0.05	0.13
15	5	5	5	5	0	20	0.14	0.23	0.03	0.12
16	7	6	4	3	0	20	0.15	0.33	0.05	0.14
17	4	5	7	1	0	17	0.14	0.26	0.04	0.13
18	4	4	6	6	0	20	0.14	0.26	0.05	0.12
19	3	8	6	2	0	19	0.13	0.25	0.04	0.12
20	4	5	6	7	0	22	0.14	0.25	0.04	0.12

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

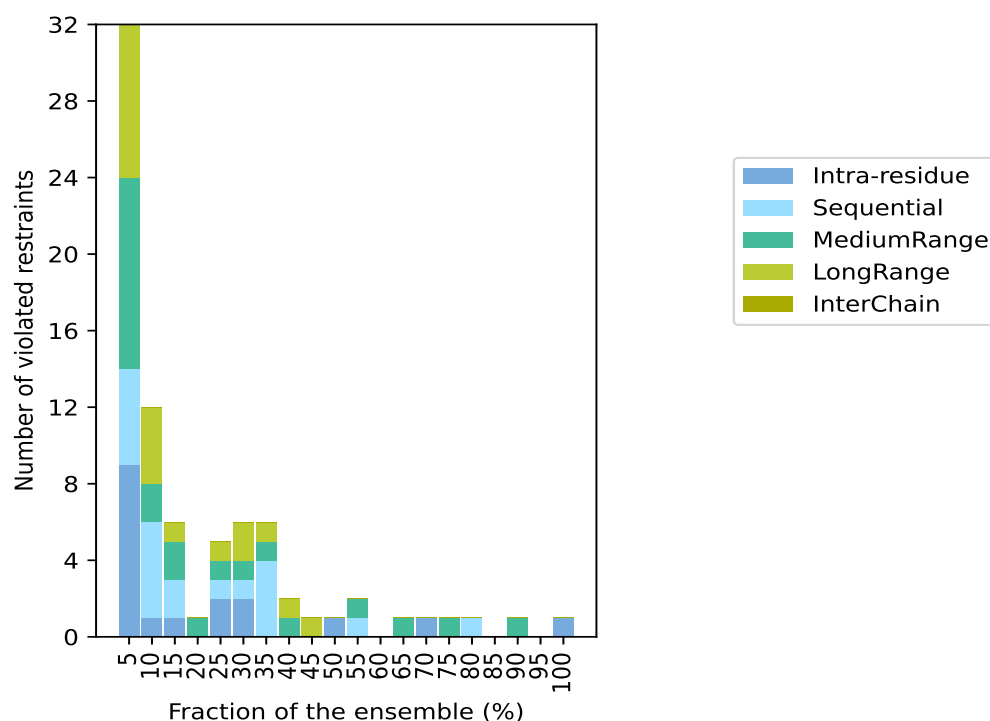
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1556(IR:342, SQ:452, MR:352, LR:410, IC:0) restraints are 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	%
9	5	10	8	0	32	1	5.0
1	5	2	4	0	12	2	10.0
1	2	2	1	0	6	3	15.0
0	0	1	0	0	1	4	20.0
2	1	1	1	0	5	5	25.0
2	1	1	2	0	6	6	30.0
0	4	1	1	0	6	7	35.0
0	0	1	1	0	2	8	40.0
0	0	0	1	0	1	9	45.0
1	0	0	0	0	1	10	50.0
0	1	1	0	0	2	11	55.0
0	0	0	0	0	0	12	60.0
0	0	1	0	0	1	13	65.0
1	0	0	0	0	1	14	70.0
0	0	1	0	0	1	15	75.0
0	1	0	0	0	1	16	80.0
0	0	0	0	0	0	17	85.0
0	0	1	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
1	0	0	0	0	1	20	100.0

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

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

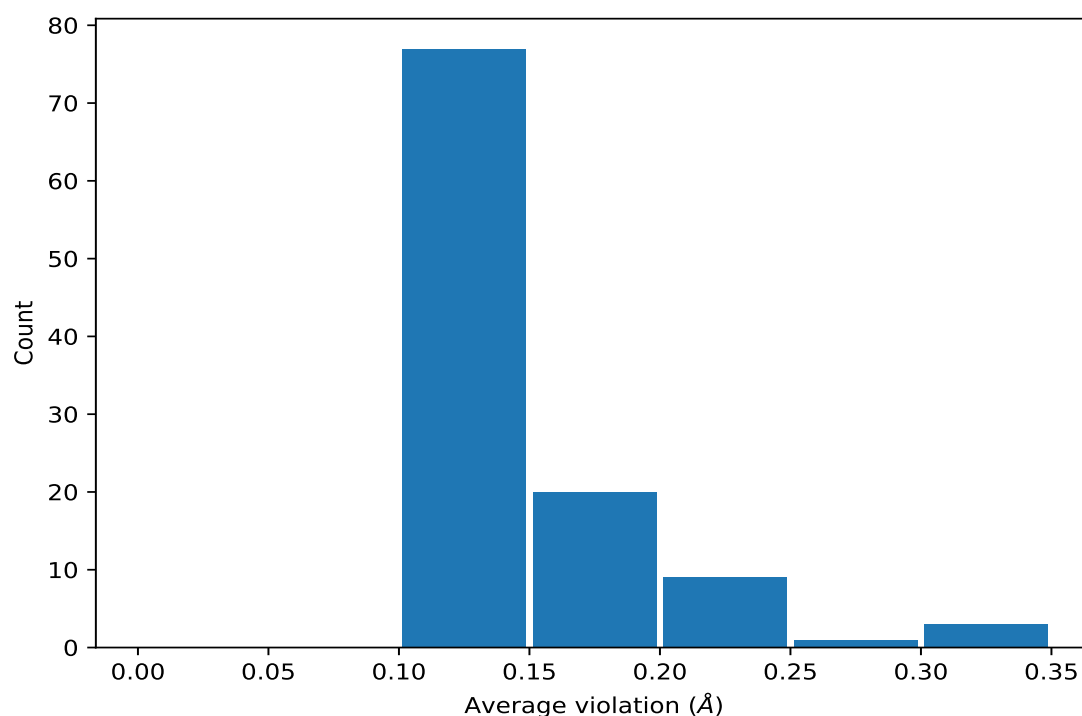
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	20	0.21	0.05	0.24
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	18	0.15	0.02	0.15
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	16	0.17	0.06	0.16
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	16	0.17	0.06	0.16
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	15	0.16	0.03	0.16
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	15	0.16	0.03	0.16
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	15	0.16	0.03	0.16
(1,762)	1:306:A:ASN:H	1:306:A:ASN:HD22	14	0.12	0.02	0.11
(1,702)	1:324:A:GLY:HA2	1:326:A:LYS:H	13	0.14	0.03	0.14
(1,702)	1:324:A:GLY:HA3	1:326:A:LYS:H	13	0.14	0.03	0.14
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE1	11	0.14	0.02	0.14
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE2	11	0.14	0.02	0.14
(1,736)	1:349:A:VAL:HG21	1:351:A:THR:H	11	0.11	0.01	0.11
(1,736)	1:349:A:VAL:HG22	1:351:A:THR:H	11	0.11	0.01	0.11
(1,736)	1:349:A:VAL:HG23	1:351:A:THR:H	11	0.11	0.01	0.11
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE1	10	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE2	10	0.11	0.01	0.11
(1,618)	1:295:A:PHE:H	1:310:A:THR:HB	9	0.11	0.01	0.11
(1,849)	1:266:A:ASP:HA	1:298:A:LEU:HG	8	0.14	0.03	0.14
(1,466)	1:282:A:ILE:HG21	1:284:A:SER:H	8	0.13	0.02	0.12
(1,466)	1:282:A:ILE:HG22	1:284:A:SER:H	8	0.13	0.02	0.12
(1,466)	1:282:A:ILE:HG23	1:284:A:SER:H	8	0.13	0.02	0.12
(1,330)	1:315:A:LEU:HG	1:316:A:GLN:H	7	0.21	0.01	0.22
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD2	7	0.16	0.02	0.16
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD3	7	0.16	0.02	0.16
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD2	7	0.16	0.02	0.16
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD3	7	0.16	0.02	0.16
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD2	7	0.16	0.02	0.16
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD3	7	0.16	0.02	0.16
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD11	7	0.14	0.02	0.13
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD12	7	0.14	0.02	0.13
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD13	7	0.14	0.02	0.13
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD1	7	0.13	0.02	0.13
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD2	7	0.13	0.02	0.13
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD1	7	0.13	0.02	0.13
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD2	7	0.13	0.02	0.13
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD1	7	0.13	0.02	0.13
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD2	7	0.13	0.02	0.13
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD11	7	0.12	0.01	0.12
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD12	7	0.12	0.01	0.12
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD13	7	0.12	0.01	0.12
(1,1405)	1:278:A:LEU:HD11	1:282:A:ILE:H	7	0.12	0.01	0.12
(1,1405)	1:278:A:LEU:HD12	1:282:A:ILE:H	7	0.12	0.01	0.12
(1,1405)	1:278:A:LEU:HD13	1:282:A:ILE:H	7	0.12	0.01	0.12
(1,1405)	1:278:A:LEU:HD21	1:282:A:ILE:H	7	0.12	0.01	0.12
(1,1405)	1:278:A:LEU:HD22	1:282:A:ILE:H	7	0.12	0.01	0.12
(1,1405)	1:278:A:LEU:HD23	1:282:A:ILE:H	7	0.12	0.01	0.12
(1,872)	1:296:A:VAL:HB	1:308:A:PRO:HA	6	0.25	0.01	0.24
(1,20)	1:266:A:ASP:H	1:267:A:GLN:H	6	0.19	0.04	0.2
(1,789)	1:290:A:GLN:HA	1:290:A:GLN:HE22	6	0.16	0.03	0.16
(1,939)	1:325:A:ASP:HB2	1:327:A:PRO:HD3	6	0.16	0.03	0.17
(1,939)	1:325:A:ASP:HB3	1:327:A:PRO:HD3	6	0.16	0.03	0.17
(1,1110)	1:326:A:LYS:HA	1:326:A:LYS:HD2	6	0.11	0.01	0.11
(1,1110)	1:326:A:LYS:HA	1:326:A:LYS:HD3	6	0.11	0.01	0.11
(1,757)	1:264:A:CYS:HA	1:299:A:TRP:HE1	6	0.11	0.01	0.11
(1,504)	1:321:A:THR:H	1:321:A:THR:HG21	5	0.3	0.04	0.32
(1,504)	1:321:A:THR:H	1:321:A:THR:HG22	5	0.3	0.04	0.32
(1,504)	1:321:A:THR:H	1:321:A:THR:HG23	5	0.3	0.04	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,261)	1:331:A:VAL:H	1:331:A:VAL:HB	5	0.12	0.01	0.12
(1,545)	1:272:A:PHE:H	1:278:A:LEU:HG	5	0.11	0.01	0.11
(1,1228)	1:348:A:HIS:HA	1:351:A:THR:H	5	0.11	0.02	0.11
(1,562)	1:275:A:SER:H	1:276:A:PRO:HB3	5	0.11	0.0	0.11
(1,548)	1:264:A:CYS:HA	1:266:A:ASP:H	4	0.18	0.04	0.16
(1,367)	1:266:A:ASP:HA	1:267:A:GLN:H	3	0.2	0.04	0.2
(1,1230)	1:280:A:ASP:HA	1:284:A:SER:HB2	3	0.13	0.01	0.12
(1,1230)	1:280:A:ASP:HA	1:284:A:SER:HB3	3	0.13	0.01	0.12
(1,612)	1:294:A:VAL:H	1:308:A:PRO:HB2	3	0.12	0.0	0.12
(1,549)	1:266:A:ASP:H	1:268:A:CYS:HB3	3	0.11	0.01	0.11
(1,818)	1:326:A:LYS:HD2	1:327:A:PRO:HD2	3	0.11	0.01	0.12
(1,818)	1:326:A:LYS:HD3	1:327:A:PRO:HD2	3	0.11	0.01	0.12
(1,925)	1:303:A:LYS:HA	1:303:A:LYS:HE2	3	0.1	0.0	0.1
(1,925)	1:303:A:LYS:HA	1:303:A:LYS:HE3	3	0.1	0.0	0.1
(1,1356)	1:259:A:ILE:HG12	1:260:A:ALA:HB1	2	0.2	0.03	0.2
(1,1356)	1:259:A:ILE:HG12	1:260:A:ALA:HB2	2	0.2	0.03	0.2
(1,1356)	1:259:A:ILE:HG12	1:260:A:ALA:HB3	2	0.2	0.03	0.2
(1,1356)	1:259:A:ILE:HG13	1:260:A:ALA:HB1	2	0.2	0.03	0.2
(1,1356)	1:259:A:ILE:HG13	1:260:A:ALA:HB2	2	0.2	0.03	0.2
(1,1356)	1:259:A:ILE:HG13	1:260:A:ALA:HB3	2	0.2	0.03	0.2
(1,543)	1:259:A:ILE:HG21	1:261:A:TYR:H	2	0.16	0.02	0.16
(1,543)	1:259:A:ILE:HG22	1:261:A:TYR:H	2	0.16	0.02	0.16
(1,543)	1:259:A:ILE:HG23	1:261:A:TYR:H	2	0.16	0.02	0.16
(1,1043)	1:346:A:ALA:HB1	1:347:A:ARG:HD2	2	0.14	0.04	0.14
(1,1043)	1:346:A:ALA:HB1	1:347:A:ARG:HD3	2	0.14	0.04	0.14
(1,1043)	1:346:A:ALA:HB2	1:347:A:ARG:HD2	2	0.14	0.04	0.14
(1,1043)	1:346:A:ALA:HB2	1:347:A:ARG:HD3	2	0.14	0.04	0.14
(1,1043)	1:346:A:ALA:HB3	1:347:A:ARG:HD2	2	0.14	0.04	0.14
(1,1043)	1:346:A:ALA:HB3	1:347:A:ARG:HD3	2	0.14	0.04	0.14
(1,1213)	1:305:A:TYR:HD1	1:306:A:ASN:HD22	2	0.12	0.0	0.12
(1,1213)	1:305:A:TYR:HD2	1:306:A:ASN:HD22	2	0.12	0.0	0.12
(1,1177)	1:310:A:THR:HA	1:353:A:PHE:HE1	2	0.12	0.0	0.12
(1,1177)	1:310:A:THR:HA	1:353:A:PHE:HE2	2	0.12	0.0	0.12
(1,443)	1:338:A:SER:H	1:339:A:PHE:HE1	2	0.11	0.01	0.11
(1,443)	1:338:A:SER:H	1:339:A:PHE:HE2	2	0.11	0.01	0.11
(1,553)	1:270:A:ALA:H	1:272:A:PHE:HE1	2	0.11	0.0	0.11
(1,553)	1:270:A:ALA:H	1:272:A:PHE:HE2	2	0.11	0.0	0.11
(1,1195)	1:300:A:LYS:H	1:305:A:TYR:HD1	2	0.11	0.01	0.11
(1,1195)	1:300:A:LYS:H	1:305:A:TYR:HD2	2	0.11	0.01	0.11
(1,972)	1:350:A:PRO:HD3	1:351:A:THR:HG21	2	0.11	0.0	0.11
(1,972)	1:350:A:PRO:HD3	1:351:A:THR:HG22	2	0.11	0.0	0.11
(1,972)	1:350:A:PRO:HD3	1:351:A:THR:HG23	2	0.11	0.0	0.11

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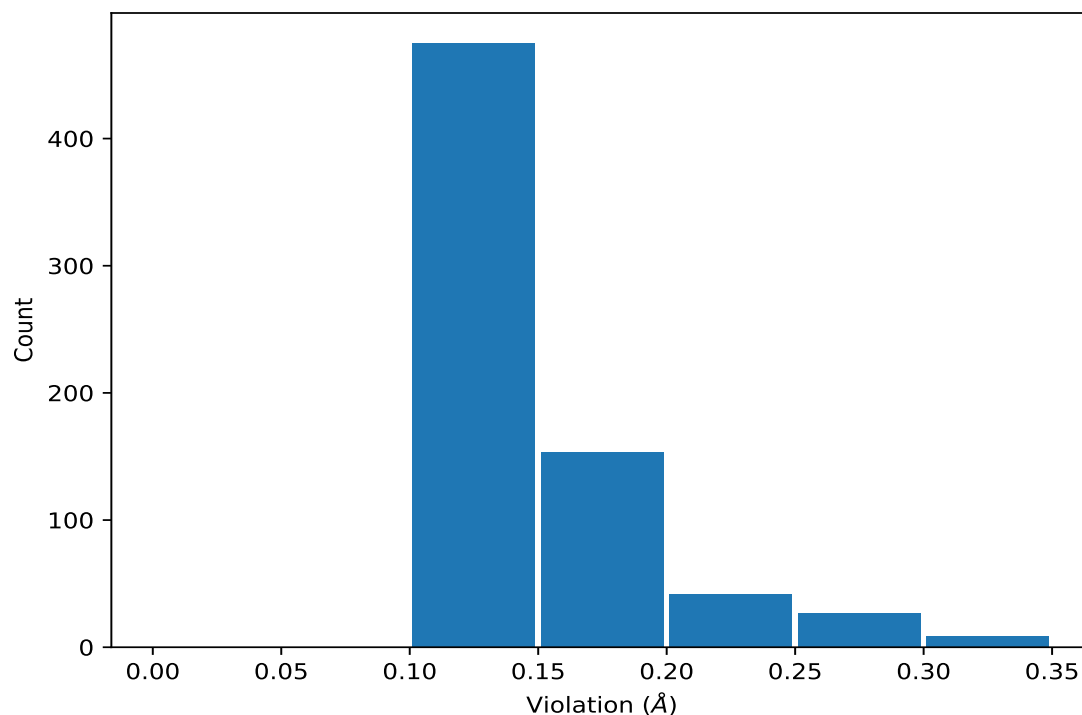
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD11	2	0.11	0.0	0.11
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD12	2	0.11	0.0	0.11
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD13	2	0.11	0.0	0.11
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD21	2	0.11	0.0	0.11
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD22	2	0.11	0.0	0.11
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD23	2	0.11	0.0	0.11
(1,1588)	1:329:A:LYS:HG2	1:338:A:SER:H	2	0.11	0.0	0.11
(1,1588)	1:329:A:LYS:HG3	1:338:A:SER:H	2	0.11	0.0	0.11
(1,936)	1:300:A:LYS:HA	1:300:A:LYS:HE2	2	0.1	0.0	0.1
(1,936)	1:300:A:LYS:HA	1:300:A:LYS:HE3	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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 [i](#)

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)
(1,504)	1:321:A:THR:H	1:321:A:THR:HG21	14	0.33
(1,504)	1:321:A:THR:H	1:321:A:THR:HG22	14	0.33
(1,504)	1:321:A:THR:H	1:321:A:THR:HG23	14	0.33
(1,504)	1:321:A:THR:H	1:321:A:THR:HG21	16	0.33
(1,504)	1:321:A:THR:H	1:321:A:THR:HG22	16	0.33
(1,504)	1:321:A:THR:H	1:321:A:THR:HG23	16	0.33
(1,504)	1:321:A:THR:H	1:321:A:THR:HG21	9	0.32
(1,504)	1:321:A:THR:H	1:321:A:THR:HG22	9	0.32
(1,504)	1:321:A:THR:H	1:321:A:THR:HG23	9	0.32
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	1	0.29
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	1	0.29
(1,872)	1:296:A:VAL:HB	1:308:A:PRO:HA	11	0.27
(1,35)	1:259:A:ILE:HA	1:260:A:ALA:H	13	0.27
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	2	0.26
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	2	0.26
(1,504)	1:321:A:THR:H	1:321:A:THR:HG21	1	0.26
(1,504)	1:321:A:THR:H	1:321:A:THR:HG22	1	0.26
(1,504)	1:321:A:THR:H	1:321:A:THR:HG23	1	0.26
(1,367)	1:266:A:ASP:HA	1:267:A:GLN:H	17	0.26
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	8	0.26
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	18	0.26
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	11	0.25
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	11	0.25
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	19	0.25
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	19	0.25
(1,872)	1:296:A:VAL:HB	1:308:A:PRO:HA	18	0.25
(1,872)	1:296:A:VAL:HB	1:308:A:PRO:HA	20	0.25
(1,548)	1:264:A:CYS:HA	1:266:A:ASP:H	12	0.25
(1,504)	1:321:A:THR:H	1:321:A:THR:HG21	11	0.25
(1,504)	1:321:A:THR:H	1:321:A:THR:HG22	11	0.25
(1,504)	1:321:A:THR:H	1:321:A:THR:HG23	11	0.25
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	2	0.25
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	6	0.25
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	9	0.25
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	11	0.25
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	13	0.25
(1,872)	1:296:A:VAL:HB	1:308:A:PRO:HA	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,872)	1:296:A:VAL:HB	1:308:A:PRO:HA	8	0.24
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	4	0.24
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	7	0.24
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	10	0.24
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	19	0.24
(1,1356)	1:259:A:ILE:HG12	1:260:A:ALA:HB1	14	0.23
(1,1356)	1:259:A:ILE:HG12	1:260:A:ALA:HB2	14	0.23
(1,1356)	1:259:A:ILE:HG12	1:260:A:ALA:HB3	14	0.23
(1,1356)	1:259:A:ILE:HG13	1:260:A:ALA:HB1	14	0.23
(1,1356)	1:259:A:ILE:HG13	1:260:A:ALA:HB2	14	0.23
(1,1356)	1:259:A:ILE:HG13	1:260:A:ALA:HB3	14	0.23
(1,872)	1:296:A:VAL:HB	1:308:A:PRO:HA	6	0.23
(1,330)	1:315:A:LEU:HG	1:316:A:GLN:H	15	0.23
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	3	0.23
(1,330)	1:315:A:LEU:HG	1:316:A:GLN:H	12	0.22
(1,330)	1:315:A:LEU:HG	1:316:A:GLN:H	14	0.22
(1,330)	1:315:A:LEU:HG	1:316:A:GLN:H	16	0.22
(1,330)	1:315:A:LEU:HG	1:316:A:GLN:H	20	0.22
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	5	0.22
(1,20)	1:266:A:ASP:H	1:267:A:GLN:H	5	0.22
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD2	7	0.21
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD3	7	0.21
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD2	7	0.21
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD3	7	0.21
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD2	7	0.21
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD3	7	0.21
(1,849)	1:266:A:ASP:HA	1:298:A:LEU:HG	12	0.21
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	4	0.21
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	4	0.21
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	4	0.21
(1,20)	1:266:A:ASP:H	1:267:A:GLN:H	18	0.21
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	6	0.2
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	6	0.2
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	6	0.2
(1,789)	1:290:A:GLN:HA	1:290:A:GLN:HE22	5	0.2
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	6	0.2
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	10	0.2
(1,367)	1:266:A:ASP:HA	1:267:A:GLN:H	12	0.2
(1,20)	1:266:A:ASP:H	1:267:A:GLN:H	3	0.2
(1,20)	1:266:A:ASP:H	1:267:A:GLN:H	8	0.2
(1,20)	1:266:A:ASP:H	1:267:A:GLN:H	9	0.2
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	8	0.19
(1,939)	1:325:A:ASP:HB2	1:327:A:PRO:HD3	8	0.19
(1,939)	1:325:A:ASP:HB3	1:327:A:PRO:HD3	8	0.19
(1,330)	1:315:A:LEU:HG	1:316:A:GLN:H	1	0.19
(1,330)	1:315:A:LEU:HG	1:316:A:GLN:H	17	0.19
(1,1356)	1:259:A:ILE:HG12	1:260:A:ALA:HB1	6	0.18
(1,1356)	1:259:A:ILE:HG12	1:260:A:ALA:HB2	6	0.18
(1,1356)	1:259:A:ILE:HG12	1:260:A:ALA:HB3	6	0.18
(1,1356)	1:259:A:ILE:HG13	1:260:A:ALA:HB1	6	0.18
(1,1356)	1:259:A:ILE:HG13	1:260:A:ALA:HB2	6	0.18
(1,1356)	1:259:A:ILE:HG13	1:260:A:ALA:HB3	6	0.18
(1,939)	1:325:A:ASP:HB2	1:327:A:PRO:HD3	14	0.18
(1,939)	1:325:A:ASP:HB3	1:327:A:PRO:HD3	14	0.18
(1,939)	1:325:A:ASP:HB2	1:327:A:PRO:HD3	20	0.18
(1,939)	1:325:A:ASP:HB3	1:327:A:PRO:HD3	20	0.18
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	3	0.18
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	3	0.18
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	3	0.18
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	19	0.18
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	19	0.18
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	19	0.18
(1,789)	1:290:A:GLN:HA	1:290:A:GLN:HE22	15	0.18
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	3	0.18
(1,702)	1:324:A:GLY:HA2	1:326:A:LYS:H	11	0.18
(1,702)	1:324:A:GLY:HA3	1:326:A:LYS:H	11	0.18
(1,702)	1:324:A:GLY:HA2	1:326:A:LYS:H	16	0.18
(1,702)	1:324:A:GLY:HA3	1:326:A:LYS:H	16	0.18
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD11	16	0.18
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD12	16	0.18
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD13	16	0.18
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE1	17	0.18
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE2	17	0.18
(1,347)	1:317:A:ARG:H	1:317:A:ARG:HB3	5	0.18
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	5	0.17
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	5	0.17
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	17	0.17
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	17	0.17
(1,1187)	1:260:A:ALA:H	1:262:A:ASN:H	4	0.17
(1,1043)	1:346:A:ALA:HB1	1:347:A:ARG:HD2	10	0.17
(1,1043)	1:346:A:ALA:HB1	1:347:A:ARG:HD3	10	0.17
(1,1043)	1:346:A:ALA:HB2	1:347:A:ARG:HD2	10	0.17
(1,1043)	1:346:A:ALA:HB2	1:347:A:ARG:HD3	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1043)	1:346:A:ALA:HB3	1:347:A:ARG:HD2	10	0.17
(1,1043)	1:346:A:ALA:HB3	1:347:A:ARG:HD3	10	0.17
(1,1013)	1:303:A:LYS:HA	1:303:A:LYS:HD2	16	0.17
(1,1013)	1:303:A:LYS:HA	1:303:A:LYS:HD3	16	0.17
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD2	3	0.17
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD3	3	0.17
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD2	3	0.17
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD3	3	0.17
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD2	3	0.17
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD3	3	0.17
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD2	15	0.17
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD3	15	0.17
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD2	15	0.17
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD3	15	0.17
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD2	15	0.17
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD3	15	0.17
(1,849)	1:266:A:ASP:HA	1:298:A:LEU:HG	1	0.17
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	2	0.17
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	2	0.17
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	2	0.17
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	10	0.17
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	10	0.17
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	10	0.17
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	15	0.17
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	15	0.17
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	15	0.17
(1,789)	1:290:A:GLN:HA	1:290:A:GLN:HE22	7	0.17
(1,762)	1:306:A:ASN:H	1:306:A:ASN:HD22	8	0.17
(1,755)	1:282:A:ILE:HD11	1:299:A:TRP:HE1	2	0.17
(1,755)	1:282:A:ILE:HD12	1:299:A:TRP:HE1	2	0.17
(1,755)	1:282:A:ILE:HD13	1:299:A:TRP:HE1	2	0.17
(1,702)	1:324:A:GLY:HA2	1:326:A:LYS:H	9	0.17
(1,702)	1:324:A:GLY:HA3	1:326:A:LYS:H	9	0.17
(1,702)	1:324:A:GLY:HA2	1:326:A:LYS:H	15	0.17
(1,702)	1:324:A:GLY:HA3	1:326:A:LYS:H	15	0.17
(1,543)	1:259:A:ILE:HG21	1:261:A:TYR:H	13	0.17
(1,543)	1:259:A:ILE:HG22	1:261:A:TYR:H	13	0.17
(1,543)	1:259:A:ILE:HG23	1:261:A:TYR:H	13	0.17
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE1	5	0.17
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE2	5	0.17
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	9	0.16
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD1	11	0.16
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD2	11	0.16
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD1	11	0.16
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD2	11	0.16
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD1	11	0.16
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD2	11	0.16
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD1	16	0.16
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD2	16	0.16
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD1	16	0.16
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD2	16	0.16
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD1	16	0.16
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD2	16	0.16
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD2	6	0.16
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD3	6	0.16
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD2	6	0.16
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD3	6	0.16
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD2	6	0.16
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD3	6	0.16
(1,939)	1:325:A:ASP:HB2	1:327:A:PRO:HD3	6	0.16
(1,939)	1:325:A:ASP:HB3	1:327:A:PRO:HD3	6	0.16
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	20	0.16
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	20	0.16
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	20	0.16
(1,789)	1:290:A:GLN:HA	1:290:A:GLN:HE22	8	0.16
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	11	0.16
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	17	0.16
(1,702)	1:324:A:GLY:HA2	1:326:A:LYS:H	4	0.16
(1,702)	1:324:A:GLY:HA3	1:326:A:LYS:H	4	0.16
(1,702)	1:324:A:GLY:HA2	1:326:A:LYS:H	17	0.16
(1,702)	1:324:A:GLY:HA3	1:326:A:LYS:H	17	0.16
(1,548)	1:264:A:CYS:HA	1:266:A:ASP:H	1	0.16
(1,548)	1:264:A:CYS:HA	1:266:A:ASP:H	11	0.16
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE1	16	0.16
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE2	16	0.16
(1,466)	1:282:A:ILE:HG21	1:284:A:SER:H	20	0.16
(1,466)	1:282:A:ILE:HG22	1:284:A:SER:H	20	0.16
(1,466)	1:282:A:ILE:HG23	1:284:A:SER:H	20	0.16
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	16	0.16
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	3	0.15
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	3	0.15
(1,1228)	1:348:A:HIS:HA	1:351:A:THR:H	15	0.15
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD2	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD3	18	0.15
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD2	18	0.15
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD3	18	0.15
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD2	18	0.15
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD3	18	0.15
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	14	0.15
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	14	0.15
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	14	0.15
(1,789)	1:290:A:GLN:HA	1:290:A:GLN:HE22	3	0.15
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	2	0.15
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	4	0.15
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	8	0.15
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	9	0.15
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	13	0.15
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	15	0.15
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD11	15	0.15
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD12	15	0.15
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD13	15	0.15
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE1	20	0.15
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE2	20	0.15
(1,466)	1:282:A:ILE:HG21	1:284:A:SER:H	17	0.15
(1,466)	1:282:A:ILE:HG22	1:284:A:SER:H	17	0.15
(1,466)	1:282:A:ILE:HG23	1:284:A:SER:H	17	0.15
(1,367)	1:266:A:ASP:HA	1:267:A:GLN:H	19	0.15
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	14	0.15
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	20	0.15
(1,1450)	1:290:A:GLN:HE21	1:296:A:VAL:HG11	4	0.14
(1,1450)	1:290:A:GLN:HE21	1:296:A:VAL:HG12	4	0.14
(1,1450)	1:290:A:GLN:HE21	1:296:A:VAL:HG13	4	0.14
(1,1450)	1:290:A:GLN:HE21	1:296:A:VAL:HG21	4	0.14
(1,1450)	1:290:A:GLN:HE21	1:296:A:VAL:HG22	4	0.14
(1,1450)	1:290:A:GLN:HE21	1:296:A:VAL:HG23	4	0.14
(1,1450)	1:290:A:GLN:HE22	1:296:A:VAL:HG11	4	0.14
(1,1450)	1:290:A:GLN:HE22	1:296:A:VAL:HG12	4	0.14
(1,1450)	1:290:A:GLN:HE22	1:296:A:VAL:HG13	4	0.14
(1,1450)	1:290:A:GLN:HE22	1:296:A:VAL:HG21	4	0.14
(1,1450)	1:290:A:GLN:HE22	1:296:A:VAL:HG22	4	0.14
(1,1450)	1:290:A:GLN:HE22	1:296:A:VAL:HG23	4	0.14
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	18	0.14
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	18	0.14
(1,1230)	1:280:A:ASP:HA	1:284:A:SER:HB2	5	0.14
(1,1230)	1:280:A:ASP:HA	1:284:A:SER:HB3	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD2	1	0.14
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD3	1	0.14
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD2	1	0.14
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD3	1	0.14
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD2	1	0.14
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD3	1	0.14
(1,849)	1:266:A:ASP:HA	1:298:A:LEU:HG	2	0.14
(1,849)	1:266:A:ASP:HA	1:298:A:LEU:HG	14	0.14
(1,849)	1:266:A:ASP:HA	1:298:A:LEU:HG	16	0.14
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD11	18	0.14
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD12	18	0.14
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD13	18	0.14
(1,812)	1:325:A:ASP:HA	1:327:A:PRO:HD2	17	0.14
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	8	0.14
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	8	0.14
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	8	0.14
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	12	0.14
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	12	0.14
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	12	0.14
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	5	0.14
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	14	0.14
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	18	0.14
(1,702)	1:324:A:GLY:HA2	1:326:A:LYS:H	12	0.14
(1,702)	1:324:A:GLY:HA3	1:326:A:LYS:H	12	0.14
(1,702)	1:324:A:GLY:HA2	1:326:A:LYS:H	20	0.14
(1,702)	1:324:A:GLY:HA3	1:326:A:LYS:H	20	0.14
(1,621)	1:290:A:GLN:HA	1:296:A:VAL:H	9	0.14
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD11	14	0.14
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD12	14	0.14
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD13	14	0.14
(1,548)	1:264:A:CYS:HA	1:266:A:ASP:H	2	0.14
(1,543)	1:259:A:ILE:HG21	1:261:A:TYR:H	4	0.14
(1,543)	1:259:A:ILE:HG22	1:261:A:TYR:H	4	0.14
(1,543)	1:259:A:ILE:HG23	1:261:A:TYR:H	4	0.14
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE1	1	0.14
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE2	1	0.14
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE1	2	0.14
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE2	2	0.14
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE1	10	0.14
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE2	10	0.14
(1,466)	1:282:A:ILE:HG21	1:284:A:SER:H	19	0.14
(1,466)	1:282:A:ILE:HG22	1:284:A:SER:H	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,466)	1:282:A:ILE:HG23	1:284:A:SER:H	19	0.14
(1,343)	1:317:A:ARG:H	1:317:A:ARG:HD3	1	0.14
(1,342)	1:317:A:ARG:H	1:317:A:ARG:HD2	16	0.14
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	1	0.14
(1,218)	1:261:A:TYR:H	1:272:A:PHE:H	12	0.14
(1,1405)	1:278:A:LEU:HD11	1:282:A:ILE:H	14	0.13
(1,1405)	1:278:A:LEU:HD12	1:282:A:ILE:H	14	0.13
(1,1405)	1:278:A:LEU:HD13	1:282:A:ILE:H	14	0.13
(1,1405)	1:278:A:LEU:HD21	1:282:A:ILE:H	14	0.13
(1,1405)	1:278:A:LEU:HD22	1:282:A:ILE:H	14	0.13
(1,1405)	1:278:A:LEU:HD23	1:282:A:ILE:H	14	0.13
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	4	0.13
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	4	0.13
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	16	0.13
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	16	0.13
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD1	8	0.13
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD2	8	0.13
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD1	8	0.13
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD2	8	0.13
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD1	8	0.13
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD2	8	0.13
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD1	19	0.13
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD2	19	0.13
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD1	19	0.13
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD2	19	0.13
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD1	19	0.13
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD2	19	0.13
(1,1150)	1:352:A:HIS:HA	1:354:A:SER:HB2	4	0.13
(1,1150)	1:352:A:HIS:HA	1:354:A:SER:HB3	4	0.13
(1,1110)	1:326:A:LYS:HA	1:326:A:LYS:HD2	2	0.13
(1,1110)	1:326:A:LYS:HA	1:326:A:LYS:HD3	2	0.13
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD2	14	0.13
(1,1010)	1:282:A:ILE:HG21	1:283:A:ARG:HD3	14	0.13
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD2	14	0.13
(1,1010)	1:282:A:ILE:HG22	1:283:A:ARG:HD3	14	0.13
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD2	14	0.13
(1,1010)	1:282:A:ILE:HG23	1:283:A:ARG:HD3	14	0.13
(1,939)	1:325:A:ASP:HB2	1:327:A:PRO:HD3	1	0.13
(1,939)	1:325:A:ASP:HB3	1:327:A:PRO:HD3	1	0.13
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	7	0.13
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	7	0.13
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,762)	1:306:A:ASN:H	1:306:A:ASN:HD22	13	0.13
(1,762)	1:306:A:ASN:H	1:306:A:ASN:HD22	14	0.13
(1,754)	1:314:A:TRP:HA	1:314:A:TRP:HE1	14	0.13
(1,702)	1:324:A:GLY:HA2	1:326:A:LYS:H	13	0.13
(1,702)	1:324:A:GLY:HA3	1:326:A:LYS:H	13	0.13
(1,702)	1:324:A:GLY:HA2	1:326:A:LYS:H	18	0.13
(1,702)	1:324:A:GLY:HA3	1:326:A:LYS:H	18	0.13
(1,618)	1:295:A:PHE:H	1:310:A:THR:HB	12	0.13
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD11	1	0.13
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD12	1	0.13
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD13	1	0.13
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD11	20	0.13
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD12	20	0.13
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD13	20	0.13
(1,549)	1:266:A:ASP:H	1:268:A:CYS:HB3	13	0.13
(1,545)	1:272:A:PHE:H	1:278:A:LEU:HG	2	0.13
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE1	3	0.13
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE2	3	0.13
(1,261)	1:331:A:VAL:H	1:331:A:VAL:HB	14	0.13
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	12	0.13
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	15	0.13
(1,253)	1:315:A:LEU:H	1:315:A:LEU:HG	17	0.13
(1,1464)	1:294:A:VAL:H	1:296:A:VAL:HG11	9	0.12
(1,1464)	1:294:A:VAL:H	1:296:A:VAL:HG12	9	0.12
(1,1464)	1:294:A:VAL:H	1:296:A:VAL:HG13	9	0.12
(1,1464)	1:294:A:VAL:H	1:296:A:VAL:HG21	9	0.12
(1,1464)	1:294:A:VAL:H	1:296:A:VAL:HG22	9	0.12
(1,1464)	1:294:A:VAL:H	1:296:A:VAL:HG23	9	0.12
(1,1405)	1:278:A:LEU:HD11	1:282:A:ILE:H	5	0.12
(1,1405)	1:278:A:LEU:HD12	1:282:A:ILE:H	5	0.12
(1,1405)	1:278:A:LEU:HD13	1:282:A:ILE:H	5	0.12
(1,1405)	1:278:A:LEU:HD21	1:282:A:ILE:H	5	0.12
(1,1405)	1:278:A:LEU:HD22	1:282:A:ILE:H	5	0.12
(1,1405)	1:278:A:LEU:HD23	1:282:A:ILE:H	5	0.12
(1,1405)	1:278:A:LEU:HD11	1:282:A:ILE:H	9	0.12
(1,1405)	1:278:A:LEU:HD12	1:282:A:ILE:H	9	0.12
(1,1405)	1:278:A:LEU:HD13	1:282:A:ILE:H	9	0.12
(1,1405)	1:278:A:LEU:HD21	1:282:A:ILE:H	9	0.12
(1,1405)	1:278:A:LEU:HD22	1:282:A:ILE:H	9	0.12
(1,1405)	1:278:A:LEU:HD23	1:282:A:ILE:H	9	0.12
(1,1405)	1:278:A:LEU:HD11	1:282:A:ILE:H	12	0.12
(1,1405)	1:278:A:LEU:HD12	1:282:A:ILE:H	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1405)	1:278:A:LEU:HD13	1:282:A:ILE:H	12	0.12
(1,1405)	1:278:A:LEU:HD21	1:282:A:ILE:H	12	0.12
(1,1405)	1:278:A:LEU:HD22	1:282:A:ILE:H	12	0.12
(1,1405)	1:278:A:LEU:HD23	1:282:A:ILE:H	12	0.12
(1,1405)	1:278:A:LEU:HD11	1:282:A:ILE:H	19	0.12
(1,1405)	1:278:A:LEU:HD12	1:282:A:ILE:H	19	0.12
(1,1405)	1:278:A:LEU:HD13	1:282:A:ILE:H	19	0.12
(1,1405)	1:278:A:LEU:HD21	1:282:A:ILE:H	19	0.12
(1,1405)	1:278:A:LEU:HD22	1:282:A:ILE:H	19	0.12
(1,1405)	1:278:A:LEU:HD23	1:282:A:ILE:H	19	0.12
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	6	0.12
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	6	0.12
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	14	0.12
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	14	0.12
(1,1348)	1:256:A:HIS:HB2	1:258:A:ASN:HB2	19	0.12
(1,1348)	1:256:A:HIS:HB2	1:258:A:ASN:HB3	19	0.12
(1,1348)	1:256:A:HIS:HB3	1:258:A:ASN:HB2	19	0.12
(1,1348)	1:256:A:HIS:HB3	1:258:A:ASN:HB3	19	0.12
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD1	1	0.12
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD2	1	0.12
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD1	1	0.12
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD2	1	0.12
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD1	1	0.12
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD2	1	0.12
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD1	4	0.12
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD2	4	0.12
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD1	4	0.12
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD2	4	0.12
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD1	4	0.12
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD2	4	0.12
(1,1230)	1:280:A:ASP:HA	1:284:A:SER:HB2	7	0.12
(1,1230)	1:280:A:ASP:HA	1:284:A:SER:HB3	7	0.12
(1,1230)	1:280:A:ASP:HA	1:284:A:SER:HB2	10	0.12
(1,1230)	1:280:A:ASP:HA	1:284:A:SER:HB3	10	0.12
(1,1213)	1:305:A:TYR:HD1	1:306:A:ASN:HD22	5	0.12
(1,1213)	1:305:A:TYR:HD2	1:306:A:ASN:HD22	5	0.12
(1,1213)	1:305:A:TYR:HD1	1:306:A:ASN:HD22	10	0.12
(1,1213)	1:305:A:TYR:HD2	1:306:A:ASN:HD22	10	0.12
(1,1195)	1:300:A:LYS:H	1:305:A:TYR:HD1	10	0.12
(1,1195)	1:300:A:LYS:H	1:305:A:TYR:HD2	10	0.12
(1,1177)	1:310:A:THR:HA	1:353:A:PHE:HE1	20	0.12
(1,1177)	1:310:A:THR:HA	1:353:A:PHE:HE2	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE1	10	0.12
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE2	10	0.12
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE1	20	0.12
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE2	20	0.12
(1,1110)	1:326:A:LYS:HA	1:326:A:LYS:HD2	18	0.12
(1,1110)	1:326:A:LYS:HA	1:326:A:LYS:HD3	18	0.12
(1,939)	1:325:A:ASP:HB2	1:327:A:PRO:HD3	7	0.12
(1,939)	1:325:A:ASP:HB3	1:327:A:PRO:HD3	7	0.12
(1,849)	1:266:A:ASP:HA	1:298:A:LEU:HG	6	0.12
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD11	3	0.12
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD12	3	0.12
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD13	3	0.12
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD11	4	0.12
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD12	4	0.12
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD13	4	0.12
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD11	15	0.12
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD12	15	0.12
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD13	15	0.12
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD11	19	0.12
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD12	19	0.12
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD13	19	0.12
(1,818)	1:326:A:LYS:HD2	1:327:A:PRO:HD2	14	0.12
(1,818)	1:326:A:LYS:HD3	1:327:A:PRO:HD2	14	0.12
(1,818)	1:326:A:LYS:HD2	1:327:A:PRO:HD2	20	0.12
(1,818)	1:326:A:LYS:HD3	1:327:A:PRO:HD2	20	0.12
(1,817)	1:262:A:ASN:HA	1:271:A:CYS:HB2	7	0.12
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	16	0.12
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	16	0.12
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	16	0.12
(1,762)	1:306:A:ASN:H	1:306:A:ASN:HD22	12	0.12
(1,762)	1:306:A:ASN:H	1:306:A:ASN:HD22	17	0.12
(1,762)	1:306:A:ASN:H	1:306:A:ASN:HD22	18	0.12
(1,757)	1:264:A:CYS:HA	1:299:A:TRP:HE1	8	0.12
(1,736)	1:349:A:VAL:HG21	1:351:A:THR:H	4	0.12
(1,736)	1:349:A:VAL:HG22	1:351:A:THR:H	4	0.12
(1,736)	1:349:A:VAL:HG23	1:351:A:THR:H	4	0.12
(1,736)	1:349:A:VAL:HG21	1:351:A:THR:H	16	0.12
(1,736)	1:349:A:VAL:HG22	1:351:A:THR:H	16	0.12
(1,736)	1:349:A:VAL:HG23	1:351:A:THR:H	16	0.12
(1,736)	1:349:A:VAL:HG21	1:351:A:THR:H	17	0.12
(1,736)	1:349:A:VAL:HG22	1:351:A:THR:H	17	0.12
(1,736)	1:349:A:VAL:HG23	1:351:A:THR:H	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	1	0.12
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	7	0.12
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	12	0.12
(1,721)	1:332:A:VAL:HB	1:336:A:ASN:H	19	0.12
(1,618)	1:295:A:PHE:H	1:310:A:THR:HB	15	0.12
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD11	12	0.12
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD12	12	0.12
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD13	12	0.12
(1,612)	1:294:A:VAL:H	1:308:A:PRO:HB2	8	0.12
(1,612)	1:294:A:VAL:H	1:308:A:PRO:HB2	20	0.12
(1,593)	1:283:A:ARG:HD2	1:287:A:VAL:H	20	0.12
(1,593)	1:283:A:ARG:HD3	1:287:A:VAL:H	20	0.12
(1,545)	1:272:A:PHE:H	1:278:A:LEU:HG	14	0.12
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE1	14	0.12
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE2	14	0.12
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE1	15	0.12
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE2	15	0.12
(1,466)	1:282:A:ILE:HG21	1:284:A:SER:H	4	0.12
(1,466)	1:282:A:ILE:HG22	1:284:A:SER:H	4	0.12
(1,466)	1:282:A:ILE:HG23	1:284:A:SER:H	4	0.12
(1,466)	1:282:A:ILE:HG21	1:284:A:SER:H	12	0.12
(1,466)	1:282:A:ILE:HG22	1:284:A:SER:H	12	0.12
(1,466)	1:282:A:ILE:HG23	1:284:A:SER:H	12	0.12
(1,466)	1:282:A:ILE:HG21	1:284:A:SER:H	16	0.12
(1,466)	1:282:A:ILE:HG22	1:284:A:SER:H	16	0.12
(1,466)	1:282:A:ILE:HG23	1:284:A:SER:H	16	0.12
(1,443)	1:338:A:SER:H	1:339:A:PHE:HE1	3	0.12
(1,443)	1:338:A:SER:H	1:339:A:PHE:HE2	3	0.12
(1,261)	1:331:A:VAL:H	1:331:A:VAL:HB	2	0.12
(1,261)	1:331:A:VAL:H	1:331:A:VAL:HB	3	0.12
(1,261)	1:331:A:VAL:H	1:331:A:VAL:HB	18	0.12
(1,84)	1:306:A:ASN:H	1:306:A:ASN:HD21	2	0.12
(1,1608)	1:341:A:SER:HB2	1:342:A:GLN:H	19	0.11
(1,1608)	1:341:A:SER:HB3	1:342:A:GLN:H	19	0.11
(1,1588)	1:329:A:LYS:HG2	1:338:A:SER:H	11	0.11
(1,1588)	1:329:A:LYS:HG3	1:338:A:SER:H	11	0.11
(1,1567)	1:326:A:LYS:H	1:326:A:LYS:HG2	20	0.11
(1,1567)	1:326:A:LYS:H	1:326:A:LYS:HG3	20	0.11
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD11	15	0.11
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD12	15	0.11
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD13	15	0.11
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD21	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD22	15	0.11
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD23	15	0.11
(1,1405)	1:278:A:LEU:HD11	1:282:A:ILE:H	1	0.11
(1,1405)	1:278:A:LEU:HD12	1:282:A:ILE:H	1	0.11
(1,1405)	1:278:A:LEU:HD13	1:282:A:ILE:H	1	0.11
(1,1405)	1:278:A:LEU:HD21	1:282:A:ILE:H	1	0.11
(1,1405)	1:278:A:LEU:HD22	1:282:A:ILE:H	1	0.11
(1,1405)	1:278:A:LEU:HD23	1:282:A:ILE:H	1	0.11
(1,1405)	1:278:A:LEU:HD11	1:282:A:ILE:H	2	0.11
(1,1405)	1:278:A:LEU:HD12	1:282:A:ILE:H	2	0.11
(1,1405)	1:278:A:LEU:HD13	1:282:A:ILE:H	2	0.11
(1,1405)	1:278:A:LEU:HD21	1:282:A:ILE:H	2	0.11
(1,1405)	1:278:A:LEU:HD22	1:282:A:ILE:H	2	0.11
(1,1405)	1:278:A:LEU:HD23	1:282:A:ILE:H	2	0.11
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	7	0.11
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	7	0.11
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE21	20	0.11
(1,1377)	1:266:A:ASP:H	1:267:A:GLN:HE22	20	0.11
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD1	3	0.11
(1,1323)	1:304:A:VAL:HG21	1:305:A:TYR:HD2	3	0.11
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD1	3	0.11
(1,1323)	1:304:A:VAL:HG22	1:305:A:TYR:HD2	3	0.11
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD1	3	0.11
(1,1323)	1:304:A:VAL:HG23	1:305:A:TYR:HD2	3	0.11
(1,1228)	1:348:A:HIS:HA	1:351:A:THR:H	9	0.11
(1,1228)	1:348:A:HIS:HA	1:351:A:THR:H	18	0.11
(1,1177)	1:310:A:THR:HA	1:353:A:PHE:HE1	11	0.11
(1,1177)	1:310:A:THR:HA	1:353:A:PHE:HE2	11	0.11
(1,1176)	1:294:A:VAL:HA	1:353:A:PHE:HE1	15	0.11
(1,1176)	1:294:A:VAL:HA	1:353:A:PHE:HE2	15	0.11
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE1	3	0.11
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE2	3	0.11
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE1	5	0.11
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE2	5	0.11
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE1	8	0.11
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE2	8	0.11
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE1	17	0.11
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE2	17	0.11
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE1	19	0.11
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE2	19	0.11
(1,1110)	1:326:A:LYS:HA	1:326:A:LYS:HD2	9	0.11
(1,1110)	1:326:A:LYS:HA	1:326:A:LYS:HD3	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1110)	1:326:A:LYS:HA	1:326:A:LYS:HD2	12	0.11
(1,1110)	1:326:A:LYS:HA	1:326:A:LYS:HD3	12	0.11
(1,1110)	1:326:A:LYS:HA	1:326:A:LYS:HD2	15	0.11
(1,1110)	1:326:A:LYS:HA	1:326:A:LYS:HD3	15	0.11
(1,1107)	1:267:A:GLN:HA	1:267:A:GLN:HG3	12	0.11
(1,1087)	1:282:A:ILE:HD11	1:299:A:TRP:HZ2	20	0.11
(1,1087)	1:282:A:ILE:HD12	1:299:A:TRP:HZ2	20	0.11
(1,1087)	1:282:A:ILE:HD13	1:299:A:TRP:HZ2	20	0.11
(1,972)	1:350:A:PRO:HD3	1:351:A:THR:HG21	19	0.11
(1,972)	1:350:A:PRO:HD3	1:351:A:THR:HG22	19	0.11
(1,972)	1:350:A:PRO:HD3	1:351:A:THR:HG23	19	0.11
(1,849)	1:266:A:ASP:HA	1:298:A:LEU:HG	15	0.11
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD11	1	0.11
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD12	1	0.11
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD13	1	0.11
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD11	16	0.11
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD12	16	0.11
(1,823)	1:284:A:SER:HA	1:285:A:ILE:HD13	16	0.11
(1,813)	1:326:A:LYS:HD2	1:327:A:PRO:HD3	10	0.11
(1,813)	1:326:A:LYS:HD3	1:327:A:PRO:HD3	10	0.11
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	9	0.11
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	9	0.11
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	9	0.11
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB1	11	0.11
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB2	11	0.11
(1,797)	1:268:A:CYS:H	1:270:A:ALA:HB3	11	0.11
(1,789)	1:290:A:GLN:HA	1:290:A:GLN:HE22	9	0.11
(1,762)	1:306:A:ASN:H	1:306:A:ASN:HD22	4	0.11
(1,762)	1:306:A:ASN:H	1:306:A:ASN:HD22	6	0.11
(1,762)	1:306:A:ASN:H	1:306:A:ASN:HD22	7	0.11
(1,762)	1:306:A:ASN:H	1:306:A:ASN:HD22	15	0.11
(1,762)	1:306:A:ASN:H	1:306:A:ASN:HD22	16	0.11
(1,762)	1:306:A:ASN:H	1:306:A:ASN:HD22	19	0.11
(1,762)	1:306:A:ASN:H	1:306:A:ASN:HD22	20	0.11
(1,757)	1:264:A:CYS:HA	1:299:A:TRP:HE1	1	0.11
(1,757)	1:264:A:CYS:HA	1:299:A:TRP:HE1	3	0.11
(1,757)	1:264:A:CYS:HA	1:299:A:TRP:HE1	7	0.11
(1,736)	1:349:A:VAL:HG21	1:351:A:THR:H	8	0.11
(1,736)	1:349:A:VAL:HG22	1:351:A:THR:H	8	0.11
(1,736)	1:349:A:VAL:HG23	1:351:A:THR:H	8	0.11
(1,736)	1:349:A:VAL:HG21	1:351:A:THR:H	10	0.11
(1,736)	1:349:A:VAL:HG22	1:351:A:THR:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:349:A:VAL:HG23	1:351:A:THR:H	10	0.11
(1,736)	1:349:A:VAL:HG21	1:351:A:THR:H	15	0.11
(1,736)	1:349:A:VAL:HG22	1:351:A:THR:H	15	0.11
(1,736)	1:349:A:VAL:HG23	1:351:A:THR:H	15	0.11
(1,736)	1:349:A:VAL:HG21	1:351:A:THR:H	18	0.11
(1,736)	1:349:A:VAL:HG22	1:351:A:THR:H	18	0.11
(1,736)	1:349:A:VAL:HG23	1:351:A:THR:H	18	0.11
(1,736)	1:349:A:VAL:HG21	1:351:A:THR:H	19	0.11
(1,736)	1:349:A:VAL:HG22	1:351:A:THR:H	19	0.11
(1,736)	1:349:A:VAL:HG23	1:351:A:THR:H	19	0.11
(1,702)	1:324:A:GLY:HA2	1:326:A:LYS:H	6	0.11
(1,702)	1:324:A:GLY:HA3	1:326:A:LYS:H	6	0.11
(1,702)	1:324:A:GLY:HA2	1:326:A:LYS:H	8	0.11
(1,702)	1:324:A:GLY:HA3	1:326:A:LYS:H	8	0.11
(1,618)	1:295:A:PHE:H	1:310:A:THR:HB	9	0.11
(1,618)	1:295:A:PHE:H	1:310:A:THR:HB	10	0.11
(1,618)	1:295:A:PHE:H	1:310:A:THR:HB	19	0.11
(1,618)	1:295:A:PHE:H	1:310:A:THR:HB	20	0.11
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD11	17	0.11
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD12	17	0.11
(1,617)	1:295:A:PHE:H	1:315:A:LEU:HD13	17	0.11
(1,612)	1:294:A:VAL:H	1:308:A:PRO:HB2	18	0.11
(1,562)	1:275:A:SER:H	1:276:A:PRO:HB3	3	0.11
(1,562)	1:275:A:SER:H	1:276:A:PRO:HB3	13	0.11
(1,562)	1:275:A:SER:H	1:276:A:PRO:HB3	19	0.11
(1,553)	1:270:A:ALA:H	1:272:A:PHE:HE1	18	0.11
(1,553)	1:270:A:ALA:H	1:272:A:PHE:HE2	18	0.11
(1,553)	1:270:A:ALA:H	1:272:A:PHE:HE1	20	0.11
(1,553)	1:270:A:ALA:H	1:272:A:PHE:HE2	20	0.11
(1,549)	1:266:A:ASP:H	1:268:A:CYS:HB3	5	0.11
(1,545)	1:272:A:PHE:H	1:278:A:LEU:HG	12	0.11
(1,545)	1:272:A:PHE:H	1:278:A:LEU:HG	19	0.11
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE1	7	0.11
(1,541)	1:260:A:ALA:H	1:261:A:TYR:HE2	7	0.11
(1,466)	1:282:A:ILE:HG21	1:284:A:SER:H	10	0.11
(1,466)	1:282:A:ILE:HG22	1:284:A:SER:H	10	0.11
(1,466)	1:282:A:ILE:HG23	1:284:A:SER:H	10	0.11
(1,466)	1:282:A:ILE:HG21	1:284:A:SER:H	18	0.11
(1,466)	1:282:A:ILE:HG22	1:284:A:SER:H	18	0.11
(1,466)	1:282:A:ILE:HG23	1:284:A:SER:H	18	0.11
(1,261)	1:331:A:VAL:H	1:331:A:VAL:HB	11	0.11
(1,233)	1:260:A:ALA:HA	1:262:A:ASN:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,198)	1:259:A:ILE:H	1:259:A:ILE:HG21	14	0.11
(1,198)	1:259:A:ILE:H	1:259:A:ILE:HG22	14	0.11
(1,198)	1:259:A:ILE:H	1:259:A:ILE:HG23	14	0.11
(1,169)	1:355:A:GLN:HA	1:356:A:GLN:H	16	0.11
(1,20)	1:266:A:ASP:H	1:267:A:GLN:H	19	0.11
(1,1588)	1:329:A:LYS:HG2	1:338:A:SER:H	20	0.1
(1,1588)	1:329:A:LYS:HG3	1:338:A:SER:H	20	0.1
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD11	12	0.1
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD12	12	0.1
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD13	12	0.1
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD21	12	0.1
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD22	12	0.1
(1,1442)	1:290:A:GLN:H	1:315:A:LEU:HD23	12	0.1
(1,1268)	1:328:A:PHE:HB2	1:342:A:GLN:HA	18	0.1
(1,1243)	1:285:A:ILE:HA	1:289:A:GLY:HA2	10	0.1
(1,1228)	1:348:A:HIS:HA	1:351:A:THR:H	14	0.1
(1,1228)	1:348:A:HIS:HA	1:351:A:THR:H	17	0.1
(1,1195)	1:300:A:LYS:H	1:305:A:TYR:HD1	4	0.1
(1,1195)	1:300:A:LYS:H	1:305:A:TYR:HD2	4	0.1
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE1	2	0.1
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE2	2	0.1
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE1	15	0.1
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE2	15	0.1
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE1	16	0.1
(1,1164)	1:305:A:TYR:HA	1:305:A:TYR:HE2	16	0.1
(1,1110)	1:326:A:LYS:HA	1:326:A:LYS:HD2	17	0.1
(1,1110)	1:326:A:LYS:HA	1:326:A:LYS:HD3	17	0.1
(1,1043)	1:346:A:ALA:HB1	1:347:A:ARG:HD2	20	0.1
(1,1043)	1:346:A:ALA:HB1	1:347:A:ARG:HD3	20	0.1
(1,1043)	1:346:A:ALA:HB2	1:347:A:ARG:HD2	20	0.1
(1,1043)	1:346:A:ALA:HB2	1:347:A:ARG:HD3	20	0.1
(1,1043)	1:346:A:ALA:HB3	1:347:A:ARG:HD2	20	0.1
(1,1043)	1:346:A:ALA:HB3	1:347:A:ARG:HD3	20	0.1
(1,987)	1:268:A:CYS:HB3	1:270:A:ALA:HB1	5	0.1
(1,987)	1:268:A:CYS:HB3	1:270:A:ALA:HB2	5	0.1
(1,987)	1:268:A:CYS:HB3	1:270:A:ALA:HB3	5	0.1
(1,972)	1:350:A:PRO:HD3	1:351:A:THR:HG21	1	0.1
(1,972)	1:350:A:PRO:HD3	1:351:A:THR:HG22	1	0.1
(1,972)	1:350:A:PRO:HD3	1:351:A:THR:HG23	1	0.1
(1,936)	1:300:A:LYS:HA	1:300:A:LYS:HE2	5	0.1
(1,936)	1:300:A:LYS:HA	1:300:A:LYS:HE3	5	0.1
(1,936)	1:300:A:LYS:HA	1:300:A:LYS:HE2	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,936)	1:300:A:LYS:HA	1:300:A:LYS:HE3	10	0.1
(1,925)	1:303:A:LYS:HA	1:303:A:LYS:HE2	7	0.1
(1,925)	1:303:A:LYS:HA	1:303:A:LYS:HE3	7	0.1
(1,925)	1:303:A:LYS:HA	1:303:A:LYS:HE2	9	0.1
(1,925)	1:303:A:LYS:HA	1:303:A:LYS:HE3	9	0.1
(1,925)	1:303:A:LYS:HA	1:303:A:LYS:HE2	16	0.1
(1,925)	1:303:A:LYS:HA	1:303:A:LYS:HE3	16	0.1
(1,915)	1:302:A:CYS:HB2	1:303:A:LYS:HE2	15	0.1
(1,915)	1:302:A:CYS:HB2	1:303:A:LYS:HE3	15	0.1
(1,915)	1:302:A:CYS:HB3	1:303:A:LYS:HE2	15	0.1
(1,915)	1:302:A:CYS:HB3	1:303:A:LYS:HE3	15	0.1
(1,849)	1:266:A:ASP:HA	1:298:A:LEU:HG	11	0.1
(1,818)	1:326:A:LYS:HD2	1:327:A:PRO:HD2	8	0.1
(1,818)	1:326:A:LYS:HD3	1:327:A:PRO:HD2	8	0.1
(1,762)	1:306:A:ASN:H	1:306:A:ASN:HD22	3	0.1
(1,757)	1:264:A:CYS:HA	1:299:A:TRP:HE1	16	0.1
(1,757)	1:264:A:CYS:HA	1:299:A:TRP:HE1	18	0.1
(1,736)	1:349:A:VAL:HG21	1:351:A:THR:H	1	0.1
(1,736)	1:349:A:VAL:HG22	1:351:A:THR:H	1	0.1
(1,736)	1:349:A:VAL:HG23	1:351:A:THR:H	1	0.1
(1,736)	1:349:A:VAL:HG21	1:351:A:THR:H	7	0.1
(1,736)	1:349:A:VAL:HG22	1:351:A:THR:H	7	0.1
(1,736)	1:349:A:VAL:HG23	1:351:A:THR:H	7	0.1
(1,736)	1:349:A:VAL:HG21	1:351:A:THR:H	13	0.1
(1,736)	1:349:A:VAL:HG22	1:351:A:THR:H	13	0.1
(1,736)	1:349:A:VAL:HG23	1:351:A:THR:H	13	0.1
(1,702)	1:324:A:GLY:HA2	1:326:A:LYS:H	3	0.1
(1,702)	1:324:A:GLY:HA3	1:326:A:LYS:H	3	0.1
(1,643)	1:303:A:LYS:HG2	1:305:A:TYR:H	8	0.1
(1,643)	1:303:A:LYS:HG3	1:305:A:TYR:H	8	0.1
(1,618)	1:295:A:PHE:H	1:310:A:THR:HB	7	0.1
(1,618)	1:295:A:PHE:H	1:310:A:THR:HB	8	0.1
(1,618)	1:295:A:PHE:H	1:310:A:THR:HB	18	0.1
(1,562)	1:275:A:SER:H	1:276:A:PRO:HB3	7	0.1
(1,562)	1:275:A:SER:H	1:276:A:PRO:HB3	9	0.1
(1,549)	1:266:A:ASP:H	1:268:A:CYS:HB3	17	0.1
(1,545)	1:272:A:PHE:H	1:278:A:LEU:HG	18	0.1
(1,443)	1:338:A:SER:H	1:339:A:PHE:HE1	17	0.1
(1,443)	1:338:A:SER:H	1:339:A:PHE:HE2	17	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found