Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 08:28 PM EDT

PDB ID	:	2N1H
BMRB ID	:	25560
Title	:	Solution structure of the GBII-beta MRH domain W409A point mutant
Authors	:	Olson, L.J.; Peterson, F.C.; Damhs, N.M.
Deposited on	:	2015-04-01

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 (i) 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 (1)) were used in the production of this report:

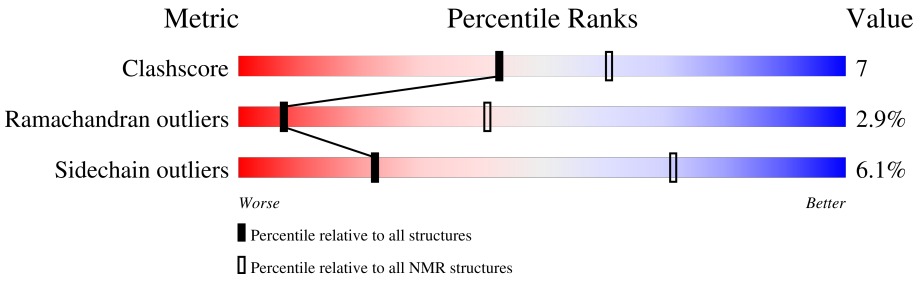
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	94	67% 14% • 18%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 5 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:365-A:408, A:414-A:446 (77)	0.47	5

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1447 atoms, of which 718 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Glucosidase 2 subunit beta.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	94	1447	458	718	122	143	6	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	ALA	TRP	engineered mutation	UNP Q9USH8

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Glucosidase 2 subunit beta

Chain A: 67% 14% • 18%

Y357 R358 A359 I360 K361 G362 M363 E364 Y374 K375 N381 V382 F383 Q384 D385 N391 K401 Y402 E403 Q406 A409 N410 G411 P412 H413 N426 V431 K436 A447 A448 C449 S450

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: Glucosidase 2 subunit beta

Chain A: 64% 17% • 18%

Y357 R358 A359 I360 K361 G362 M363 E364 T365 K366 R367 E368 I369 Y374 K375 V382 F383 Q384 D385 N391 K401 Y402 Q406 A409 N410 G411 P412 H413 N426 V431 K436 L440 K444 A447 A448 C449 S450

4.2.2 Score per residue for model 2

• Molecule 1: Glucosidase 2 subunit beta

Chain A: 60% 20% • 18%

Y357 R358 A359 I360 K361 G362 M363 E364 T365 K366 G370 Y374 F378 L389 G390 N391 K401 Y402 E403 N404 G405 Q406 A409 N410 G411 P412 H413 R414 S415 C422 N426 V431 L432 E433 K436 C437 E438 Y439 L440 K444 A447 A448 C449 S450

4.2.3 Score per residue for model 3

- Molecule 1: Glucosidase 2 subunit beta

Chain A: 65% 15% • 18%

Y357 R358 A359 I360 K361 G362 M363 E364 Y374 F383 L388 N391 Q395 V399 L400 K401 Y402 E403 A409 N410 G411 P412 H413 V418 C422 N426 K436 K442 M443 K444 A447 A448 C449 S450

4.2.4 Score per residue for model 4

- Molecule 1: Glucosidase 2 subunit beta

Chain A: 62% 20% 18%

Y357 R358 A359 I360 K361 G362 M363 E364 T365 K366 R367 E368 Y374 K375 V376 V377 F378 Y379 V382 F383 N391 L400 K401 Y402 E403 A409 N410 G411 P412 H413 R414 S415 V418 C422 E425 K436 A447 A448 C449 S450

4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Glucosidase 2 subunit beta

Chain A: 63% 17% • 18%

Y357 R358 A359 I360 K361 G362 M363 E364 T365 K366 Y374 K375 V376 V377 V382 F383 Q384 D385 L388 N391 K401 Y402 E403 Q406 A409 N410 G411 P412 H413 I417 N426 V431 K436 K444 A447 A448 C449 S450

4.2.6 Score per residue for model 6

- Molecule 1: Glucosidase 2 subunit beta

Chain A: 65% 15% • 18%

Y357 R358 A359 I360 K361 G362 M363 E364 E368 T373 Y374 K375 V376 V377 E380 N381 V382 F383 Q384 D385 K401 Y402 E403 Q406 A409 N410 G411 P412 H413 R414 S415 A434 Q435 K436 A447 A448 C449 S450

4.2.7 Score per residue for model 7

- Molecule 1: Glucosidase 2 subunit beta

Chain A: 63% 15% • 18%

Y357 R358 A359 I360 K361 G362 M363 E364 T365 K366 G370 T373 Y374 N381 V382 F383 Q384 D385 L388 L389 G390 N391 K401 Q406 S407 C408 A409 N410 G411 P412 H413 I417 V431 K436 L440 A447 A448 C449 S450

4.2.8 Score per residue for model 8

- Molecule 1: Glucosidase 2 subunit beta

Chain A: 60% 21% • 18%

Y357 R358 A359 I360 K361 G362 M363 E364 T365 E368 I369 Y374 K375 V376 V377 V382 F383 Q384 D385 L389 G390 N391 Q395 Y402 G405 Q406 A409 N410 G411 P412 H413 V420 N426 E427 I428 V431 K436 M443 A447 A448 C449 S450

4.2.9 Score per residue for model 9

- Molecule 1: Glucosidase 2 subunit beta

Chain A: 62% 17% • 18%

Y357 R358 A359 I360 K361 G362 M363 E364 T365 K366 Y372 T373 Y374 F378 Y379 E380 N381 V382 F383 L388 N391 K401 Y402 E403 N404 A409 N410 G411 P412 H413 C422 N426 V431 K436 L440 K444 A447 A448 C449 S450

4.2.10 Score per residue for model 10

- Molecule 1: Glucosidase 2 subunit beta

Chain A: 61% 18% • 18%

Y357 R358 A359 I360 K361 G362 M363 E364 E368 I369 Y374 K375 Y379 E380 N381 V382 F383 Q384 D385 G390 N391 K401 Y402 E403 N404 A409 N410 G411 P412 H413 V420 V431 L432 E433 K436 C437 A447 A448 C449 S450

4.2.11 Score per residue for model 11

- Molecule 1: Glucosidase 2 subunit beta

Chain A: 53% 29% 18%

Y357 R358 A359 I360 K361 G362 M363 E364 T365 K366 G370 Y374 V377 F378 Y379 E380 N381 V382 F383 Q384 D385 S386 I387 L388 L389 G390 N391 K401 Y402 E403 N404 G405 Q406 A409 N410 G411 P412 H413 R414 S415 E425 N426 V431 K436 C437 E438 Y439 L440 K444 A447 A448 C449 S450

4.2.12 Score per residue for model 12

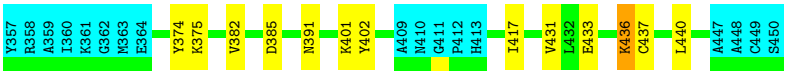
- Molecule 1: Glucosidase 2 subunit beta

Chain A: 67% 14% • 18%

4.2.13 Score per residue for model 13

- Molecule 1: Glucosidase 2 subunit beta

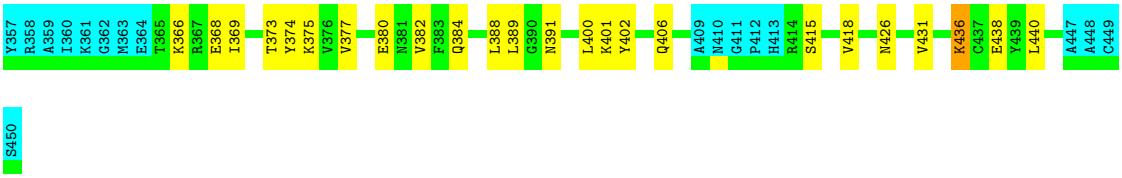
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: Glucosidase 2 subunit beta

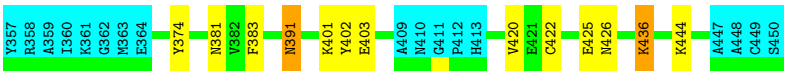
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: Glucosidase 2 subunit beta

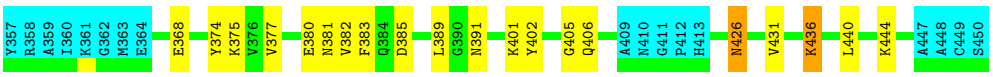
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: Glucosidase 2 subunit beta

Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: Glucosidase 2 subunit beta

Chain A: 64% 16% • 18%

Y357 R358 A359 I360 K361 G362 M363 E364 Y374 K375 Y379 V382 F383 Q384 D385 N391 Q395 K401 Y402 E403 A409 N410 G411 P412 H413 C422 N426 E427 I428 K436 M443 K444 A447 A448 C449 S450

4.2.18 Score per residue for model 18

- Molecule 1: Glucosidase 2 subunit beta

Chain A: 64% 16% • 18%

Y357 R358 A359 I360 K361 G362 M363 E364 Y374 K375 F378 Y379 E380 N381 V382 F383 Q384 D385 N391 K401 Y402 E403 A409 N410 G411 P412 H413 C422 E425 V431 K436 L440 A447 A448 C449 S450

4.2.19 Score per residue for model 19

- Molecule 1: Glucosidase 2 subunit beta

Chain A: 62% 17% • 18%

Y357 R358 A359 I360 K361 G362 M363 E364 E368 T373 Y374 K375 V376 V377 E380 N381 V382 F383 Q384 L389 G390 N391 Y402 G405 Q406 A409 N410 G411 P412 H413 C422 V431 K436 A447 A448 C449 S450

4.2.20 Score per residue for model 20

- Molecule 1: Glucosidase 2 subunit beta

Chain A: 63% 18% • 18%

Y357 R358 A359 I360 K361 G362 M363 E364 T365 K366 R367 E368 I369 T373 Y374 F378 N381 Q384 N391 K401 Y402 Q406 A409 N410 G411 P412 H413 V420 E421 C422 V431 K436 L440 M443 A447 A448 C449 S450

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	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	1071
Number of shifts mapped to atoms	1071
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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	606	599	599	8±2
All	All	12120	11980	11980	170

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:401:LYS:HE3	1:A:415:SER:OG	0.64	1.93	4	3
1:A:426:ASN:HA	1:A:444:LYS:O	0.60	1.96	15	9
1:A:374:TYR:HA	1:A:383:PHE:O	0.59	1.96	16	15
1:A:391:ASN:O	1:A:402:TYR:HA	0.56	2.00	5	18
1:A:400:LEU:HB2	1:A:418:VAL:CG1	0.55	2.31	4	3
1:A:431:VAL:HA	1:A:440:LEU:O	0.55	2.01	2	10
1:A:401:LYS:HE2	1:A:403:GLU:HB2	0.53	1.79	15	1
1:A:366:LYS:HA	1:A:374:TYR:O	0.53	2.04	7	8
1:A:381:ASN:HA	1:A:402:TYR:CE1	0.51	2.40	19	2
1:A:369:ILE:HB	1:A:374:TYR:CE1	0.51	2.39	1	5
1:A:377:VAL:HG11	1:A:380:GLU:OE1	0.51	2.04	19	1
1:A:381:ASN:HA	1:A:402:TYR:CD2	0.50	2.42	11	4
1:A:401:LYS:HE2	1:A:403:GLU:HB3	0.49	1.83	5	3
1:A:401:LYS:HG2	1:A:417:ILE:HD13	0.49	1.83	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:389:LEU:O	1:A:405:GLY:HA3	0.49	2.08	8	5
1:A:375:LYS:O	1:A:382:VAL:HA	0.48	2.09	4	13
1:A:401:LYS:HD2	1:A:402:TYR:N	0.48	2.24	4	5
1:A:369:ILE:HB	1:A:374:TYR:CD1	0.48	2.44	20	2
1:A:373:THR:O	1:A:384:GLN:HA	0.47	2.09	6	4
1:A:401:LYS:HE3	1:A:403:GLU:HB3	0.47	1.85	17	3
1:A:374:TYR:CE2	1:A:431:VAL:HG11	0.47	2.44	13	9
1:A:415:SER:O	1:A:438:GLU:HA	0.47	2.08	14	2
1:A:374:TYR:CE2	1:A:389:LEU:HD11	0.47	2.44	2	1
1:A:381:ASN:HD22	1:A:381:ASN:N	0.47	2.07	6	5
1:A:365:THR:OG1	1:A:426:ASN:HB3	0.47	2.09	8	1
1:A:401:LYS:CE	1:A:403:GLU:HB3	0.47	2.39	5	1
1:A:400:LEU:HB2	1:A:418:VAL:HG12	0.47	1.86	3	2
1:A:381:ASN:HA	1:A:402:TYR:CD1	0.46	2.45	16	3
1:A:433:GLU:HB2	1:A:439:TYR:CE2	0.45	2.47	2	1
1:A:433:GLU:OE2	1:A:437:CYS:HA	0.45	2.11	13	3
1:A:401:LYS:HE3	1:A:403:GLU:HB2	0.45	1.88	18	1
1:A:381:ASN:HB2	1:A:390:GLY:O	0.44	2.12	10	3
1:A:399:VAL:HG13	1:A:418:VAL:O	0.44	2.13	3	1
1:A:388:LEU:HD21	1:A:391:ASN:HD21	0.44	1.73	5	4
1:A:381:ASN:HB3	1:A:391:ASN:HA	0.43	1.91	7	1
1:A:377:VAL:HG11	1:A:380:GLU:OE2	0.42	2.14	11	3
1:A:389:LEU:HD22	1:A:439:TYR:CD1	0.42	2.49	11	1
1:A:365:THR:CG2	1:A:428:ILE:HG13	0.42	2.45	8	1
1:A:377:VAL:HB	1:A:380:GLU:HB2	0.42	1.92	14	1
1:A:428:ILE:HA	1:A:443:MET:HG2	0.41	1.92	8	2
1:A:384:GLN:CD	1:A:389:LEU:HD21	0.41	2.35	14	1
1:A:383:PHE:CE1	1:A:388:LEU:HD13	0.41	2.51	3	1
1:A:420:VAL:HG12	1:A:422:CYS:H	0.41	1.75	15	1
1:A:381:ASN:CB	1:A:391:ASN:HA	0.40	2.46	10	1
1:A:368:GLU:HA	1:A:373:THR:HA	0.40	1.93	14	1
1:A:378:PHE:HD2	1:A:379:TYR:CE2	0.40	2.35	4	1
1:A:384:GLN:HG3	1:A:387:ILE:HB	0.40	1.92	11	1
1:A:420:VAL:HA	1:A:443:MET:O	0.40	2.16	20	1
1:A:378:PHE:HD2	1:A:379:TYR:CE1	0.40	2.34	18	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	77/94 (82%)	68±2 (88±2%)	7±2 (9±2%)	2±1 (3±1%)	7 41
All	All	1540/1880 (82%)	1354 (88%)	142 (9%)	44 (3%)	7 41

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	436	LYS	16
1	A	385	ASP	12
1	A	422	CYS	8
1	A	370	GLY	3
1	A	378	PHE	3
1	A	434	ALA	1
1	A	380	GLU	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	68/79 (86%)	64±1 (94±1%)	4±1 (6±1%)	22 71
All	All	1360/1580 (86%)	1277 (94%)	83 (6%)	22 71

All 15 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	436	LYS	20
1	A	406	GLN	12
1	A	401	LYS	11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	368	GLU	8
1	A	426	ASN	5
1	A	381	ASN	5
1	A	395	GLN	4
1	A	425	GLU	4
1	A	391	ASN	4
1	A	403	GLU	3
1	A	417	ILE	2
1	A	404	ASN	2
1	A	442	LYS	1
1	A	372	TYR	1
1	A	366	LYS	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

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 92% for the well-defined parts and 86% 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	1071
Number of shifts mapped to atoms	1071
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	89	-0.81 ± 0.16	Should be applied
$^{13}C_{\beta}$	81	-0.12 ± 0.34	None needed (< 0.5 ppm)
$^{13}C'$	77	0.13 ± 0.15	None needed (< 0.5 ppm)
^{15}N	86	-0.54 ± 0.38	None needed (imprecise)

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 92%, i.e. 960 atoms were assigned a chemical shift out of a possible 1040. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	381/389 (98%)	159/159 (100%)	146/154 (95%)	76/76 (100%)
Sidechain	527/576 (91%)	363/373 (97%)	155/182 (85%)	9/21 (43%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Aromatic	52/75 (69%)	34/35 (97%)	18/40 (45%)	0/0 (—%)
Overall	960/1040 (92%)	556/567 (98%)	319/376 (85%)	85/97 (88%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1071 atoms were assigned a chemical shift out of a possible 1247. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	435/474 (92%)	183/194 (94%)	166/188 (88%)	86/92 (93%)
Sidechain	580/681 (85%)	400/442 (90%)	170/213 (80%)	10/26 (38%)
Aromatic	56/92 (61%)	36/43 (84%)	20/47 (43%)	0/2 (0%)
Overall	1071/1247 (86%)	619/679 (91%)	356/448 (79%)	96/120 (80%)

7.1.4 Statistically unusual chemical shifts (i)

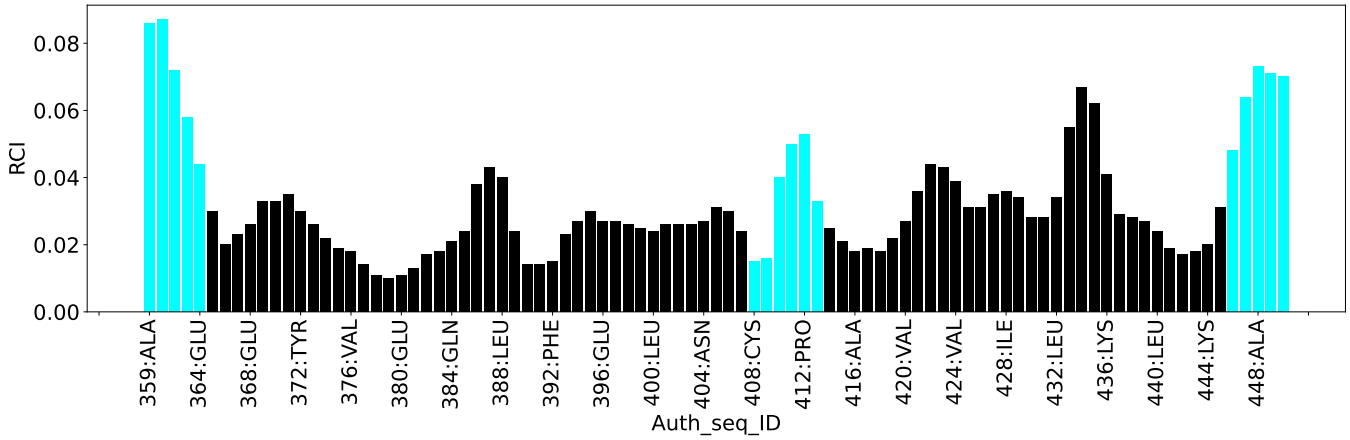
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	409	ALA	CB	60.31	10.19 – 27.75	23.5
1	A	390	GLY	N	129.22	91.59 – 127.52	5.5

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.00
0.02
0.04
0.06
0.08
359:ALA
364:GLU
368:GLU
372:TYR
376:VAL
380:GLU
384:GLN
388:LEU
392:PHE
396:GLU
400:LEU
404:ASN
408:CYS
412:PRO
416:ALA
420:VAL
424:VAL
428:ILE
432:LEU
436:LYS
440:LEU
444:LYS
448:ALA
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	1367
Intra-residue (|i-j|=0)	263
Sequential (|i-j|=1)	351
Medium range (|i-j|>1 and |i-j|<5)	146
Long range (|i-j|≥5)	601
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	6
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	14.5
Number of long range restraints per residue[1]	6.5

[1]Long 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 (i)

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 (i)

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)	6.5	0.2
0.2-0.5 (Medium)	1.0	0.42
>0.5 (Large)	0.1	0.97

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 (i)

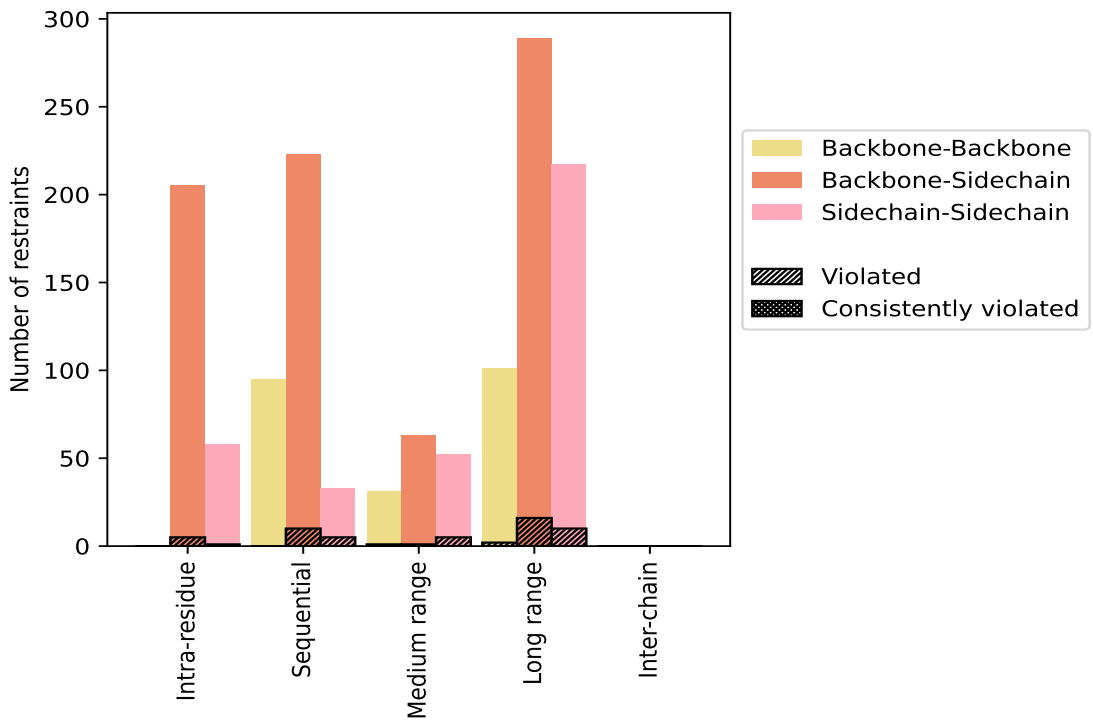
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	263	19.2	6	2.3	0.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	205	15.0	5	2.4	0.4	0	0.0	0.0
Sidechain-Sidechain	58	4.2	1	1.7	0.1	0	0.0	0.0
Sequential (|i-j|=1)	351	25.7	15	4.3	1.1	0	0.0	0.0
Backbone-Backbone	95	6.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	223	16.3	10	4.5	0.7	0	0.0	0.0
Sidechain-Sidechain	33	2.4	5	15.2	0.4	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	146	10.7	7	4.8	0.5	0	0.0	0.0
Backbone-Backbone	31	2.3	1	3.2	0.1	0	0.0	0.0
Backbone-Sidechain	63	4.6	1	1.6	0.1	0	0.0	0.0
Sidechain-Sidechain	52	3.8	5	9.6	0.4	0	0.0	0.0
Long range (|i-j|≥5)	601	44.0	28	4.7	2.0	0	0.0	0.0
Backbone-Backbone	101	7.4	2	2.0	0.1	0	0.0	0.0
Backbone-Sidechain	289	21.1	16	5.5	1.2	0	0.0	0.0
Sidechain-Sidechain	211	15.4	10	4.7	0.7	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	6	0.4	0	0.0	0.0	0	0.0	0.0
Total	1367	100.0	56	4.1	4.1	0	0.0	0.0
Backbone-Backbone	227	16.6	3	1.3	0.2	0	0.0	0.0
Backbone-Sidechain	780	57.1	32	4.1	2.3	0	0.0	0.0
Sidechain-Sidechain	360	26.3	21	5.8	1.5	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	2	1	3	0	6	0.17	0.28	0.07	0.12
2	0	2	0	6	0	8	0.15	0.23	0.04	0.14
3	1	5	1	4	0	11	0.13	0.19	0.02	0.12
4	0	2	0	5	0	7	0.25	0.97	0.29	0.13
5	0	3	1	3	0	7	0.14	0.29	0.06	0.11
6	0	1	1	4	0	6	0.17	0.35	0.08	0.13
7	0	1	2	4	0	7	0.15	0.23	0.04	0.14
8	1	2	1	4	0	8	0.15	0.21	0.03	0.13
9	1	0	1	5	0	7	0.17	0.28	0.06	0.15
10	1	3	0	3	0	7	0.14	0.23	0.05	0.12
11	0	1	0	4	0	5	0.16	0.24	0.05	0.13

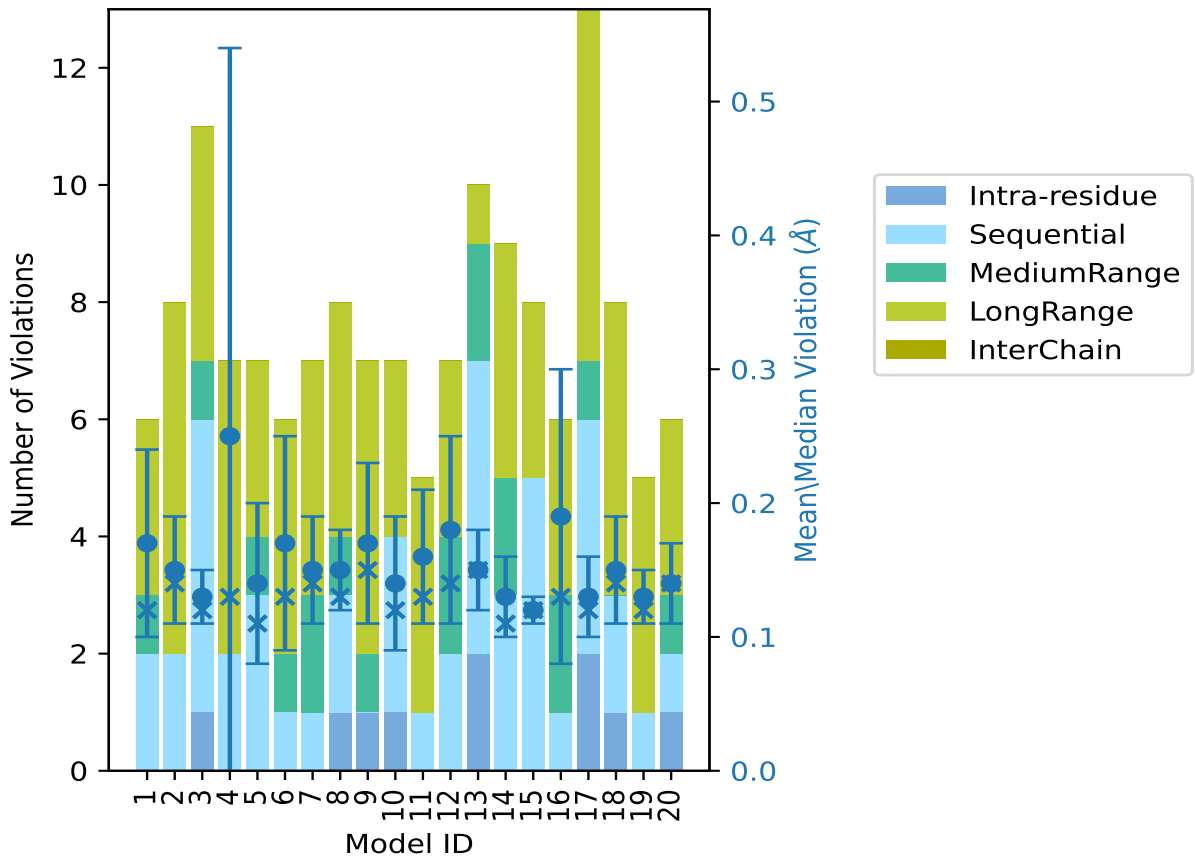
Continued on next page...

Continued from previous page...

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				
12	0	2	2	3	0	7	0.18	0.29	0.07	0.14
13	2	5	2	1	0	10	0.15	0.21	0.03	0.15
14	0	3	2	4	0	9	0.13	0.18	0.03	0.11
15	0	5	0	3	0	8	0.12	0.13	0.01	0.12
16	0	1	2	3	0	6	0.19	0.42	0.11	0.13
17	2	4	1	6	0	13	0.13	0.23	0.03	0.12
18	1	2	0	5	0	8	0.15	0.23	0.04	0.14
19	0	1	0	4	0	5	0.13	0.16	0.02	0.12
20	1	1	1	3	0	6	0.14	0.2	0.03	0.14

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

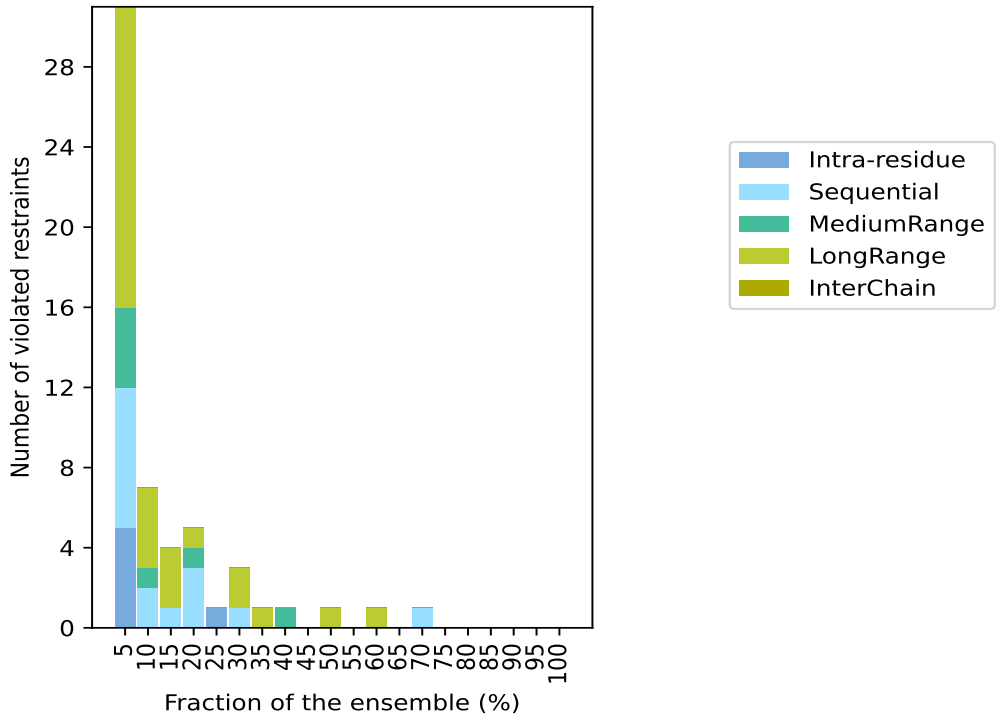
9.3 Distance violation statistics for the ensemble (i)

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, 1305(IR:257, SQ:336, MR:139, LR:573, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
5	7	4	15	0	31	1	5.0
0	2	1	4	0	7	2	10.0
0	1	0	3	0	4	3	15.0
0	3	1	1	0	5	4	20.0
1	0	0	0	0	1	5	25.0
0	1	0	2	0	3	6	30.0
0	0	0	1	0	1	7	35.0
0	0	1	0	0	1	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	1	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	1	0	1	12	60.0
0	0	0	0	0	0	13	65.0
0	1	0	0	0	1	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	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

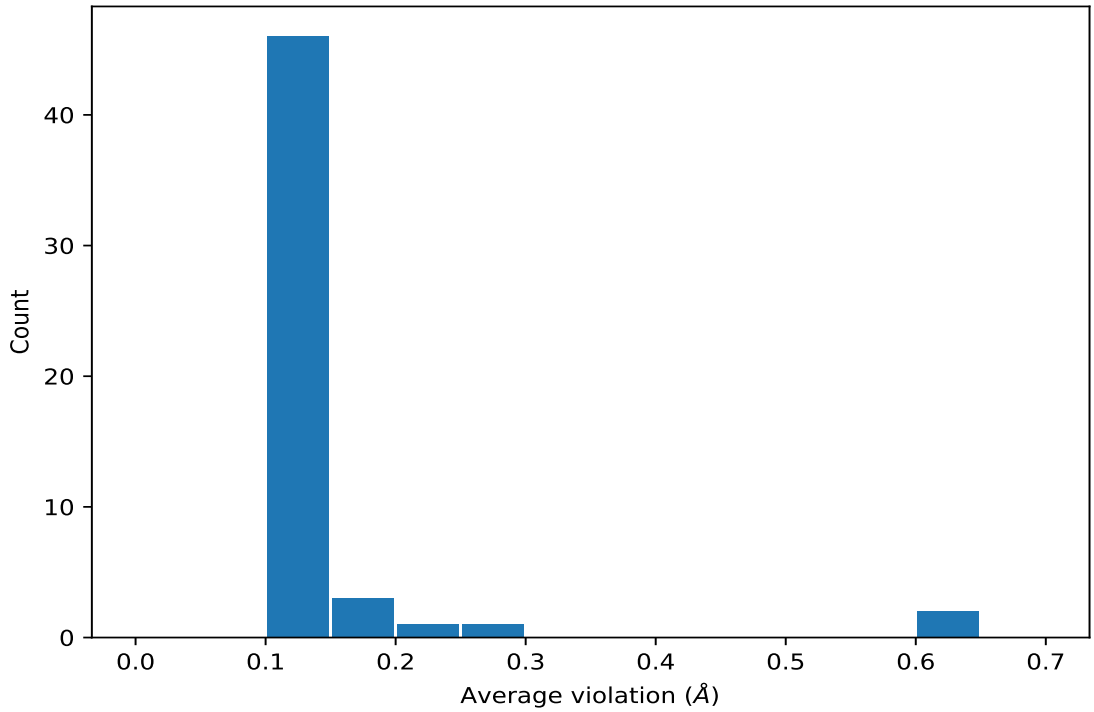
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,709)	1:A:391:ASN:HD22	1:A:392:PHE:H	14	0.21	0.03	0.22
(1,708)	1:A:381:ASN:HD22	1:A:392:PHE:H	12	0.16	0.03	0.15
(1,317)	1:A:418:VAL:HB	1:A:441:ILE:HG13	10	0.12	0.01	0.12
(1,548)	1:A:423:GLY:HA2	1:A:425:GLU:H	8	0.28	0.07	0.28
(1,859)	1:A:373:THR:H	1:A:384:GLN:HB3	7	0.12	0.01	0.13
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE1	6	0.14	0.02	0.14
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE2	6	0.14	0.02	0.14
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE3	6	0.14	0.02	0.14
(1,546)	1:A:422:CYS:HB2	1:A:448:ALA:H	6	0.13	0.01	0.13
(1,1050)	1:A:443:MET:H	1:A:444:LYS:HB3	6	0.12	0.0	0.12
(1,1256)	1:A:401:LYS:HB2	1:A:401:LYS:HD2	5	0.11	0.0	0.11
(1,1256)	1:A:401:LYS:HB2	1:A:401:LYS:HD3	5	0.11	0.0	0.11
(1,1256)	1:A:401:LYS:HB3	1:A:401:LYS:HD2	5	0.11	0.0	0.11
(1,1256)	1:A:401:LYS:HB3	1:A:401:LYS:HD3	5	0.11	0.0	0.11
(1,1122)	1:A:371:GLY:HA2	1:A:372:TYR:HD1	4	0.17	0.07	0.14
(1,1122)	1:A:371:GLY:HA2	1:A:372:TYR:HD2	4	0.17	0.07	0.14

Continued on next page...

Continued from previous page...

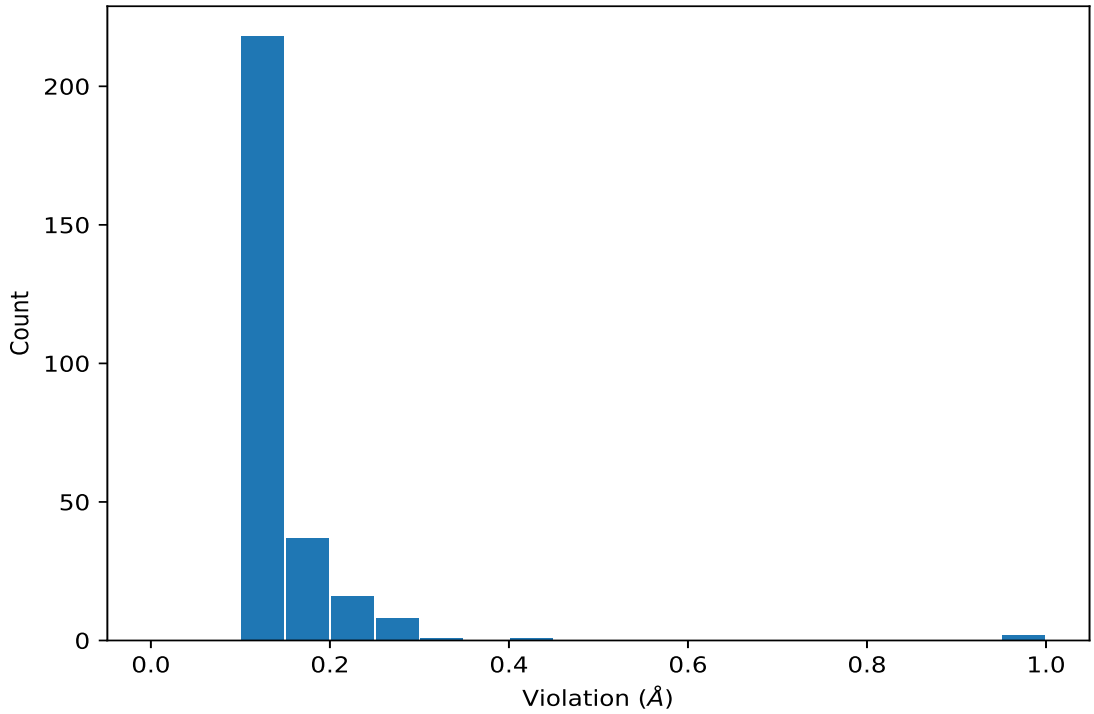
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG11	4	0.14	0.02	0.15
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG12	4	0.14	0.02	0.15
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG13	4	0.14	0.02	0.15
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG21	4	0.14	0.02	0.15
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG22	4	0.14	0.02	0.15
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG23	4	0.14	0.02	0.15
(1,360)	1:A:366:LYS:H	1:A:367:ARG:HD2	4	0.14	0.02	0.13
(1,174)	1:A:377:VAL:HA	1:A:380:GLU:HB2	4	0.12	0.01	0.12
(1,118)	1:A:366:LYS:HG2	1:A:367:ARG:HA	4	0.11	0.0	0.11
(1,118)	1:A:366:LYS:HG3	1:A:367:ARG:HA	4	0.11	0.0	0.11
(1,1261)	1:A:402:TYR:H	1:A:403:GLU:HG2	3	0.14	0.01	0.14
(1,1261)	1:A:402:TYR:H	1:A:403:GLU:HG3	3	0.14	0.01	0.14
(1,727)	1:A:402:TYR:H	1:A:415:SER:HA	3	0.12	0.0	0.12
(1,106)	1:A:417:ILE:HB	1:A:440:LEU:HA	3	0.12	0.01	0.12
(1,1161)	1:A:362:GLY:HA2	1:A:377:VAL:HG11	3	0.12	0.01	0.11
(1,1161)	1:A:362:GLY:HA2	1:A:377:VAL:HG12	3	0.12	0.01	0.11
(1,1161)	1:A:362:GLY:HA2	1:A:377:VAL:HG13	3	0.12	0.01	0.11
(1,1161)	1:A:362:GLY:HA3	1:A:377:VAL:HG11	3	0.12	0.01	0.11
(1,1161)	1:A:362:GLY:HA3	1:A:377:VAL:HG12	3	0.12	0.01	0.11
(1,1161)	1:A:362:GLY:HA3	1:A:377:VAL:HG13	3	0.12	0.01	0.11
(1,1276)	1:A:405:GLY:HA2	1:A:413:HIS:HB2	2	0.62	0.34	0.62
(1,1276)	1:A:405:GLY:HA2	1:A:413:HIS:HB3	2	0.62	0.34	0.62
(1,223)	1:A:390:GLY:HA2	1:A:416:ALA:HB1	2	0.14	0.03	0.14
(1,223)	1:A:390:GLY:HA2	1:A:416:ALA:HB2	2	0.14	0.03	0.14
(1,223)	1:A:390:GLY:HA2	1:A:416:ALA:HB3	2	0.14	0.03	0.14
(1,846)	1:A:365:THR:H	1:A:376:VAL:HA	2	0.13	0.02	0.13
(1,1099)	1:A:378:PHE:HE1	1:A:379:TYR:HE1	2	0.13	0.01	0.13
(1,1099)	1:A:378:PHE:HE1	1:A:379:TYR:HE2	2	0.13	0.01	0.13
(1,1099)	1:A:378:PHE:HE2	1:A:379:TYR:HE1	2	0.13	0.01	0.13
(1,1099)	1:A:378:PHE:HE2	1:A:379:TYR:HE2	2	0.13	0.01	0.13
(1,170)	1:A:379:TYR:HB2	1:A:380:GLU:HB2	2	0.12	0.01	0.12
(1,170)	1:A:379:TYR:HB3	1:A:380:GLU:HB2	2	0.12	0.01	0.12
(1,1259)	1:A:401:LYS:HD2	1:A:403:GLU:HB2	2	0.12	0.01	0.12
(1,1259)	1:A:401:LYS:HD2	1:A:403:GLU:HB3	2	0.12	0.01	0.12
(1,1259)	1:A:401:LYS:HD3	1:A:403:GLU:HB2	2	0.12	0.01	0.12
(1,1259)	1:A:401:LYS:HD3	1:A:403:GLU:HB3	2	0.12	0.01	0.12
(1,245)	1:A:388:LEU:HG	1:A:406:GLN:HG3	2	0.12	0.0	0.12

[1]Number of violated models, [2]Standard 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)
(1,1276)	1:A:405:GLY:HA2	1:A:413:HIS:HB2	4	0.97
(1,1276)	1:A:405:GLY:HA2	1:A:413:HIS:HB3	4	0.97
(1,548)	1:A:423:GLY:HA2	1:A:425:GLU:H	16	0.42
(1,548)	1:A:423:GLY:HA2	1:A:425:GLU:H	6	0.35
(1,548)	1:A:423:GLY:HA2	1:A:425:GLU:H	12	0.29
(1,1122)	1:A:371:GLY:HA2	1:A:372:TYR:HD1	5	0.29
(1,1122)	1:A:371:GLY:HA2	1:A:372:TYR:HD2	5	0.29
(1,548)	1:A:423:GLY:HA2	1:A:425:GLU:H	1	0.28
(1,548)	1:A:423:GLY:HA2	1:A:425:GLU:H	9	0.28
(1,1276)	1:A:405:GLY:HA2	1:A:413:HIS:HB2	12	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1276)	1:A:405:GLY:HA2	1:A:413:HIS:HB3	12	0.28
(1,709)	1:A:391:ASN:HD22	1:A:392:PHE:H	1	0.25
(1,709)	1:A:391:ASN:HD22	1:A:392:PHE:H	11	0.24
(1,709)	1:A:391:ASN:HD22	1:A:392:PHE:H	2	0.23
(1,709)	1:A:391:ASN:HD22	1:A:392:PHE:H	10	0.23
(1,709)	1:A:391:ASN:HD22	1:A:392:PHE:H	16	0.23
(1,709)	1:A:391:ASN:HD22	1:A:392:PHE:H	17	0.23
(1,709)	1:A:391:ASN:HD22	1:A:392:PHE:H	18	0.23
(1,708)	1:A:381:ASN:HD22	1:A:392:PHE:H	9	0.23
(1,548)	1:A:423:GLY:HA2	1:A:425:GLU:H	7	0.23
(1,709)	1:A:391:ASN:HD22	1:A:392:PHE:H	12	0.21
(1,709)	1:A:391:ASN:HD22	1:A:392:PHE:H	13	0.21
(1,548)	1:A:423:GLY:HA2	1:A:425:GLU:H	8	0.21
(1,548)	1:A:423:GLY:HA2	1:A:425:GLU:H	13	0.21
(1,709)	1:A:391:ASN:HD22	1:A:392:PHE:H	8	0.2
(1,709)	1:A:391:ASN:HD22	1:A:392:PHE:H	20	0.2
(1,708)	1:A:381:ASN:HD22	1:A:392:PHE:H	6	0.2
(1,708)	1:A:381:ASN:HD22	1:A:392:PHE:H	10	0.2
(1,782)	1:A:425:GLU:HA	1:A:426:ASN:HD21	2	0.19
(1,709)	1:A:391:ASN:HD22	1:A:392:PHE:H	3	0.19
(1,709)	1:A:391:ASN:HD22	1:A:392:PHE:H	4	0.18
(1,708)	1:A:381:ASN:HD22	1:A:392:PHE:H	7	0.18
(1,438)	1:A:374:TYR:HD1	1:A:384:GLN:HB3	14	0.18
(1,438)	1:A:374:TYR:HD2	1:A:384:GLN:HB3	14	0.18
(1,360)	1:A:366:LYS:H	1:A:367:ARG:HD2	14	0.17
(1,223)	1:A:390:GLY:HA2	1:A:416:ALA:HB1	9	0.17
(1,223)	1:A:390:GLY:HA2	1:A:416:ALA:HB2	9	0.17
(1,223)	1:A:390:GLY:HA2	1:A:416:ALA:HB3	9	0.17
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG11	2	0.17
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG12	2	0.17
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG13	2	0.17
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG21	2	0.17
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG22	2	0.17
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG23	2	0.17
(1,1153)	1:A:412:PRO:HB3	1:A:413:HIS:HD2	13	0.17
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE1	11	0.17
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE2	11	0.17
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE3	11	0.17
(1,708)	1:A:381:ASN:HD22	1:A:392:PHE:H	19	0.16
(1,1267)	1:A:403:GLU:HB2	1:A:404:ASN:HD21	13	0.16
(1,1267)	1:A:403:GLU:HB2	1:A:404:ASN:HD22	13	0.16
(1,1267)	1:A:403:GLU:HB3	1:A:404:ASN:HD21	13	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1267)	1:A:403:GLU:HB3	1:A:404:ASN:HD22	13	0.16
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG11	7	0.16
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG12	7	0.16
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG13	7	0.16
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG21	7	0.16
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG22	7	0.16
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG23	7	0.16
(1,1039)	1:A:389:LEU:HD11	1:A:440:LEU:H	18	0.16
(1,1039)	1:A:389:LEU:HD12	1:A:440:LEU:H	18	0.16
(1,1039)	1:A:389:LEU:HD13	1:A:440:LEU:H	18	0.16
(1,1039)	1:A:389:LEU:HD21	1:A:440:LEU:H	18	0.16
(1,1039)	1:A:389:LEU:HD22	1:A:440:LEU:H	18	0.16
(1,1039)	1:A:389:LEU:HD23	1:A:440:LEU:H	18	0.16
(1,846)	1:A:365:THR:H	1:A:376:VAL:HA	2	0.15
(1,708)	1:A:381:ASN:HD22	1:A:392:PHE:H	5	0.15
(1,708)	1:A:381:ASN:HD22	1:A:392:PHE:H	20	0.15
(1,546)	1:A:422:CYS:HB2	1:A:448:ALA:H	18	0.15
(1,1261)	1:A:402:TYR:H	1:A:403:GLU:HG2	13	0.15
(1,1261)	1:A:402:TYR:H	1:A:403:GLU:HG3	13	0.15
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE1	9	0.15
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE2	9	0.15
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE3	9	0.15
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE1	13	0.15
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE2	13	0.15
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE3	13	0.15
(1,859)	1:A:373:THR:H	1:A:384:GLN:HB3	9	0.14
(1,745)	1:A:406:GLN:HE22	1:A:407:SER:H	4	0.14
(1,708)	1:A:381:ASN:HD22	1:A:392:PHE:H	1	0.14
(1,360)	1:A:366:LYS:H	1:A:367:ARG:HD2	7	0.14
(1,128)	1:A:365:THR:HG21	1:A:367:ARG:HD3	7	0.14
(1,128)	1:A:365:THR:HG22	1:A:367:ARG:HD3	7	0.14
(1,128)	1:A:365:THR:HG23	1:A:367:ARG:HD3	7	0.14
(1,1261)	1:A:402:TYR:H	1:A:403:GLU:HG2	18	0.14
(1,1261)	1:A:402:TYR:H	1:A:403:GLU:HG3	18	0.14
(1,1161)	1:A:362:GLY:HA2	1:A:377:VAL:HG11	20	0.14
(1,1161)	1:A:362:GLY:HA2	1:A:377:VAL:HG12	20	0.14
(1,1161)	1:A:362:GLY:HA2	1:A:377:VAL:HG13	20	0.14
(1,1161)	1:A:362:GLY:HA3	1:A:377:VAL:HG11	20	0.14
(1,1161)	1:A:362:GLY:HA3	1:A:377:VAL:HG12	20	0.14
(1,1161)	1:A:362:GLY:HA3	1:A:377:VAL:HG13	20	0.14
(1,1158)	1:A:360:ILE:HA	1:A:360:ILE:HG12	13	0.14
(1,1158)	1:A:360:ILE:HA	1:A:360:ILE:HG13	13	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	1:A:371:GLY:HA2	1:A:372:TYR:HD1	12	0.14
(1,1122)	1:A:371:GLY:HA2	1:A:372:TYR:HD2	12	0.14
(1,1122)	1:A:371:GLY:HA2	1:A:372:TYR:HD1	17	0.14
(1,1122)	1:A:371:GLY:HA2	1:A:372:TYR:HD2	17	0.14
(1,1099)	1:A:378:PHE:HE1	1:A:379:TYR:HE1	3	0.14
(1,1099)	1:A:378:PHE:HE1	1:A:379:TYR:HE2	3	0.14
(1,1099)	1:A:378:PHE:HE2	1:A:379:TYR:HE1	3	0.14
(1,1099)	1:A:378:PHE:HE2	1:A:379:TYR:HE2	3	0.14
(1,1029)	1:A:433:GLU:HG3	1:A:438:GLU:H	6	0.14
(1,859)	1:A:373:THR:H	1:A:384:GLN:HB3	3	0.13
(1,859)	1:A:373:THR:H	1:A:384:GLN:HB3	8	0.13
(1,859)	1:A:373:THR:H	1:A:384:GLN:HB3	16	0.13
(1,75)	1:A:436:LYS:HD2	1:A:438:GLU:HB2	20	0.13
(1,75)	1:A:436:LYS:HD3	1:A:438:GLU:HB2	20	0.13
(1,727)	1:A:402:TYR:H	1:A:415:SER:HA	11	0.13
(1,709)	1:A:391:ASN:HD22	1:A:392:PHE:H	14	0.13
(1,708)	1:A:381:ASN:HD22	1:A:392:PHE:H	4	0.13
(1,708)	1:A:381:ASN:HD22	1:A:392:PHE:H	8	0.13
(1,708)	1:A:381:ASN:HD22	1:A:392:PHE:H	17	0.13
(1,563)	1:A:376:VAL:H	1:A:428:ILE:HG12	8	0.13
(1,546)	1:A:422:CYS:HB2	1:A:448:ALA:H	8	0.13
(1,546)	1:A:422:CYS:HB2	1:A:448:ALA:H	17	0.13
(1,546)	1:A:422:CYS:HB2	1:A:448:ALA:H	19	0.13
(1,317)	1:A:418:VAL:HB	1:A:441:ILE:HG13	9	0.13
(1,317)	1:A:418:VAL:HB	1:A:441:ILE:HG13	18	0.13
(1,259)	1:A:419:THR:HB	1:A:442:LYS:HD2	2	0.13
(1,259)	1:A:419:THR:HB	1:A:442:LYS:HD3	2	0.13
(1,174)	1:A:377:VAL:HA	1:A:380:GLU:HB2	5	0.13
(1,170)	1:A:379:TYR:HB2	1:A:380:GLU:HB2	15	0.13
(1,170)	1:A:379:TYR:HB3	1:A:380:GLU:HB2	15	0.13
(1,1353)	1:A:435:GLN:H	1:A:435:GLN:HG2	8	0.13
(1,1353)	1:A:435:GLN:H	1:A:435:GLN:HG3	8	0.13
(1,1259)	1:A:401:LYS:HD2	1:A:403:GLU:HB2	16	0.13
(1,1259)	1:A:401:LYS:HD2	1:A:403:GLU:HB3	16	0.13
(1,1259)	1:A:401:LYS:HD3	1:A:403:GLU:HB2	16	0.13
(1,1259)	1:A:401:LYS:HD3	1:A:403:GLU:HB3	16	0.13
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG11	15	0.13
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG12	15	0.13
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG13	15	0.13
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG21	15	0.13
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG22	15	0.13
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG23	15	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1123)	1:A:372:TYR:HD1	1:A:385:ASP:HB2	18	0.13
(1,1123)	1:A:372:TYR:HD2	1:A:385:ASP:HB2	18	0.13
(1,106)	1:A:417:ILE:HB	1:A:440:LEU:HA	12	0.13
(1,1003)	1:A:431:VAL:H	1:A:442:LYS:HB2	11	0.13
(1,998)	1:A:368:GLU:H	1:A:368:GLU:HB2	3	0.12
(1,859)	1:A:373:THR:H	1:A:384:GLN:HB3	17	0.12
(1,854)	1:A:368:GLU:H	1:A:368:GLU:HB3	17	0.12
(1,727)	1:A:402:TYR:H	1:A:415:SER:HA	3	0.12
(1,727)	1:A:402:TYR:H	1:A:415:SER:HA	15	0.12
(1,360)	1:A:366:LYS:H	1:A:367:ARG:HD2	10	0.12
(1,317)	1:A:418:VAL:HB	1:A:441:ILE:HG13	6	0.12
(1,317)	1:A:418:VAL:HB	1:A:441:ILE:HG13	15	0.12
(1,317)	1:A:418:VAL:HB	1:A:441:ILE:HG13	20	0.12
(1,245)	1:A:388:LEU:HG	1:A:406:GLN:HG3	12	0.12
(1,174)	1:A:377:VAL:HA	1:A:380:GLU:HB2	13	0.12
(1,170)	1:A:379:TYR:HB2	1:A:380:GLU:HB2	3	0.12
(1,170)	1:A:379:TYR:HB3	1:A:380:GLU:HB2	3	0.12
(1,1350)	1:A:434:ALA:H	1:A:435:GLN:HG2	15	0.12
(1,1350)	1:A:434:ALA:H	1:A:435:GLN:HG3	15	0.12
(1,1261)	1:A:402:TYR:H	1:A:403:GLU:HG2	15	0.12
(1,1261)	1:A:402:TYR:H	1:A:403:GLU:HG3	15	0.12
(1,1256)	1:A:401:LYS:HB2	1:A:401:LYS:HD2	20	0.12
(1,1256)	1:A:401:LYS:HB2	1:A:401:LYS:HD3	20	0.12
(1,1256)	1:A:401:LYS:HB3	1:A:401:LYS:HD2	20	0.12
(1,1256)	1:A:401:LYS:HB3	1:A:401:LYS:HD3	20	0.12
(1,118)	1:A:366:LYS:HG2	1:A:367:ARG:HA	17	0.12
(1,118)	1:A:366:LYS:HG3	1:A:367:ARG:HA	17	0.12
(1,1142)	1:A:380:GLU:HB2	1:A:383:PHE:HE1	3	0.12
(1,1142)	1:A:380:GLU:HB2	1:A:383:PHE:HE2	3	0.12
(1,1122)	1:A:371:GLY:HA2	1:A:372:TYR:HD1	19	0.12
(1,1122)	1:A:371:GLY:HA2	1:A:372:TYR:HD2	19	0.12
(1,1099)	1:A:378:PHE:HE1	1:A:379:TYR:HE1	6	0.12
(1,1099)	1:A:378:PHE:HE1	1:A:379:TYR:HE2	6	0.12
(1,1099)	1:A:378:PHE:HE2	1:A:379:TYR:HE1	6	0.12
(1,1099)	1:A:378:PHE:HE2	1:A:379:TYR:HE2	6	0.12
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE1	4	0.12
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE2	4	0.12
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE3	4	0.12
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE1	19	0.12
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE2	19	0.12
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE3	19	0.12
(1,106)	1:A:417:ILE:HB	1:A:440:LEU:HA	14	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1050)	1:A:443:MET:H	1:A:444:LYS:HB3	8	0.12
(1,1050)	1:A:443:MET:H	1:A:444:LYS:HB3	10	0.12
(1,1050)	1:A:443:MET:H	1:A:444:LYS:HB3	17	0.12
(1,888)	1:A:382:VAL:H	1:A:416:ALA:HB1	10	0.11
(1,888)	1:A:382:VAL:H	1:A:416:ALA:HB2	10	0.11
(1,888)	1:A:382:VAL:H	1:A:416:ALA:HB3	10	0.11
(1,859)	1:A:373:THR:H	1:A:384:GLN:HB3	4	0.11
(1,859)	1:A:373:THR:H	1:A:384:GLN:HB3	5	0.11
(1,846)	1:A:365:THR:H	1:A:376:VAL:HA	3	0.11
(1,722)	1:A:398:ASN:HD21	1:A:420:VAL:H	2	0.11
(1,708)	1:A:381:ASN:HD22	1:A:392:PHE:H	14	0.11
(1,546)	1:A:422:CYS:HB2	1:A:448:ALA:H	4	0.11
(1,546)	1:A:422:CYS:HB2	1:A:448:ALA:H	10	0.11
(1,396)	1:A:375:LYS:HE2	1:A:383:PHE:HE1	3	0.11
(1,396)	1:A:375:LYS:HE2	1:A:383:PHE:HE2	3	0.11
(1,396)	1:A:375:LYS:HE3	1:A:383:PHE:HE1	3	0.11
(1,396)	1:A:375:LYS:HE3	1:A:383:PHE:HE2	3	0.11
(1,360)	1:A:366:LYS:H	1:A:367:ARG:HD2	3	0.11
(1,336)	1:A:389:LEU:HA	1:A:439:TYR:HB2	7	0.11
(1,317)	1:A:418:VAL:HB	1:A:441:ILE:HG13	2	0.11
(1,317)	1:A:418:VAL:HB	1:A:441:ILE:HG13	7	0.11
(1,317)	1:A:418:VAL:HB	1:A:441:ILE:HG13	11	0.11
(1,317)	1:A:418:VAL:HB	1:A:441:ILE:HG13	16	0.11
(1,317)	1:A:418:VAL:HB	1:A:441:ILE:HG13	19	0.11
(1,264)	1:A:422:CYS:HB3	1:A:449:CYS:HA	16	0.11
(1,245)	1:A:388:LEU:HG	1:A:406:GLN:HG3	1	0.11
(1,223)	1:A:390:GLY:HA2	1:A:416:ALA:HB1	18	0.11
(1,223)	1:A:390:GLY:HA2	1:A:416:ALA:HB2	18	0.11
(1,223)	1:A:390:GLY:HA2	1:A:416:ALA:HB3	18	0.11
(1,174)	1:A:377:VAL:HA	1:A:380:GLU:HB2	12	0.11
(1,174)	1:A:377:VAL:HA	1:A:380:GLU:HB2	17	0.11
(1,1286)	1:A:413:HIS:H	1:A:413:HIS:HB2	18	0.11
(1,1286)	1:A:413:HIS:H	1:A:413:HIS:HB3	18	0.11
(1,1259)	1:A:401:LYS:HD2	1:A:403:GLU:HB2	14	0.11
(1,1259)	1:A:401:LYS:HD2	1:A:403:GLU:HB3	14	0.11
(1,1259)	1:A:401:LYS:HD3	1:A:403:GLU:HB2	14	0.11
(1,1259)	1:A:401:LYS:HD3	1:A:403:GLU:HB3	14	0.11
(1,1256)	1:A:401:LYS:HB2	1:A:401:LYS:HD2	9	0.11
(1,1256)	1:A:401:LYS:HB2	1:A:401:LYS:HD3	9	0.11
(1,1256)	1:A:401:LYS:HB3	1:A:401:LYS:HD2	9	0.11
(1,1256)	1:A:401:LYS:HB3	1:A:401:LYS:HD3	9	0.11
(1,1256)	1:A:401:LYS:HB2	1:A:401:LYS:HD2	10	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1256)	1:A:401:LYS:HB2	1:A:401:LYS:HD3	10	0.11
(1,1256)	1:A:401:LYS:HB3	1:A:401:LYS:HD2	10	0.11
(1,1256)	1:A:401:LYS:HB3	1:A:401:LYS:HD3	10	0.11
(1,1256)	1:A:401:LYS:HB2	1:A:401:LYS:HD2	13	0.11
(1,1256)	1:A:401:LYS:HB2	1:A:401:LYS:HD3	13	0.11
(1,1256)	1:A:401:LYS:HB3	1:A:401:LYS:HD2	13	0.11
(1,1256)	1:A:401:LYS:HB3	1:A:401:LYS:HD3	13	0.11
(1,1256)	1:A:401:LYS:HB2	1:A:401:LYS:HD2	17	0.11
(1,1256)	1:A:401:LYS:HB2	1:A:401:LYS:HD3	17	0.11
(1,1256)	1:A:401:LYS:HB3	1:A:401:LYS:HD2	17	0.11
(1,1256)	1:A:401:LYS:HB3	1:A:401:LYS:HD3	17	0.11
(1,1223)	1:A:384:GLN:HG2	1:A:389:LEU:H	1	0.11
(1,1223)	1:A:384:GLN:HG3	1:A:389:LEU:H	1	0.11
(1,1219)	1:A:383:PHE:HD1	1:A:384:GLN:HG2	14	0.11
(1,1219)	1:A:383:PHE:HD1	1:A:384:GLN:HG3	14	0.11
(1,1219)	1:A:383:PHE:HD2	1:A:384:GLN:HG2	14	0.11
(1,1219)	1:A:383:PHE:HD2	1:A:384:GLN:HG3	14	0.11
(1,1216)	1:A:382:VAL:HG11	1:A:384:GLN:HE21	14	0.11
(1,1216)	1:A:382:VAL:HG11	1:A:384:GLN:HE22	14	0.11
(1,1216)	1:A:382:VAL:HG12	1:A:384:GLN:HE21	14	0.11
(1,1216)	1:A:382:VAL:HG12	1:A:384:GLN:HE22	14	0.11
(1,1216)	1:A:382:VAL:HG13	1:A:384:GLN:HE21	14	0.11
(1,1216)	1:A:382:VAL:HG13	1:A:384:GLN:HE22	14	0.11
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG11	6	0.11
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG12	6	0.11
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG13	6	0.11
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG21	6	0.11
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG22	6	0.11
(1,1199)	1:A:378:PHE:HB2	1:A:418:VAL:HG23	6	0.11
(1,118)	1:A:366:LYS:HG2	1:A:367:ARG:HA	5	0.11
(1,118)	1:A:366:LYS:HG3	1:A:367:ARG:HA	5	0.11
(1,118)	1:A:366:LYS:HG2	1:A:367:ARG:HA	13	0.11
(1,118)	1:A:366:LYS:HG3	1:A:367:ARG:HA	13	0.11
(1,118)	1:A:366:LYS:HG2	1:A:367:ARG:HA	15	0.11
(1,118)	1:A:366:LYS:HG3	1:A:367:ARG:HA	15	0.11
(1,1175)	1:A:372:TYR:HB3	1:A:384:GLN:HG2	14	0.11
(1,1175)	1:A:372:TYR:HB3	1:A:384:GLN:HG3	14	0.11
(1,1161)	1:A:362:GLY:HA2	1:A:377:VAL:HG11	5	0.11
(1,1161)	1:A:362:GLY:HA2	1:A:377:VAL:HG12	5	0.11
(1,1161)	1:A:362:GLY:HA2	1:A:377:VAL:HG13	5	0.11
(1,1161)	1:A:362:GLY:HA3	1:A:377:VAL:HG11	5	0.11
(1,1161)	1:A:362:GLY:HA3	1:A:377:VAL:HG12	5	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1161)	1:A:362:GLY:HA3	1:A:377:VAL:HG13	5	0.11
(1,1161)	1:A:362:GLY:HA2	1:A:377:VAL:HG11	17	0.11
(1,1161)	1:A:362:GLY:HA2	1:A:377:VAL:HG12	17	0.11
(1,1161)	1:A:362:GLY:HA2	1:A:377:VAL:HG13	17	0.11
(1,1161)	1:A:362:GLY:HA3	1:A:377:VAL:HG11	17	0.11
(1,1161)	1:A:362:GLY:HA3	1:A:377:VAL:HG12	17	0.11
(1,1161)	1:A:362:GLY:HA3	1:A:377:VAL:HG13	17	0.11
(1,1127)	1:A:369:ILE:HG21	1:A:374:TYR:HD1	2	0.11
(1,1127)	1:A:369:ILE:HG21	1:A:374:TYR:HD2	2	0.11
(1,1127)	1:A:369:ILE:HG22	1:A:374:TYR:HD1	2	0.11
(1,1127)	1:A:369:ILE:HG22	1:A:374:TYR:HD2	2	0.11
(1,1127)	1:A:369:ILE:HG23	1:A:374:TYR:HD1	2	0.11
(1,1127)	1:A:369:ILE:HG23	1:A:374:TYR:HD2	2	0.11
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE1	17	0.11
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE2	17	0.11
(1,1087)	1:A:426:ASN:HD22	1:A:443:MET:HE3	17	0.11
(1,106)	1:A:417:ILE:HB	1:A:440:LEU:HA	17	0.11
(1,1050)	1:A:443:MET:H	1:A:444:LYS:HB3	1	0.11
(1,1050)	1:A:443:MET:H	1:A:444:LYS:HB3	5	0.11
(1,1050)	1:A:443:MET:H	1:A:444:LYS:HB3	15	0.11
(1,1044)	1:A:441:ILE:HG12	1:A:442:LYS:H	3	0.11

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value