



Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 12:02 AM UTC

PDB ID : 2LVQ / pdb_00002lvq
BMRB ID : 18584
Title : gp78CUE domain bound to the proximal ubiquitin of K48-linked diubiquitin
Authors : Liu, S.; Chen, Y.; Huang, T.; Tarasov, S.G.; King, A.; Li, J.; Weissman, A.M.;
Byrd, R.A.; Das, R.
Deposited on : 2012-07-09

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

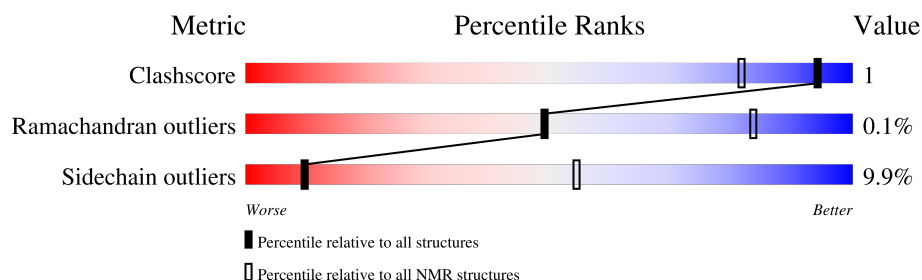
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 8%.

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	76	87% 7% 7%
1	B	76	87% 8% 5%
2	D	52	79% 8% 13%

2 Ensemble composition and analysis ⓘ

This entry contains 24 models. Model 21 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:1-A:71 (71)	0.34	13
2	B:1-B:72, D:455-D:499 (117)	0.63	21

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 4 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 9, 10, 11, 12, 13, 14, 15, 16
2	21, 22, 23, 24
3	17, 18, 19, 20
4	5, 6, 7, 8

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3298 atoms, of which 1675 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms						Trace
1	A	76	Total	C	H	N	O	S	0
			1231	378	629	105	118	1	
1	B	76	Total	C	H	N	O	S	0
			1231	378	629	105	118	1	

- Molecule 2 is a protein called E3 ubiquitin-protein ligase AMFR.

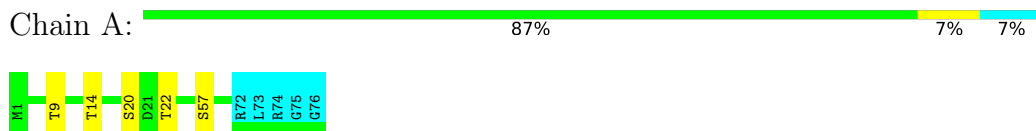
Mol	Chain	Residues	Atoms						Trace
2	D	52	Total	C	H	N	O	S	0
			836	264	417	72	81	2	

4 Residue-property plots

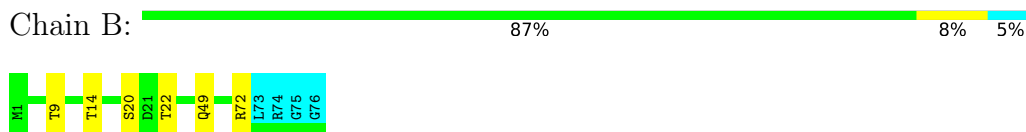
4.1 Average score per residue in the NMR ensemble

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.

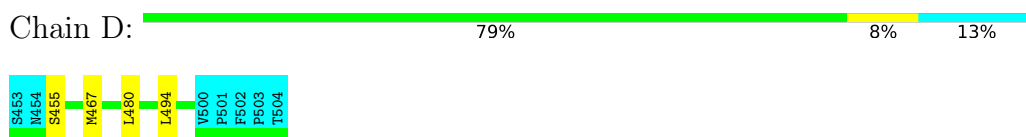
- Molecule 1: Ubiquitin



- Molecule 1: Ubiquitin



- Molecule 2: E3 ubiquitin-protein ligase AMFR

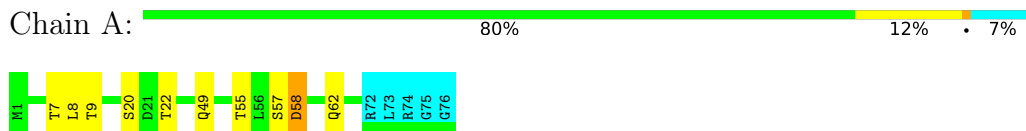


4.2 Scores per residue for each member of the ensemble

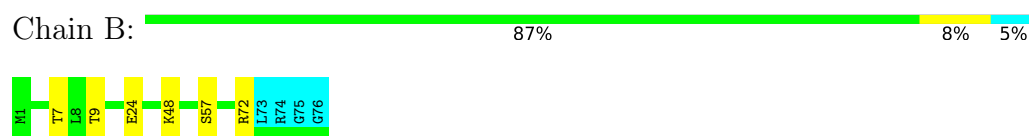
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

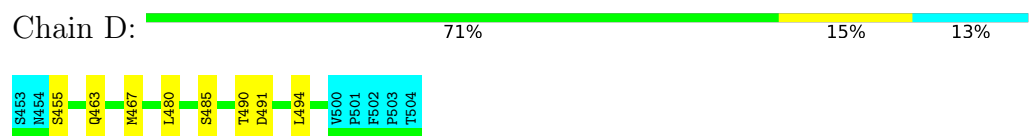
- Molecule 1: Ubiquitin



- Molecule 1: Ubiquitin

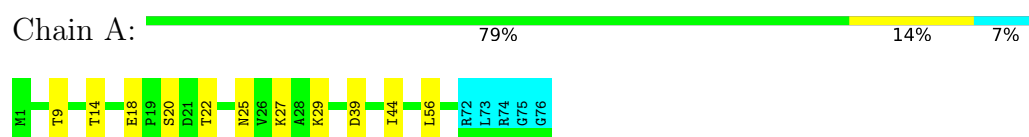


- Molecule 2: E3 ubiquitin-protein ligase AMFR

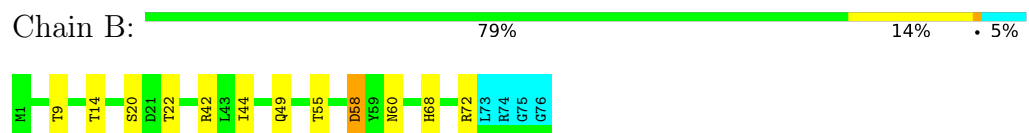


4.2.2 Score per residue for model 2

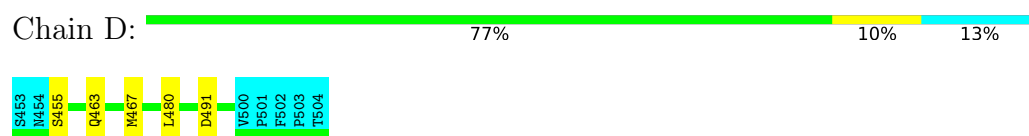
- Molecule 1: Ubiquitin



- Molecule 1: Ubiquitin

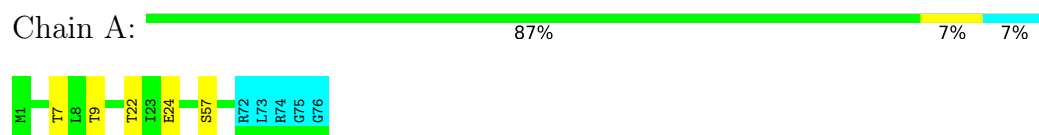


- Molecule 2: E3 ubiquitin-protein ligase AMFR



4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin



- Molecule 1: Ubiquitin

Chain B:  83% 12% 5%



- Molecule 2: E3 ubiquitin-protein ligase AMFR

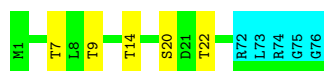
Chain D:  75% 12% 13%



4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin

Chain A:  87% 7% 7%



- Molecule 1: Ubiquitin

Chain B:  80% 12% 5%



- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain D:  73% 13% 13%



4.2.5 Score per residue for model 5

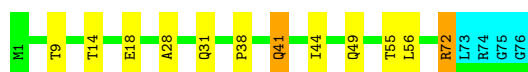
- Molecule 1: Ubiquitin

Chain A:  87% 7% 7%



- Molecule 1: Ubiquitin

Chain B:  79% 13% 5%

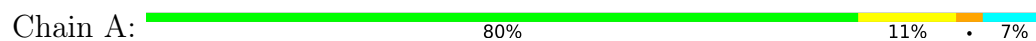


- Molecule 2: E3 ubiquitin-protein ligase AMFR

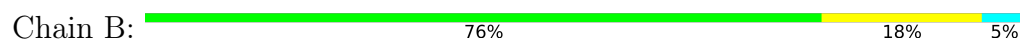


4.2.6 Score per residue for model 6

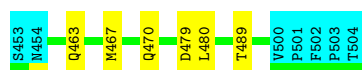
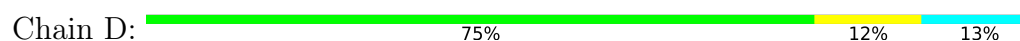
- Molecule 1: Ubiquitin



- Molecule 1: Ubiquitin

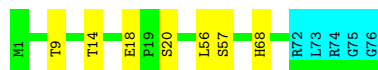
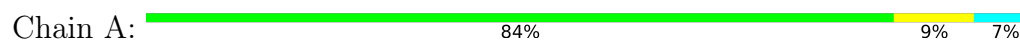


- Molecule 2: E3 ubiquitin-protein ligase AMFR

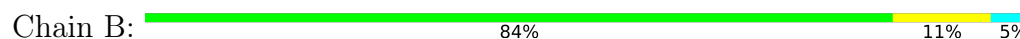


4.2.7 Score per residue for model 7

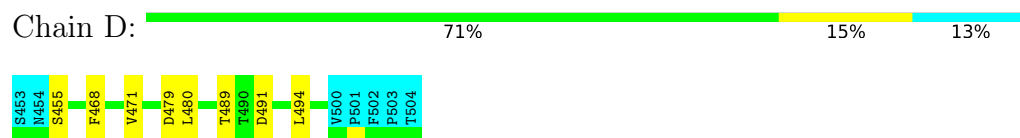
- Molecule 1: Ubiquitin



- Molecule 1: Ubiquitin

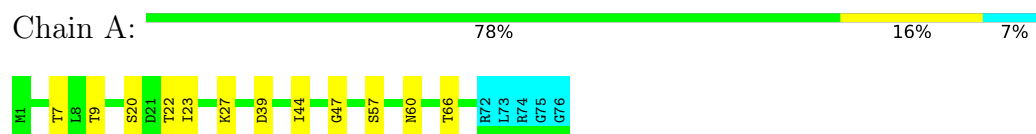


- Molecule 2: E3 ubiquitin-protein ligase AMFR

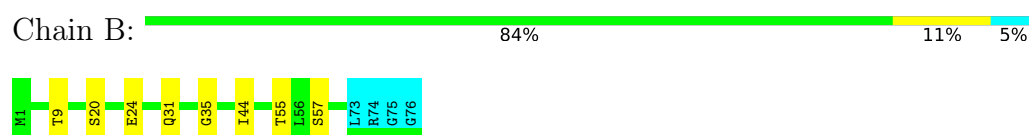


4.2.8 Score per residue for model 8

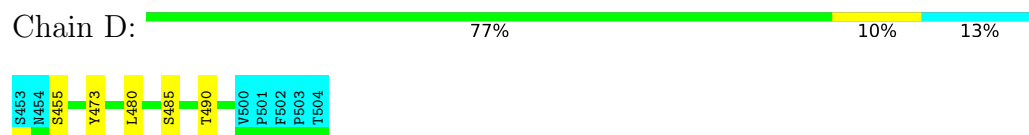
- Molecule 1: Ubiquitin



- Molecule 1: Ubiquitin

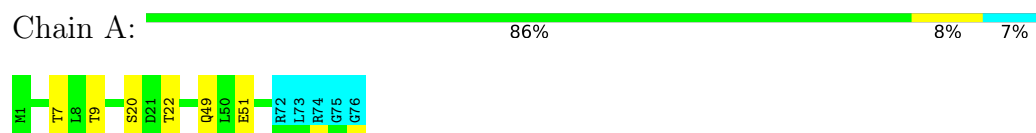


- Molecule 2: E3 ubiquitin-protein ligase AMFR

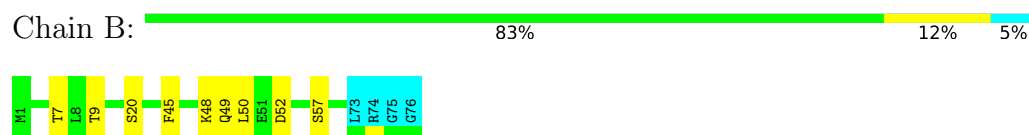


4.2.9 Score per residue for model 9

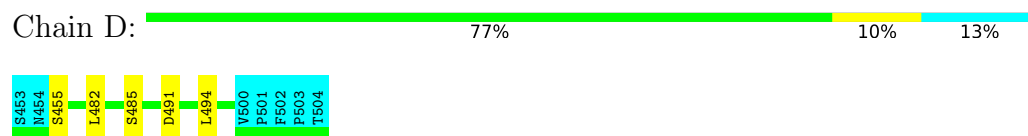
- Molecule 1: Ubiquitin



- Molecule 1: Ubiquitin

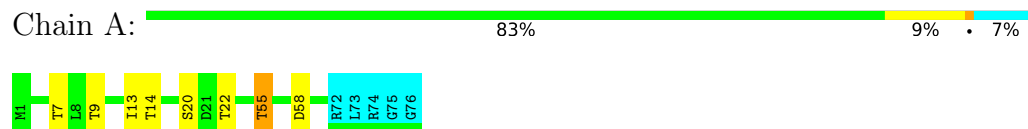


- Molecule 2: E3 ubiquitin-protein ligase AMFR

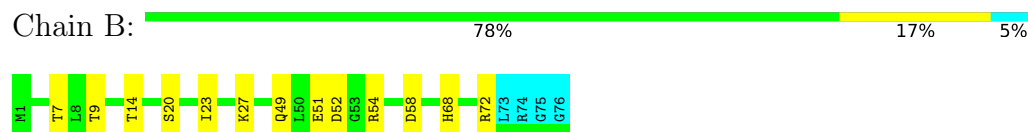


4.2.10 Score per residue for model 10

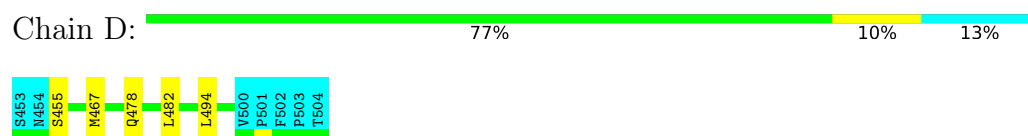
- Molecule 1: Ubiquitin



- Molecule 1: Ubiquitin

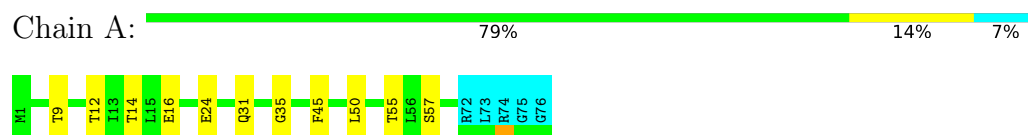


- Molecule 2: E3 ubiquitin-protein ligase AMFR

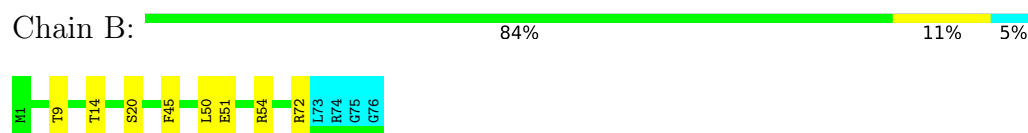


4.2.11 Score per residue for model 11

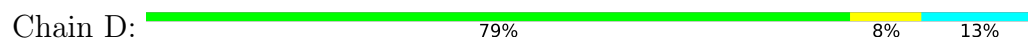
- Molecule 1: Ubiquitin



- Molecule 1: Ubiquitin



- Molecule 2: E3 ubiquitin-protein ligase AMFR





4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin

Chain A: 78% 12% 7%



- Molecule 1: Ubiquitin

Chain B: 82% 13% 5%



- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain D: 81% 6% 13%



4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin

Chain A: 83% 11% 7%



- Molecule 1: Ubiquitin

Chain B: 86% 9% 5%



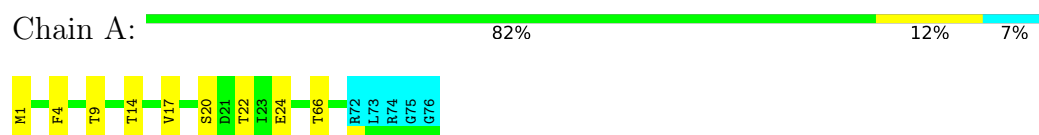
- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain D: 71% 15% 13%

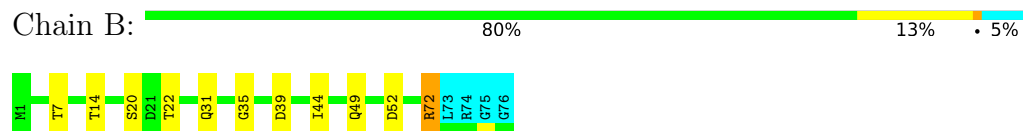


4.2.14 Score per residue for model 14

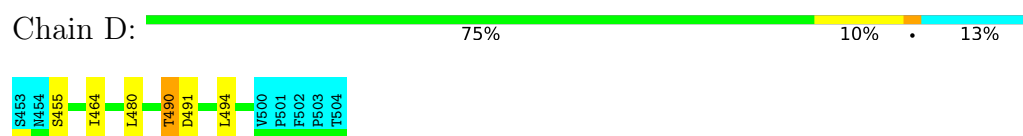
- Molecule 1: Ubiquitin



- Molecule 1: Ubiquitin

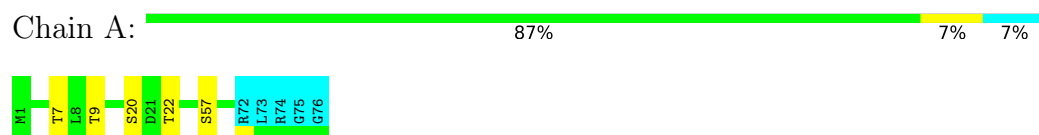


- Molecule 2: E3 ubiquitin-protein ligase AMFR

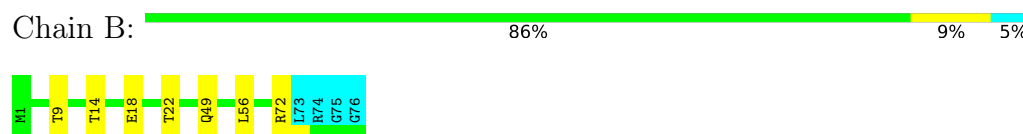


4.2.15 Score per residue for model 15

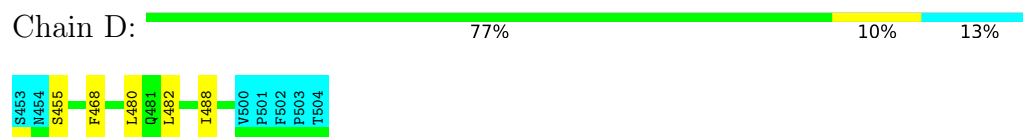
- Molecule 1: Ubiquitin



- Molecule 1: Ubiquitin



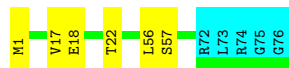
- Molecule 2: E3 ubiquitin-protein ligase AMFR



4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin

Chain A:  86% 8% 7%



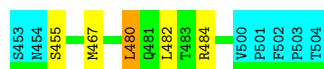
- Molecule 1: Ubiquitin

Chain B:  82% 12% 5%



- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain D:  77% 8% 13%



4.2.17 Score per residue for model 17

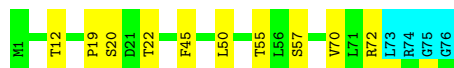
- Molecule 1: Ubiquitin

Chain A:  84% 9% 7%



- Molecule 1: Ubiquitin

Chain B:  82% 13% 5%



- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain D:  79% 6% 13%



4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin

Chain A:  86% 8% 7%



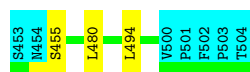
- Molecule 1: Ubiquitin

Chain B:  75% 18% 5%



- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain D:  81% 6% 13%



4.2.19 Score per residue for model 19

- Molecule 1: Ubiquitin

Chain A:  83% 11% 7%



- Molecule 1: Ubiquitin

Chain B:  83% 12% 5%



- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain D:  71% 15% 13%



4.2.20 Score per residue for model 20

- Molecule 1: Ubiquitin

Chain A:  88% 5% 7%



- Molecule 1: Ubiquitin

Chain B:  82% 13% 5%



- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain D:  77% 10% 13%



4.2.21 Score per residue for model 21 (medoid)

- Molecule 1: Ubiquitin

Chain A:  86% 8% 7%



- Molecule 1: Ubiquitin

Chain B:  80% 14% 5%



- Molecule 2: E3 ubiquitin-protein ligase AMFR

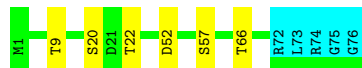
Chain D:  77% 10% 13%



4.2.22 Score per residue for model 22

- Molecule 1: Ubiquitin

Chain A:  86% 8% 7%



- Molecule 1: Ubiquitin

Chain B:  76% 18% 5%



- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain D:  73% 13% 13%



4.2.23 Score per residue for model 23

- Molecule 1: Ubiquitin

Chain A:  84% 9% 7%



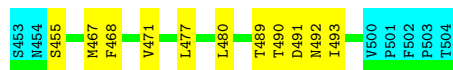
- Molecule 1: Ubiquitin

Chain B:  79% 16% 5%



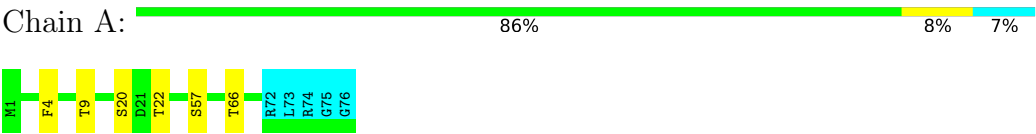
- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain D:  65% 21% 13%

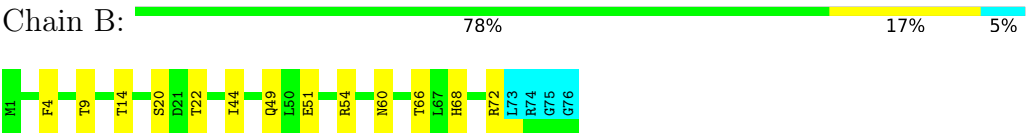


4.2.24 Score per residue for model 24

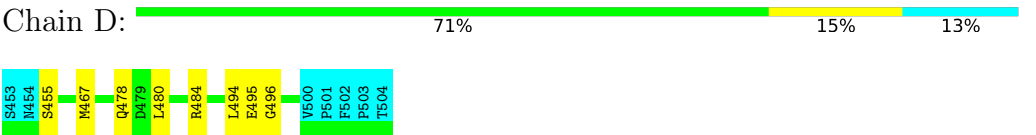
● Molecule 1: Ubiquitin



● Molecule 1: Ubiquitin



● Molecule 2: E3 ubiquitin-protein ligase AMFR



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 24 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	structure solution	
CNS	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	2
Total number of shifts	222
Number of shifts mapped to atoms	222
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	8%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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	563	586	586	1±1
1	B	574	599	599	2±1
2	D	365	365	365	1±1
All	All	36048	37200	37200	90

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:70:VAL:HG13	2:D:490:THR:HB	0.67	1.67	17	1
1:B:1:MET:SD	1:B:63:LYS:HA	0.64	2.32	6	1
1:B:45:PHE:HB3	1:B:50:LEU:HD21	0.56	1.75	20	5
1:A:55:THR:O	1:A:58:ASP:HB2	0.53	2.03	10	4
1:B:38:PRO:HA	1:B:41:GLN:CD	0.51	2.31	5	1
1:B:68:HIS:CD2	2:D:467:MET:HA	0.50	2.41	3	11
1:A:23:ILE:O	1:A:27:LYS:HG2	0.50	2.07	8	2
1:B:72:ARG:HB2	2:D:491:ASP:OD1	0.49	2.07	7	2
1:B:1:MET:HG2	1:B:17:VAL:O	0.49	2.08	22	2
1:A:4:PHE:O	1:A:66:THR:HA	0.47	2.09	14	2
1:A:18:GLU:O	1:A:56:LEU:HD12	0.47	2.10	13	4
1:B:18:GLU:O	1:B:21:ASP:HB2	0.47	2.10	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:468:PHE:O	2:D:471:VAL:HG12	0.47	2.09	5	4
2:D:479:ASP:HB3	2:D:489:THR:HG23	0.47	1.86	6	2
1:B:55:THR:O	1:B:58:ASP:HB2	0.46	2.11	18	5
1:B:18:GLU:O	1:B:56:LEU:HD12	0.46	2.11	5	5
2:D:463:GLN:O	2:D:467:MET:HG2	0.46	2.11	5	3
1:B:72:ARG:HA	2:D:491:ASP:CG	0.46	2.36	4	1
1:B:72:ARG:HE	2:D:491:ASP:CG	0.45	2.19	5	1
1:A:18:GLU:O	1:A:21:ASP:HB2	0.45	2.10	6	3
2:D:480:LEU:O	2:D:484:ARG:HG3	0.45	2.11	16	1
2:D:491:ASP:O	2:D:495:GLU:HG2	0.45	2.11	17	1
1:B:72:ARG:HG3	2:D:491:ASP:OD1	0.45	2.12	1	1
2:D:489:THR:O	2:D:493:ILE:HG13	0.44	2.12	22	2
1:B:31:GLN:O	1:B:35:GLY:HA2	0.44	2.12	8	5
1:A:1:MET:HG2	1:A:17:VAL:O	0.44	2.11	16	3
1:B:44:ILE:HG21	2:D:468:PHE:CZ	0.44	2.48	20	1
1:B:23:ILE:O	1:B:27:LYS:HG2	0.44	2.13	10	1
1:A:25:ASN:O	1:A:29:LYS:HG3	0.43	2.13	2	1
1:B:51:GLU:HB2	1:B:54:ARG:CG	0.43	2.44	24	2
1:A:51:GLU:HB2	1:A:54:ARG:CG	0.42	2.44	19	1
1:B:45:PHE:O	1:B:48:LYS:HE3	0.42	2.14	18	1
1:A:31:GLN:O	1:A:35:GLY:HA2	0.41	2.15	11	1
1:B:28:ALA:O	1:B:31:GLN:HG2	0.41	2.16	5	1
1:B:72:ARG:HG3	2:D:491:ASP:OD2	0.41	2.16	2	1
1:B:4:PHE:O	1:B:66:THR:HA	0.41	2.15	24	1
2:D:464:ILE:HG23	2:D:490:THR:HG23	0.41	1.93	14	1
1:A:22:THR:O	1:A:26:VAL:HG23	0.41	2.16	12	1
1:A:45:PHE:HB3	1:A:50:LEU:HD21	0.40	1.93	11	1
1:B:19:PRO:O	1:B:55:THR:HB	0.40	2.17	17	1
1:A:47:GLY:HA2	2:D:473:TYR:HB3	0.40	1.94	8	1
1:B:51:GLU:HB2	1:B:54:ARG:HG2	0.40	1.94	11	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	70/76 (92%)	68±1 (97±2%)	2±1 (3±2%)	0±0 (0±0%)	100	100
1	B	71/76 (93%)	70±1 (98±1%)	1±1 (2±1%)	0±0 (0±0%)	100	100
2	D	45/52 (87%)	43±2 (95±4%)	2±2 (5±4%)	0±0 (0±1%)	37	78
All	All	4464/4896 (91%)	4331 (97%)	130 (3%)	3 (0%)	49	83

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
2	D	496	GLY	3

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	65/68 (96%)	59±2 (91±3%)	6±2 (9±3%)	11	57
1	B	66/68 (97%)	59±2 (89±3%)	7±2 (11±3%)	8	52
2	D	42/49 (86%)	38±1 (90±3%)	4±1 (10±3%)	10	55
All	All	4152/4440 (94%)	3743 (90%)	409 (10%)	10	54

All 72 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	D	455	SER	23
1	B	9	THR	21
2	D	480	LEU	21
1	A	9	THR	20
1	A	20	SER	19
1	B	20	SER	19
1	A	22	THR	17
1	B	14	THR	16
1	B	49	GLN	16
2	D	494	LEU	15
1	B	72	ARG	15
1	A	57	SER	14
1	B	22	THR	14

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Mol	Chain	Res	Type	Models (Total)
1	A	14	THR	13
1	A	7	THR	11
1	B	57	SER	11
1	B	44	ILE	9
2	D	482	LEU	8
1	B	52	ASP	7
1	B	7	THR	6
1	B	55	THR	6
2	D	490	THR	5
1	A	24	GLU	5
2	D	478	GLN	5
1	B	12	THR	5
1	A	49	GLN	4
1	B	24	GLU	4
2	D	485	SER	4
1	A	39	ASP	4
1	A	55	THR	4
1	A	62	GLN	3
1	B	48	LYS	3
1	A	44	ILE	3
1	B	58	ASP	3
1	B	39	ASP	3
2	D	463	GLN	3
1	A	66	THR	3
1	A	58	ASP	2
1	A	27	LYS	2
1	B	60	ASN	2
1	B	66	THR	2
1	A	68	HIS	2
1	A	21	ASP	2
1	A	51	GLU	2
1	A	12	THR	2
2	D	468	PHE	2
1	B	13	ILE	2
1	A	52	ASP	2
2	D	495	GLU	2
1	A	8	LEU	1
1	B	42	ARG	1
2	D	483	THR	1
1	B	41	GLN	1
1	B	51	GLU	1
2	D	470	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	60	ASN	1
1	A	13	ILE	1
1	A	16	GLU	1
2	D	486	VAL	1
1	B	16	GLU	1
2	D	498	ILE	1
1	B	21	ASP	1
1	B	69	LEU	1
2	D	462	HIS	1
2	D	466	GLU	1
1	B	64	GLU	1
1	A	15	LEU	1
1	A	64	GLU	1
2	D	477	LEU	1
2	D	491	ASP	1
2	D	492	ASN	1
2	D	484	ARG	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

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 8% for the well-defined parts and 8% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *gp78CUE_amides_in_gp78-K48Ub2*

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	90
Number of shifts mapped to atoms	90
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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	45	1.54 ± 0.38	Should be applied

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 3%, i.e. 84 atoms were assigned a chemical shift out of a possible 2659. 0 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	84/933 (9%)	42/377 (11%)	0/376 (0%)	42/180 (23%)
Sidechain	0/1621 (0%)	0/1050 (0%)	0/511 (0%)	0/60 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/105 (0%)	0/53 (0%)	0/48 (0%)	0/4 (0%)
Overall	84/2659 (3%)	42/1480 (3%)	0/935 (0%)	42/244 (17%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 90 atoms were assigned a chemical shift out of a possible 2876. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	90/1013 (9%)	45/411 (11%)	0/408 (0%)	45/194 (23%)
Sidechain	0/1748 (0%)	0/1132 (0%)	0/546 (0%)	0/70 (0%)
Aromatic	0/115 (0%)	0/58 (0%)	0/53 (0%)	0/4 (0%)
Overall	90/2876 (3%)	45/1601 (3%)	0/1007 (0%)	45/268 (17%)

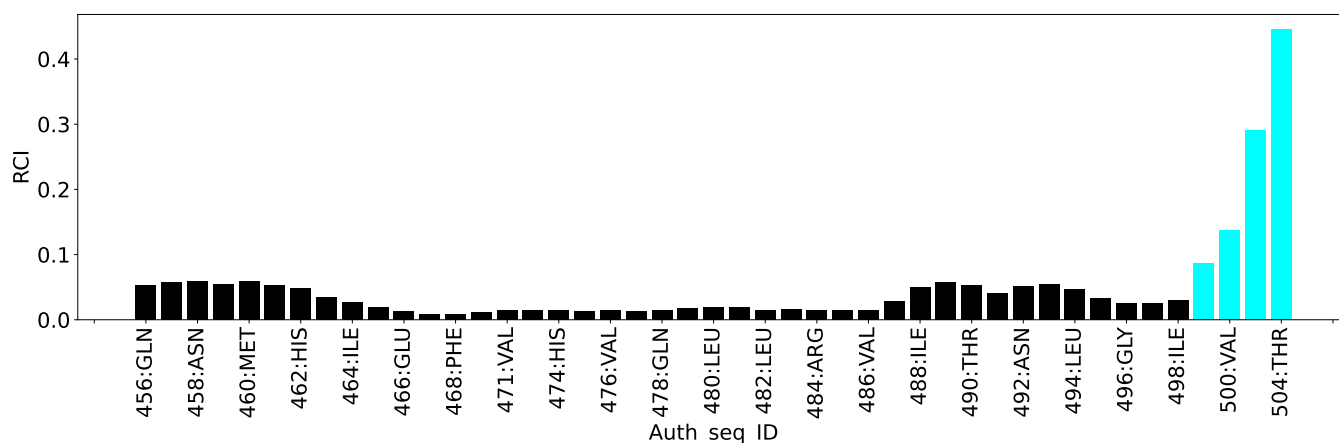
7.1.4 Statistically unusual chemical shifts [i](#)

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 D:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *ProximalUb_amides_in_gp78-K48Ub2*

7.2.1 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	132
Number of shifts mapped to atoms	132
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

7.2.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	66	0.53 ± 0.49	None needed (imprecise)

7.2.3 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 5%, i.e. 124 atoms were assigned a chemical shift out of a possible 2659. 0 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	124/933 (13%)	62/377 (16%)	0/376 (0%)	62/180 (34%)
Sidechain	0/1621 (0%)	0/1050 (0%)	0/511 (0%)	0/60 (0%)
Aromatic	0/105 (0%)	0/53 (0%)	0/48 (0%)	0/4 (0%)
Overall	124/2659 (5%)	62/1480 (4%)	0/935 (0%)	62/244 (25%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 5%, i.e. 132 atoms were assigned a chemical shift out of a possible 2876. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	132/1013 (13%)	66/411 (16%)	0/408 (0%)	66/194 (34%)
Sidechain	0/1748 (0%)	0/1132 (0%)	0/546 (0%)	0/70 (0%)
Aromatic	0/115 (0%)	0/58 (0%)	0/53 (0%)	0/4 (0%)
Overall	132/2876 (5%)	66/1601 (4%)	0/1007 (0%)	66/268 (25%)

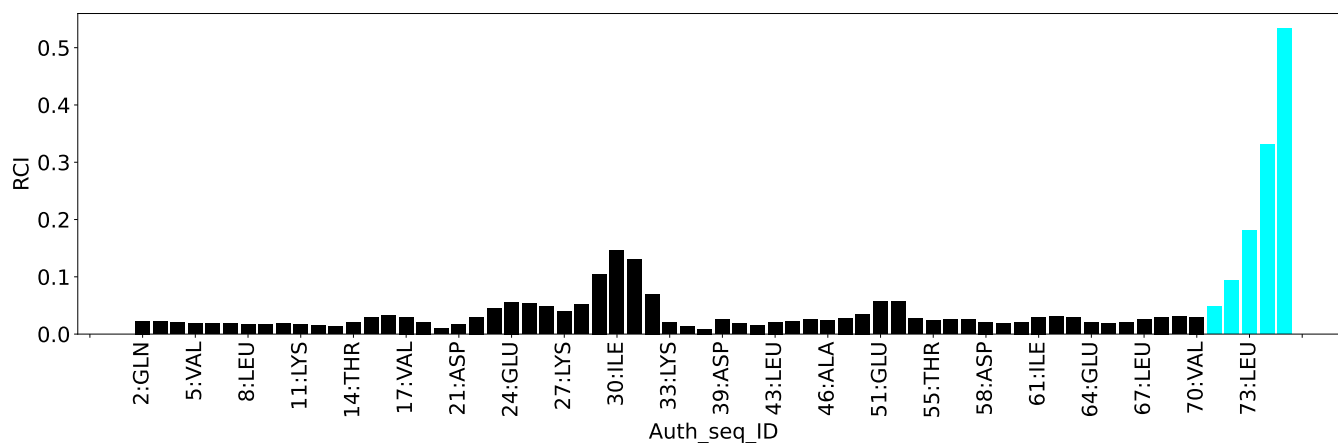
7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 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	64
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	64
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.3
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)	4.3	0.2
0.2-0.5 (Medium)	4.0	0.5
>0.5 (Large)	15.0	8.32

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 ⓘ

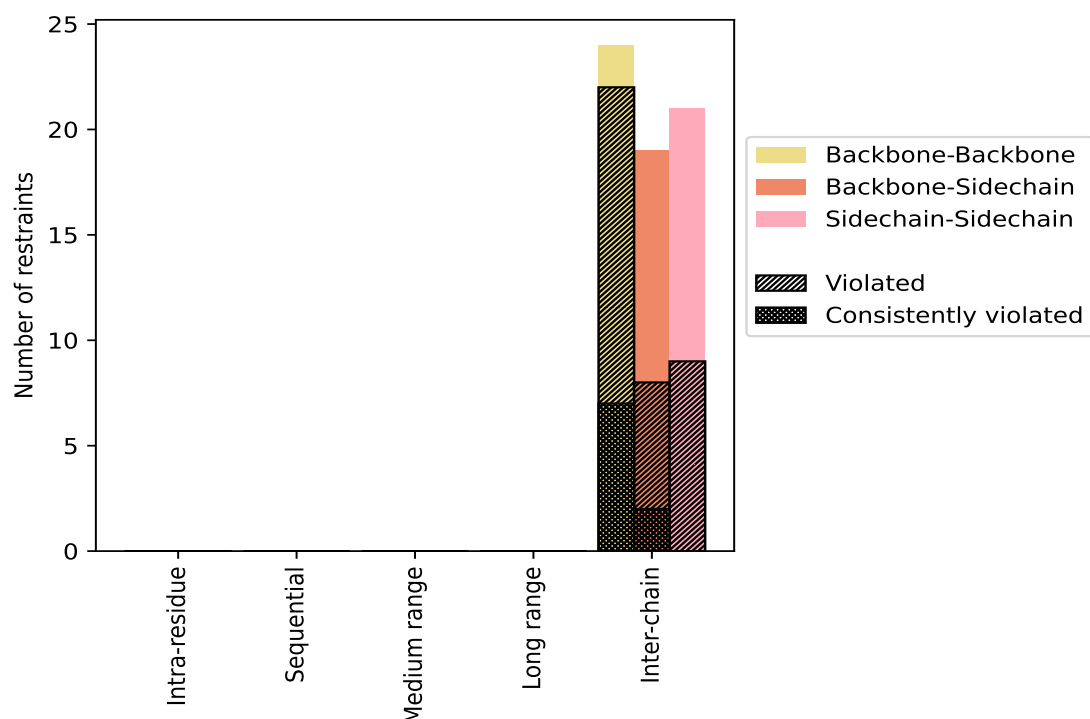
9.1 Summary of distance violations ⓘ

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	64	100.0	39	60.9	60.9	9	14.1	14.1
Backbone-Backbone	24	37.5	22	91.7	34.4	7	29.2	10.9
Backbone-Sidechain	19	29.7	8	42.1	12.5	2	10.5	3.1
Sidechain-Sidechain	21	32.8	9	42.9	14.1	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	64	100.0	39	60.9	60.9	9	14.1	14.1
Backbone-Backbone	24	37.5	22	91.7	34.4	7	29.2	10.9
Backbone-Sidechain	19	29.7	8	42.1	12.5	2	10.5	3.1
Sidechain-Sidechain	21	32.8	9	42.9	14.1	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	22	22	1.42	4.0	1.3	1.04
2	0	0	0	0	22	22	1.53	4.61	1.42	1.03
3	0	0	0	0	29	29	1.23	4.38	1.34	0.55
4	0	0	0	0	23	23	1.18	3.54	1.06	0.87
5	0	0	0	0	23	23	1.6	4.58	1.44	1.23
6	0	0	0	0	22	22	1.54	4.21	1.39	1.12
7	0	0	0	0	21	21	1.53	3.74	1.25	1.61
8	0	0	0	0	28	28	1.27	3.86	1.33	0.36
9	0	0	0	0	23	23	1.57	4.56	1.35	1.29
10	0	0	0	0	24	24	1.85	7.13	1.75	1.53

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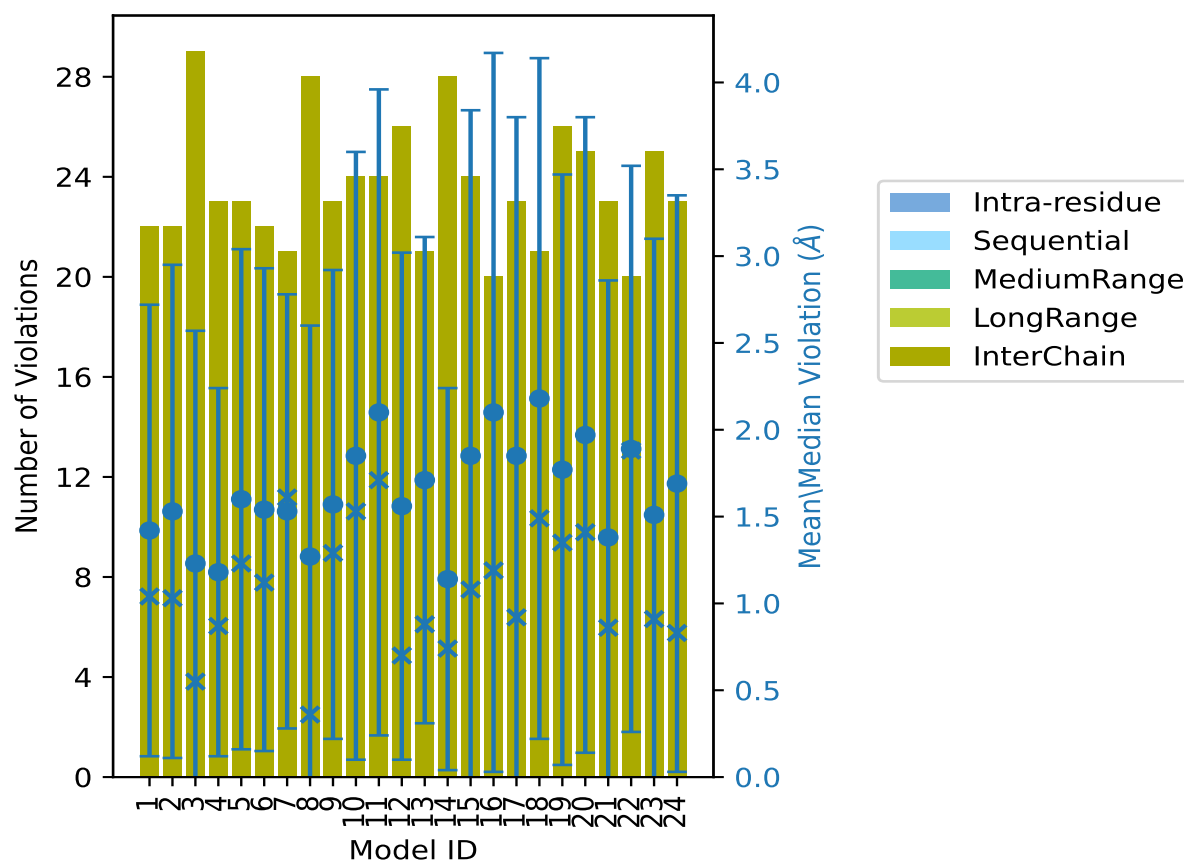
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	0	24	24	2.1	8.06	1.86	1.71
12	0	0	0	0	26	26	1.56	4.6	1.46	0.7
13	0	0	0	0	21	21	1.71	4.46	1.4	0.88
14	0	0	0	0	28	28	1.14	3.78	1.1	0.74
15	0	0	0	0	24	24	1.85	8.0	1.99	1.08
16	0	0	0	0	20	20	2.1	8.13	2.07	1.19
17	0	0	0	0	23	23	1.85	7.75	1.95	0.92
18	0	0	0	0	21	21	2.18	8.32	1.96	1.49
19	0	0	0	0	26	26	1.77	7.07	1.7	1.35
20	0	0	0	0	25	25	1.97	7.5	1.83	1.41
21	0	0	0	0	23	23	1.38	4.49	1.48	0.86
22	0	0	0	0	20	20	1.89	6.38	1.63	1.88
23	0	0	0	0	25	25	1.51	6.08	1.59	0.91
24	0	0	0	0	23	23	1.69	5.05	1.66	0.83

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 [i](#)



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 [i](#)

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, 25(IR:0, SQ:0, MR:0, LR:0, IC:25) 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	4	4	1	4.2
0	0	0	0	3	3	2	8.3
0	0	0	0	0	0	3	12.5
0	0	0	0	2	2	4	16.7
0	0	0	0	1	1	5	20.8
0	0	0	0	0	0	6	25.0

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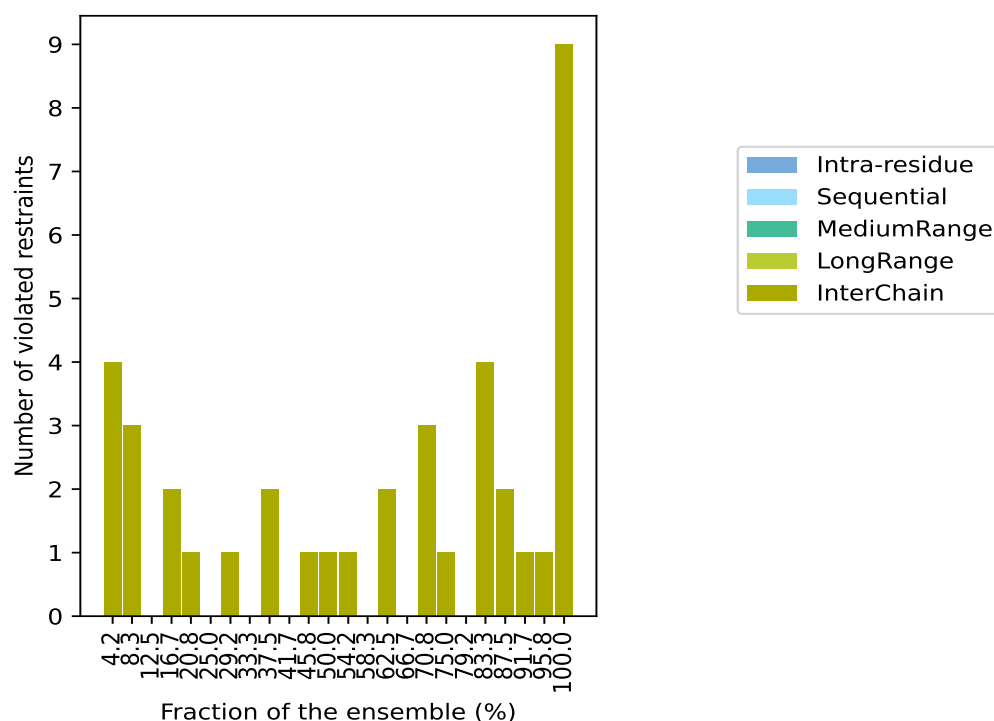
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	1	1	7	29.2
0	0	0	0	0	0	8	33.3
0	0	0	0	2	2	9	37.5
0	0	0	0	0	0	10	41.7
0	0	0	0	1	1	11	45.8
0	0	0	0	1	1	12	50.0
0	0	0	0	1	1	13	54.2
0	0	0	0	0	0	14	58.3
0	0	0	0	2	2	15	62.5
0	0	0	0	0	0	16	66.7
0	0	0	0	3	3	17	70.8
0	0	0	0	1	1	18	75.0
0	0	0	0	0	0	19	79.2
0	0	0	0	4	4	20	83.3
0	0	0	0	2	2	21	87.5
0	0	0	0	1	1	22	91.7
0	0	0	0	1	1	23	95.8
0	0	0	0	9	9	24	100.0

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

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

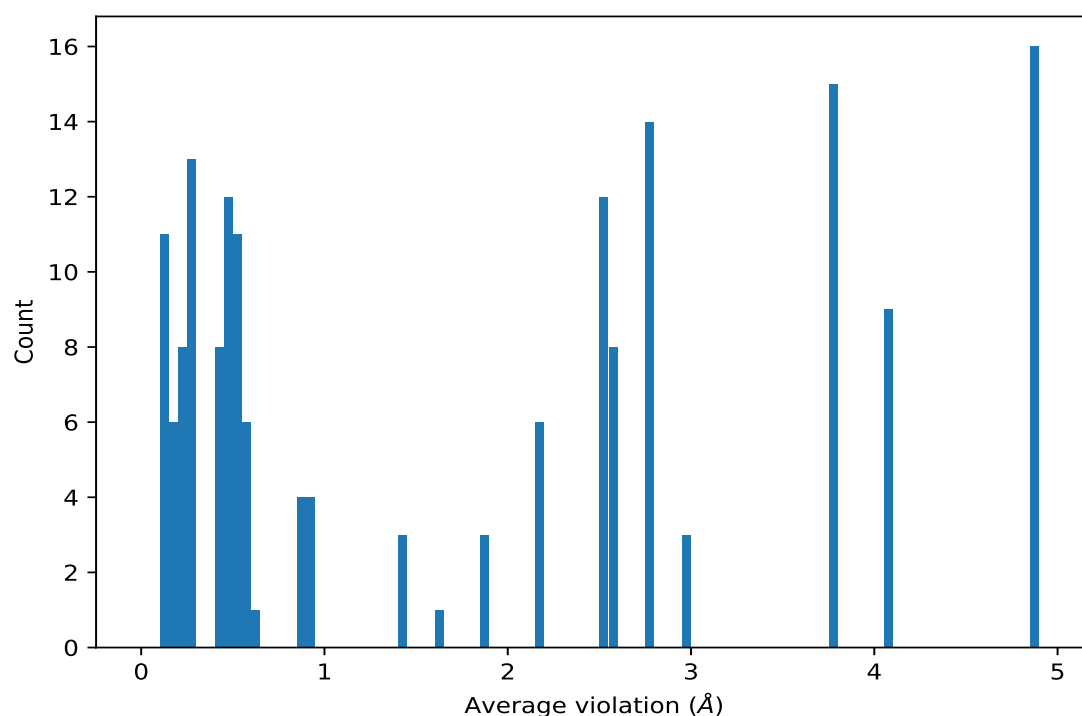
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,5)	1:45:B:PHE:C	2:467:D:MET:O	24	4.05	0.69	4.03
(1,5)	1:45:B:PHE:H	2:468:D:PHE:HE1	24	4.05	0.69	4.03
(1,5)	1:45:B:PHE:H	2:468:D:PHE:HZ	24	4.05	0.69	4.03
(1,5)	1:45:B:PHE:HA	2:467:D:MET:O	24	4.05	0.69	4.03
(1,5)	1:45:B:PHE:N	2:468:D:PHE:HE1	24	4.05	0.69	4.03
(1,5)	1:45:B:PHE:C	2:469:D:PRO:HG3	24	4.05	0.69	4.03
(1,5)	1:45:B:PHE:N	2:467:D:MET:O	24	4.05	0.69	4.03
(1,5)	1:45:B:PHE:H	2:494:D:LEU:HD22	24	4.05	0.69	4.03
(1,5)	1:45:B:PHE:C	2:469:D:PRO:HD2	24	4.05	0.69	4.03
(1,13)	1:73:B:LEU:HD11	2:486:D:VAL:C	24	3.8	0.81	3.95
(1,13)	1:73:B:LEU:O	2:492:D:ASN:HD22	24	3.8	0.81	3.95
(1,13)	1:73:B:LEU:HD12	2:486:D:VAL:C	24	3.8	0.81	3.95
(1,13)	1:73:B:LEU:HD13	2:492:D:ASN:H	24	3.8	0.81	3.95
(1,13)	1:73:B:LEU:H	2:492:D:ASN:H	24	3.8	0.81	3.95
(1,13)	1:73:B:LEU:H	2:492:D:ASN:HD21	24	3.8	0.81	3.95
(1,13)	1:73:B:LEU:HD21	2:486:D:VAL:N	24	3.8	0.81	3.95

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,13)	1:73:B:LEU:HD11	2:492:D:ASN:OD1	24	3.8	0.81	3.95
(1,13)	1:73:B:LEU:HD13	2:486:D:VAL:C	24	3.8	0.81	3.95
(1,13)	1:73:B:LEU:HD21	2:486:D:VAL:C	24	3.8	0.81	3.95
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	24	3.77	0.25	3.78
(1,3)	1:43:B:LEU:C	2:468:D:PHE:HZ	24	3.77	0.25	3.78
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD23	24	3.77	0.25	3.78
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD11	24	3.77	0.25	3.78
(1,3)	1:43:B:LEU:N	2:494:D:LEU:HD11	24	3.77	0.25	3.78
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	24	2.97	0.73	2.88
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	24	2.97	0.73	2.88
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	24	2.97	0.73	2.88
(1,12)	1:72:B:ARG:HE	2:494:D:LEU:HB3	24	2.79	0.71	3.01
(1,12)	1:72:B:ARG:HD2	2:494:D:LEU:HB3	24	2.79	0.71	3.01
(1,12)	1:72:B:ARG:HB2	2:494:D:LEU:HD13	24	2.79	0.71	3.01
(1,12)	1:72:B:ARG:HH21	2:492:D:ASN:HA	24	2.79	0.71	3.01
(1,12)	1:72:B:ARG:HG3	2:494:D:LEU:HD12	24	2.79	0.71	3.01
(1,12)	1:72:B:ARG:HH21	2:494:D:LEU:HB2	24	2.79	0.71	3.01
(1,12)	1:72:B:ARG:HH21	2:494:D:LEU:HB3	24	2.79	0.71	3.01
(1,12)	1:72:B:ARG:HE	2:494:D:LEU:HB2	24	2.79	0.71	3.01
(1,12)	1:72:B:ARG:HH21	2:492:D:ASN:HD21	24	2.79	0.71	3.01
(1,12)	1:72:B:ARG:HH21	2:492:D:ASN:N	24	2.79	0.71	3.01
(1,12)	1:72:B:ARG:HB3	2:494:D:LEU:HD12	24	2.79	0.71	3.01
(1,12)	1:72:B:ARG:HH12	2:492:D:ASN:HA	24	2.79	0.71	3.01
(1,12)	1:72:B:ARG:HE	2:492:D:ASN:HD21	24	2.79	0.71	3.01
(1,12)	1:72:B:ARG:HH21	2:494:D:LEU:O	24	2.79	0.71	3.01
(1,6)	1:48:B:LYS:HA	2:468:D:PHE:HE2	24	2.59	0.83	2.69
(1,6)	1:48:B:LYS:HA	2:468:D:PHE:HE1	24	2.59	0.83	2.69
(1,6)	1:48:B:LYS:N	2:468:D:PHE:HE2	24	2.59	0.83	2.69
(1,6)	1:48:B:LYS:N	2:468:D:PHE:HE1	24	2.59	0.83	2.69
(1,6)	1:48:B:LYS:O	2:468:D:PHE:HE1	24	2.59	0.83	2.69
(1,6)	1:48:B:LYS:N	2:468:D:PHE:HZ	24	2.59	0.83	2.69
(1,6)	1:48:B:LYS:HA	2:494:D:LEU:HD23	24	2.59	0.83	2.69
(1,6)	1:48:B:LYS:H	2:469:D:PRO:HD2	24	2.59	0.83	2.69
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG21	24	2.18	1.03	2.54
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG22	24	2.18	1.03	2.54
(1,11)	1:71:B:LEU:H	2:467:D:MET:HE3	24	2.18	1.03	2.54
(1,11)	1:71:B:LEU:O	2:486:D:VAL:O	24	2.18	1.03	2.54
(1,11)	1:71:B:LEU:H	2:467:D:MET:HE2	24	2.18	1.03	2.54
(1,11)	1:71:B:LEU:H	2:486:D:VAL:O	24	2.18	1.03	2.54
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	24	1.88	0.71	1.98
(1,18)	2:469:D:PRO:HG2	1:68:B:HIS:HE1	24	1.88	0.71	1.98
(1,18)	2:469:D:PRO:HG3	1:68:B:HIS:HE1	24	1.88	0.71	1.98

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	24	1.62	0.07	1.63
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	23	0.6	0.33	0.61
(1,7)	1:49:B:GLN:HB2	2:494:D:LEU:HD22	23	0.6	0.33	0.61
(1,7)	1:49:B:GLN:HB2	2:494:D:LEU:HD23	23	0.6	0.33	0.61
(1,7)	1:49:B:GLN:OE1	2:494:D:LEU:HD21	23	0.6	0.33	0.61
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD23	23	0.6	0.33	0.61
(1,2)	1:42:B:ARG:HD3	2:494:D:LEU:HD12	22	0.51	0.12	0.52
(1,2)	1:42:B:ARG:HG2	2:494:D:LEU:HD12	22	0.51	0.12	0.52
(1,2)	1:42:B:ARG:HD3	2:494:D:LEU:HD13	22	0.51	0.12	0.52
(1,2)	1:42:B:ARG:CZ	2:494:D:LEU:HD21	22	0.51	0.12	0.52
(1,2)	1:42:B:ARG:HE	2:494:D:LEU:HD22	22	0.51	0.12	0.52
(1,2)	1:42:B:ARG:HH21	2:494:D:LEU:HD21	22	0.51	0.12	0.52
(1,2)	1:42:B:ARG:HH12	2:494:D:LEU:HB3	22	0.51	0.12	0.52
(1,2)	1:42:B:ARG:HD3	2:494:D:LEU:HD22	22	0.51	0.12	0.52
(1,2)	1:42:B:ARG:HH22	2:494:D:LEU:HB3	22	0.51	0.12	0.52
(1,2)	1:42:B:ARG:NH2	2:494:D:LEU:HD21	22	0.51	0.12	0.52
(1,2)	1:42:B:ARG:HG2	2:494:D:LEU:HD22	22	0.51	0.12	0.52
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	21	0.86	0.41	0.91
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	21	0.86	0.41	0.91
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	21	0.86	0.41	0.91
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	21	0.45	0.39	0.32
(1,14)	1:74:B:ARG:HH22	2:492:D:ASN:OD1	20	4.88	2.8	5.56
(1,14)	1:74:B:ARG:O	2:492:D:ASN:OD1	20	4.88	2.8	5.56
(1,14)	1:74:B:ARG:HH21	2:492:D:ASN:HA	20	4.88	2.8	5.56
(1,14)	1:74:B:ARG:HH12	2:492:D:ASN:OD1	20	4.88	2.8	5.56
(1,14)	1:74:B:ARG:HD2	2:492:D:ASN:OD1	20	4.88	2.8	5.56
(1,14)	1:74:B:ARG:HA	2:492:D:ASN:HA	20	4.88	2.8	5.56
(1,14)	1:74:B:ARG:HA	2:492:D:ASN:OD1	20	4.88	2.8	5.56
(1,14)	1:74:B:ARG:HH22	2:492:D:ASN:H	20	4.88	2.8	5.56
(1,14)	1:74:B:ARG:HH22	2:492:D:ASN:HA	20	4.88	2.8	5.56
(1,14)	1:74:B:ARG:C	2:492:D:ASN:HD22	20	4.88	2.8	5.56
(1,14)	1:74:B:ARG:HD3	2:494:D:LEU:HD12	20	4.88	2.8	5.56
(1,14)	1:74:B:ARG:HA	2:492:D:ASN:H	20	4.88	2.8	5.56
(1,14)	1:74:B:ARG:N	2:492:D:ASN:H	20	4.88	2.8	5.56
(1,14)	1:74:B:ARG:HB3	2:492:D:ASN:OD1	20	4.88	2.8	5.56
(1,14)	1:74:B:ARG:C	2:492:D:ASN:HB2	20	4.88	2.8	5.56
(1,14)	1:74:B:ARG:HH22	2:492:D:ASN:N	20	4.88	2.8	5.56
(1,20)	2:492:D:ASN:OD1	1:74:B:ARG:HH22	20	2.51	1.07	2.98
(1,20)	2:492:D:ASN:HA	1:72:B:ARG:HH21	20	2.51	1.07	2.98
(1,20)	2:492:D:ASN:HA	1:74:B:ARG:HH21	20	2.51	1.07	2.98
(1,20)	2:492:D:ASN:OD1	1:74:B:ARG:HH12	20	2.51	1.07	2.98
(1,20)	2:492:D:ASN:OD1	1:74:B:ARG:HD2	20	2.51	1.07	2.98

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,20)	2:492:D:ASN:N	1:72:B:ARG:HH21	20	2.51	1.07	2.98
(1,20)	2:492:D:ASN:H	1:74:B:ARG:HH22	20	2.51	1.07	2.98
(1,20)	2:492:D:ASN:HA	1:74:B:ARG:HH22	20	2.51	1.07	2.98
(1,20)	2:492:D:ASN:HD21	1:72:B:ARG:HH21	20	2.51	1.07	2.98
(1,20)	2:492:D:ASN:N	1:42:B:ARG:HH12	20	2.51	1.07	2.98
(1,20)	2:492:D:ASN:H	1:70:B:VAL:HG11	20	2.51	1.07	2.98
(1,20)	2:492:D:ASN:HA	1:72:B:ARG:HH12	20	2.51	1.07	2.98
(1,9)	1:69:B:LEU:H	2:467:D:MET:HE3	20	0.92	0.8	0.62
(1,9)	1:69:B:LEU:O	2:467:D:MET:HE3	20	0.92	0.8	0.62
(1,9)	1:69:B:LEU:O	2:467:D:MET:SD	20	0.92	0.8	0.62
(1,9)	1:69:B:LEU:H	2:467:D:MET:SD	20	0.92	0.8	0.62
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	20	0.55	0.68	0.27
(1,19)	2:486:D:VAL:HG23	1:8:B:LEU:HB3	18	0.29	0.17	0.24
(1,19)	2:486:D:VAL:O	1:8:B:LEU:HD11	18	0.29	0.17	0.24
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HD23	18	0.29	0.17	0.24
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HB3	18	0.29	0.17	0.24
(1,19)	2:486:D:VAL:HG21	1:8:B:LEU:HB3	18	0.29	0.17	0.24
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HD11	18	0.29	0.17	0.24
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HD13	18	0.29	0.17	0.24
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	17	1.41	0.37	1.51
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	17	1.41	0.37	1.51
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	17	1.41	0.37	1.51
(1,10)	1:70:B:VAL:HG12	2:494:D:LEU:HD12	17	0.48	0.33	0.38
(1,10)	1:70:B:VAL:HG23	2:468:D:PHE:HE1	17	0.48	0.33	0.38
(1,10)	1:70:B:VAL:HG13	2:494:D:LEU:HD12	17	0.48	0.33	0.38
(1,10)	1:70:B:VAL:HG22	2:467:D:MET:HE3	17	0.48	0.33	0.38
(1,10)	1:70:B:VAL:HG23	2:468:D:PHE:HE2	17	0.48	0.33	0.38
(1,10)	1:70:B:VAL:HG11	2:494:D:LEU:HD12	17	0.48	0.33	0.38
(1,10)	1:70:B:VAL:HG13	2:494:D:LEU:HD13	17	0.48	0.33	0.38
(1,10)	1:70:B:VAL:HG23	2:468:D:PHE:HZ	17	0.48	0.33	0.38
(1,10)	1:70:B:VAL:HG11	2:494:D:LEU:HD13	17	0.48	0.33	0.38
(1,10)	1:70:B:VAL:HA	2:467:D:MET:HE3	17	0.48	0.33	0.38
(1,8)	1:68:B:HIS:HB3	2:467:D:MET:HE1	17	0.26	0.18	0.2
(1,8)	1:68:B:HIS:HE2	2:467:D:MET:HA	17	0.26	0.18	0.2
(1,8)	1:68:B:HIS:HE2	2:466:D:GLU:O	17	0.26	0.18	0.2
(1,8)	1:68:B:HIS:HB3	2:467:D:MET:HG2	17	0.26	0.18	0.2
(1,8)	1:68:B:HIS:HB3	2:467:D:MET:HB3	17	0.26	0.18	0.2
(1,8)	1:68:B:HIS:HD2	2:467:D:MET:HG2	17	0.26	0.18	0.2
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	15	0.47	0.27	0.41
(1,17)	2:468:D:PHE:HE1	1:70:B:VAL:HG23	15	0.44	0.51	0.32
(1,17)	2:468:D:PHE:HE2	1:44:B:ILE:HG12	15	0.44	0.51	0.32
(1,17)	2:468:D:PHE:HE1	1:44:B:ILE:HG12	15	0.44	0.51	0.32

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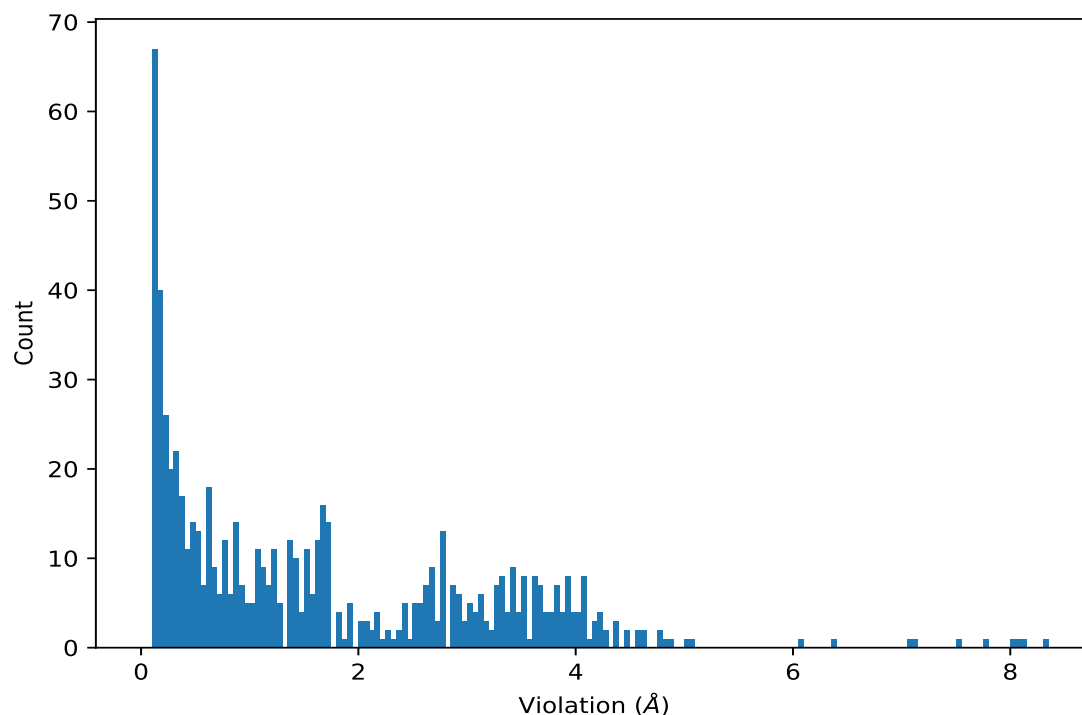
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,17)	2:468:D:PHE:HZ	1:44:B:ILE:HG12	15	0.44	0.51	0.32
(1,17)	2:468:D:PHE:HD2	1:70:B:VAL:HG21	15	0.44	0.51	0.32
(1,17)	2:468:D:PHE:HE2	1:70:B:VAL:HG23	15	0.44	0.51	0.32
(1,17)	2:468:D:PHE:HZ	1:70:B:VAL:HG23	15	0.44	0.51	0.32
(1,4)	1:44:B:ILE:HD13	2:494:D:LEU:HD11	13	0.15	0.06	0.14
(1,4)	1:44:B:ILE:HD12	2:494:D:LEU:HD22	13	0.15	0.06	0.14
(1,4)	1:44:B:ILE:HG12	2:468:D:PHE:HZ	13	0.15	0.06	0.14
(1,4)	1:44:B:ILE:HD13	2:494:D:LEU:HD22	13	0.15	0.06	0.14
(1,21)	2:494:D:LEU:HD11	1:44:B:ILE:HD13	12	0.14	0.04	0.14
(1,21)	2:494:D:LEU:HD22	1:49:B:GLN:HG3	12	0.14	0.04	0.14
(1,21)	2:494:D:LEU:HD11	1:44:B:ILE:HG12	12	0.14	0.04	0.14
(1,1)	1:8:B:LEU:HB3	2:486:D:VAL:HG23	11	0.18	0.07	0.15
(1,1)	1:8:B:LEU:HD22	2:467:D:MET:HG3	11	0.18	0.07	0.15
(1,1)	1:8:B:LEU:HD23	2:486:D:VAL:HB	11	0.18	0.07	0.15
(1,1)	1:8:B:LEU:HD22	2:467:D:MET:HE2	11	0.18	0.07	0.15
(1,1)	1:8:B:LEU:HD11	2:486:D:VAL:HB	11	0.18	0.07	0.15
(1,28)	2:486:D:VAL:HG12	1:8:B:LEU:HB3	9	0.62	0.36	0.52
(1,16)	2:467:D:MET:HA	1:68:B:HIS:HE2	9	0.21	0.06	0.21
(1,16)	2:467:D:MET:HE3	1:70:B:VAL:HG22	9	0.21	0.06	0.21
(1,16)	2:467:D:MET:HE1	1:68:B:HIS:HB3	9	0.21	0.06	0.21
(1,16)	2:467:D:MET:HE2	1:8:B:LEU:HG	9	0.21	0.06	0.21
(1,16)	2:467:D:MET:HG3	1:8:B:LEU:HD21	9	0.21	0.06	0.21
(1,16)	2:467:D:MET:HG3	1:8:B:LEU:HD22	9	0.21	0.06	0.21
(1,16)	2:467:D:MET:HE3	1:8:B:LEU:HD22	9	0.21	0.06	0.21
(1,16)	2:467:D:MET:HB3	1:68:B:HIS:HB3	9	0.21	0.06	0.21
(1,54)	2:489:D:THR:H	1:72:B:ARG:HA	7	0.14	0.03	0.13
(1,57)	2:492:D:ASN:H	1:73:B:LEU:HD11	5	0.4	0.57	0.13
(1,35)	2:494:D:LEU:HD13	1:42:B:ARG:HG3	4	0.88	0.58	0.72
(1,40)	2:494:D:LEU:HD22	1:42:B:ARG:HG3	4	0.17	0.06	0.15
(1,52)	2:494:D:LEU:HD22	1:43:B:LEU:H	2	0.12	0.01	0.12
(1,36)	2:494:D:LEU:HD11	1:48:B:LYS:HA	2	0.12	0.0	0.12
(1,50)	2:494:D:LEU:HD22	1:70:B:VAL:H	2	0.12	0.0	0.12

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)
(1,14)	1:74:B:ARG:N	2:492:D:ASN:H	18	8.32
(1,14)	1:74:B:ARG:HD3	2:494:D:LEU:HD12	16	8.13
(1,14)	1:74:B:ARG:HA	2:492:D:ASN:OD1	11	8.06
(1,14)	1:74:B:ARG:HA	2:492:D:ASN:OD1	15	8.0
(1,14)	1:74:B:ARG:HA	2:492:D:ASN:H	17	7.75
(1,14)	1:74:B:ARG:HA	2:492:D:ASN:OD1	20	7.5
(1,14)	1:74:B:ARG:HA	2:492:D:ASN:HA	10	7.13
(1,14)	1:74:B:ARG:HB3	2:492:D:ASN:OD1	19	7.07
(1,14)	1:74:B:ARG:C	2:492:D:ASN:HB2	22	6.38
(1,14)	1:74:B:ARG:C	2:492:D:ASN:HD22	23	6.08
(1,14)	1:74:B:ARG:HH22	2:492:D:ASN:N	24	5.05
(1,5)	1:45:B:PHE:H	2:468:D:PHE:HE1	15	5.03
(1,5)	1:45:B:PHE:H	2:494:D:LEU:HD22	17	4.87
(1,13)	1:73:B:LEU:HD12	2:486:D:VAL:C	20	4.8
(1,5)	1:45:B:PHE:H	2:494:D:LEU:HD22	16	4.78
(1,13)	1:73:B:LEU:H	2:492:D:ASN:H	11	4.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:45:B:PHE:H	2:468:D:PHE:HE1	2	4.61
(1,5)	1:45:B:PHE:C	2:467:D:MET:O	12	4.6
(1,5)	1:45:B:PHE:H	2:468:D:PHE:HE1	5	4.58
(1,5)	1:45:B:PHE:H	2:468:D:PHE:HZ	9	4.56
(1,5)	1:45:B:PHE:HA	2:467:D:MET:O	21	4.49
(1,5)	1:45:B:PHE:C	2:469:D:PRO:HG3	13	4.46
(1,5)	1:45:B:PHE:H	2:468:D:PHE:HZ	3	4.38
(1,5)	1:45:B:PHE:H	2:468:D:PHE:HZ	18	4.38
(1,13)	1:73:B:LEU:HD21	2:486:D:VAL:C	24	4.36
(1,3)	1:43:B:LEU:N	2:494:D:LEU:HD11	21	4.29
(1,13)	1:73:B:LEU:HD11	2:492:D:ASN:OD1	16	4.27
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	6	4.21
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	6	4.21
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	6	4.21
(1,6)	1:48:B:LYS:N	2:468:D:PHE:HZ	12	4.2
(1,13)	1:73:B:LEU:HD13	2:486:D:VAL:C	19	4.18
(1,13)	1:73:B:LEU:HD12	2:486:D:VAL:C	10	4.16
(1,5)	1:45:B:PHE:H	2:468:D:PHE:HZ	19	4.15
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	9	4.1
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	21	4.09
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	21	4.09
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	21	4.09
(1,13)	1:73:B:LEU:HD13	2:486:D:VAL:C	18	4.07
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	18	4.06
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	24	4.05
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	24	4.05
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	24	4.05
(1,13)	1:73:B:LEU:HD11	2:486:D:VAL:C	5	4.04
(1,6)	1:48:B:LYS:HA	2:494:D:LEU:HD23	13	4.02
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	23	4.01
(1,13)	1:73:B:LEU:HD11	2:486:D:VAL:C	1	4.0
(1,13)	1:73:B:LEU:H	2:492:D:ASN:HD21	23	3.97
(1,13)	1:73:B:LEU:HD12	2:486:D:VAL:C	6	3.96
(1,13)	1:73:B:LEU:HD12	2:486:D:VAL:C	21	3.96
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	15	3.96
(1,13)	1:73:B:LEU:HD21	2:486:D:VAL:N	15	3.94
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	3	3.94
(1,3)	1:43:B:LEU:C	2:468:D:PHE:HZ	11	3.94
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	2	3.92
(1,5)	1:45:B:PHE:HA	2:467:D:MET:O	10	3.91
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	16	3.9
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	16	3.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	16	3.9
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	1	3.88
(1,12)	1:72:B:ARG:HE	2:494:D:LEU:HB2	8	3.86
(1,5)	1:45:B:PHE:H	2:468:D:PHE:HE1	20	3.86
(1,13)	1:73:B:LEU:HD13	2:486:D:VAL:C	22	3.85
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	10	3.83
(1,5)	1:45:B:PHE:H	2:468:D:PHE:HE1	23	3.82
(1,5)	1:45:B:PHE:C	2:469:D:PRO:HD2	24	3.82
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	13	3.82
(1,13)	1:73:B:LEU:HD11	2:486:D:VAL:C	3	3.81
(1,20)	2:492:D:ASN:N	1:42:B:ARG:HH12	17	3.8
(1,13)	1:73:B:LEU:HD12	2:486:D:VAL:C	17	3.8
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	17	3.79
(1,14)	1:74:B:ARG:C	2:492:D:ASN:HD22	14	3.78
(1,13)	1:73:B:LEU:HD12	2:486:D:VAL:C	12	3.78
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	5	3.78
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	7	3.74
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	16	3.74
(1,13)	1:73:B:LEU:H	2:492:D:ASN:H	13	3.71
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	6	3.71
(1,13)	1:73:B:LEU:HD11	2:486:D:VAL:C	2	3.69
(1,5)	1:45:B:PHE:C	2:467:D:MET:O	22	3.68
(1,13)	1:73:B:LEU:H	2:492:D:ASN:H	9	3.67
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	24	3.67
(1,5)	1:45:B:PHE:C	2:467:D:MET:O	1	3.66
(1,5)	1:45:B:PHE:N	2:467:D:MET:O	14	3.66
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD11	20	3.66
(1,11)	1:71:B:LEU:O	2:486:D:VAL:O	10	3.64
(1,5)	1:45:B:PHE:H	2:468:D:PHE:HE1	6	3.62
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	12	3.62
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	5	3.61
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	5	3.61
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	5	3.61
(1,20)	2:492:D:ASN:H	1:70:B:VAL:HG11	20	3.6
(1,11)	1:71:B:LEU:H	2:486:D:VAL:O	20	3.6
(1,12)	1:72:B:ARG:HH21	2:494:D:LEU:HB3	20	3.57
(1,5)	1:45:B:PHE:H	2:468:D:PHE:HZ	4	3.54
(1,5)	1:45:B:PHE:C	2:467:D:MET:O	8	3.54
(1,13)	1:73:B:LEU:HD11	2:486:D:VAL:C	8	3.52
(1,11)	1:71:B:LEU:H	2:486:D:VAL:O	19	3.52
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	14	3.52
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	12	3.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	12	3.51
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	12	3.51
(1,5)	1:45:B:PHE:N	2:468:D:PHE:HE1	11	3.48
(1,13)	1:73:B:LEU:HD13	2:492:D:ASN:H	7	3.47
(1,20)	2:492:D:ASN:N	1:72:B:ARG:HH21	15	3.45
(1,12)	1:72:B:ARG:HH21	2:492:D:ASN:N	15	3.45
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	8	3.44
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	17	3.43
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	17	3.43
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	17	3.43
(1,20)	2:492:D:ASN:N	1:42:B:ARG:HH12	16	3.43
(1,20)	2:492:D:ASN:HA	1:72:B:ARG:HH21	11	3.41
(1,12)	1:72:B:ARG:HH21	2:492:D:ASN:HA	11	3.41
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	4	3.41
(1,6)	1:48:B:LYS:H	2:469:D:PRO:HD2	24	3.4
(1,6)	1:48:B:LYS:HA	2:494:D:LEU:HD23	15	3.39
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	15	3.35
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	15	3.35
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	15	3.35
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	22	3.34
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	22	3.34
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	22	3.34
(1,20)	2:492:D:ASN:N	1:72:B:ARG:HH21	10	3.34
(1,20)	2:492:D:ASN:HA	1:72:B:ARG:HH21	18	3.34
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG21	11	3.34
(1,12)	1:72:B:ARG:HH21	2:494:D:LEU:HB3	7	3.33
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD23	19	3.32
(1,12)	1:72:B:ARG:HH21	2:494:D:LEU:HB2	16	3.29
(1,12)	1:72:B:ARG:HH21	2:494:D:LEU:O	24	3.29
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	3	3.27
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	3	3.27
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	3	3.27
(1,20)	2:492:D:ASN:HA	1:72:B:ARG:HH21	19	3.27
(1,12)	1:72:B:ARG:HH21	2:492:D:ASN:HA	19	3.27
(1,14)	1:74:B:ARG:O	2:492:D:ASN:OD1	5	3.23
(1,3)	1:43:B:LEU:O	2:494:D:LEU:HD22	22	3.23
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	8	3.18
(1,6)	1:48:B:LYS:HA	2:468:D:PHE:HE2	9	3.17
(1,20)	2:492:D:ASN:N	1:42:B:ARG:HH12	24	3.15
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	23	3.13
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	23	3.13
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	23	3.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	11	3.13
(1,12)	1:72:B:ARG:HD2	2:494:D:LEU:HB3	2	3.13
(1,12)	1:72:B:ARG:HH21	2:494:D:LEU:HB3	18	3.13
(1,12)	1:72:B:ARG:HE	2:494:D:LEU:HB3	1	3.09
(1,11)	1:71:B:LEU:H	2:467:D:MET:HE2	18	3.09
(1,6)	1:48:B:LYS:N	2:468:D:PHE:HE1	11	3.09
(1,20)	2:492:D:ASN:HA	1:72:B:ARG:HH21	5	3.07
(1,12)	1:72:B:ARG:HB2	2:494:D:LEU:HD13	3	3.02
(1,6)	1:48:B:LYS:HA	2:468:D:PHE:HE1	5	3.02
(1,13)	1:73:B:LEU:H	2:492:D:ASN:HD21	14	3.01
(1,12)	1:72:B:ARG:HE	2:492:D:ASN:HD21	23	3.0
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG22	4	3.0
(1,12)	1:72:B:ARG:HB3	2:494:D:LEU:HD12	17	2.99
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG21	13	2.99
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG21	9	2.95
(1,9)	1:69:B:LEU:O	2:467:D:MET:HE3	20	2.93
(1,6)	1:48:B:LYS:HA	2:494:D:LEU:HD23	21	2.91
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	13	2.9
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	13	2.9
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	13	2.9
(1,6)	1:48:B:LYS:HA	2:468:D:PHE:HE2	1	2.9
(1,20)	2:492:D:ASN:HA	1:74:B:ARG:HH21	6	2.89
(1,14)	1:74:B:ARG:HH21	2:492:D:ASN:HA	6	2.89
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	7	2.86
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	7	2.86
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	7	2.86
(1,12)	1:72:B:ARG:HH21	2:494:D:LEU:HB3	12	2.85
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG21	2	2.85
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	2	2.77
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	2	2.77
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	2	2.77
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	18	2.77
(1,11)	1:71:B:LEU:H	2:467:D:MET:HE3	7	2.77
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG21	3	2.76
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	8	2.75
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	8	2.75
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	8	2.75
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	18	2.75
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	18	2.75
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	18	2.75
(1,6)	1:48:B:LYS:HA	2:494:D:LEU:HD23	17	2.75
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	20	2.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:48:B:LYS:HA	2:494:D:LEU:HD23	16	2.72
(1,6)	1:48:B:LYS:N	2:468:D:PHE:HE1	10	2.7
(1,6)	1:48:B:LYS:N	2:468:D:PHE:HE1	19	2.68
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	1	2.67
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	1	2.67
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	1	2.67
(1,9)	1:69:B:LEU:H	2:467:D:MET:SD	8	2.67
(1,6)	1:48:B:LYS:HA	2:468:D:PHE:HE2	8	2.66
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	4	2.65
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	4	2.65
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	4	2.65
(1,20)	2:492:D:ASN:OD1	1:74:B:ARG:HH12	7	2.64
(1,14)	1:74:B:ARG:HH12	2:492:D:ASN:OD1	7	2.64
(1,6)	1:48:B:LYS:HA	2:468:D:PHE:HE1	2	2.64
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	12	2.63
(1,12)	1:72:B:ARG:HH21	2:494:D:LEU:HB3	10	2.63
(1,6)	1:48:B:LYS:N	2:468:D:PHE:HE2	3	2.63
(1,6)	1:48:B:LYS:HA	2:468:D:PHE:HE2	22	2.63
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	22	2.59
(1,12)	1:72:B:ARG:HH21	2:494:D:LEU:HB2	6	2.58
(1,20)	2:492:D:ASN:H	1:74:B:ARG:HH22	12	2.57
(1,14)	1:74:B:ARG:HH22	2:492:D:ASN:H	12	2.57
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	11	2.55
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	9	2.54
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	9	2.54
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	9	2.54
(1,11)	1:71:B:LEU:H	2:467:D:MET:HE3	12	2.54
(1,11)	1:71:B:LEU:H	2:467:D:MET:HE3	22	2.53
(1,6)	1:48:B:LYS:N	2:468:D:PHE:HE1	18	2.45
(1,12)	1:72:B:ARG:HH21	2:494:D:LEU:HB3	13	2.42
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	10	2.41
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	10	2.41
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	10	2.41
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	20	2.4
(1,12)	1:72:B:ARG:HH21	2:494:D:LEU:HB3	9	2.39
(1,12)	1:72:B:ARG:HH21	2:494:D:LEU:HB2	21	2.39
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	9	2.31
(1,17)	2:468:D:PHE:HD2	1:70:B:VAL:HG21	13	2.28
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	4	2.26
(1,9)	1:69:B:LEU:O	2:467:D:MET:SD	7	2.24
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	14	2.15
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	14	2.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	14	2.15
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	3	2.15
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	2	2.1
(1,11)	1:71:B:LEU:H	2:467:D:MET:HE2	17	2.1
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	23	2.08
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG21	8	2.08
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	19	2.06
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	11	2.0
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	11	2.0
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	11	2.0
(1,6)	1:48:B:LYS:N	2:468:D:PHE:HE1	20	1.92
(1,20)	2:492:D:ASN:N	1:42:B:ARG:HH12	23	1.91
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	10	1.91
(1,20)	2:492:D:ASN:HA	1:72:B:ARG:HH12	22	1.9
(1,12)	1:72:B:ARG:HH12	2:492:D:ASN:HA	22	1.9
(1,9)	1:69:B:LEU:H	2:467:D:MET:SD	22	1.85
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	11	1.84
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	11	1.84
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	11	1.84
(1,35)	2:494:D:LEU:HD13	1:42:B:ARG:HG3	19	1.81
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	19	1.74
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	19	1.74
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	19	1.74
(1,6)	1:48:B:LYS:N	2:468:D:PHE:HE1	6	1.74
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	10	1.73
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	13	1.73
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	13	1.73
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	13	1.73
(1,12)	1:72:B:ARG:HG3	2:494:D:LEU:HD12	5	1.72
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	1	1.71
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	3	1.71
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	2	1.71
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	2	1.71
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	2	1.71
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	10	1.69
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	10	1.69
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	10	1.69
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	7	1.68
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	14	1.68
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	14	1.68
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	14	1.68
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	2	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	20	1.67
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	19	1.67
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	19	1.67
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	19	1.67
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	14	1.66
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	15	1.66
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	5	1.65
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	12	1.65
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	4	1.64
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	7	1.64
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	13	1.63
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	17	1.63
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	23	1.63
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	16	1.62
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	19	1.62
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	1	1.61
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	1	1.61
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	1	1.61
(1,5)	1:45:B:PHE:H	2:468:D:PHE:HE1	7	1.61
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	8	1.6
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	22	1.59
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	11	1.58
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	9	1.58
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	9	1.58
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	9	1.58
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	24	1.55
(1,57)	2:492:D:ASN:H	1:73:B:LEU:HD11	8	1.54
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	24	1.54
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	5	1.54
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	5	1.54
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	5	1.54
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	21	1.53
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	9	1.51
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	15	1.51
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	15	1.51
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	15	1.51
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	6	1.5
(1,64)	1:76:A:GLY:C	1:48:B:LYS:NZ	18	1.49
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	18	1.45
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	18	1.45
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	18	1.45
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	4	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	4	1.44
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	4	1.44
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	23	1.43
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	23	1.43
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	23	1.43
(1,26)	2:467:D:MET:HE1	1:70:B:VAL:HA	20	1.41
(1,26)	2:467:D:MET:HE2	1:70:B:VAL:HA	20	1.41
(1,26)	2:467:D:MET:HE3	1:70:B:VAL:HA	20	1.41
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	1	1.41
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	14	1.38
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	10	1.37
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	10	1.37
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	10	1.37
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	4	1.36
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	4	1.36
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	4	1.36
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	17	1.36
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	17	1.36
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	17	1.36
(1,20)	2:492:D:ASN:HD21	1:72:B:ARG:HH21	14	1.36
(1,12)	1:72:B:ARG:HH21	2:492:D:ASN:HD21	14	1.36
(1,20)	2:492:D:ASN:OD1	1:74:B:ARG:HD2	9	1.29
(1,14)	1:74:B:ARG:HD2	2:492:D:ASN:OD1	9	1.29
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	15	1.27
(1,18)	2:469:D:PRO:HG2	1:68:B:HIS:HE1	5	1.27
(1,6)	1:48:B:LYS:N	2:468:D:PHE:HE1	23	1.27
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG21	1	1.24
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	5	1.23
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	4	1.23
(1,28)	2:486:D:VAL:HG12	1:8:B:LEU:HB3	23	1.23
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG22	15	1.23
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	16	1.22
(1,7)	1:49:B:GLN:HB2	2:494:D:LEU:HD22	21	1.22
(1,6)	1:48:B:LYS:HA	2:468:D:PHE:HE1	14	1.21
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	18	1.2
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	18	1.2
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	18	1.2
(1,10)	1:70:B:VAL:HG23	2:468:D:PHE:HZ	20	1.19
(1,7)	1:49:B:GLN:HB2	2:494:D:LEU:HD22	6	1.19
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	21	1.18
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	24	1.16
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	16	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	2:469:D:PRO:HD3	1:68:B:HIS:HE1	6	1.15
(1,6)	1:48:B:LYS:N	2:468:D:PHE:HE1	4	1.15
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	9	1.14
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	9	1.14
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	9	1.14
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	20	1.12
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	20	1.12
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	20	1.12
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	2	1.11
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	2	1.11
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	2	1.11
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	19	1.08
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	19	1.08
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	19	1.08
(1,11)	1:71:B:LEU:H	2:467:D:MET:HE3	6	1.08
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	3	1.07
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	3	1.07
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	3	1.07
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	11	1.05
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	11	1.05
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	11	1.05
(1,10)	1:70:B:VAL:HG23	2:468:D:PHE:HE2	19	1.05
(1,28)	2:486:D:VAL:HG12	1:8:B:LEU:HB3	1	1.04
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	1	1.03
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	1	1.03
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	1	1.03
(1,6)	1:48:B:LYS:O	2:468:D:PHE:HE1	7	1.01
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG21	16	0.99
(1,9)	1:69:B:LEU:O	2:467:D:MET:HE3	6	0.98
(1,7)	1:49:B:GLN:HB2	2:494:D:LEU:HD23	11	0.98
(1,28)	2:486:D:VAL:HG12	1:8:B:LEU:HB3	21	0.95
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	2	0.95
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	8	0.93
(1,18)	2:469:D:PRO:HG2	1:68:B:HIS:HE1	15	0.92
(1,18)	2:469:D:PRO:HG3	1:68:B:HIS:HE1	17	0.92
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	23	0.91
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	23	0.91
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	23	0.91
(1,10)	1:70:B:VAL:HG13	2:494:D:LEU:HD12	4	0.9
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG21	21	0.89
(1,9)	1:69:B:LEU:H	2:467:D:MET:HE3	14	0.89
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	16	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	16	0.88
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	16	0.88
(1,18)	2:469:D:PRO:HG3	1:68:B:HIS:HE1	13	0.88
(1,20)	2:492:D:ASN:OD1	1:74:B:ARG:HH22	3	0.87
(1,14)	1:74:B:ARG:HH22	2:492:D:ASN:OD1	3	0.87
(1,12)	1:72:B:ARG:HH21	2:492:D:ASN:HA	4	0.87
(1,9)	1:69:B:LEU:H	2:467:D:MET:HE3	19	0.87
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	21	0.86
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	12	0.86
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	3	0.86
(1,10)	1:70:B:VAL:HG11	2:494:D:LEU:HD12	13	0.85
(1,35)	2:494:D:LEU:HD13	1:42:B:ARG:HG3	11	0.84
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	14	0.83
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	14	0.83
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	14	0.83
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG21	5	0.83
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG22	24	0.83
(1,20)	2:492:D:ASN:HA	1:74:B:ARG:HH22	13	0.79
(1,14)	1:74:B:ARG:HH22	2:492:D:ASN:HA	13	0.79
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG21	14	0.79
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	5	0.79
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	12	0.78
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	12	0.78
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	12	0.78
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	13	0.78
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	13	0.78
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	13	0.78
(1,8)	1:68:B:HIS:HE2	2:467:D:MET:HA	20	0.78
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	2	0.76
(1,9)	1:69:B:LEU:O	2:467:D:MET:HE3	24	0.73
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	3	0.72
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	3	0.72
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	3	0.72
(1,9)	1:69:B:LEU:H	2:467:D:MET:HE3	4	0.72
(1,28)	2:486:D:VAL:HG12	1:8:B:LEU:HB3	14	0.7
(1,2)	1:42:B:ARG:HD3	2:494:D:LEU:HD12	8	0.69
(1,11)	1:71:B:LEU:HD12	2:486:D:VAL:HG21	23	0.67
(1,2)	1:42:B:ARG:CZ	2:494:D:LEU:HD21	4	0.67
(1,10)	1:70:B:VAL:HG23	2:468:D:PHE:HE2	11	0.66
(1,2)	1:42:B:ARG:HD3	2:494:D:LEU:HD12	22	0.66
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	15	0.65
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	15	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	15	0.65
(1,10)	1:70:B:VAL:HG23	2:468:D:PHE:HE2	10	0.65
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HB3	18	0.64
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	18	0.64
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	24	0.64
(1,2)	1:42:B:ARG:HE	2:494:D:LEU:HD22	7	0.64
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	9	0.63
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HD23	10	0.63
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	7	0.63
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	9	0.63
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	6	0.62
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	6	0.62
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	6	0.62
(1,17)	2:468:D:PHE:HE1	1:44:B:ILE:HG12	5	0.62
(1,9)	1:69:B:LEU:O	2:467:D:MET:HE3	12	0.62
(1,2)	1:42:B:ARG:HD3	2:494:D:LEU:HD22	11	0.62
(1,35)	2:494:D:LEU:HD13	1:42:B:ARG:HG3	4	0.61
(1,17)	2:468:D:PHE:HE2	1:70:B:VAL:HG23	21	0.61
(1,9)	1:69:B:LEU:H	2:467:D:MET:HE3	10	0.61
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	13	0.61
(1,2)	1:42:B:ARG:HD3	2:494:D:LEU:HD12	16	0.59
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	14	0.58
(1,8)	1:68:B:HIS:HE2	2:466:D:GLU:O	14	0.58
(1,2)	1:42:B:ARG:HH21	2:494:D:LEU:HD21	14	0.58
(1,10)	1:70:B:VAL:HG23	2:468:D:PHE:HE1	12	0.55
(1,9)	1:69:B:LEU:H	2:467:D:MET:HE3	3	0.55
(1,2)	1:42:B:ARG:HH22	2:494:D:LEU:HB3	15	0.55
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HB3	13	0.54
(1,2)	1:42:B:ARG:NH2	2:494:D:LEU:HD21	18	0.53
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	12	0.52
(1,28)	2:486:D:VAL:HG12	1:8:B:LEU:HB3	5	0.52
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	17	0.52
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	17	0.52
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	17	0.52
(1,2)	1:42:B:ARG:HD3	2:494:D:LEU:HD12	1	0.52
(1,2)	1:42:B:ARG:HH12	2:494:D:LEU:HB3	10	0.52
(1,2)	1:42:B:ARG:HD3	2:494:D:LEU:HD12	12	0.52
(1,2)	1:42:B:ARG:HG2	2:494:D:LEU:HD22	20	0.52
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	23	0.51
(1,2)	1:42:B:ARG:NH2	2:494:D:LEU:HD21	19	0.5
(1,2)	1:42:B:ARG:HH22	2:494:D:LEU:HB3	17	0.49
(1,24)	2:467:D:MET:HE1	1:68:B:HIS:HA	12	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,24)	2:467:D:MET:HE2	1:68:B:HIS:HA	12	0.48
(1,24)	2:467:D:MET:HE3	1:68:B:HIS:HA	12	0.48
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	17	0.47
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	3	0.46
(1,7)	1:49:B:GLN:OE1	2:494:D:LEU:HD21	14	0.46
(1,2)	1:42:B:ARG:HH21	2:494:D:LEU:HD21	9	0.46
(1,2)	1:42:B:ARG:HD3	2:494:D:LEU:HD12	23	0.46
(1,28)	2:486:D:VAL:HG12	1:8:B:LEU:HB3	6	0.45
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	1	0.45
(1,9)	1:69:B:LEU:H	2:467:D:MET:HE3	18	0.45
(1,8)	1:68:B:HIS:HB3	2:467:D:MET:HB3	12	0.45
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD23	19	0.45
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	9	0.44
(1,10)	1:70:B:VAL:HG11	2:494:D:LEU:HD13	23	0.44
(1,9)	1:69:B:LEU:H	2:467:D:MET:HE3	11	0.43
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	15	0.43
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	1	0.41
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	19	0.41
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	21	0.41
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	21	0.41
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	21	0.41
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HB3	11	0.41
(1,7)	1:49:B:GLN:HB2	2:494:D:LEU:HD23	20	0.41
(1,9)	1:69:B:LEU:O	2:467:D:MET:HE3	16	0.39
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	10	0.39
(1,2)	1:42:B:ARG:CZ	2:494:D:LEU:HD21	13	0.39
(1,19)	2:486:D:VAL:HG23	1:8:B:LEU:HB3	19	0.38
(1,17)	2:468:D:PHE:HE1	1:44:B:ILE:HG12	15	0.38
(1,13)	1:73:B:LEU:O	2:492:D:ASN:HD22	4	0.38
(1,10)	1:70:B:VAL:HG23	2:468:D:PHE:HE2	14	0.38
(1,2)	1:42:B:ARG:HD3	2:494:D:LEU:HD12	5	0.38
(1,17)	2:468:D:PHE:HE1	1:44:B:ILE:HG12	8	0.37
(1,17)	2:468:D:PHE:HE1	1:70:B:VAL:HG23	1	0.36
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	17	0.36
(1,2)	1:42:B:ARG:HG2	2:494:D:LEU:HD12	2	0.36
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	1	0.35
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HD23	3	0.35
(1,17)	2:468:D:PHE:HZ	1:44:B:ILE:HG12	22	0.35
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	22	0.35
(1,2)	1:42:B:ARG:HD3	2:494:D:LEU:HD13	3	0.35
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	8	0.34
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	24	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	8	0.34
(1,28)	2:486:D:VAL:HG12	1:8:B:LEU:HB3	7	0.34
(1,9)	1:69:B:LEU:O	2:467:D:MET:HE3	21	0.34
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	12	0.34
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	5	0.33
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HD23	15	0.33
(1,16)	2:467:D:MET:HE3	1:8:B:LEU:HD22	20	0.33
(1,9)	1:69:B:LEU:H	2:467:D:MET:HE3	9	0.33
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	6	0.32
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	21	0.32
(1,17)	2:468:D:PHE:HZ	1:70:B:VAL:HG23	24	0.32
(1,4)	1:44:B:ILE:HD13	2:494:D:LEU:HD11	21	0.32
(1,9)	1:69:B:LEU:H	2:467:D:MET:HE3	23	0.31
(1,1)	1:8:B:LEU:HD22	2:467:D:MET:HG3	3	0.31
(1,1)	1:8:B:LEU:HD22	2:467:D:MET:HE2	11	0.31
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	6	0.3
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HB3	4	0.3
(1,17)	2:468:D:PHE:HE2	1:44:B:ILE:HG12	4	0.3
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	10	0.3
(1,8)	1:68:B:HIS:HB3	2:467:D:MET:HG2	8	0.3
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	18	0.29
(1,19)	2:486:D:VAL:O	1:8:B:LEU:HD11	2	0.29
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	18	0.29
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	19	0.29
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	20	0.28
(1,16)	2:467:D:MET:HE2	1:8:B:LEU:HG	12	0.28
(1,10)	1:70:B:VAL:HG23	2:468:D:PHE:HE1	9	0.28
(1,8)	1:68:B:HIS:HE2	2:467:D:MET:HA	18	0.28
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	2	0.27
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	3	0.27
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	16	0.27
(1,9)	1:69:B:LEU:H	2:467:D:MET:HE3	17	0.27
(1,8)	1:68:B:HIS:HD2	2:467:D:MET:HG2	22	0.27
(1,40)	2:494:D:LEU:HD22	1:42:B:ARG:HG3	20	0.26
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	14	0.26
(1,35)	2:494:D:LEU:HD13	1:42:B:ARG:HG3	20	0.25
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	8	0.25
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	8	0.25
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	8	0.25
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	3	0.25
(1,28)	2:486:D:VAL:HG12	1:8:B:LEU:HB3	16	0.24
(1,16)	2:467:D:MET:HG3	1:8:B:LEU:HD21	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	7	0.24
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	24	0.24
(1,10)	1:70:B:VAL:HG13	2:494:D:LEU:HD13	15	0.24
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	15	0.23
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	17	0.23
(1,21)	2:494:D:LEU:HD11	1:44:B:ILE:HD13	20	0.23
(1,17)	2:468:D:PHE:HZ	1:44:B:ILE:HG12	10	0.23
(1,10)	1:70:B:VAL:HG12	2:494:D:LEU:HD12	1	0.23
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	22	0.22
(1,16)	2:467:D:MET:HE1	1:68:B:HIS:HB3	11	0.22
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	2	0.22
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	9	0.22
(1,8)	1:68:B:HIS:HB3	2:467:D:MET:HE1	11	0.22
(1,17)	2:468:D:PHE:HZ	1:44:B:ILE:HG12	14	0.21
(1,16)	2:467:D:MET:HG3	1:8:B:LEU:HD22	17	0.21
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	1	0.21
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	23	0.2
(1,19)	2:486:D:VAL:HG21	1:8:B:LEU:HB3	9	0.2
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HD23	17	0.2
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	6	0.2
(1,8)	1:68:B:HIS:HB3	2:467:D:MET:HE1	1	0.2
(1,8)	1:68:B:HIS:HE2	2:466:D:GLU:O	6	0.2
(1,4)	1:44:B:ILE:HD13	2:494:D:LEU:HD11	4	0.2
(1,1)	1:8:B:LEU:HD23	2:486:D:VAL:HB	17	0.2
(1,54)	2:489:D:THR:H	1:72:B:ARG:HA	2	0.19
(1,33)	2:494:D:LEU:HD11	1:42:B:ARG:HB3	22	0.19
(1,10)	1:70:B:VAL:HG23	2:468:D:PHE:HE2	18	0.19
(1,10)	1:70:B:VAL:HA	2:467:D:MET:HE3	24	0.19
(1,8)	1:68:B:HIS:HB3	2:467:D:MET:HG2	7	0.19
(1,54)	2:489:D:THR:H	1:72:B:ARG:HA	9	0.18
(1,43)	2:494:D:LEU:HD22	1:49:B:GLN:HE21	8	0.18
(1,43)	2:494:D:LEU:HD22	1:49:B:GLN:HE22	8	0.18
(1,21)	2:494:D:LEU:HD11	1:44:B:ILE:HG12	11	0.18
(1,21)	2:494:D:LEU:HD11	1:44:B:ILE:HD13	14	0.18
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HD11	21	0.18
(1,16)	2:467:D:MET:HA	1:68:B:HIS:HE2	3	0.18
(1,16)	2:467:D:MET:HE3	1:70:B:VAL:HG22	8	0.18
(1,10)	1:70:B:VAL:HG22	2:467:D:MET:HE3	8	0.18
(1,8)	1:68:B:HIS:HE2	2:467:D:MET:HA	3	0.18
(1,4)	1:44:B:ILE:HD13	2:494:D:LEU:HD11	14	0.18
(1,1)	1:8:B:LEU:HD22	2:467:D:MET:HG3	10	0.18
(1,1)	1:8:B:LEU:HD11	2:486:D:VAL:HB	21	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	2:494:D:LEU:HD22	1:42:B:ARG:HG3	14	0.16
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	13	0.16
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	5	0.16
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	5	0.16
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	5	0.16
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	21	0.16
(1,4)	1:44:B:ILE:HD12	2:494:D:LEU:HD22	8	0.16
(1,2)	1:42:B:ARG:HH12	2:494:D:LEU:HB3	21	0.16
(1,54)	2:489:D:THR:H	1:72:B:ARG:HA	3	0.15
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	10	0.15
(1,21)	2:494:D:LEU:HD22	1:49:B:GLN:HG3	8	0.15
(1,21)	2:494:D:LEU:HD11	1:44:B:ILE:HD13	12	0.15
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HD23	7	0.15
(1,17)	2:468:D:PHE:HE2	1:70:B:VAL:HG23	17	0.15
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	4	0.15
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	15	0.15
(1,10)	1:70:B:VAL:HG23	2:468:D:PHE:HE2	17	0.15
(1,8)	1:68:B:HIS:HB3	2:467:D:MET:HE1	9	0.15
(1,8)	1:68:B:HIS:HE2	2:466:D:GLU:O	15	0.15
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	8	0.15
(1,4)	1:44:B:ILE:HD13	2:494:D:LEU:HD11	22	0.15
(1,1)	1:8:B:LEU:HD23	2:486:D:VAL:HB	7	0.15
(1,57)	2:492:D:ASN:H	1:73:B:LEU:HD11	14	0.14
(1,21)	2:494:D:LEU:HD11	1:44:B:ILE:HD13	19	0.14
(1,21)	2:494:D:LEU:HD22	1:49:B:GLN:HG3	23	0.14
(1,20)	2:492:D:ASN:HA	1:74:B:ARG:HH21	8	0.14
(1,19)	2:486:D:VAL:HG23	1:8:B:LEU:HB3	1	0.14
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HD23	12	0.14
(1,17)	2:468:D:PHE:HZ	1:44:B:ILE:HG12	12	0.14
(1,16)	2:467:D:MET:HG3	1:8:B:LEU:HD22	23	0.14
(1,14)	1:74:B:ARG:HH21	2:492:D:ASN:HA	8	0.14
(1,9)	1:69:B:LEU:H	2:467:D:MET:HE3	2	0.14
(1,8)	1:68:B:HIS:HB3	2:467:D:MET:HE1	2	0.14
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	23	0.14
(1,4)	1:44:B:ILE:HD13	2:494:D:LEU:HD11	5	0.14
(1,4)	1:44:B:ILE:HG12	2:468:D:PHE:HZ	12	0.14
(1,1)	1:8:B:LEU:HB3	2:486:D:VAL:HG23	1	0.14
(1,1)	1:8:B:LEU:HD23	2:486:D:VAL:HB	12	0.14
(1,57)	2:492:D:ASN:H	1:73:B:LEU:HD11	6	0.13
(1,54)	2:489:D:THR:H	1:72:B:ARG:HA	4	0.13
(1,52)	2:494:D:LEU:HD22	1:43:B:LEU:H	6	0.13
(1,40)	2:494:D:LEU:HD22	1:42:B:ARG:HG3	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	2:486:D:VAL:HG22	1:8:B:LEU:HB3	7	0.13
(1,23)	2:467:D:MET:HE1	1:44:B:ILE:HD11	24	0.13
(1,23)	2:467:D:MET:HE2	1:44:B:ILE:HD11	24	0.13
(1,23)	2:467:D:MET:HE3	1:44:B:ILE:HD11	24	0.13
(1,21)	2:494:D:LEU:HD11	1:44:B:ILE:HD13	3	0.13
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HD23	5	0.13
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HD13	24	0.13
(1,17)	2:468:D:PHE:HE1	1:70:B:VAL:HG23	16	0.13
(1,17)	2:468:D:PHE:HZ	1:44:B:ILE:HG12	19	0.13
(1,16)	2:467:D:MET:HB3	1:68:B:HIS:HB3	21	0.13
(1,15)	2:466:D:GLU:O	1:68:B:HIS:HE2	23	0.13
(1,8)	1:68:B:HIS:HB3	2:467:D:MET:HB3	21	0.13
(1,8)	1:68:B:HIS:HE2	2:466:D:GLU:O	23	0.13
(1,4)	1:44:B:ILE:HD13	2:494:D:LEU:HD22	16	0.13
(1,4)	1:44:B:ILE:HG12	2:468:D:PHE:HZ	19	0.13
(1,1)	1:8:B:LEU:HD23	2:486:D:VAL:HB	5	0.13
(1,1)	1:8:B:LEU:HD22	2:467:D:MET:HE2	19	0.13
(1,54)	2:489:D:THR:H	1:72:B:ARG:HA	5	0.12
(1,52)	2:494:D:LEU:HD22	1:43:B:LEU:H	16	0.12
(1,50)	2:494:D:LEU:HD22	1:70:B:VAL:H	7	0.12
(1,40)	2:494:D:LEU:HD22	1:42:B:ARG:HG3	3	0.12
(1,36)	2:494:D:LEU:HD11	1:48:B:LYS:HA	3	0.12
(1,28)	2:486:D:VAL:HG12	1:8:B:LEU:HB3	24	0.12
(1,25)	2:467:D:MET:HE1	1:8:B:LEU:HA	22	0.12
(1,25)	2:467:D:MET:HE2	1:8:B:LEU:HA	22	0.12
(1,25)	2:467:D:MET:HE3	1:8:B:LEU:HA	22	0.12
(1,19)	2:486:D:VAL:HB	1:8:B:LEU:HD23	20	0.12
(1,1)	1:8:B:LEU:HD23	2:486:D:VAL:HB	20	0.12
(1,54)	2:489:D:THR:H	1:72:B:ARG:HA	14	0.11
(1,54)	2:489:D:THR:H	1:72:B:ARG:HA	19	0.11
(1,50)	2:494:D:LEU:HD22	1:70:B:VAL:H	8	0.11
(1,42)	2:494:D:LEU:HD21	1:49:B:GLN:HB2	6	0.11
(1,36)	2:494:D:LEU:HD11	1:48:B:LYS:HA	2	0.11
(1,21)	2:494:D:LEU:HD22	1:49:B:GLN:HG3	4	0.11
(1,21)	2:494:D:LEU:HD11	1:44:B:ILE:HD13	13	0.11
(1,21)	2:494:D:LEU:HD11	1:44:B:ILE:HD13	15	0.11
(1,10)	1:70:B:VAL:HG23	2:468:D:PHE:HE1	3	0.11
(1,8)	1:68:B:HIS:HB3	2:467:D:MET:HB3	24	0.11
(1,7)	1:49:B:GLN:HG3	2:494:D:LEU:HD22	4	0.11
(1,4)	1:44:B:ILE:HD13	2:494:D:LEU:HD11	13	0.11
(1,4)	1:44:B:ILE:HD13	2:494:D:LEU:HD11	15	0.11
(1,4)	1:44:B:ILE:HD13	2:494:D:LEU:HD11	24	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,57)	2:492:D:ASN:H	1:73:B:LEU:HD11	2	0.1
(1,57)	2:492:D:ASN:H	1:73:B:LEU:HD11	23	0.1
(1,34)	2:494:D:LEU:HD12	1:42:B:ARG:HD2	3	0.1
(1,21)	2:494:D:LEU:HD11	1:44:B:ILE:HD13	10	0.1
(1,4)	1:44:B:ILE:HD13	2:494:D:LEU:HD11	10	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found