



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 06:29 PM UTC

PDB ID : 2LXP / pdb_00002lxp
BMRB ID : 18688
Title : NMR structure of two domains in ubiquitin ligase gp78, RING and G2BR, bound to its conjugating enzyme Ube2g
Authors : Das, R.; Linag, Y.; Mariano, J.; Li, J.; Huang, T.; King, A.; Weissman, A.; Ji, X.; Byrd, R.
Deposited on : 2012-08-30

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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

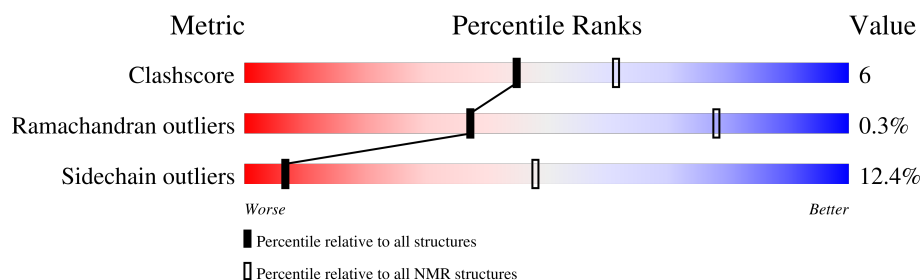
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 3%.

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	164	 79% 13% .. 5%
2	B	27	 52% 48%
3	C	58	 83% 17%

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 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:2-A:96, A:108-A:165, B:574-B:600, C:327-C:384 (238)	0.48	14

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

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

The models can be grouped into 5 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3795 atoms, of which 1880 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin-conjugating enzyme E2 G2.

Mol	Chain	Residues	Atoms						Trace
1	A	156	Total	C	H	N	O	S	0
			2444	793	1213	200	228	10	

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

Mol	Chain	Residues	Atoms						Trace
2	B	27	Total	C	H	N	O	S	0
			483	142	248	50	42	1	

- Molecule 3 is a protein called E3 ubiquitin-protein ligase AMFR.

Mol	Chain	Residues	Atoms						Trace
3	C	58	Total	C	H	N	O	S	0
			866	272	419	80	87	8	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

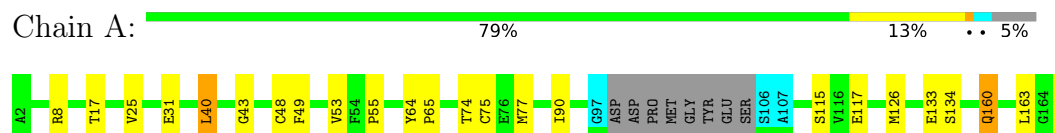
Mol	Chain	Residues	Atoms	
4	C	2	Total	Zn
			2	2

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.

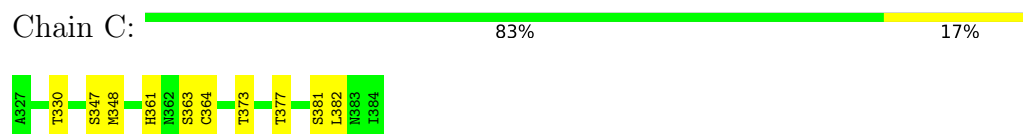
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR



- Molecule 3: E3 ubiquitin-protein ligase AMFR

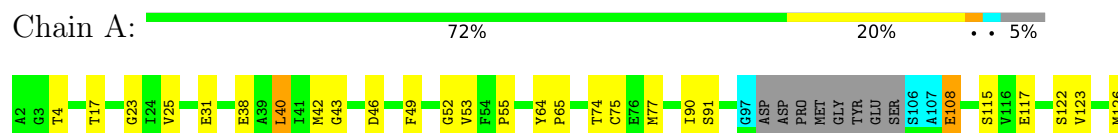


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

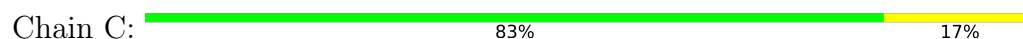




- Molecule 2: E3 ubiquitin-protein ligase AMFR

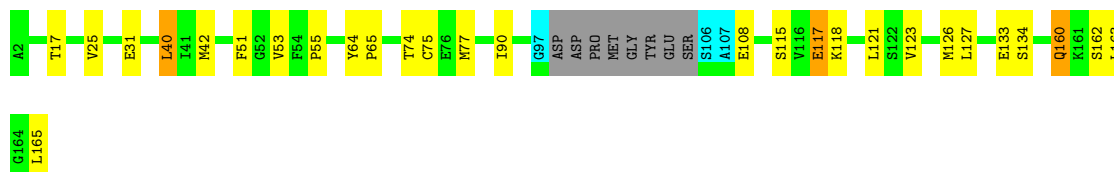
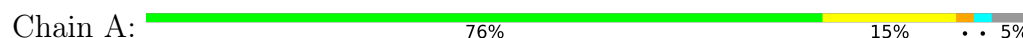


- Molecule 3: E3 ubiquitin-protein ligase AMFR



4.2.2 Score per residue for model 2

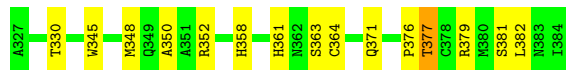
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR



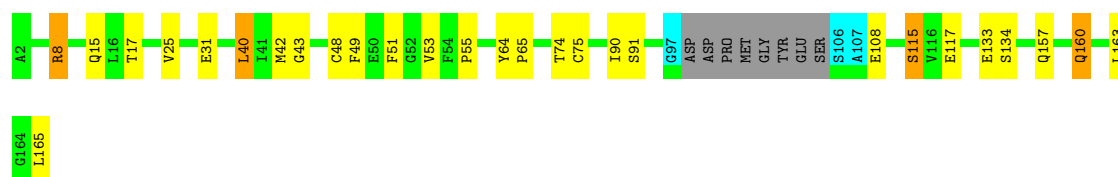
- Molecule 3: E3 ubiquitin-protein ligase AMFR



4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

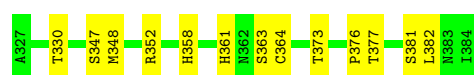
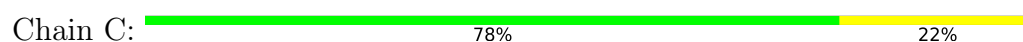




- Molecule 2: E3 ubiquitin-protein ligase AMFR

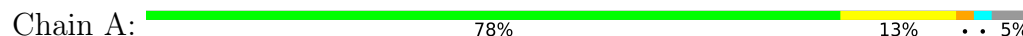


- Molecule 3: E3 ubiquitin-protein ligase AMFR



4.2.4 Score per residue for model 4

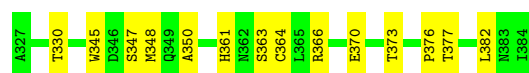
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR



- Molecule 3: E3 ubiquitin-protein ligase AMFR



4.2.5 Score per residue for model 5

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2





- Molecule 2: E3 ubiquitin-protein ligase AMFR

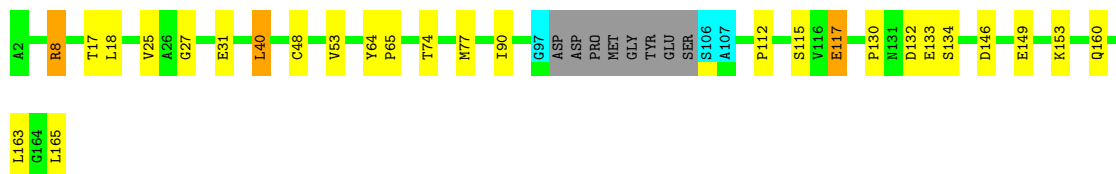
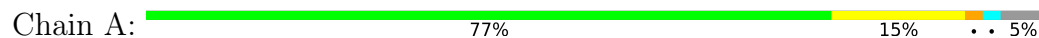


- Molecule 3: E3 ubiquitin-protein ligase AMFR



4.2.6 Score per residue for model 6

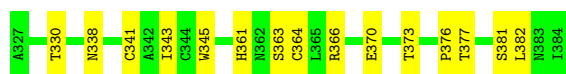
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR

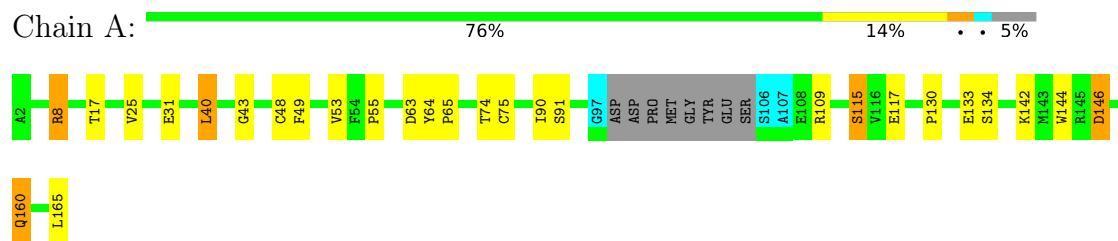


- Molecule 3: E3 ubiquitin-protein ligase AMFR



4.2.7 Score per residue for model 7

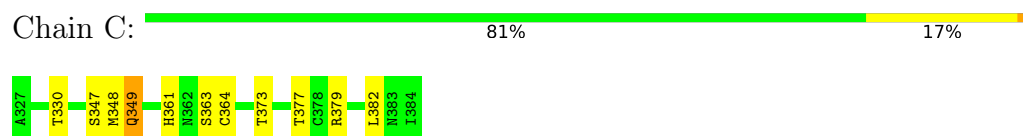
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR

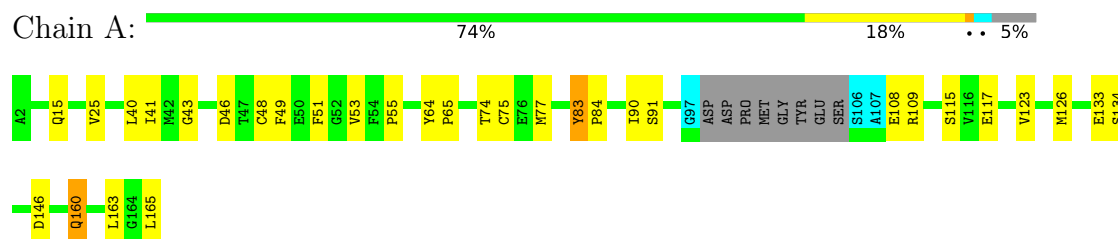


- Molecule 3: E3 ubiquitin-protein ligase AMFR

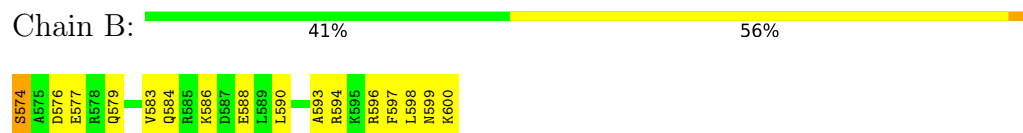


4.2.8 Score per residue for model 8

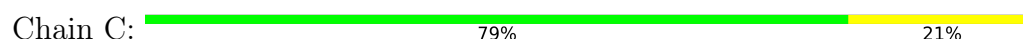
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR



- Molecule 3: E3 ubiquitin-protein ligase AMFR

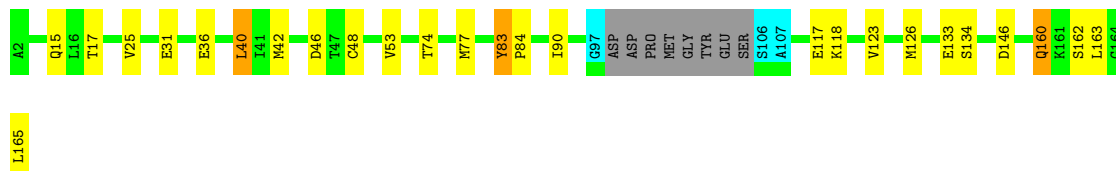




4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

Chain A: 77% 14% 5%



- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain B: 52% 48%



- Molecule 3: E3 ubiquitin-protein ligase AMFR

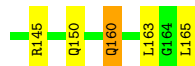
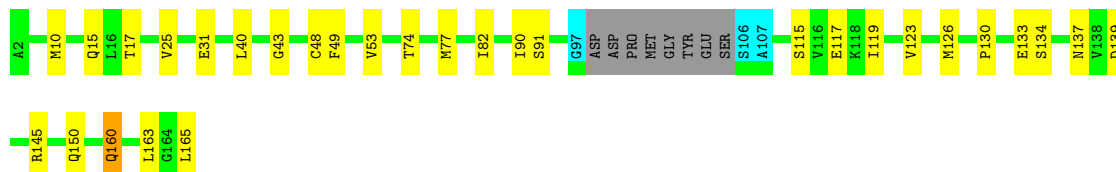
Chain C: 83% 17%



4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

Chain A: 75% 18% 5%

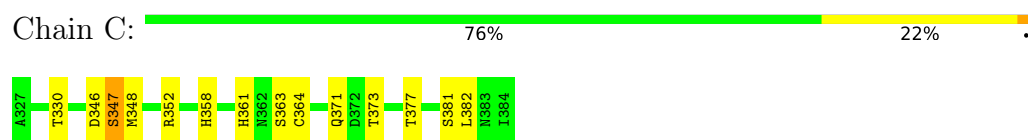


- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain B: 56% 44%

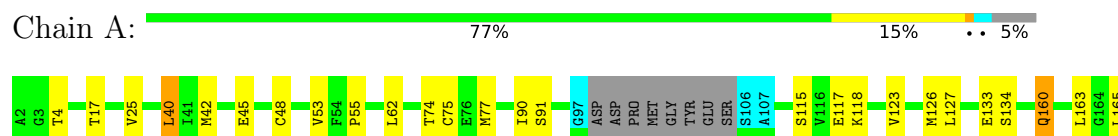


- Molecule 3: E3 ubiquitin-protein ligase AMFR

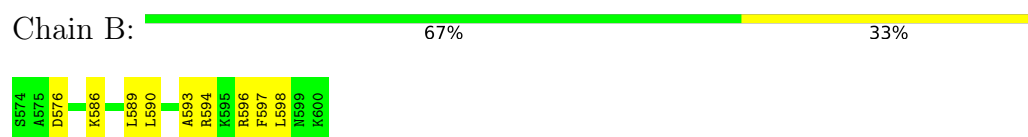


4.2.11 Score per residue for model 11

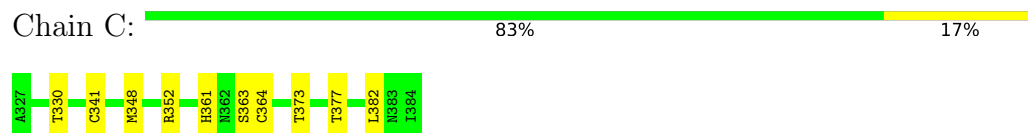
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR

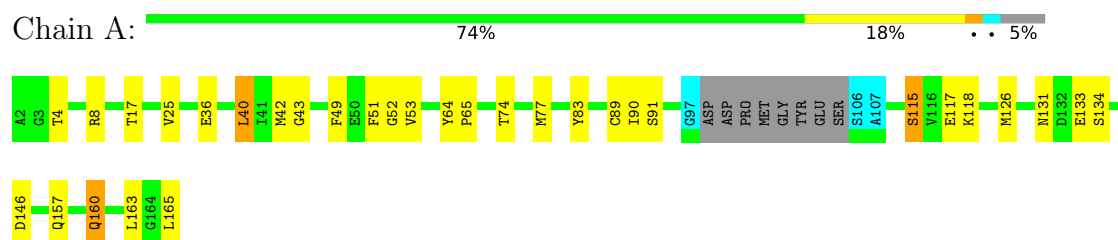


- Molecule 3: E3 ubiquitin-protein ligase AMFR



4.2.12 Score per residue for model 12

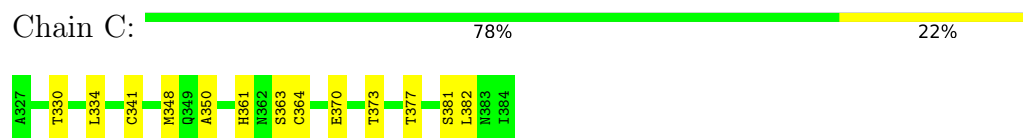
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR

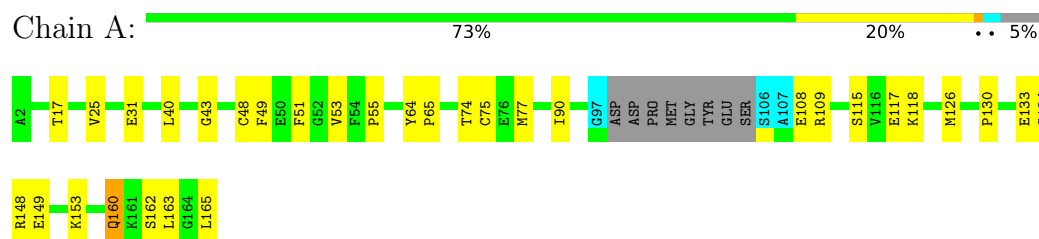


- Molecule 3: E3 ubiquitin-protein ligase AMFR

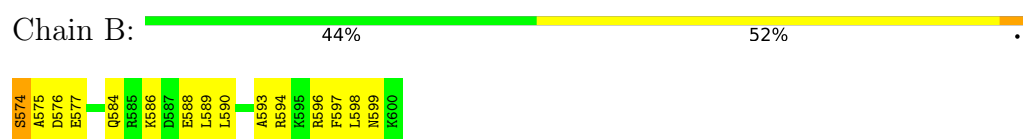


4.2.13 Score per residue for model 13

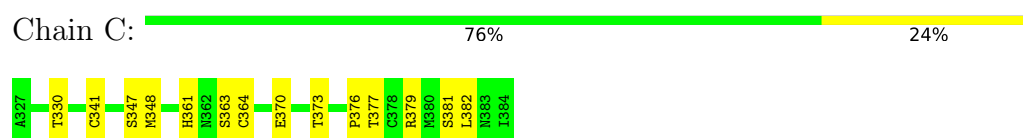
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR

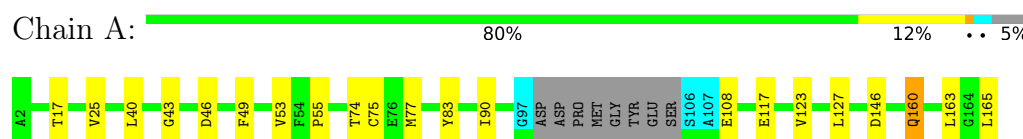


- Molecule 3: E3 ubiquitin-protein ligase AMFR



4.2.14 Score per residue for model 14 (medoid)

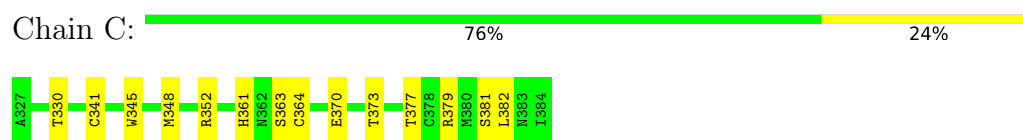
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR

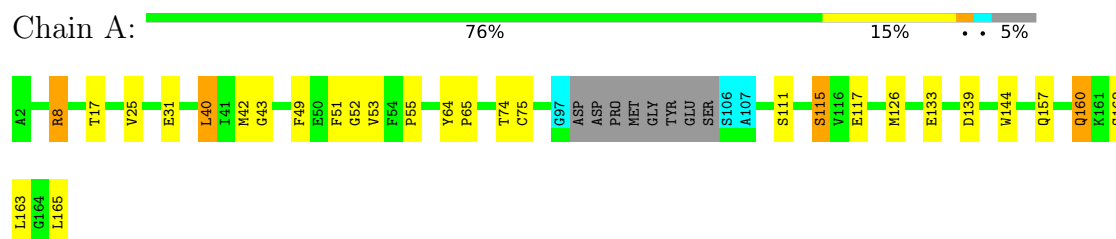


- Molecule 3: E3 ubiquitin-protein ligase AMFR



4.2.15 Score per residue for model 15

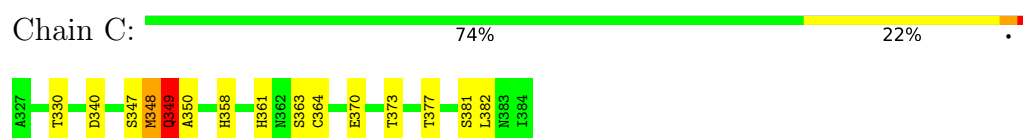
- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR

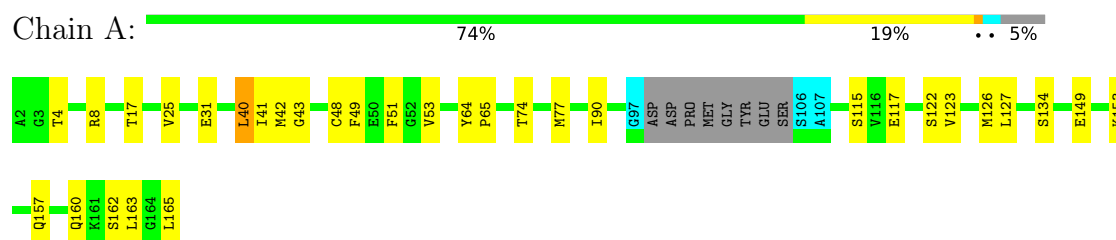


- Molecule 3: E3 ubiquitin-protein ligase AMFR



4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2



- Molecule 2: E3 ubiquitin-protein ligase AMFR





- Molecule 3: E3 ubiquitin-protein ligase AMFR

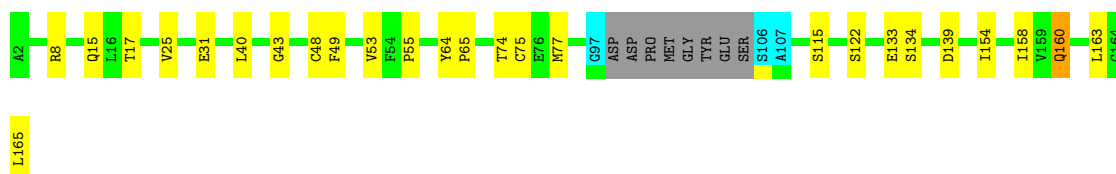
Chain C: 74% 26%



4.2.17 Score per residue for model 17

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

Chain A: 77% 15% 5%



- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain B: 56% 44%



- Molecule 3: E3 ubiquitin-protein ligase AMFR

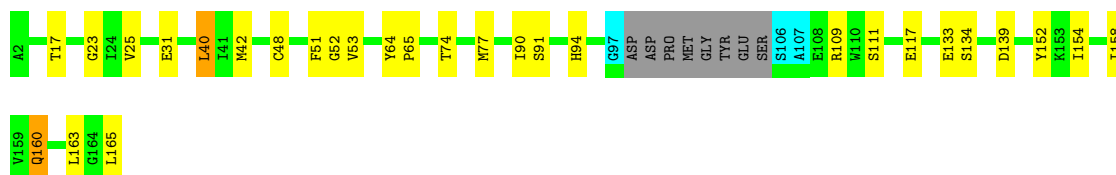
Chain C: 74% 26%



4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

Chain A: 76% 16% 5%



- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain B:  52% 44% .



- Molecule 3: E3 ubiquitin-protein ligase AMFR

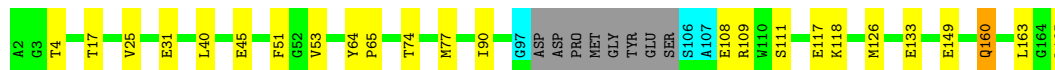
Chain C:  79% 21%



4.2.19 Score per residue for model 19

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

Chain A:  79% 14% .. 5%



- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain B:  56% 41% .



- Molecule 3: E3 ubiquitin-protein ligase AMFR

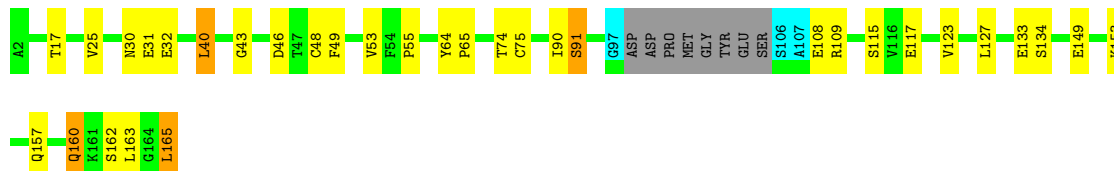
Chain C:  78% 22%



4.2.20 Score per residue for model 20

- Molecule 1: Ubiquitin-conjugating enzyme E2 G2

Chain A:  73% 18% .. 5%



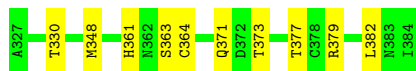
- Molecule 2: E3 ubiquitin-protein ligase AMFR

Chain B:  67% 33%



- Molecule 3: E3 ubiquitin-protein ligase AMFR

Chain C:  83% 17%



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *Lowest Haddock Scores*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
CNS	structure solution	
X-PLOR NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	110
Number of shifts mapped to atoms	110
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

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.

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 ⓘ

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	1216	1200	1197	20±3
2	B	235	248	247	16±2
3	C	447	419	416	3±3
All	All	38000	37340	37200	477

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:348:MET:HE2	3:C:349:GLN:N	1.25	1.41	15	1
3:C:348:MET:CE	3:C:349:GLN:HB2	1.06	1.80	15	1
1:A:53:VAL:HG21	2:B:590:LEU:HA	1.03	1.28	2	20
3:C:348:MET:CE	3:C:349:GLN:CB	1.02	2.37	15	1
3:C:348:MET:HE2	3:C:349:GLN:CA	1.00	1.84	15	1
3:C:348:MET:HE3	3:C:349:GLN:HB2	0.98	1.34	15	1
3:C:348:MET:CE	3:C:349:GLN:N	0.88	2.34	15	1
3:C:348:MET:HE1	3:C:350:ALA:H	0.87	1.26	15	1
3:C:348:MET:HE2	3:C:349:GLN:H	0.78	1.35	15	1
3:C:348:MET:CE	3:C:350:ALA:H	0.77	1.91	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:348:MET:CE	3:C:349:GLN:CA	0.76	2.63	15	1
2:B:574:SER:N	2:B:577:GLU:HB2	0.71	2.00	15	13
1:A:25:VAL:HG23	2:B:589:LEU:HD22	0.69	1.61	9	6
1:A:165:LEU:HD21	2:B:594:ARG:HD3	0.69	1.64	20	15
3:C:361:HIS:HB2	3:C:364:CYS:SG	0.68	2.28	14	20
1:A:163:LEU:HD22	2:B:594:ARG:HG3	0.68	1.65	2	18
1:A:42:MET:HB2	2:B:589:LEU:HD11	0.67	1.65	12	9
1:A:40:LEU:HD12	2:B:586:LYS:HG2	0.65	1.68	4	17
1:A:163:LEU:HD21	2:B:593:ALA:HB3	0.64	1.68	10	18
3:C:348:MET:CE	3:C:350:ALA:N	0.63	2.62	15	1
1:A:31:GLU:HG3	2:B:575:ALA:O	0.62	1.94	2	15
1:A:165:LEU:HD13	2:B:598:LEU:HD21	0.62	1.72	12	20
1:A:25:VAL:HG11	2:B:586:LYS:HG3	0.61	1.71	17	20
1:A:55:PRO:HD2	1:A:75:CYS:SG	0.60	2.36	20	13
1:A:163:LEU:HD22	2:B:594:ARG:CG	0.60	2.27	11	19
1:A:25:VAL:CG1	2:B:586:LYS:HG3	0.58	2.27	1	16
1:A:40:LEU:CG	2:B:586:LYS:HG2	0.58	2.28	1	16
1:A:40:LEU:HD11	2:B:586:LYS:HG2	0.58	1.74	12	3
1:A:51:PHE:CE1	2:B:596:ARG:HB3	0.57	2.34	8	7
1:A:40:LEU:CD1	2:B:586:LYS:HG2	0.57	2.29	4	17
1:A:108:GLU:OE2	3:C:379:ARG:NH2	0.57	2.30	2	1
1:A:163:LEU:HD21	2:B:593:ALA:CB	0.57	2.29	10	8
3:C:348:MET:HE1	3:C:350:ALA:N	0.56	2.09	15	1
1:A:160:GLN:NE2	2:B:597:PHE:HZ	0.56	1.99	9	17
2:B:595:LYS:O	2:B:599:ASN:HB3	0.55	2.01	15	1
1:A:53:VAL:HB	2:B:590:LEU:HD13	0.54	1.79	7	10
1:A:23:GLY:HA2	2:B:589:LEU:CD1	0.54	2.33	18	2
1:A:64:TYR:CD1	1:A:65:PRO:HA	0.53	2.39	6	16
1:A:149:GLU:O	1:A:153:LYS:HG2	0.52	2.04	6	4
1:A:43:GLY:HA3	1:A:49:PHE:O	0.51	2.05	12	14
1:A:8:ARG:NH2	1:A:115:SER:HA	0.51	2.21	5	7
3:C:348:MET:HE2	3:C:349:GLN:CB	0.51	2.11	15	1
1:A:40:LEU:HD12	2:B:589:LEU:HD23	0.51	1.83	3	2
1:A:53:VAL:CB	2:B:590:LEU:HD13	0.50	2.36	7	6
3:C:341:CYS:HB2	3:C:361:HIS:CE1	0.50	2.41	17	9
1:A:91:SER:O	1:A:109:ARG:HA	0.50	2.06	20	4
1:A:115:SER:HB2	1:A:117:GLU:OE1	0.50	2.06	6	1
1:A:123:VAL:O	1:A:127:LEU:HG	0.49	2.07	16	6
1:A:108:GLU:HA	3:C:379:ARG:NH1	0.47	2.23	13	5
3:C:366:ARG:O	3:C:370:GLU:HG3	0.47	2.10	16	1
1:A:30:ASN:OD1	1:A:32:GLU:HG2	0.47	2.10	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:GLU:O	1:A:121:LEU:HG	0.46	2.10	2	1
1:A:42:MET:HA	1:A:52:GLY:O	0.46	2.11	15	4
1:A:40:LEU:HD12	2:B:586:LYS:CG	0.45	2.39	4	11
1:A:130:PRO:HD2	1:A:144:TRP:CH2	0.45	2.46	7	1
1:A:157:GLN:HA	1:A:160:GLN:OE1	0.45	2.12	20	2
1:A:94:HIS:O	1:A:109:ARG:HG2	0.45	2.12	18	1
1:A:82:ILE:O	1:A:137:ASN:HB2	0.45	2.12	10	1
1:A:31:GLU:OE2	2:B:578:ARG:HB2	0.45	2.12	16	1
1:A:83:TYR:CD1	1:A:84:PRO:HD2	0.44	2.48	9	1
2:B:587:ASP:O	2:B:591:GLN:HG2	0.44	2.13	12	1
2:B:596:ARG:HA	2:B:599:ASN:ND2	0.44	2.27	13	2
1:A:25:VAL:HB	1:A:40:LEU:HB2	0.44	1.88	20	1
1:A:123:VAL:O	1:A:126:MET:HG2	0.44	2.13	1	6
1:A:53:VAL:HG21	2:B:590:LEU:CA	0.44	2.33	3	1
3:C:350:ALA:O	3:C:361:HIS:HA	0.43	2.13	9	5
1:A:83:TYR:CD2	1:A:84:PRO:HD2	0.43	2.49	8	1
1:A:31:GLU:HG2	2:B:579:GLN:CG	0.43	2.44	16	1
1:A:112:PRO:CB	3:C:343:ILE:HA	0.43	2.44	5	2
1:A:160:GLN:NE2	2:B:597:PHE:CZ	0.42	2.87	17	3
3:C:346:ASP:CG	3:C:347:SER:H	0.42	2.22	10	1
2:B:579:GLN:O	2:B:583:VAL:HG23	0.42	2.15	8	2
1:A:51:PHE:O	2:B:593:ALA:HB1	0.42	2.13	13	2
1:A:154:ILE:O	1:A:158:ILE:HG12	0.42	2.14	18	3
1:A:108:GLU:HB2	3:C:379:ARG:CZ	0.41	2.45	19	1
1:A:150:GLN:OE1	1:A:150:GLN:HA	0.41	2.15	10	1
3:C:358:HIS:CE1	3:C:377:THR:HB	0.41	2.51	2	1
3:C:366:ARG:O	3:C:370:GLU:HB2	0.41	2.16	4	1
1:A:114:GLN:HE21	1:A:114:GLN:HA	0.41	1.74	4	1
1:A:40:LEU:HG	2:B:586:LYS:HG2	0.41	1.93	5	1
1:A:142:LYS:O	1:A:146:ASP:HB2	0.41	2.16	7	1
1:A:27:GLY:HA3	2:B:582:LEU:HD21	0.40	1.92	6	1
1:A:119:ILE:O	1:A:123:VAL:HG23	0.40	2.16	10	1
1:A:83:TYR:HE2	1:A:89:CYS:SG	0.40	2.39	12	1
2:B:584:GLN:O	2:B:588:GLU:HG3	0.40	2.16	8	1
2:B:584:GLN:O	2:B:588:GLU:HG2	0.40	2.16	13	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	151/164 (92%)	143±2 (95±1%)	8±2 (5±1%)	0±1 (0±0%)	44	80
2	B	25/27 (93%)	21±0 (82±2%)	4±0 (18±2%)	0±0 (0±0%)	100	100
3	C	56/58 (97%)	47±2 (83±4%)	9±2 (16±4%)	0±0 (1±1%)	16	66
All	All	4640/4980 (93%)	4200 (91%)	425 (9%)	15 (0%)	37	78

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	C	376	PRO	8
1	A	130	PRO	3
3	C	349	GLN	2
1	A	132	ASP	1
1	A	148	ARG	1

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/142 (94%)	120±2 (89±2%)	14±2 (11±2%)	9	52
2	B	25/25 (100%)	22±1 (89±5%)	3±1 (11±5%)	8	51
3	C	51/51 (100%)	42±2 (82±3%)	9±2 (18±3%)	4	37
All	All	4200/4360 (96%)	3679 (88%)	521 (12%)	7	48

All 74 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	160	GLN	20
3	C	330	THR	20
3	C	377	THR	20
1	A	17	THR	19
1	A	74	THR	19
1	A	117	GLU	19
3	C	363	SER	19
1	A	90	ILE	18
1	A	133	GLU	18
3	C	348	MET	18
3	C	382	LEU	18
1	A	134	SER	17
3	C	373	THR	17
1	A	77	MET	16
1	A	115	SER	15
1	A	48	CYS	13
1	A	40	LEU	12
2	B	576	ASP	12
3	C	381	SER	12
2	B	599	ASN	11
3	C	347	SER	11
3	C	352	ARG	8
1	A	146	ASP	8
3	C	370	GLU	8
2	B	574	SER	7
1	A	118	LYS	7
3	C	345	TRP	7
1	A	8	ARG	7
1	A	4	THR	6
1	A	91	SER	6
1	A	126	MET	6
1	A	162	SER	6
2	B	587	ASP	6
1	A	15	GLN	6
1	A	46	ASP	5
3	C	358	HIS	5
2	B	596	ARG	5
2	B	589	LEU	4
1	A	157	GLN	4
1	A	83	TYR	4
2	B	600	LYS	4
1	A	139	ASP	4
1	A	108	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	122	SER	3
3	C	371	GLN	3
2	B	595	LYS	3
3	C	338	ASN	3
3	C	367	SER	3
1	A	111	SER	3
3	C	349	GLN	2
3	C	379	ARG	2
1	A	41	ILE	2
1	A	36	GLU	2
1	A	145	ARG	2
1	A	45	GLU	2
1	A	109	ARG	2
3	C	340	ASP	2
1	A	38	GLU	1
2	B	592	GLN	1
1	A	114	GLN	1
1	A	18	LEU	1
2	B	581	MET	1
3	C	366	ARG	1
1	A	63	ASP	1
3	C	369	LEU	1
1	A	10	MET	1
1	A	62	LEU	1
1	A	131	ASN	1
2	B	577	GLU	1
3	C	334	LEU	1
1	A	144	TRP	1
1	A	152	TYR	1
1	A	149	GLU	1
1	A	165	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 3% for the well-defined parts and 3% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	110
Number of shifts mapped to atoms	110
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	55	0.45 ± 0.36	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 3%, i.e. 109 atoms were assigned a chemical shift out of a possible 3272. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	109/1165 (9%)	54/468 (12%)	0/476 (0%)	55/221 (25%)
Sidechain	0/1873 (0%)	0/1216 (0%)	0/581 (0%)	0/76 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/234 (0%)	0/117 (0%)	0/108 (0%)	0/9 (0%)
Overall	109/3272 (3%)	54/1801 (3%)	0/1165 (0%)	55/306 (18%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 109 atoms were assigned a chemical shift out of a possible 3295. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	109/1181 (9%)	54/475 (11%)	0/482 (0%)	55/224 (25%)
Sidechain	0/1880 (0%)	0/1221 (0%)	0/583 (0%)	0/76 (0%)
Aromatic	0/234 (0%)	0/117 (0%)	0/108 (0%)	0/9 (0%)
Overall	109/3295 (3%)	54/1813 (3%)	0/1173 (0%)	55/309 (18%)

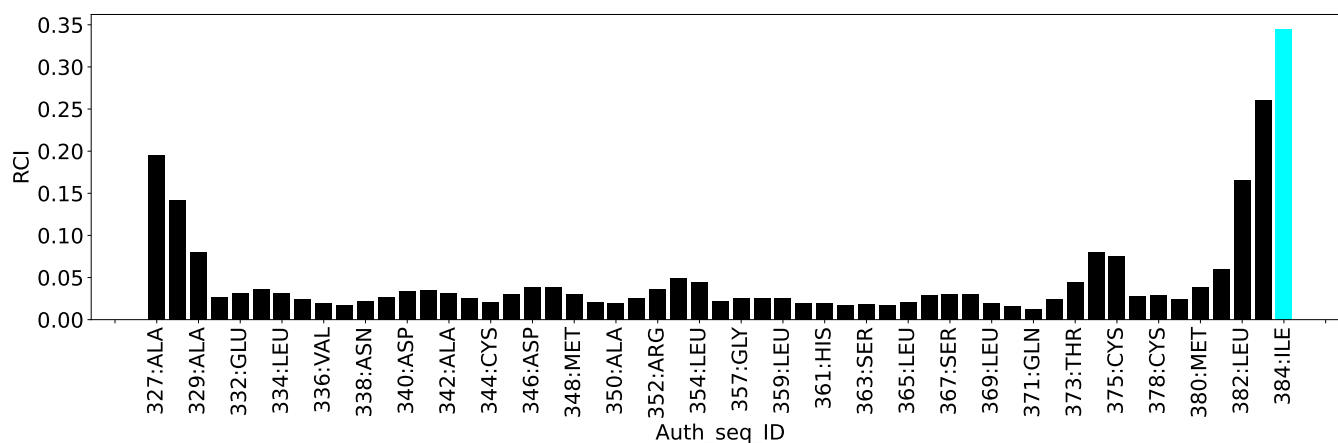
7.1.4 Statistically unusual chemical shifts [i](#)

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 C:



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	65
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	2
Long range ($ i-j \geq 5$)	4
Inter-chain	45
Hydrogen bond restraints	0
Disulfide bond restraints	6
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)	2.4	0.2
0.2-0.5 (Medium)	3.6	0.5
>0.5 (Large)	10.1	7.22

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 ⓘ

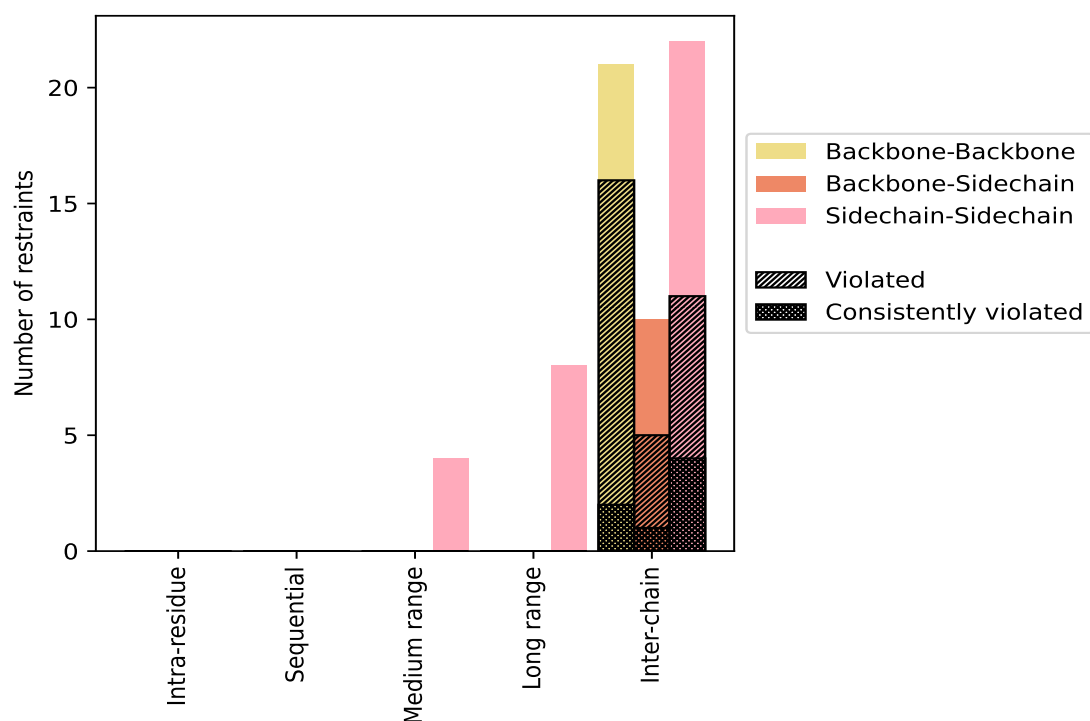
9.1 Summary of distance violations ⓘ

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)	2	3.1	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	2	3.1	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	4	6.2	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	4	6.2	0	0.0	0.0	0	0.0	0.0
Inter-chain	45	69.2	30	66.7	46.2	7	15.6	10.8
Backbone-Backbone	21	32.3	16	76.2	24.6	2	9.5	3.1
Backbone-Sidechain	10	15.4	5	50.0	7.7	1	10.0	1.5
Sidechain-Sidechain	14	21.5	9	64.3	13.8	4	28.6	6.2
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	6	9.2	0	0.0	0.0	0	0.0	0.0
Total	65	100.0	32	49.2	49.2	7	10.8	10.8
Backbone-Backbone	21	32.3	16	76.2	24.6	2	9.5	3.1
Backbone-Sidechain	10	15.4	5	50.0	7.7	1	10.0	1.5
Sidechain-Sidechain	34	52.3	11	32.4	16.9	4	11.8	6.2

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	0	0	0	0	15	15	1.42	5.88	1.78	0.57
2	0	0	0	0	15	15	1.47	5.93	1.61	1.01
3	0	0	0	0	17	17	1.46	6.17	1.76	0.57
4	0	0	0	0	21	21	1.42	6.01	1.73	0.66
5	0	0	0	0	15	15	1.53	6.24	1.8	0.66
6	0	0	0	0	16	16	1.67	6.12	1.84	0.84
7	0	0	0	0	18	18	1.65	7.11	2.19	0.5
8	0	0	0	0	18	18	1.76	7.22	2.12	0.68
9	0	0	0	0	16	16	1.56	5.95	1.75	0.7
10	0	0	0	0	21	21	1.09	6.0	1.61	0.38

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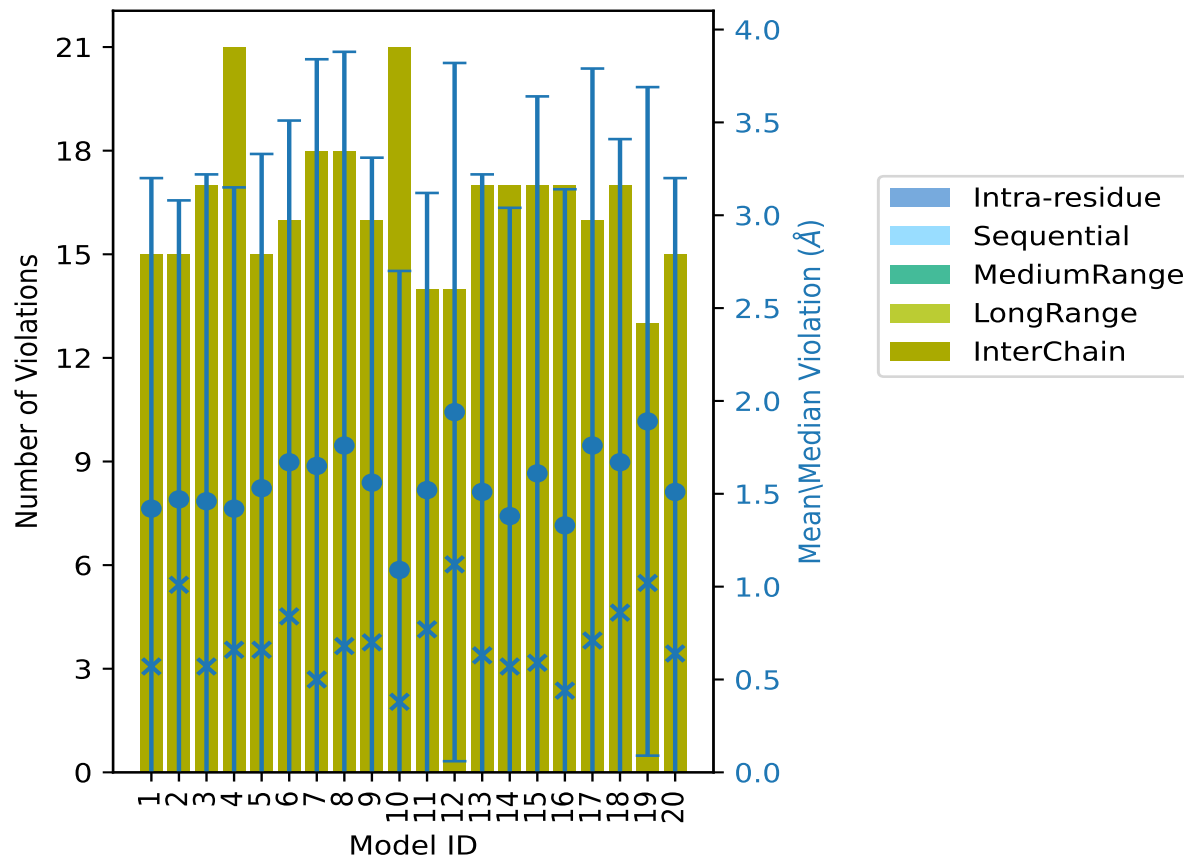
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	0	14	14	1.52	5.78	1.6	0.77
12	0	0	0	0	14	14	1.94	5.82	1.88	1.12
13	0	0	0	0	17	17	1.51	5.71	1.71	0.63
14	0	0	0	0	17	17	1.38	6.03	1.66	0.57
15	0	0	0	0	17	17	1.61	6.3	2.03	0.59
16	0	0	0	0	17	17	1.33	6.32	1.81	0.44
17	0	0	0	0	16	16	1.76	6.03	2.03	0.71
18	0	0	0	0	17	17	1.67	6.35	1.74	0.86
19	0	0	0	0	13	13	1.89	6.03	1.8	1.02
20	0	0	0	0	15	15	1.51	6.17	1.69	0.64

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

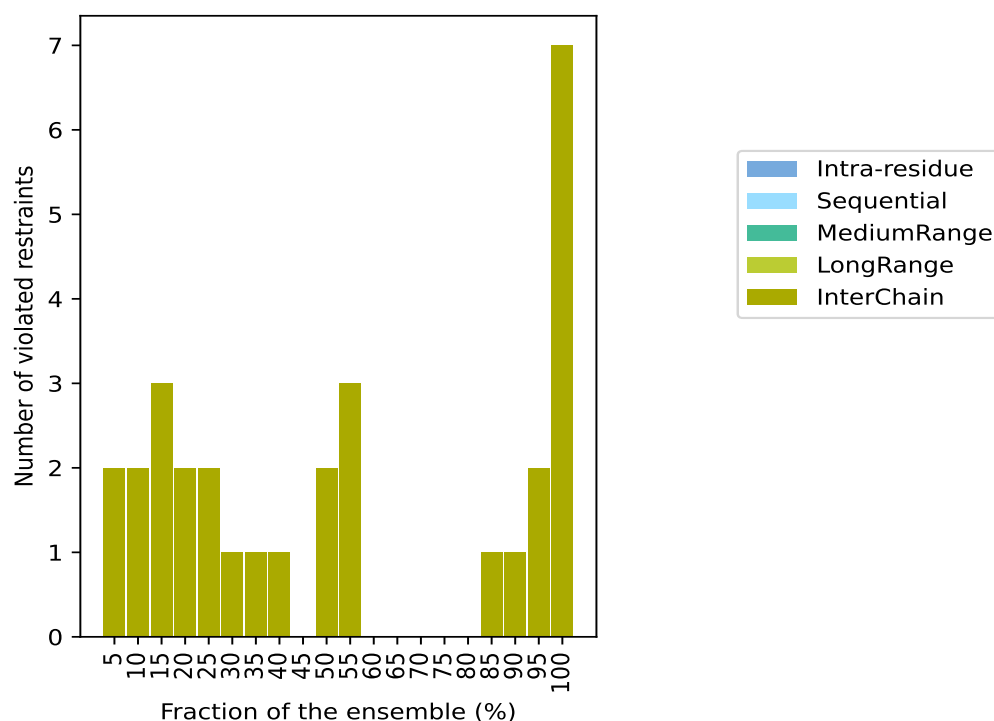
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 21(IR:0, SQ:0, MR:2, LR:4, IC:15) restraints are not violated in the ensemble.

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

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

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

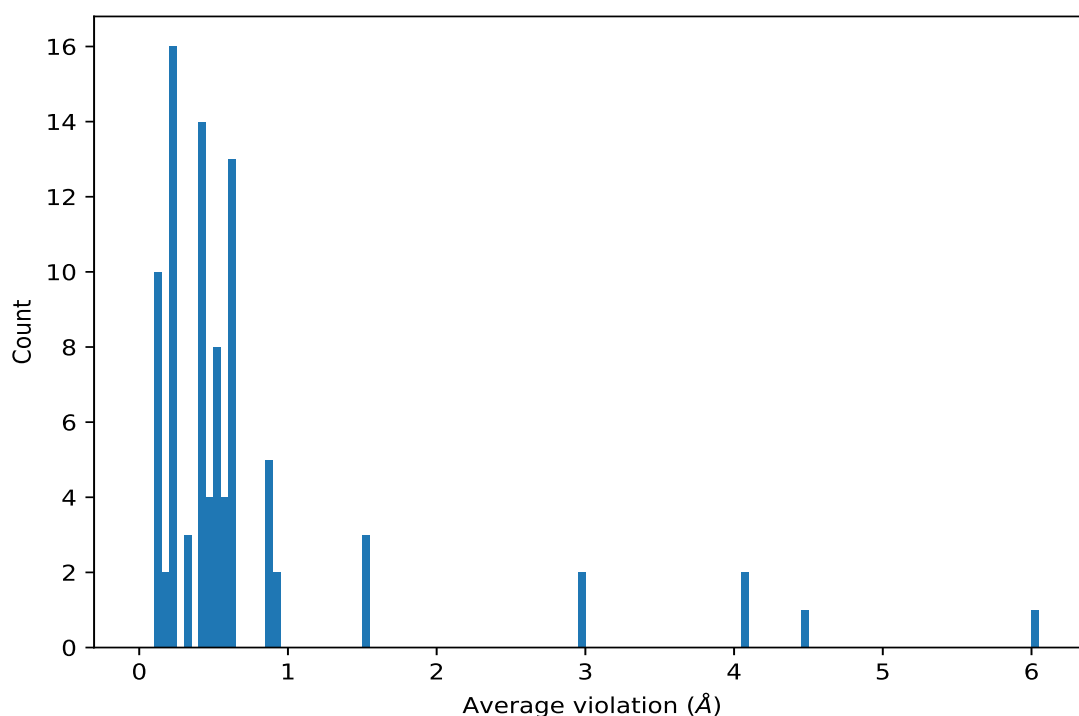
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	20	6.03	0.16	6.02
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	20	4.46	0.17	4.42
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	20	4.05	1.52	3.54
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	20	4.05	1.52	3.54
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	20	1.53	0.38	1.64
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	20	1.53	0.38	1.64
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	20	1.51	0.5	1.54
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	20	0.9	0.44	0.78
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	20	0.9	0.44	0.78
(3,34)	1:8:A:ARG:HH11	3:345:C:TRP:HD1	20	0.88	0.29	0.88
(3,34)	1:8:A:ARG:HB2	3:345:C:TRP:HB2	20	0.88	0.29	0.88
(3,34)	1:8:A:ARG:HD3	3:345:C:TRP:HB2	20	0.88	0.29	0.88
(3,34)	1:8:A:ARG:HH12	3:342:C:ALA:O	20	0.88	0.29	0.88
(3,34)	1:8:A:ARG:HD3	3:345:C:TRP:HD1	20	0.88	0.29	0.88
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	19	2.98	1.41	3.5
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:OE1	19	2.98	1.41	3.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,45)	3:368:C:TRP:HE3	1:66:A:LEU:HD23	19	0.61	0.09	0.62
(3,45)	3:368:C:TRP:HE3	1:66:A:LEU:HD21	19	0.61	0.09	0.62
(3,45)	3:368:C:TRP:CH2	1:112:A:PRO:HD3	19	0.61	0.09	0.62
(3,45)	3:368:C:TRP:HH2	1:111:A:SER:HA	19	0.61	0.09	0.62
(3,45)	3:368:C:TRP:HH2	1:112:A:PRO:HD3	19	0.61	0.09	0.62
(3,45)	3:368:C:TRP:CZ3	1:112:A:PRO:HD3	19	0.61	0.09	0.62
(3,45)	3:368:C:TRP:HE3	1:66:A:LEU:HD22	19	0.61	0.09	0.62
(3,48)	3:377:C:THR:HG22	1:113:A:VAL:HG23	18	0.41	0.1	0.4
(3,48)	3:377:C:THR:HG1	1:113:A:VAL:HG21	18	0.41	0.1	0.4
(3,48)	3:377:C:THR:HG1	1:113:A:VAL:HG23	18	0.41	0.1	0.4
(3,48)	3:377:C:THR:HG21	1:113:A:VAL:HG21	18	0.41	0.1	0.4
(3,48)	3:377:C:THR:HG21	1:113:A:VAL:HG23	18	0.41	0.1	0.4
(3,48)	3:377:C:THR:HG22	1:113:A:VAL:HG22	18	0.41	0.1	0.4
(3,48)	3:377:C:THR:HA	1:113:A:VAL:HG12	18	0.41	0.1	0.4
(3,48)	3:377:C:THR:HG21	1:113:A:VAL:HG22	18	0.41	0.1	0.4
(3,48)	3:377:C:THR:HG21	1:113:A:VAL:HG12	18	0.41	0.1	0.4
(3,43)	3:345:C:TRP:HD1	1:8:A:ARG:HH11	17	0.5	0.26	0.47
(3,43)	3:345:C:TRP:HE3	1:7:A:LYS:HG2	17	0.5	0.26	0.47
(3,43)	3:345:C:TRP:HH2	1:11:A:ALA:HB3	17	0.5	0.26	0.47
(3,43)	3:345:C:TRP:HZ3	1:7:A:LYS:HE2	17	0.5	0.26	0.47
(3,43)	3:345:C:TRP:HE3	1:7:A:LYS:HB3	17	0.5	0.26	0.47
(3,43)	3:345:C:TRP:HZ3	1:11:A:ALA:HB2	17	0.5	0.26	0.47
(3,43)	3:345:C:TRP:HZ3	1:7:A:LYS:HG2	17	0.5	0.26	0.47
(3,43)	3:345:C:TRP:HD1	1:8:A:ARG:HD3	17	0.5	0.26	0.47
(3,36)	1:66:A:LEU:HB3	3:371:C:GLN:HE22	11	0.62	0.37	0.63
(3,36)	1:66:A:LEU:HD22	3:368:C:TRP:HE3	11	0.62	0.37	0.63
(3,36)	1:66:A:LEU:HD21	3:343:C:ILE:HG22	11	0.62	0.37	0.63
(3,36)	1:66:A:LEU:O	3:371:C:GLN:HE22	11	0.62	0.37	0.63
(3,36)	1:66:A:LEU:O	3:371:C:GLN:HE21	11	0.62	0.37	0.63
(3,36)	1:66:A:LEU:HD12	3:367:C:SER:HG	11	0.62	0.37	0.63
(3,13)	3:377:C:THR:HA	1:113:A:VAL:HG11	11	0.49	0.45	0.37
(3,40)	1:113:A:VAL:HG22	3:342:C:ALA:HB2	11	0.23	0.06	0.24
(3,40)	1:113:A:VAL:HG21	3:342:C:ALA:HB2	11	0.23	0.06	0.24
(3,40)	1:113:A:VAL:HG22	3:377:C:THR:HG22	11	0.23	0.06	0.24
(3,40)	1:113:A:VAL:HG23	3:342:C:ALA:HB2	11	0.23	0.06	0.24
(3,40)	1:113:A:VAL:HG22	3:342:C:ALA:HB3	11	0.23	0.06	0.24
(3,40)	1:113:A:VAL:HG21	3:377:C:THR:HG1	11	0.23	0.06	0.24
(3,46)	3:371:C:GLN:HE22	1:66:A:LEU:HB3	10	0.4	0.28	0.3
(3,46)	3:371:C:GLN:HG2	1:96:A:PRO:O	10	0.4	0.28	0.3
(3,46)	3:371:C:GLN:HE21	1:96:A:PRO:O	10	0.4	0.28	0.3
(3,46)	3:371:C:GLN:HE22	1:66:A:LEU:O	10	0.4	0.28	0.3
(3,46)	3:371:C:GLN:HE21	1:66:A:LEU:O	10	0.4	0.28	0.3

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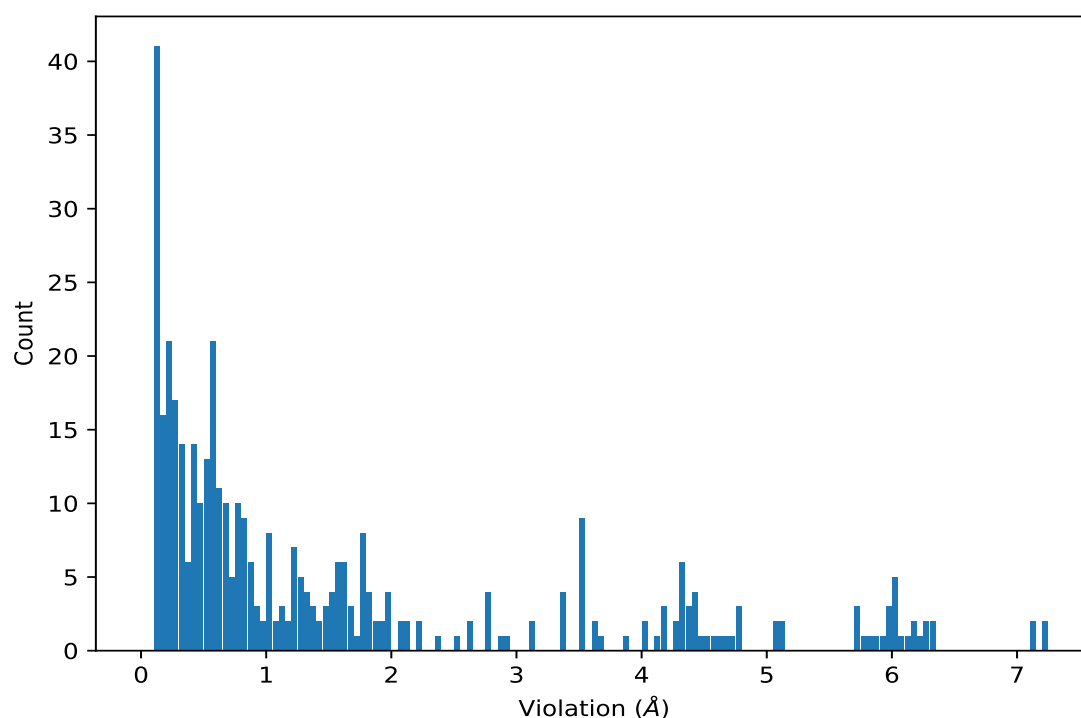
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,41)	3:342:C:ALA:HB2	1:113:A:VAL:HG21	10	0.23	0.1	0.2
(3,41)	3:342:C:ALA:O	1:112:A:PRO:HB2	10	0.23	0.1	0.2
(3,41)	3:342:C:ALA:HB2	1:113:A:VAL:HG23	10	0.23	0.1	0.2
(3,41)	3:342:C:ALA:HB3	1:113:A:VAL:HG22	10	0.23	0.1	0.2
(3,38)	1:111:A:SER:HB3	3:376:C:PRO:HA	8	0.21	0.11	0.18
(3,38)	1:111:A:SER:HB3	3:376:C:PRO:HB3	8	0.21	0.11	0.18
(3,38)	1:111:A:SER:OG	3:379:C:ARG:HE	8	0.21	0.11	0.18
(3,38)	1:111:A:SER:HB2	3:376:C:PRO:HB3	8	0.21	0.11	0.18
(3,7)	3:342:C:ALA:HA	1:113:A:VAL:HG21	7	0.32	0.09	0.32
(1,1)	3:341:C:CYS:SG	4:900:C:ZN:ZN	7	0.11	0.01	0.11
(3,42)	3:343:C:ILE:HA	1:112:A:PRO:HB2	6	0.19	0.06	0.16
(3,42)	3:343:C:ILE:HG12	1:112:A:PRO:HB2	6	0.19	0.06	0.16
(3,37)	1:108:A:GLU:HA	3:379:C:ARG:HH11	5	0.14	0.04	0.13
(3,37)	1:108:A:GLU:OE1	3:379:C:ARG:HH22	5	0.14	0.04	0.13
(3,37)	1:108:A:GLU:OE2	3:379:C:ARG:HH12	5	0.14	0.04	0.13
(3,49)	3:379:C:ARG:HH11	1:108:A:GLU:HA	5	0.14	0.04	0.13
(3,49)	3:379:C:ARG:HH22	1:108:A:GLU:OE1	5	0.14	0.04	0.13
(3,49)	3:379:C:ARG:HH12	1:108:A:GLU:OE2	5	0.14	0.04	0.13
(3,9)	3:376:C:PRO:HB2	1:113:A:VAL:HG21	4	0.31	0.13	0.31
(3,9)	3:376:C:PRO:HB3	1:113:A:VAL:HG21	4	0.31	0.13	0.31
(3,47)	3:376:C:PRO:HA	1:111:A:SER:HB3	4	0.23	0.06	0.23
(3,47)	3:376:C:PRO:HB3	1:112:A:PRO:HD2	4	0.23	0.06	0.23
(3,19)	3:367:C:SER:HG	1:66:A:LEU:HD11	3	0.58	0.23	0.68
(3,19)	3:367:C:SER:HG	1:66:A:LEU:HD12	3	0.58	0.23	0.68
(3,19)	3:367:C:SER:HG	1:66:A:LEU:HD13	3	0.58	0.23	0.68
(3,8)	3:377:C:THR:HA	1:113:A:VAL:HG21	3	0.48	0.23	0.62
(3,39)	1:112:A:PRO:HD2	3:376:C:PRO:HG3	3	0.13	0.02	0.13
(3,39)	1:112:A:PRO:HB2	3:343:C:ILE:HA	3	0.13	0.02	0.13
(3,32)	3:379:C:ARG:HD3	1:109:A:ARG:H	2	0.58	0.09	0.58
(3,12)	3:376:C:PRO:HG2	1:113:A:VAL:HG11	2	0.46	0.09	0.46
(3,12)	3:376:C:PRO:HG3	1:113:A:VAL:HG11	2	0.46	0.09	0.46
(1,6)	3:375:C:CYS:SG	4:901:C:ZN:ZN	2	0.11	0.0	0.11

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)
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	8	7.22
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	8	7.22
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	7	7.11
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	7	7.11
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	18	6.35
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	16	6.32
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	15	6.3
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	15	6.3
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	5	6.24
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	3	6.17
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	20	6.17
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	6	6.12
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	15	6.06
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	14	6.03
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	17	6.03
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	19	6.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	4	6.01
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	10	6.0
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	7	5.98
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	8	5.96
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	9	5.95
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	2	5.93
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	1	5.88
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	12	5.82
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	11	5.78
(3,30)	3:343:C:ILE:HB	1:9:A:LEU:H	13	5.71
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	17	5.71
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	17	5.71
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	4	5.14
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	4	5.14
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	12	5.1
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	12	5.1
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	18	4.78
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	16	4.77
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	7	4.76
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	3	4.71
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	5	4.67
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	20	4.62
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	15	4.57
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	10	4.53
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	17	4.45
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	8	4.43
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	6	4.42
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	7	4.42
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	19	4.42
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	2	4.39
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	13	4.38
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	14	4.38
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	19	4.35
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	1	4.33
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	4	4.32
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	11	4.32
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	9	4.31
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:OE1	17	4.3
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	12	4.29
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	6	4.27
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	8	4.16
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	1	4.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	1	4.16
(3,29)	3:343:C:ILE:HA	1:9:A:LEU:H	13	4.12
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	10	4.04
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	10	4.04
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	9	3.9
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	12	3.66
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	6	3.65
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	6	3.65
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	18	3.54
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	3	3.54
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	3	3.54
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	18	3.54
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	18	3.54
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	4	3.5
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	5	3.5
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	16	3.5
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	16	3.5
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	13	3.4
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	13	3.4
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	9	3.37
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	9	3.37
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	14	3.13
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	14	3.13
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	15	2.92
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	3	2.86
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	20	2.8
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	20	2.8
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	2	2.78
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	2	2.78
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	19	2.64
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	19	2.64
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	16	2.54
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	14	2.35
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	12	2.23
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	12	2.23
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	11	2.13
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	11	2.13
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	4	2.08
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	11	2.07
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	8	1.98
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	17	1.98
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	6	1.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	6	1.97
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	8	1.95
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	8	1.95
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	1	1.87
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	1	1.87
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH11	5	1.81
(3,28)	3:379:C:ARG:HD3	1:109:A:ARG:HH12	5	1.81
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	3	1.81
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	3	1.81
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	14	1.79
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	14	1.79
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	18	1.78
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	18	1.78
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	15	1.77
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	15	1.77
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	5	1.76
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	5	1.76
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	15	1.74
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	11	1.7
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	11	1.7
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	5	1.66
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	13	1.65
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	13	1.65
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	2	1.63
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	6	1.62
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	7	1.62
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	7	1.62
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	20	1.58
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	4	1.58
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	4	1.58
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	16	1.58
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	16	1.58
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	14	1.56
(3,13)	3:377:C:THR:HA	1:113:A:VAL:HG11	20	1.54
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	10	1.52
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	10	1.52
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	13	1.51
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	11	1.48
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	9	1.48
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	9	1.48
(3,34)	1:8:A:ARG:HB2	3:345:C:TRP:HB2	3	1.44
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	18	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	9	1.39
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	8	1.35
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	8	1.35
(3,34)	1:8:A:ARG:HD3	3:345:C:TRP:HB2	19	1.33
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	1	1.33
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	12	1.33
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	12	1.33
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	20	1.27
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	20	1.27
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	7	1.27
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	7	1.27
(3,36)	1:66:A:LEU:HD21	3:343:C:ILE:HG22	6	1.26
(3,34)	1:8:A:ARG:HB2	3:345:C:TRP:HB2	9	1.23
(3,13)	3:377:C:THR:HA	1:113:A:VAL:HG11	2	1.23
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	2	1.22
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	2	1.22
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	12	1.21
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	19	1.21
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	19	1.21
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	17	1.19
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	17	1.19
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	20	1.15
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	20	1.15
(3,34)	1:8:A:ARG:HH12	3:342:C:ALA:O	13	1.1
(3,36)	1:66:A:LEU:HD21	3:343:C:ILE:HG22	17	1.07
(3,34)	1:8:A:ARG:HD3	3:345:C:TRP:HB2	14	1.06
(3,34)	1:8:A:ARG:HB2	3:345:C:TRP:HB2	12	1.04
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	19	1.02
(3,43)	3:345:C:TRP:HD1	1:8:A:ARG:HH11	2	1.01
(3,34)	1:8:A:ARG:HH11	3:345:C:TRP:HD1	2	1.01
(3,36)	1:66:A:LEU:HD22	3:368:C:TRP:HE3	19	1.0
(3,34)	1:8:A:ARG:HD3	3:345:C:TRP:HB2	10	1.0
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	18	1.0
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	18	1.0
(3,46)	3:371:C:GLN:HG2	1:96:A:PRO:O	4	0.99
(3,34)	1:8:A:ARG:HB2	3:345:C:TRP:HB2	18	0.99
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	1	0.93
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	10	0.93
(3,34)	1:8:A:ARG:HD3	3:345:C:TRP:HB2	11	0.91
(3,43)	3:345:C:TRP:HZ3	1:11:A:ALA:HB2	10	0.89
(3,45)	3:368:C:TRP:CH2	1:112:A:PRO:HD3	18	0.86
(3,34)	1:8:A:ARG:HH11	3:345:C:TRP:HD1	4	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	7	0.86
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	6	0.86
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	6	0.86
(3,43)	3:345:C:TRP:HE3	1:7:A:LYS:HG2	18	0.84
(3,34)	1:8:A:ARG:HB2	3:345:C:TRP:HB2	8	0.83
(3,36)	1:66:A:LEU:HD22	3:368:C:TRP:HE3	4	0.82
(3,34)	1:8:A:ARG:HB2	3:345:C:TRP:HB2	6	0.81
(3,19)	3:367:C:SER:HG	1:66:A:LEU:HD11	18	0.81
(3,19)	3:367:C:SER:HG	1:66:A:LEU:HD12	18	0.81
(3,19)	3:367:C:SER:HG	1:66:A:LEU:HD13	18	0.81
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	3	0.81
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	3	0.81
(3,43)	3:345:C:TRP:HH2	1:11:A:ALA:HB3	4	0.79
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	17	0.78
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	17	0.78
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	19	0.78
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	19	0.78
(3,45)	3:368:C:TRP:CZ3	1:112:A:PRO:HD3	14	0.76
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	9	0.76
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	9	0.76
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	2	0.75
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	2	0.75
(3,36)	1:66:A:LEU:O	3:371:C:GLN:HE22	8	0.73
(3,34)	1:8:A:ARG:HB2	3:345:C:TRP:HB2	16	0.72
(3,34)	1:8:A:ARG:HB2	3:345:C:TRP:HB2	5	0.71
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	16	0.71
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	16	0.71
(3,45)	3:368:C:TRP:HH2	1:112:A:PRO:HD3	12	0.7
(3,19)	3:367:C:SER:HG	1:66:A:LEU:HD11	15	0.68
(3,19)	3:367:C:SER:HG	1:66:A:LEU:HD12	15	0.68
(3,19)	3:367:C:SER:HG	1:66:A:LEU:HD13	15	0.68
(3,32)	3:379:C:ARG:HD3	1:109:A:ARG:H	7	0.67
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	5	0.66
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	5	0.66
(3,8)	3:377:C:THR:HA	1:113:A:VAL:HG21	4	0.66
(3,45)	3:368:C:TRP:CH2	1:112:A:PRO:HD3	4	0.65
(3,45)	3:368:C:TRP:CH2	1:112:A:PRO:HD3	9	0.65
(3,45)	3:368:C:TRP:CH2	1:112:A:PRO:HD3	15	0.64
(3,45)	3:368:C:TRP:HH2	1:111:A:SER:HA	17	0.64
(3,45)	3:368:C:TRP:CH2	1:112:A:PRO:HD3	19	0.64
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	20	0.64
(3,46)	3:371:C:GLN:HE22	1:66:A:LEU:O	13	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,43)	3:345:C:TRP:HE3	1:7:A:LYS:HG2	11	0.63
(3,36)	1:66:A:LEU:O	3:371:C:GLN:HE22	13	0.63
(3,46)	3:371:C:GLN:HG2	1:96:A:PRO:O	8	0.62
(3,45)	3:368:C:TRP:HE3	1:66:A:LEU:HD21	2	0.62
(3,45)	3:368:C:TRP:CH2	1:112:A:PRO:HD3	13	0.62
(3,8)	3:377:C:THR:HA	1:113:A:VAL:HG21	11	0.62
(3,45)	3:368:C:TRP:HH2	1:111:A:SER:HA	8	0.6
(3,45)	3:368:C:TRP:CH2	1:112:A:PRO:HD3	11	0.6
(3,43)	3:345:C:TRP:HD1	1:8:A:ARG:HD3	20	0.6
(3,34)	1:8:A:ARG:HD3	3:345:C:TRP:HD1	20	0.6
(3,48)	3:377:C:THR:HG21	1:113:A:VAL:HG22	12	0.59
(3,34)	1:8:A:ARG:HB2	3:345:C:TRP:HB2	15	0.59
(3,48)	3:377:C:THR:HG22	1:113:A:VAL:HG23	1	0.58
(3,46)	3:371:C:GLN:HE22	1:66:A:LEU:O	18	0.58
(3,45)	3:368:C:TRP:HE3	1:66:A:LEU:HD22	16	0.58
(3,43)	3:345:C:TRP:HE3	1:7:A:LYS:HG2	3	0.58
(3,45)	3:368:C:TRP:CH2	1:112:A:PRO:HD3	3	0.57
(3,43)	3:345:C:TRP:HE3	1:7:A:LYS:HB3	9	0.57
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	1	0.57
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	1	0.57
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	14	0.57
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	14	0.57
(3,13)	3:377:C:THR:HA	1:113:A:VAL:HG11	19	0.55
(3,12)	3:376:C:PRO:HG2	1:113:A:VAL:HG11	10	0.55
(3,12)	3:376:C:PRO:HG3	1:113:A:VAL:HG11	10	0.55
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	15	0.55
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	15	0.55
(3,45)	3:368:C:TRP:HE3	1:66:A:LEU:HD23	1	0.54
(3,45)	3:368:C:TRP:CH2	1:112:A:PRO:HD3	20	0.54
(3,34)	1:8:A:ARG:HB2	3:345:C:TRP:HB2	17	0.54
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	4	0.54
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	4	0.54
(3,48)	3:377:C:THR:HG21	1:113:A:VAL:HG21	13	0.53
(3,34)	1:8:A:ARG:HB2	3:345:C:TRP:HB2	7	0.53
(3,11)	3:376:C:PRO:HB2	1:113:A:VAL:HG11	10	0.52
(3,11)	3:376:C:PRO:HB3	1:113:A:VAL:HG11	10	0.52
(3,45)	3:368:C:TRP:HH2	1:111:A:SER:HA	6	0.51
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	3	0.51
(3,7)	3:342:C:ALA:HA	1:113:A:VAL:HG21	18	0.51
(3,48)	3:377:C:THR:HG21	1:113:A:VAL:HG12	14	0.5
(3,32)	3:379:C:ARG:HD3	1:109:A:ARG:H	8	0.49
(3,13)	3:377:C:THR:HA	1:113:A:VAL:HG11	10	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,45)	3:368:C:TRP:HH2	1:111:A:SER:HA	5	0.48
(3,48)	3:377:C:THR:HG21	1:113:A:VAL:HG23	7	0.47
(3,43)	3:345:C:TRP:HZ3	1:7:A:LYS:HE2	5	0.47
(3,41)	3:342:C:ALA:O	1:112:A:PRO:HB2	8	0.47
(3,36)	1:66:A:LEU:HD12	3:367:C:SER:HG	18	0.47
(3,9)	3:376:C:PRO:HB2	1:113:A:VAL:HG21	4	0.46
(3,9)	3:376:C:PRO:HB3	1:113:A:VAL:HG21	4	0.46
(3,48)	3:377:C:THR:HG1	1:113:A:VAL:HG23	3	0.45
(3,48)	3:377:C:THR:HG21	1:113:A:VAL:HG23	18	0.44
(3,48)	3:377:C:THR:HG21	1:113:A:VAL:HG23	20	0.44
(3,45)	3:368:C:TRP:HH2	1:111:A:SER:HA	7	0.44
(3,38)	1:111:A:SER:HB2	3:376:C:PRO:HB3	19	0.44
(3,27)	3:379:C:ARG:HD3	1:108:A:GLU:HG3	16	0.44
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	13	0.44
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	13	0.44
(3,43)	3:345:C:TRP:HZ3	1:7:A:LYS:HE2	17	0.43
(3,9)	3:376:C:PRO:HB2	1:113:A:VAL:HG21	13	0.43
(3,9)	3:376:C:PRO:HB3	1:113:A:VAL:HG21	13	0.43
(3,35)	1:63:A:ASP:OD2	3:371:C:GLN:HE22	2	0.42
(3,13)	3:377:C:THR:HA	1:113:A:VAL:HG11	17	0.42
(3,48)	3:377:C:THR:HA	1:113:A:VAL:HG12	15	0.4
(3,43)	3:345:C:TRP:HE3	1:7:A:LYS:HB3	7	0.4
(3,48)	3:377:C:THR:HG21	1:113:A:VAL:HG21	4	0.39
(3,48)	3:377:C:THR:HG1	1:113:A:VAL:HG23	5	0.38
(3,48)	3:377:C:THR:HA	1:113:A:VAL:HG12	10	0.38
(3,12)	3:376:C:PRO:HG2	1:113:A:VAL:HG11	2	0.38
(3,12)	3:376:C:PRO:HG3	1:113:A:VAL:HG11	2	0.38
(3,13)	3:377:C:THR:HA	1:113:A:VAL:HG11	15	0.37
(3,41)	3:342:C:ALA:HB2	1:113:A:VAL:HG23	12	0.35
(3,40)	1:113:A:VAL:HG23	3:342:C:ALA:HB2	12	0.35
(3,7)	3:342:C:ALA:HA	1:113:A:VAL:HG21	3	0.35
(3,48)	3:377:C:THR:HG22	1:113:A:VAL:HG23	6	0.34
(3,43)	3:345:C:TRP:HE3	1:7:A:LYS:HB3	6	0.34
(3,7)	3:342:C:ALA:HA	1:113:A:VAL:HG21	10	0.34
(3,48)	3:377:C:THR:HG1	1:113:A:VAL:HG21	2	0.32
(3,46)	3:371:C:GLN:HE22	1:66:A:LEU:HB3	3	0.32
(3,43)	3:345:C:TRP:HE3	1:7:A:LYS:HB3	14	0.32
(3,36)	1:66:A:LEU:HB3	3:371:C:GLN:HE22	3	0.32
(3,7)	3:342:C:ALA:HA	1:113:A:VAL:HG21	1	0.32
(3,48)	3:377:C:THR:HG21	1:113:A:VAL:HG21	11	0.31
(3,47)	3:376:C:PRO:HA	1:111:A:SER:HB3	4	0.31
(3,38)	1:111:A:SER:HB3	3:376:C:PRO:HA	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,48)	3:377:C:THR:HG21	1:113:A:VAL:HG23	9	0.3
(3,42)	3:343:C:ILE:HA	1:112:A:PRO:HB2	9	0.3
(3,20)	3:368:C:TRP:HE3	1:66:A:LEU:HD11	10	0.29
(3,20)	3:368:C:TRP:HE3	1:66:A:LEU:HD12	10	0.29
(3,20)	3:368:C:TRP:HE3	1:66:A:LEU:HD13	10	0.29
(3,46)	3:371:C:GLN:HE21	1:66:A:LEU:O	11	0.28
(3,36)	1:66:A:LEU:O	3:371:C:GLN:HE21	11	0.28
(3,40)	1:113:A:VAL:HG21	3:342:C:ALA:HB2	7	0.27
(3,13)	3:377:C:THR:HA	1:113:A:VAL:HG11	18	0.27
(3,41)	3:342:C:ALA:HB2	1:113:A:VAL:HG21	9	0.26
(3,40)	1:113:A:VAL:HG21	3:342:C:ALA:HB2	9	0.26
(3,19)	3:367:C:SER:HG	1:66:A:LEU:HD11	5	0.26
(3,19)	3:367:C:SER:HG	1:66:A:LEU:HD12	5	0.26
(3,19)	3:367:C:SER:HG	1:66:A:LEU:HD13	5	0.26
(3,7)	3:342:C:ALA:HA	1:113:A:VAL:HG21	15	0.26
(3,38)	1:111:A:SER:HB3	3:376:C:PRO:HB3	12	0.25
(3,7)	3:342:C:ALA:HA	1:113:A:VAL:HG21	20	0.25
(3,48)	3:377:C:THR:HG22	1:113:A:VAL:HG22	8	0.24
(3,48)	3:377:C:THR:HG1	1:113:A:VAL:HG21	16	0.24
(3,47)	3:376:C:PRO:HB3	1:112:A:PRO:HD2	10	0.24
(3,42)	3:343:C:ILE:HA	1:112:A:PRO:HB2	12	0.24
(3,40)	1:113:A:VAL:HG22	3:377:C:THR:HG22	8	0.24
(3,40)	1:113:A:VAL:HG21	3:377:C:THR:HG1	16	0.24
(3,40)	1:113:A:VAL:HG21	3:342:C:ALA:HB2	20	0.24
(3,10)	3:376:C:PRO:HG2	1:113:A:VAL:HG21	11	0.24
(3,10)	3:376:C:PRO:HG3	1:113:A:VAL:HG21	11	0.24
(3,43)	3:345:C:TRP:HE3	1:7:A:LYS:HB3	16	0.23
(3,41)	3:342:C:ALA:O	1:112:A:PRO:HB2	7	0.23
(3,40)	1:113:A:VAL:HG22	3:342:C:ALA:HB2	2	0.23
(3,47)	3:376:C:PRO:HA	1:111:A:SER:HB3	18	0.22
(3,43)	3:345:C:TRP:HD1	1:8:A:ARG:HH11	1	0.22
(3,41)	3:342:C:ALA:HB2	1:113:A:VAL:HG21	10	0.22
(3,40)	1:113:A:VAL:HG21	3:342:C:ALA:HB2	10	0.22
(3,34)	1:8:A:ARG:HH11	3:345:C:TRP:HD1	1	0.22
(3,7)	3:342:C:ALA:HA	1:113:A:VAL:HG21	5	0.22
(3,49)	3:379:C:ARG:HH12	1:108:A:GLU:OE2	7	0.21
(3,37)	1:108:A:GLU:OE2	3:379:C:ARG:HH12	7	0.21
(3,38)	1:111:A:SER:HB3	3:376:C:PRO:HB3	8	0.2
(3,41)	3:342:C:ALA:HB3	1:113:A:VAL:HG22	14	0.19
(3,41)	3:342:C:ALA:HB2	1:113:A:VAL:HG21	17	0.19
(3,40)	1:113:A:VAL:HG22	3:342:C:ALA:HB3	14	0.19
(3,13)	3:377:C:THR:HA	1:113:A:VAL:HG11	16	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,9)	3:376:C:PRO:HB2	1:113:A:VAL:HG21	16	0.19
(3,9)	3:376:C:PRO:HB3	1:113:A:VAL:HG21	16	0.19
(3,41)	3:342:C:ALA:O	1:112:A:PRO:HB2	20	0.18
(3,46)	3:371:C:GLN:HE21	1:96:A:PRO:O	17	0.17
(3,40)	1:113:A:VAL:HG21	3:342:C:ALA:HB2	6	0.17
(3,18)	3:367:C:SER:HB2	1:66:A:LEU:HD11	13	0.17
(3,18)	3:367:C:SER:HB2	1:66:A:LEU:HD12	13	0.17
(3,18)	3:367:C:SER:HB2	1:66:A:LEU:HD13	13	0.17
(3,9)	3:376:C:PRO:HB2	1:113:A:VAL:HG21	14	0.17
(3,9)	3:376:C:PRO:HB3	1:113:A:VAL:HG21	14	0.17
(3,42)	3:343:C:ILE:HG12	1:112:A:PRO:HB2	19	0.16
(3,8)	3:377:C:THR:HA	1:113:A:VAL:HG21	13	0.16
(3,47)	3:376:C:PRO:HA	1:111:A:SER:HB3	16	0.15
(3,43)	3:345:C:TRP:HE3	1:7:A:LYS:HB3	8	0.15
(3,42)	3:343:C:ILE:HA	1:112:A:PRO:HB2	10	0.15
(3,41)	3:342:C:ALA:O	1:112:A:PRO:HB2	6	0.15
(3,39)	1:112:A:PRO:HB2	3:343:C:ILE:HA	10	0.15
(3,38)	1:111:A:SER:HB3	3:376:C:PRO:HA	16	0.15
(3,13)	3:377:C:THR:HA	1:113:A:VAL:HG11	9	0.15
(3,49)	3:379:C:ARG:HH12	1:108:A:GLU:OE2	15	0.14
(3,42)	3:343:C:ILE:HA	1:112:A:PRO:HB2	14	0.14
(3,38)	1:111:A:SER:HB3	3:376:C:PRO:HB3	17	0.14
(3,37)	1:108:A:GLU:OE2	3:379:C:ARG:HH12	15	0.14
(3,49)	3:379:C:ARG:HH11	1:108:A:GLU:HA	1	0.13
(3,42)	3:343:C:ILE:HA	1:112:A:PRO:HB2	13	0.13
(3,39)	1:112:A:PRO:HD2	3:376:C:PRO:HG3	13	0.13
(3,37)	1:108:A:GLU:HA	3:379:C:ARG:HH11	1	0.13
(3,46)	3:371:C:GLN:HE21	1:96:A:PRO:O	6	0.12
(3,46)	3:371:C:GLN:HE22	1:66:A:LEU:O	7	0.12
(3,46)	3:371:C:GLN:HE22	1:66:A:LEU:HB3	14	0.12
(3,36)	1:66:A:LEU:O	3:371:C:GLN:HE22	7	0.12
(3,36)	1:66:A:LEU:HB3	3:371:C:GLN:HE22	14	0.12
(3,13)	3:377:C:THR:HA	1:113:A:VAL:HG11	4	0.12
(1,1)	3:341:C:CYS:SG	4:900:C:ZN:ZN	1	0.12
(1,1)	3:341:C:CYS:SG	4:900:C:ZN:ZN	10	0.12
(3,49)	3:379:C:ARG:HH22	1:108:A:GLU:OE1	3	0.11
(3,49)	3:379:C:ARG:HH12	1:108:A:GLU:OE2	4	0.11
(3,38)	1:111:A:SER:HB3	3:376:C:PRO:HA	15	0.11
(3,37)	1:108:A:GLU:OE1	3:379:C:ARG:HH22	3	0.11
(3,37)	1:108:A:GLU:OE2	3:379:C:ARG:HH12	4	0.11
(3,13)	3:377:C:THR:HA	1:113:A:VAL:HG11	3	0.11
(1,6)	3:375:C:CYS:SG	4:901:C:ZN:ZN	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	3:341:C:CYS:SG	4:900:C:ZN:ZN	2	0.11
(1,1)	3:341:C:CYS:SG	4:900:C:ZN:ZN	6	0.11
(1,1)	3:341:C:CYS:SG	4:900:C:ZN:ZN	8	0.11
(1,1)	3:341:C:CYS:SG	4:900:C:ZN:ZN	17	0.11
(3,43)	3:345:C:TRP:HZ3	1:7:A:LYS:HG2	15	0.1
(3,41)	3:342:C:ALA:HB2	1:113:A:VAL:HG21	5	0.1
(3,40)	1:113:A:VAL:HG21	3:342:C:ALA:HB2	5	0.1
(3,39)	1:112:A:PRO:HD2	3:376:C:PRO:HG3	9	0.1
(3,38)	1:111:A:SER:OG	3:379:C:ARG:HE	10	0.1
(1,6)	3:375:C:CYS:SG	4:901:C:ZN:ZN	16	0.1
(1,1)	3:341:C:CYS:SG	4:900:C:ZN:ZN	4	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found