Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 08:02 AM EDT

PDB ID	:	2KZK
BMRB ID	:	17007
Title	:	Solution structure of alpha-mannosidase binding domain of Atg34
Authors	:	Watanabe, Y.; Noda, N.; Kumeta, H.; Suzuki, K.; Ohsumi, Y.; Inagaki, F.
Deposited on	:	2010-06-18

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (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 (i)) were used in the production of this report:

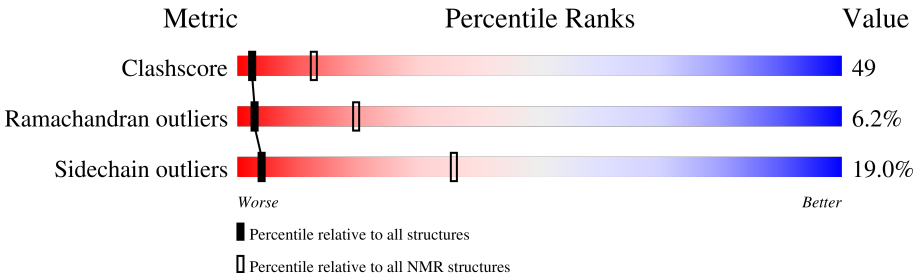
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 94%.

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	107	28% 51% 10% 7% .

2 Ensemble composition and analysis

This entry contains 20 models. Model 20 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:249-A:283, A:288-A:348 (96)	0.69	20

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1617 atoms, of which 807 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein YOL083W.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	103	1617	520	807	129	157	4	0

There are 4 discrepancies between the modelled and reference sequences:

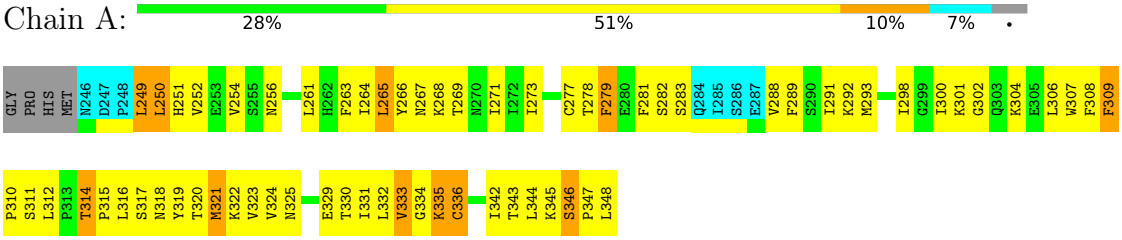
Chain	Residue	Modelled	Actual	Comment	Reference
A	242	GLY	-	expression tag	UNP Q12292
A	243	PRO	-	expression tag	UNP Q12292
A	244	HIS	-	expression tag	UNP Q12292
A	245	MET	-	expression tag	UNP Q12292

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: Uncharacterized protein YOL083W

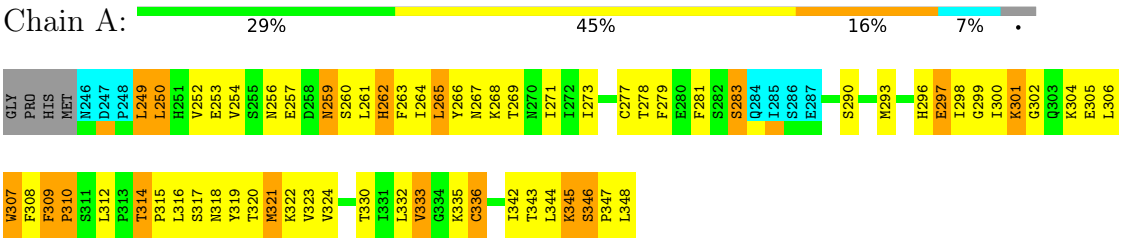


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

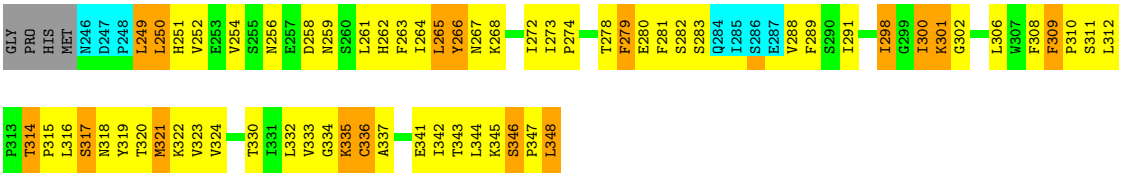
4.2.1 Score per residue for model 1

• Molecule 1: Uncharacterized protein YOL083W



4.2.2 Score per residue for model 2

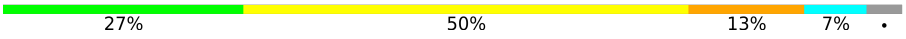
• Molecule 1: Uncharacterized protein YOL083W



4.2.3 Score per residue for model 3

• Molecule 1: Uncharacterized protein YOL083W

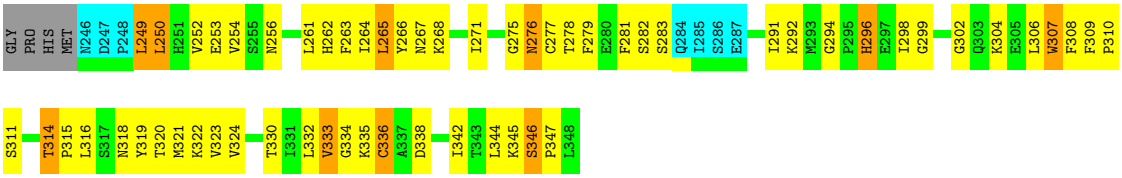
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Uncharacterized protein YOL083W

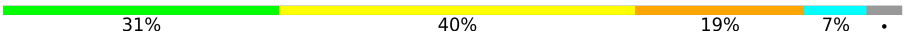
Chain A:

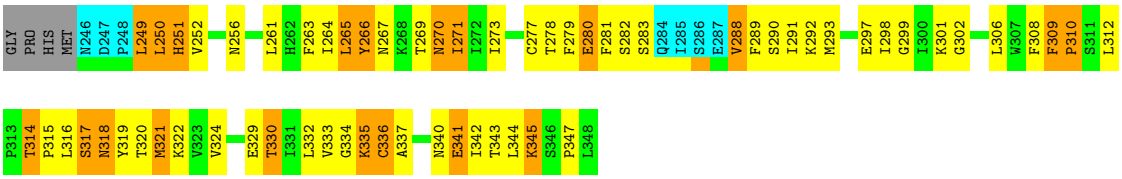


4.2.5 Score per residue for model 5

• Molecule 1: Uncharacterized protein YOL083W

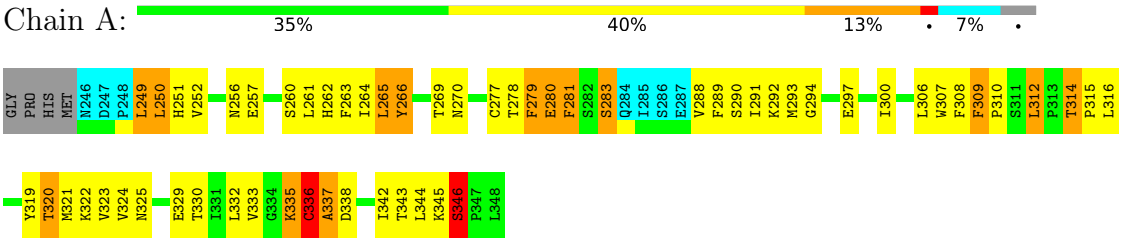
Chain A:





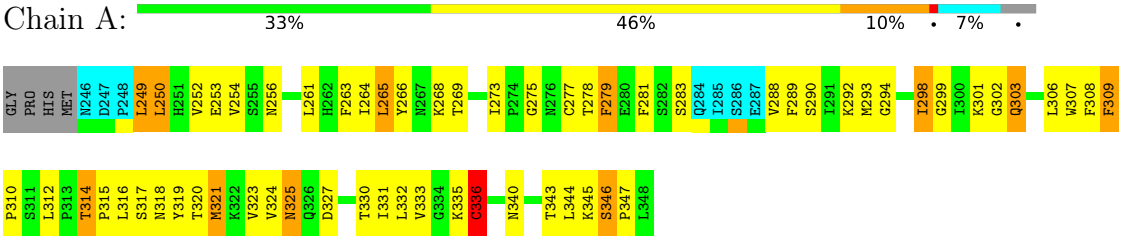
4.2.6 Score per residue for model 6

• Molecule 1: Uncharacterized protein YOL083W



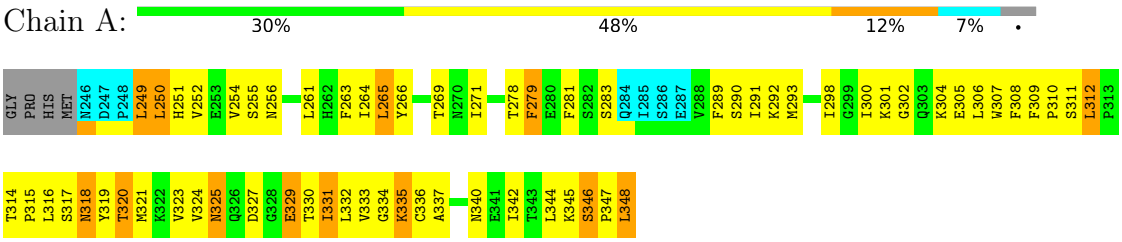
4.2.7 Score per residue for model 7

• Molecule 1: Uncharacterized protein YOL083W



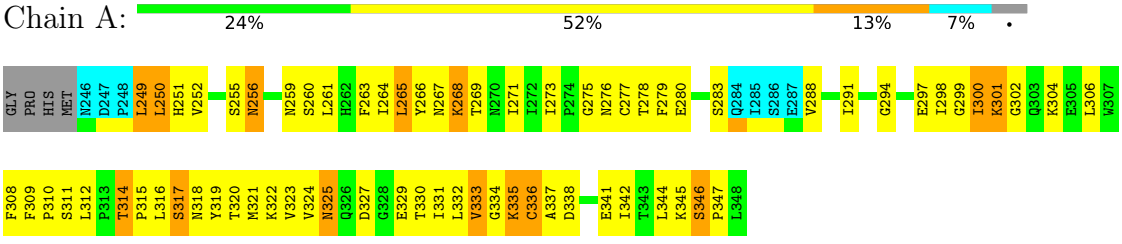
4.2.8 Score per residue for model 8

• Molecule 1: Uncharacterized protein YOL083W



4.2.9 Score per residue for model 9

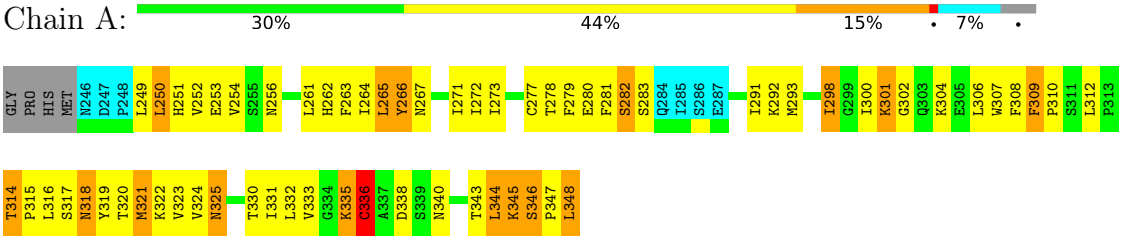
• Molecule 1: Uncharacterized protein YOL083W



4.2.10 Score per residue for model 10

• Molecule 1: Uncharacterized protein YOL083W

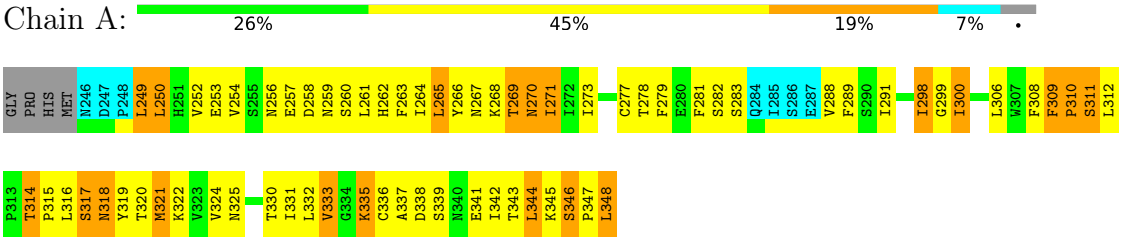
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Uncharacterized protein YOL083W

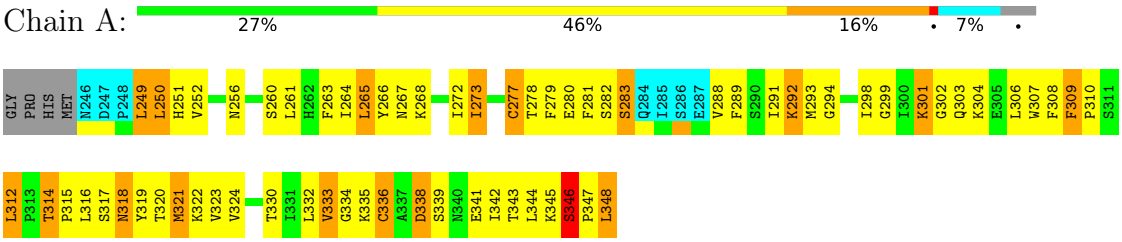
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Uncharacterized protein YOL083W

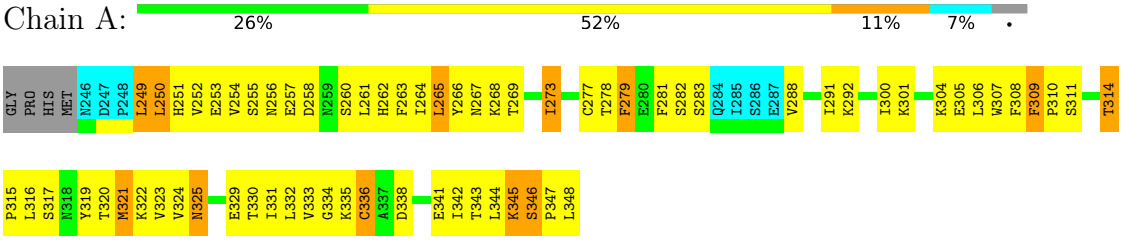
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Uncharacterized protein YOL083W

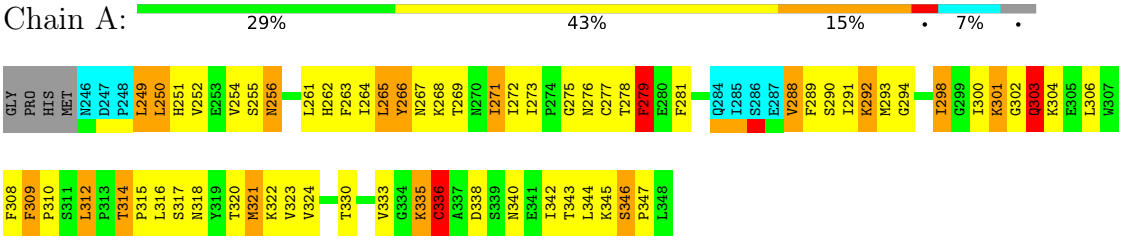
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Uncharacterized protein YOL083W

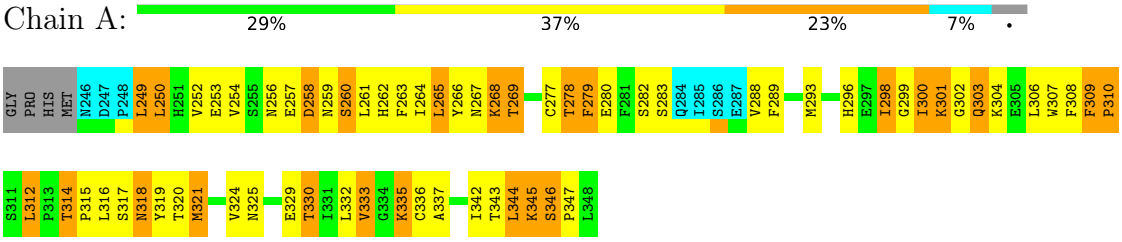
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Uncharacterized protein YOL083W

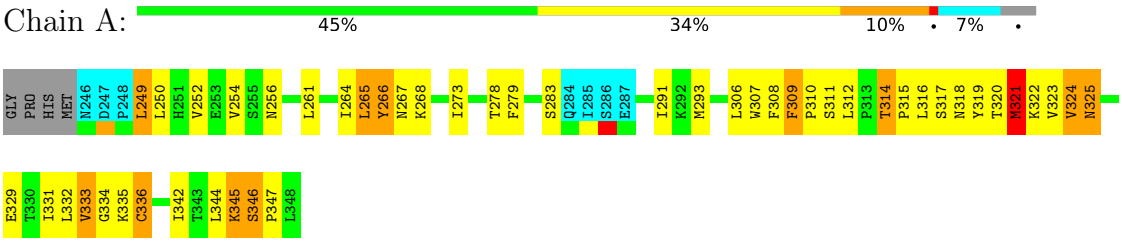
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Uncharacterized protein YOL083W

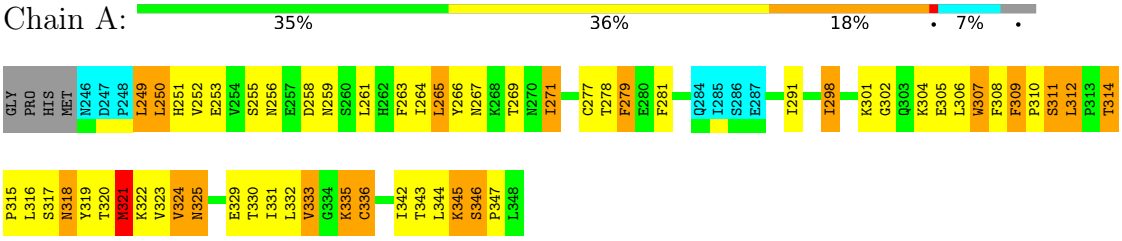
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Uncharacterized protein YOL083W

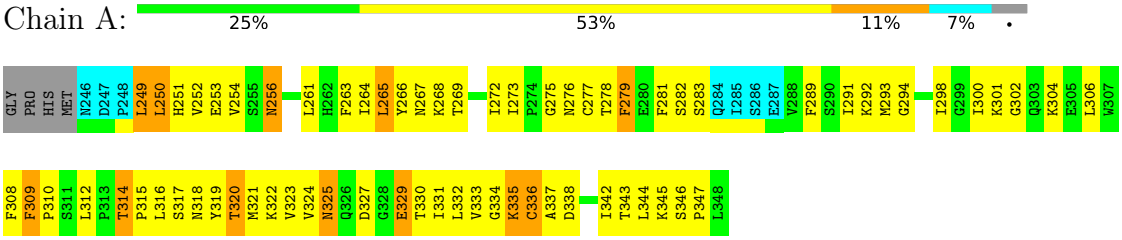
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Uncharacterized protein YOL083W

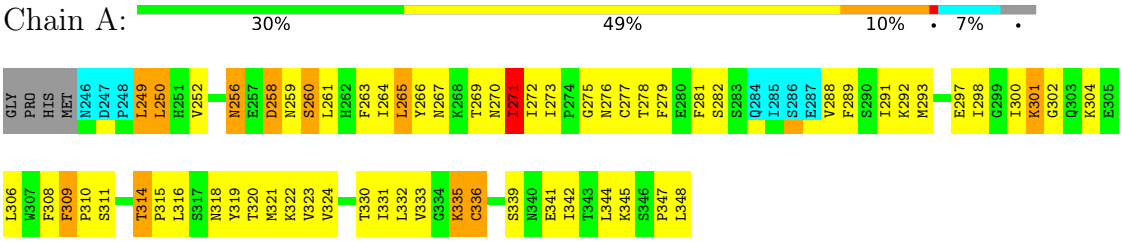
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Uncharacterized protein YOL083W

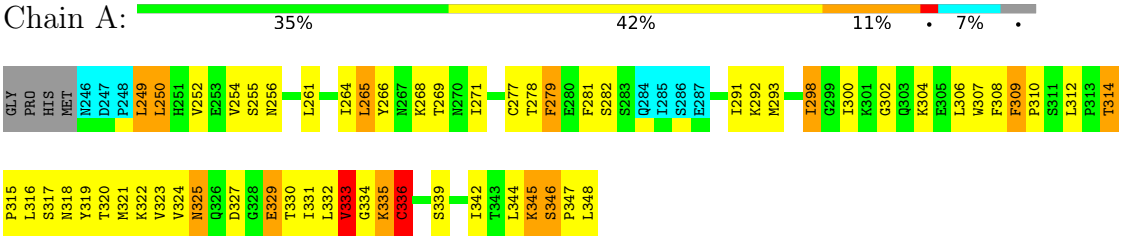
Chain A:



4.2.20 Score per residue for model 20 (medoid)

• Molecule 1: Uncharacterized protein YOL083W

Chain A:



5 Refinement protocol and experimental data overview

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
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	1303
Number of shifts mapped to atoms	1303
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

6 Model quality

6.1 Standard geometry

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	755	758	755	74±8
All	All	15100	15160	15100	1471

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 49.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:265:LEU:HD11	1:A:306:LEU:HD12	1.05	1.28	20	11
1:A:252:VAL:HG13	1:A:265:LEU:HD23	0.97	1.36	11	3
1:A:261:LEU:CD1	1:A:312:LEU:HD12	0.94	1.92	12	7
1:A:279:PHE:CG	1:A:306:LEU:HD13	0.92	2.00	15	12
1:A:316:LEU:HD13	1:A:321:MET:SD	0.91	2.05	9	5
1:A:249:LEU:HD23	1:A:249:LEU:O	0.91	1.65	3	2
1:A:283:SER:O	1:A:312:LEU:HD22	0.91	1.66	8	2
1:A:249:LEU:HD13	1:A:249:LEU:O	0.88	1.69	19	5
1:A:291:ILE:HD11	1:A:308:PHE:CD1	0.86	2.06	18	4
1:A:335:LYS:HZ3	1:A:337:ALA:H	0.85	1.04	18	1
1:A:278:THR:O	1:A:324:VAL:HG22	0.84	1.72	9	18
1:A:265:LEU:HD11	1:A:306:LEU:CD1	0.83	2.03	20	7
1:A:252:VAL:CG2	1:A:265:LEU:HD23	0.81	2.05	5	7
1:A:263:PHE:CE1	1:A:308:PHE:CD2	0.81	2.68	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:256:ASN:HA	1:A:261:LEU:HD23	0.81	1.53	11	20
1:A:279:PHE:CD1	1:A:323:VAL:HG22	0.81	2.11	12	7
1:A:250:LEU:HD22	1:A:344:LEU:HD22	0.80	1.53	19	7
1:A:298:ILE:HG23	1:A:302:GLY:O	0.80	1.75	15	4
1:A:278:THR:HG22	1:A:290:SER:OG	0.79	1.78	6	5
1:A:332:LEU:HB3	1:A:344:LEU:HD23	0.79	1.54	17	18
1:A:281:PHE:CE2	1:A:308:PHE:CD2	0.79	2.70	11	5
1:A:321:MET:SD	1:A:342:ILE:HD13	0.79	2.18	19	5
1:A:298:ILE:HG22	1:A:299:GLY:N	0.78	1.93	15	3
1:A:261:LEU:HD11	1:A:312:LEU:HG	0.78	1.54	14	1
1:A:252:VAL:HG21	1:A:265:LEU:HD23	0.78	1.55	5	8
1:A:261:LEU:HD11	1:A:312:LEU:HB2	0.77	1.54	7	6
1:A:293:MET:HG2	1:A:306:LEU:HD21	0.77	1.57	15	13
1:A:264:ILE:HG22	1:A:266:TYR:CZ	0.76	2.15	12	17
1:A:300:ILE:HG22	1:A:301:LYS:HD3	0.76	1.58	2	3
1:A:324:VAL:HG12	1:A:330:THR:N	0.75	1.97	20	12
1:A:250:LEU:CD2	1:A:344:LEU:HD22	0.75	2.12	2	5
1:A:316:LEU:HD23	1:A:319:TYR:CE2	0.75	2.15	1	10
1:A:279:PHE:CD1	1:A:306:LEU:HD13	0.75	2.15	5	4
1:A:325:ASN:OD1	1:A:331:ILE:HG21	0.75	1.82	10	3
1:A:264:ILE:HG22	1:A:266:TYR:CE1	0.74	2.16	20	4
1:A:321:MET:HE3	1:A:342:ILE:CD1	0.74	2.10	2	6
1:A:308:PHE:CE2	1:A:312:LEU:HD11	0.74	2.17	16	2
1:A:281:PHE:CZ	1:A:308:PHE:CG	0.74	2.75	3	4
1:A:264:ILE:HG22	1:A:266:TYR:CE2	0.74	2.18	13	10
1:A:325:ASN:ND2	1:A:331:ILE:HG23	0.74	1.97	3	1
1:A:265:LEU:N	1:A:265:LEU:HD12	0.74	1.97	15	1
1:A:283:SER:HB2	1:A:312:LEU:HD23	0.73	1.60	11	1
1:A:271:ILE:C	1:A:271:ILE:HD13	0.73	2.03	19	1
1:A:252:VAL:CG1	1:A:265:LEU:HD23	0.73	2.14	11	2
1:A:254:VAL:HG23	1:A:340:ASN:O	0.73	1.84	10	3
1:A:335:LYS:HZ2	1:A:337:ALA:HB2	0.72	1.44	9	7
1:A:251:HIS:CD2	1:A:343:THR:HG22	0.71	2.20	10	5
1:A:273:ILE:HG21	1:A:298:ILE:HD12	0.71	1.61	7	1
1:A:249:LEU:HD12	1:A:249:LEU:N	0.71	1.99	5	2
1:A:249:LEU:HD22	1:A:343:THR:HB	0.71	1.62	5	1
1:A:291:ILE:CD1	1:A:308:PHE:CD1	0.71	2.74	6	11
1:A:249:LEU:C	1:A:249:LEU:HD22	0.69	2.07	11	5
1:A:320:THR:HG22	1:A:322:LYS:HG2	0.69	1.64	16	1
1:A:281:PHE:CD1	1:A:308:PHE:CE2	0.69	2.81	8	2
1:A:332:LEU:CB	1:A:344:LEU:HD23	0.69	2.17	15	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:314:THR:HG22	1:A:316:LEU:HD12	0.69	1.63	13	5
1:A:254:VAL:CG1	1:A:314:THR:HG21	0.69	2.18	4	10
1:A:348:LEU:HD13	1:A:348:LEU:O	0.69	1.87	13	2
1:A:300:ILE:HG22	1:A:301:LYS:CD	0.68	2.17	14	2
1:A:273:ILE:HG13	1:A:298:ILE:HD12	0.68	1.64	18	2
1:A:254:VAL:HG22	1:A:263:PHE:CE2	0.68	2.24	15	1
1:A:250:LEU:HD12	1:A:250:LEU:C	0.67	2.10	11	7
1:A:316:LEU:HD13	1:A:321:MET:CE	0.67	2.18	18	6
1:A:309:PHE:CD1	1:A:309:PHE:N	0.67	2.63	1	15
1:A:293:MET:CG	1:A:306:LEU:HD21	0.67	2.19	20	8
1:A:249:LEU:HD22	1:A:251:HIS:NE2	0.67	2.04	6	2
1:A:348:LEU:C	1:A:348:LEU:HD22	0.67	2.11	3	4
1:A:281:PHE:CZ	1:A:308:PHE:CD2	0.67	2.82	10	9
1:A:334:GLY:CA	1:A:344:LEU:HD12	0.66	2.19	12	4
1:A:320:THR:HG23	1:A:322:LYS:HD3	0.66	1.65	13	1
1:A:263:PHE:CE2	1:A:308:PHE:CD2	0.66	2.83	3	4
1:A:249:LEU:HD12	1:A:249:LEU:O	0.66	1.91	4	8
1:A:279:PHE:CD1	1:A:306:LEU:CD1	0.66	2.80	12	6
1:A:252:VAL:HG22	1:A:265:LEU:HD23	0.66	1.67	20	2
1:A:321:MET:HE1	1:A:342:ILE:HD11	0.65	1.66	15	2
1:A:266:TYR:N	1:A:266:TYR:CD1	0.65	2.64	14	6
1:A:249:LEU:HD23	1:A:249:LEU:C	0.65	2.11	3	2
1:A:261:LEU:HD12	1:A:312:LEU:HD12	0.65	1.67	1	4
1:A:323:VAL:CG2	1:A:344:LEU:HD21	0.65	2.21	1	4
1:A:265:LEU:CD1	1:A:306:LEU:HD12	0.65	2.15	20	2
1:A:252:VAL:HG22	1:A:265:LEU:HB3	0.65	1.67	6	4
1:A:300:ILE:HG22	1:A:301:LYS:N	0.64	2.07	9	2
1:A:264:ILE:CG2	1:A:266:TYR:CZ	0.64	2.80	4	14
1:A:321:MET:HE3	1:A:342:ILE:HD13	0.64	1.67	2	1
1:A:316:LEU:O	1:A:319:TYR:CD1	0.64	2.51	11	2
1:A:273:ILE:HD13	1:A:273:ILE:N	0.64	2.07	2	1
1:A:264:ILE:CG2	1:A:266:TYR:CE2	0.64	2.81	13	9
1:A:251:HIS:NE2	1:A:343:THR:HG22	0.64	2.07	10	1
1:A:264:ILE:CG2	1:A:266:TYR:CE1	0.64	2.81	19	4
1:A:321:MET:HE1	1:A:342:ILE:CD1	0.64	2.23	15	5
1:A:325:ASN:OD1	1:A:331:ILE:HD13	0.64	1.93	16	1
1:A:261:LEU:CD1	1:A:312:LEU:CD1	0.63	2.77	6	3
1:A:263:PHE:CD2	1:A:308:PHE:CE2	0.63	2.87	2	3
1:A:291:ILE:CD1	1:A:308:PHE:CE1	0.63	2.81	17	6
1:A:281:PHE:CE1	1:A:308:PHE:CD2	0.63	2.87	8	1
1:A:283:SER:OG	1:A:312:LEU:HD22	0.63	1.94	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:264:ILE:HG23	1:A:304:LYS:O	0.63	1.94	10	3
1:A:324:VAL:HG12	1:A:330:THR:HA	0.62	1.68	6	8
1:A:281:PHE:CE1	1:A:308:PHE:CE2	0.62	2.87	8	4
1:A:316:LEU:HD12	1:A:321:MET:CE	0.62	2.25	4	2
1:A:336:CYS:O	1:A:337:ALA:HB2	0.62	1.94	6	1
1:A:267:ASN:HB2	1:A:273:ILE:HD13	0.62	1.70	1	2
1:A:325:ASN:ND2	1:A:331:ILE:HD13	0.62	2.09	17	1
1:A:249:LEU:HD22	1:A:343:THR:CB	0.61	2.24	5	1
1:A:314:THR:HG22	1:A:316:LEU:CD1	0.61	2.25	13	3
1:A:261:LEU:HD11	1:A:312:LEU:CG	0.61	2.26	14	1
1:A:281:PHE:CD1	1:A:281:PHE:N	0.61	2.68	6	9
1:A:324:VAL:HG12	1:A:330:THR:CA	0.61	2.26	6	12
1:A:321:MET:CE	1:A:342:ILE:CD1	0.61	2.79	1	8
1:A:316:LEU:HD23	1:A:319:TYR:CD2	0.61	2.30	19	6
1:A:251:HIS:O	1:A:266:TYR:CD2	0.61	2.54	10	1
1:A:316:LEU:HD12	1:A:321:MET:HE2	0.60	1.72	3	2
1:A:265:LEU:HD12	1:A:265:LEU:H	0.60	1.56	15	1
1:A:264:ILE:O	1:A:266:TYR:CE1	0.60	2.54	14	9
1:A:282:SER:O	1:A:319:TYR:CD2	0.60	2.55	4	9
1:A:254:VAL:HG22	1:A:263:PHE:CE1	0.60	2.31	13	2
1:A:301:LYS:N	1:A:301:LYS:CD	0.60	2.64	2	2
1:A:291:ILE:HD12	1:A:308:PHE:CE1	0.60	2.32	13	8
1:A:264:ILE:O	1:A:266:TYR:CE2	0.60	2.54	20	2
1:A:279:PHE:CD2	1:A:306:LEU:HD13	0.60	2.29	15	3
1:A:291:ILE:HD12	1:A:308:PHE:CD1	0.60	2.31	19	7
1:A:256:ASN:CA	1:A:261:LEU:HD23	0.60	2.27	15	6
1:A:306:LEU:O	1:A:308:PHE:CE1	0.60	2.55	10	7
1:A:298:ILE:CG2	1:A:299:GLY:N	0.60	2.64	15	2
1:A:256:ASN:OD1	1:A:314:THR:HG23	0.60	1.96	9	4
1:A:282:SER:OG	1:A:319:TYR:CD2	0.60	2.53	5	2
1:A:261:LEU:HD13	1:A:263:PHE:CZ	0.60	2.32	18	4
1:A:308:PHE:CE2	1:A:312:LEU:CD1	0.60	2.83	16	2
1:A:308:PHE:CE2	1:A:309:PHE:O	0.60	2.55	16	1
1:A:298:ILE:HG23	1:A:302:GLY:C	0.60	2.16	15	5
1:A:300:ILE:HD13	1:A:300:ILE:N	0.60	2.10	20	2
1:A:291:ILE:HD13	1:A:308:PHE:CE1	0.59	2.32	17	3
1:A:282:SER:O	1:A:319:TYR:CE2	0.59	2.55	11	4
1:A:267:ASN:HB3	1:A:298:ILE:HG22	0.59	1.73	4	1
1:A:254:VAL:HG11	1:A:314:THR:CG2	0.59	2.27	1	4
1:A:271:ILE:C	1:A:272:ILE:HD12	0.59	2.17	14	1
1:A:261:LEU:HD12	1:A:308:PHE:CD1	0.59	2.32	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:263:PHE:CE1	1:A:321:MET:SD	0.59	2.96	2	1
1:A:307:TRP:CD1	1:A:307:TRP:O	0.59	2.55	8	3
1:A:317:SER:O	1:A:318:ASN:CB	0.58	2.51	12	15
1:A:291:ILE:HD13	1:A:308:PHE:CD1	0.58	2.34	17	4
1:A:335:LYS:HZ2	1:A:337:ALA:CB	0.58	2.12	2	6
1:A:291:ILE:HD11	1:A:308:PHE:HD1	0.57	1.58	5	3
1:A:254:VAL:HG13	1:A:263:PHE:CE1	0.57	2.33	11	1
1:A:308:PHE:CE1	1:A:312:LEU:HD11	0.57	2.33	1	1
1:A:252:VAL:HG13	1:A:265:LEU:CD2	0.57	2.24	11	2
1:A:316:LEU:HD22	1:A:321:MET:HE3	0.57	1.76	17	1
1:A:345:LYS:O	1:A:346:SER:CB	0.56	2.52	17	17
1:A:329:GLU:CG	1:A:329:GLU:O	0.56	2.53	17	4
1:A:254:VAL:HG11	1:A:314:THR:HG21	0.56	1.75	1	7
1:A:320:THR:O	1:A:321:MET:C	0.56	2.44	11	20
1:A:250:LEU:C	1:A:250:LEU:CD1	0.56	2.73	11	10
1:A:261:LEU:HD13	1:A:263:PHE:HE2	0.56	1.58	7	2
1:A:249:LEU:CD2	1:A:249:LEU:N	0.56	2.68	12	1
1:A:296:HIS:CE1	1:A:297:GLU:OE1	0.56	2.58	1	1
1:A:320:THR:HG23	1:A:322:LYS:HD2	0.56	1.77	18	1
1:A:294:GLY:HA3	1:A:304:LYS:HZ2	0.56	1.61	18	1
1:A:267:ASN:ND2	1:A:273:ILE:HD11	0.56	2.15	2	1
1:A:283:SER:OG	1:A:319:TYR:CE2	0.56	2.55	6	1
1:A:334:GLY:HA2	1:A:344:LEU:HD12	0.55	1.76	5	3
1:A:308:PHE:CE1	1:A:312:LEU:CD1	0.55	2.89	1	1
1:A:251:HIS:O	1:A:252:VAL:HG23	0.55	2.02	14	2
1:A:332:LEU:HD21	1:A:345:LYS:O	0.55	2.01	20	1
1:A:261:LEU:HD13	1:A:312:LEU:HD12	0.55	1.73	12	2
1:A:262:HIS:NE2	1:A:264:ILE:CD1	0.55	2.70	13	1
1:A:267:ASN:CG	1:A:273:ILE:HD13	0.55	2.22	13	1
1:A:262:HIS:NE2	1:A:307:TRP:CD1	0.55	2.74	4	2
1:A:308:PHE:CD2	1:A:312:LEU:CD1	0.55	2.89	16	1
1:A:281:PHE:HE1	1:A:291:ILE:HD12	0.55	1.61	3	1
1:A:322:LYS:HZ2	1:A:333:VAL:HB	0.55	1.62	4	2
1:A:294:GLY:CA	1:A:304:LYS:NZ	0.55	2.70	18	1
1:A:279:PHE:CE1	1:A:323:VAL:HG22	0.55	2.36	3	3
1:A:332:LEU:HD23	1:A:346:SER:HA	0.55	1.78	4	5
1:A:250:LEU:C	1:A:250:LEU:HD12	0.55	2.21	17	3
1:A:308:PHE:CZ	1:A:309:PHE:O	0.55	2.59	16	3
1:A:308:PHE:C	1:A:309:PHE:CD1	0.54	2.81	10	4
1:A:335:LYS:HZ3	1:A:337:ALA:N	0.54	1.88	18	1
1:A:324:VAL:HG23	1:A:329:GLU:H	0.54	1.61	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:335:LYS:C	1:A:336:CYS:SG	0.54	2.86	20	1
1:A:281:PHE:CZ	1:A:308:PHE:CE2	0.53	2.96	6	2
1:A:263:PHE:O	1:A:265:LEU:HD23	0.53	2.03	9	1
1:A:298:ILE:HG22	1:A:298:ILE:O	0.53	2.04	4	1
1:A:252:VAL:CG1	1:A:265:LEU:CD2	0.53	2.86	11	1
1:A:308:PHE:CG	1:A:309:PHE:N	0.53	2.76	7	6
1:A:269:THR:O	1:A:270:ASN:CB	0.53	2.57	11	2
1:A:292:LYS:CD	1:A:292:LYS:N	0.53	2.72	14	2
1:A:324:VAL:HG23	1:A:329:GLU:N	0.53	2.18	16	1
1:A:252:VAL:HG13	1:A:265:LEU:HB3	0.53	1.80	9	1
1:A:262:HIS:CD2	1:A:307:TRP:CD1	0.52	2.97	4	1
1:A:320:THR:CG2	1:A:321:MET:N	0.52	2.72	8	2
1:A:325:ASN:OD1	1:A:331:ILE:HG22	0.52	2.04	8	2
1:A:325:ASN:ND2	1:A:325:ASN:N	0.52	2.57	3	4
1:A:325:ASN:CG	1:A:331:ILE:HD13	0.52	2.25	16	2
1:A:279:PHE:HD1	1:A:323:VAL:HG22	0.52	1.59	12	1
1:A:261:LEU:HD13	1:A:263:PHE:CE2	0.52	2.39	7	3
1:A:298:ILE:CG2	1:A:302:GLY:O	0.52	2.58	14	7
1:A:251:HIS:CD2	1:A:341:GLU:OE1	0.52	2.62	5	1
1:A:263:PHE:CD1	1:A:308:PHE:CE2	0.52	2.98	19	4
1:A:270:ASN:O	1:A:300:ILE:HD11	0.52	2.04	19	2
1:A:252:VAL:HG13	1:A:265:LEU:HG	0.52	1.80	16	1
1:A:279:PHE:CG	1:A:306:LEU:CD1	0.52	2.85	15	3
1:A:278:THR:HG23	1:A:291:ILE:O	0.52	2.05	16	3
1:A:333:VAL:HG11	1:A:347:PRO:HA	0.52	1.80	15	2
1:A:283:SER:CB	1:A:312:LEU:HD23	0.52	2.35	9	5
1:A:251:HIS:ND1	1:A:343:THR:HG22	0.52	2.19	2	1
1:A:281:PHE:CZ	1:A:308:PHE:HB3	0.51	2.40	3	2
1:A:265:LEU:HD21	1:A:306:LEU:HD12	0.51	1.82	9	3
1:A:316:LEU:HD23	1:A:319:TYR:HD2	0.51	1.65	15	2
1:A:316:LEU:HD22	1:A:319:TYR:CE2	0.51	2.40	2	2
1:A:278:THR:HG22	1:A:290:SER:HB3	0.51	1.82	7	1
1:A:325:ASN:ND2	1:A:325:ASN:H	0.51	2.03	9	5
1:A:336:CYS:SG	1:A:342:ILE:CD1	0.51	2.98	17	1
1:A:336:CYS:SG	1:A:342:ILE:HD13	0.51	2.45	8	2
1:A:335:LYS:NZ	1:A:337:ALA:HB2	0.51	2.18	9	2
1:A:269:THR:OG1	1:A:271:ILE:CD1	0.51	2.59	11	1
1:A:269:THR:O	1:A:300:ILE:HD12	0.51	2.05	20	1
1:A:258:ASP:O	1:A:259:ASN:CB	0.51	2.59	11	2
1:A:312:LEU:HD12	1:A:312:LEU:O	0.51	2.04	14	1
1:A:332:LEU:C	1:A:333:VAL:HG12	0.51	2.26	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:316:LEU:CD2	1:A:319:TYR:CD2	0.51	2.94	7	3
1:A:280:GLU:CG	1:A:288:VAL:HG21	0.51	2.36	2	2
1:A:294:GLY:CA	1:A:304:LYS:HZ2	0.51	2.18	18	1
1:A:325:ASN:OD1	1:A:331:ILE:CG2	0.50	2.60	18	6
1:A:261:LEU:HD22	1:A:263:PHE:CE1	0.50	2.42	10	1
1:A:280:GLU:HG3	1:A:288:VAL:HG21	0.50	1.83	2	4
1:A:280:GLU:HG2	1:A:288:VAL:HG21	0.50	1.82	5	1
1:A:271:ILE:C	1:A:271:ILE:CD1	0.50	2.74	19	1
1:A:306:LEU:O	1:A:308:PHE:CD1	0.50	2.64	12	2
1:A:316:LEU:CD2	1:A:319:TYR:CE2	0.50	2.93	1	5
1:A:251:HIS:O	1:A:252:VAL:CG2	0.50	2.59	14	2
1:A:263:PHE:CE1	1:A:308:PHE:CE2	0.50	3.00	9	3
1:A:320:THR:HG23	1:A:322:LYS:HZ3	0.50	1.67	20	1
1:A:320:THR:HG22	1:A:322:LYS:HG3	0.50	1.83	2	5
1:A:256:ASN:OD1	1:A:314:THR:CG2	0.50	2.60	9	3
1:A:308:PHE:C	1:A:309:PHE:CG	0.49	2.86	10	1
1:A:275:GLY:O	1:A:276:ASN:CB	0.49	2.60	18	3
1:A:332:LEU:CD2	1:A:345:LYS:C	0.49	2.80	20	1
1:A:268:LYS:CE	1:A:300:ILE:O	0.49	2.60	1	2
1:A:261:LEU:HD13	1:A:263:PHE:HZ	0.49	1.67	5	2
1:A:316:LEU:C	1:A:319:TYR:CD1	0.49	2.85	17	2
1:A:282:SER:HB3	1:A:288:VAL:HG23	0.49	1.84	15	1
1:A:267:ASN:CG	1:A:298:ILE:CG2	0.49	2.79	18	1
1:A:316:LEU:HD22	1:A:321:MET:CE	0.49	2.38	6	3
1:A:321:MET:CE	1:A:342:ILE:HD11	0.49	2.37	16	2
1:A:322:LYS:HG2	1:A:333:VAL:HG23	0.49	1.85	12	1
1:A:320:THR:HG23	1:A:322:LYS:CD	0.49	2.38	18	1
1:A:252:VAL:HG12	1:A:253:GLU:N	0.49	2.23	11	10
1:A:316:LEU:O	1:A:319:TYR:HB2	0.49	2.07	12	2
1:A:261:LEU:HD21	1:A:312:LEU:CD1	0.49	2.38	14	1
1:A:322:LYS:HG2	1:A:333:VAL:HG12	0.49	1.84	19	1
1:A:283:SER:HA	1:A:319:TYR:CE2	0.49	2.42	4	8
1:A:251:HIS:CD2	1:A:252:VAL:N	0.49	2.81	5	2
1:A:249:LEU:O	1:A:249:LEU:CD1	0.49	2.60	14	8
1:A:335:LYS:O	1:A:336:CYS:CB	0.49	2.60	6	1
1:A:249:LEU:N	1:A:249:LEU:HD23	0.49	2.22	12	1
1:A:249:LEU:HD22	1:A:250:LEU:N	0.49	2.23	7	2
1:A:288:VAL:HG22	1:A:289:PHE:N	0.49	2.23	11	8
1:A:294:GLY:N	1:A:304:LYS:NZ	0.49	2.60	18	2
1:A:267:ASN:OD1	1:A:273:ILE:CD1	0.49	2.60	16	3
1:A:305:GLU:HB2	1:A:307:TRP:CZ2	0.49	2.43	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:294:GLY:H	1:A:304:LYS:NZ	0.49	2.06	4	2
1:A:267:ASN:OD1	1:A:273:ILE:HD13	0.49	2.08	13	1
1:A:254:VAL:CG2	1:A:340:ASN:O	0.49	2.61	14	1
1:A:279:PHE:CD1	1:A:322:LYS:O	0.49	2.66	16	1
1:A:335:LYS:NZ	1:A:337:ALA:CB	0.48	2.76	5	5
1:A:281:PHE:CE1	1:A:291:ILE:HD12	0.48	2.43	3	1
1:A:316:LEU:HD13	1:A:321:MET:HE3	0.48	1.85	12	5
1:A:283:SER:O	1:A:319:TYR:CE2	0.48	2.66	9	1
1:A:321:MET:CE	1:A:336:CYS:SG	0.48	3.01	16	2
1:A:279:PHE:CD2	1:A:281:PHE:CD1	0.48	3.02	7	5
1:A:277:CYS:SG	1:A:293:MET:CE	0.48	3.01	12	1
1:A:324:VAL:HG12	1:A:329:GLU:C	0.48	2.28	20	2
1:A:336:CYS:O	1:A:337:ALA:CB	0.48	2.60	6	1
1:A:252:VAL:HG22	1:A:265:LEU:CD2	0.48	2.35	20	1
1:A:279:PHE:CE2	1:A:321:MET:HG2	0.48	2.43	4	3
1:A:316:LEU:HD13	1:A:321:MET:HE1	0.48	1.85	18	2
1:A:307:TRP:CE3	1:A:307:TRP:O	0.48	2.67	16	2
1:A:281:PHE:CD2	1:A:312:LEU:HD11	0.48	2.44	8	2
1:A:273:ILE:HG22	1:A:274:PRO:HD2	0.48	1.85	2	1
1:A:306:LEU:HB3	1:A:308:PHE:CE1	0.48	2.43	2	12
1:A:312:LEU:HD12	1:A:312:LEU:H	0.48	1.69	11	1
1:A:251:HIS:CE1	1:A:341:GLU:CD	0.48	2.87	9	1
1:A:332:LEU:C	1:A:333:VAL:CG1	0.48	2.82	3	9
1:A:271:ILE:HD13	1:A:271:ILE:O	0.48	2.09	19	1
1:A:298:ILE:CG2	1:A:302:GLY:C	0.47	2.82	1	6
1:A:298:ILE:HG22	1:A:299:GLY:H	0.47	1.63	15	2
1:A:249:LEU:CD1	1:A:249:LEU:C	0.47	2.82	9	1
1:A:259:ASN:ND2	1:A:260:SER:N	0.47	2.63	9	1
1:A:281:PHE:CZ	1:A:308:PHE:CB	0.47	2.97	3	1
1:A:296:HIS:CE1	1:A:304:LYS:HD3	0.47	2.44	4	1
1:A:267:ASN:OD1	1:A:271:ILE:HD13	0.47	2.09	11	1
1:A:263:PHE:CD1	1:A:263:PHE:N	0.47	2.78	14	2
1:A:305:GLU:CB	1:A:307:TRP:CZ2	0.47	2.97	1	1
1:A:281:PHE:CE2	1:A:308:PHE:HB3	0.47	2.45	3	2
1:A:279:PHE:CD2	1:A:308:PHE:CZ	0.47	3.02	12	1
1:A:310:PRO:O	1:A:311:SER:CB	0.47	2.63	17	1
1:A:321:MET:HE3	1:A:342:ILE:HD11	0.47	1.84	18	1
1:A:314:THR:CB	1:A:315:PRO:HA	0.47	2.39	14	10
1:A:252:VAL:N	1:A:342:ILE:O	0.47	2.48	14	2
1:A:316:LEU:HD13	1:A:321:MET:HE2	0.47	1.84	18	2
1:A:312:LEU:CD1	1:A:312:LEU:C	0.47	2.83	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:322:LYS:CG	1:A:333:VAL:HG12	0.47	2.40	19	2
1:A:323:VAL:HG21	1:A:344:LEU:HD21	0.47	1.83	1	1
1:A:270:ASN:C	1:A:271:ILE:CG2	0.47	2.83	11	1
1:A:330:THR:HG22	1:A:347:PRO:HG3	0.47	1.86	12	1
1:A:267:ASN:CG	1:A:267:ASN:O	0.47	2.51	15	2
1:A:316:LEU:CD1	1:A:321:MET:CE	0.47	2.93	12	1
1:A:277:CYS:SG	1:A:331:ILE:CD1	0.47	3.03	19	1
1:A:306:LEU:HB3	1:A:308:PHE:CZ	0.47	2.45	17	8
1:A:267:ASN:ND2	1:A:271:ILE:O	0.46	2.48	11	2
1:A:278:THR:HG23	1:A:292:LYS:HA	0.46	1.87	8	1
1:A:272:ILE:HD12	1:A:272:ILE:N	0.46	2.25	18	3
1:A:336:CYS:SG	1:A:337:ALA:N	0.46	2.88	6	1
1:A:261:LEU:HD21	1:A:312:LEU:HD12	0.46	1.87	14	1
1:A:254:VAL:HG12	1:A:314:THR:HG21	0.46	1.87	2	1
1:A:294:GLY:H	1:A:304:LYS:HZ1	0.46	1.54	4	2
1:A:278:THR:CG2	1:A:290:SER:OG	0.46	2.60	8	2
1:A:252:VAL:HG13	1:A:265:LEU:CB	0.46	2.40	9	1
1:A:316:LEU:O	1:A:319:TYR:CG	0.46	2.69	11	2
1:A:269:THR:O	1:A:300:ILE:CD1	0.46	2.64	19	1
1:A:314:THR:HA	1:A:315:PRO:C	0.46	2.31	8	20
1:A:348:LEU:HD13	1:A:348:LEU:C	0.46	2.30	13	1
1:A:278:THR:O	1:A:324:VAL:CG2	0.46	2.64	5	6
1:A:267:ASN:ND2	1:A:299:GLY:O	0.46	2.49	9	1
1:A:325:ASN:HB3	1:A:331:ILE:HG21	0.46	1.87	11	1
1:A:305:GLU:HG2	1:A:307:TRP:CZ3	0.46	2.46	13	1
1:A:320:THR:O	1:A:322:LYS:N	0.46	2.49	2	2
1:A:325:ASN:ND2	1:A:329:GLU:O	0.46	2.49	3	1
1:A:288:VAL:CG2	1:A:289:PHE:N	0.46	2.79	19	4
1:A:298:ILE:HD11	1:A:304:LYS:HB2	0.46	1.88	9	2
1:A:267:ASN:CG	1:A:273:ILE:CD1	0.46	2.85	19	1
1:A:251:HIS:CE1	1:A:341:GLU:HG2	0.46	2.46	2	2
1:A:266:TYR:CD1	1:A:266:TYR:N	0.45	2.85	5	4
1:A:329:GLU:O	1:A:329:GLU:CG	0.45	2.64	5	2
1:A:261:LEU:HD22	1:A:263:PHE:CZ	0.45	2.46	18	1
1:A:300:ILE:CG2	1:A:301:LYS:N	0.45	2.76	9	2
1:A:252:VAL:CG1	1:A:253:GLU:N	0.45	2.79	17	6
1:A:249:LEU:CD1	1:A:249:LEU:O	0.45	2.64	9	1
1:A:260:SER:CB	1:A:310:PRO:O	0.45	2.64	12	1
1:A:251:HIS:CD2	1:A:341:GLU:CD	0.45	2.89	5	1
1:A:281:PHE:CE2	1:A:312:LEU:HD11	0.45	2.47	8	2
1:A:249:LEU:O	1:A:269:THR:CG2	0.45	2.64	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:298:ILE:N	1:A:298:ILE:HD13	0.45	2.25	14	1
1:A:309:PHE:HA	1:A:310:PRO:C	0.45	2.32	10	20
1:A:279:PHE:CZ	1:A:321:MET:HG2	0.45	2.47	4	2
1:A:312:LEU:HD22	1:A:316:LEU:HD21	0.45	1.89	14	1
1:A:312:LEU:CD2	1:A:316:LEU:HD21	0.45	2.40	14	1
1:A:323:VAL:HG23	1:A:344:LEU:HD21	0.45	1.88	2	2
1:A:267:ASN:O	1:A:267:ASN:ND2	0.45	2.50	4	1
1:A:283:SER:CB	1:A:319:TYR:OH	0.45	2.65	6	1
1:A:300:ILE:C	1:A:302:GLY:N	0.45	2.70	8	1
1:A:333:VAL:CG2	1:A:333:VAL:O	0.45	2.64	17	1
1:A:249:LEU:N	1:A:249:LEU:CD1	0.45	2.70	5	2
1:A:267:ASN:ND2	1:A:300:ILE:O	0.45	2.50	9	1
1:A:266:TYR:O	1:A:268:LYS:N	0.45	2.50	12	3
1:A:265:LEU:O	1:A:304:LYS:N	0.44	2.50	13	6
1:A:263:PHE:CE2	1:A:308:PHE:CE2	0.44	3.05	3	3
1:A:254:VAL:O	1:A:340:ASN:ND2	0.44	2.50	3	2
1:A:262:HIS:CD2	1:A:264:ILE:HG13	0.44	2.46	13	1
1:A:275:GLY:O	1:A:276:ASN:ND2	0.44	2.49	4	1
1:A:256:ASN:HB2	1:A:314:THR:HG21	0.44	1.88	8	1
1:A:280:GLU:O	1:A:321:MET:N	0.44	2.50	2	2
1:A:281:PHE:CE1	1:A:289:PHE:HB3	0.44	2.47	2	1
1:A:322:LYS:C	1:A:323:VAL:CG2	0.44	2.86	6	6
1:A:335:LYS:O	1:A:336:CYS:SG	0.44	2.76	6	3
1:A:335:LYS:NZ	1:A:336:CYS:O	0.44	2.49	6	1
1:A:265:LEU:N	1:A:265:LEU:CD1	0.44	2.69	15	1
1:A:278:THR:N	1:A:293:MET:SD	0.44	2.91	16	2
1:A:283:SER:HB2	1:A:312:LEU:HD21	0.44	1.89	5	1
1:A:273:ILE:O	1:A:297:GLU:CG	0.44	2.65	9	2
1:A:305:GLU:HG2	1:A:307:TRP:CH2	0.44	2.47	13	1
1:A:335:LYS:CE	1:A:336:CYS:O	0.44	2.65	6	1
1:A:291:ILE:CG2	1:A:306:LEU:HD23	0.44	2.42	16	1
1:A:267:ASN:OD1	1:A:273:ILE:HD12	0.44	2.12	1	1
1:A:281:PHE:O	1:A:281:PHE:CG	0.44	2.70	2	1
1:A:316:LEU:C	1:A:336:CYS:HG	0.44	2.16	11	1
1:A:282:SER:OG	1:A:288:VAL:N	0.44	2.51	13	1
1:A:267:ASN:OD1	1:A:299:GLY:O	0.44	2.36	15	1
1:A:305:GLU:HB3	1:A:307:TRP:CE2	0.44	2.48	17	2
1:A:265:LEU:H	1:A:265:LEU:HD12	0.44	1.72	3	2
1:A:264:ILE:HG21	1:A:266:TYR:CE2	0.44	2.48	17	1
1:A:325:ASN:ND2	1:A:331:ILE:CG2	0.43	2.76	3	1
1:A:250:LEU:HD12	1:A:267:ASN:HA	0.43	1.90	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:281:PHE:CZ	1:A:308:PHE:CD1	0.43	3.06	11	1
1:A:299:GLY:O	1:A:300:ILE:O	0.43	2.36	15	1
1:A:316:LEU:HB3	1:A:319:TYR:CG	0.43	2.48	17	1
1:A:275:GLY:C	1:A:277:CYS:N	0.43	2.71	4	2
1:A:275:GLY:O	1:A:294:GLY:O	0.43	2.37	7	1
1:A:251:HIS:NE2	1:A:341:GLU:CG	0.43	2.81	9	1
1:A:299:GLY:O	1:A:300:ILE:C	0.43	2.57	15	2
1:A:296:HIS:NE2	1:A:297:GLU:OE1	0.43	2.51	1	1
1:A:254:VAL:HG22	1:A:263:PHE:CD1	0.43	2.47	2	1
1:A:316:LEU:HD22	1:A:321:MET:HE2	0.43	1.89	15	1
1:A:333:VAL:CG1	1:A:347:PRO:HA	0.43	2.43	17	2
1:A:320:THR:HG23	1:A:322:LYS:HG3	0.43	1.90	20	7
1:A:302:GLY:O	1:A:303:GLN:O	0.43	2.37	15	3
1:A:259:ASN:OD1	1:A:259:ASN:N	0.43	2.50	1	1
1:A:334:GLY:C	1:A:336:CYS:N	0.43	2.72	8	9
1:A:334:GLY:CA	1:A:344:LEU:CD1	0.43	2.96	5	1
1:A:300:ILE:HG22	1:A:301:LYS:HG2	0.43	1.90	19	1
1:A:330:THR:HG23	1:A:332:LEU:O	0.43	2.14	20	1
1:A:283:SER:CB	1:A:312:LEU:HD21	0.43	2.43	5	1
1:A:293:MET:O	1:A:294:GLY:C	0.43	2.57	18	1
1:A:269:THR:OG1	1:A:270:ASN:N	0.43	2.52	5	1
1:A:280:GLU:O	1:A:322:LYS:N	0.43	2.52	6	1
1:A:249:LEU:HD13	1:A:249:LEU:C	0.43	2.31	7	1
1:A:261:LEU:HD11	1:A:312:LEU:CB	0.43	2.37	7	1
1:A:335:LYS:O	1:A:336:CYS:C	0.43	2.57	17	4
1:A:268:LYS:HZ1	1:A:301:LYS:HA	0.43	1.73	13	1
1:A:333:VAL:HG22	1:A:346:SER:C	0.43	2.34	14	1
1:A:272:ILE:CG2	1:A:273:ILE:N	0.43	2.82	18	1
1:A:265:LEU:HD21	1:A:279:PHE:CE1	0.43	2.49	2	1
1:A:288:VAL:HG22	1:A:289:PHE:H	0.43	1.74	14	1
1:A:249:LEU:C	1:A:249:LEU:CD2	0.43	2.83	1	2
1:A:278:THR:CA	1:A:293:MET:SD	0.43	3.07	16	1
1:A:283:SER:OG	1:A:319:TYR:CZ	0.42	2.65	8	1
1:A:251:HIS:NE2	1:A:343:THR:CG2	0.42	2.82	10	1
1:A:257:GLU:N	1:A:260:SER:O	0.42	2.52	6	1
1:A:308:PHE:CD1	1:A:308:PHE:N	0.42	2.83	2	3
1:A:338:ASP:OD2	1:A:338:ASP:N	0.42	2.50	12	1
1:A:338:ASP:CG	1:A:338:ASP:O	0.42	2.57	14	1
1:A:289:PHE:CD2	1:A:308:PHE:CE1	0.42	3.07	18	1
1:A:270:ASN:O	1:A:271:ILE:O	0.42	2.37	19	1
1:A:257:GLU:O	1:A:260:SER:O	0.42	2.38	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:316:LEU:O	1:A:336:CYS:SG	0.42	2.78	17	3
1:A:343:THR:O	1:A:344:LEU:C	0.42	2.58	13	8
1:A:256:ASN:CG	1:A:314:THR:HG1	0.42	2.17	9	1
1:A:324:VAL:CG1	1:A:330:THR:N	0.42	2.82	17	1
1:A:283:SER:HB2	1:A:312:LEU:CD2	0.42	2.44	1	1
1:A:333:VAL:O	1:A:333:VAL:CG2	0.42	2.68	3	2
1:A:252:VAL:CG2	1:A:265:LEU:CD2	0.42	2.98	10	2
1:A:278:THR:HB	1:A:324:VAL:HG13	0.42	1.90	16	1
1:A:265:LEU:CD1	1:A:306:LEU:CD1	0.42	2.89	20	1
1:A:275:GLY:O	1:A:277:CYS:N	0.42	2.53	4	1
1:A:249:LEU:O	1:A:269:THR:HG23	0.42	2.15	11	1
1:A:269:THR:OG1	1:A:271:ILE:HD12	0.42	2.13	11	1
1:A:250:LEU:HD21	1:A:265:LEU:HB3	0.42	1.92	14	1
1:A:335:LYS:O	1:A:336:CYS:O	0.42	2.38	14	2
1:A:250:LEU:O	1:A:342:ILE:O	0.42	2.38	19	3
1:A:316:LEU:HD13	1:A:319:TYR:CD2	0.42	2.49	2	1
1:A:256:ASN:O	1:A:256:ASN:CG	0.42	2.58	12	2
1:A:327:ASP:OD2	1:A:327:ASP:N	0.42	2.51	7	1
1:A:249:LEU:O	1:A:249:LEU:HD12	0.42	2.15	9	1
1:A:271:ILE:HG12	1:A:272:ILE:N	0.42	2.29	19	1
1:A:277:CYS:C	1:A:278:THR:OG1	0.42	2.59	13	10
1:A:273:ILE:N	1:A:273:ILE:CD1	0.42	2.75	2	1
1:A:261:LEU:HD12	1:A:312:LEU:HG	0.42	1.92	8	1
1:A:281:PHE:CE1	1:A:308:PHE:CZ	0.42	3.08	11	1
1:A:266:TYR:CD1	1:A:303:GLN:HG2	0.42	2.49	14	1
1:A:348:LEU:C	1:A:348:LEU:HD12	0.42	2.34	20	1
1:A:252:VAL:HG12	1:A:253:GLU:H	0.41	1.75	3	1
1:A:278:THR:HB	1:A:324:VAL:CG2	0.41	2.45	8	1
1:A:300:ILE:O	1:A:302:GLY:N	0.41	2.53	8	1
1:A:249:LEU:HD22	1:A:251:HIS:CE1	0.41	2.50	13	1
1:A:339:SER:C	1:A:341:GLU:N	0.41	2.72	19	3
1:A:268:LYS:O	1:A:269:THR:O	0.41	2.38	15	1
1:A:277:CYS:CB	1:A:293:MET:SD	0.41	3.08	15	2
1:A:321:MET:SD	1:A:342:ILE:CD1	0.41	3.08	15	1
1:A:261:LEU:CD1	1:A:312:LEU:HG	0.41	2.45	8	1
1:A:283:SER:OG	1:A:312:LEU:CD2	0.41	2.67	12	1
1:A:299:GLY:C	1:A:301:LYS:N	0.41	2.73	1	2
1:A:301:LYS:N	1:A:301:LYS:HD3	0.41	2.30	7	1
1:A:347:PRO:O	1:A:348:LEU:C	0.41	2.58	12	2
1:A:270:ASN:O	1:A:271:ILE:C	0.41	2.58	19	1
1:A:335:LYS:HB3	1:A:345:LYS:CE	0.41	2.46	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:294:GLY:HA3	1:A:304:LYS:HZ3	0.41	1.75	12	1
1:A:267:ASN:CG	1:A:298:ILE:HG21	0.41	2.34	18	1
1:A:256:ASN:ND2	1:A:312:LEU:O	0.41	2.53	2	1
1:A:320:THR:C	1:A:322:LYS:N	0.41	2.73	17	2
1:A:348:LEU:C	1:A:348:LEU:HD13	0.41	2.36	2	1
1:A:316:LEU:HD22	1:A:319:TYR:CD2	0.41	2.49	12	1
1:A:298:ILE:CD1	1:A:304:LYS:HB2	0.41	2.46	14	1
1:A:267:ASN:ND2	1:A:298:ILE:CG2	0.41	2.83	18	1
1:A:298:ILE:CG2	1:A:302:GLY:HA3	0.41	2.45	18	1
1:A:316:LEU:HA	1:A:319:TYR:CD1	0.41	2.50	8	1
1:A:261:LEU:CD1	1:A:312:LEU:CG	0.41	2.98	6	1
1:A:281:PHE:O	1:A:288:VAL:HG23	0.41	2.15	6	1
1:A:336:CYS:H	1:A:342:ILE:HG23	0.41	1.76	17	1
1:A:283:SER:CB	1:A:312:LEU:CD2	0.41	2.99	1	1
1:A:258:ASP:O	1:A:259:ASN:C	0.41	2.59	17	3
1:A:275:GLY:O	1:A:276:ASN:C	0.41	2.59	4	2
1:A:277:CYS:SG	1:A:324:VAL:O	0.41	2.79	7	2
1:A:277:CYS:O	1:A:278:THR:OG1	0.41	2.39	9	1
1:A:252:VAL:HG22	1:A:265:LEU:CB	0.41	2.46	14	1
1:A:256:ASN:OD1	1:A:312:LEU:O	0.41	2.39	18	1
1:A:319:TYR:O	1:A:320:THR:C	0.41	2.59	18	1
1:A:316:LEU:HB3	1:A:319:TYR:CD2	0.41	2.51	19	1
1:A:308:PHE:O	1:A:309:PHE:O	0.41	2.39	3	1
1:A:251:HIS:C	1:A:252:VAL:CG2	0.41	2.90	8	1
1:A:257:GLU:O	1:A:258:ASP:C	0.41	2.60	13	1
1:A:279:PHE:CE1	1:A:323:VAL:CG2	0.40	3.04	12	1
1:A:301:LYS:HG2	1:A:301:LYS:O	0.40	2.16	15	1
1:A:317:SER:OG	1:A:337:ALA:C	0.40	2.60	5	1
1:A:317:SER:OG	1:A:338:ASP:OD2	0.40	2.39	12	1
1:A:251:HIS:C	1:A:252:VAL:HG23	0.40	2.36	14	1
1:A:283:SER:HB3	1:A:312:LEU:CD2	0.40	2.46	2	3
1:A:256:ASN:OD1	1:A:314:THR:OG1	0.40	2.40	4	1
1:A:259:ASN:C	1:A:260:SER:OG	0.40	2.60	19	1
1:A:267:ASN:O	1:A:300:ILE:O	0.40	2.40	3	1
1:A:314:THR:CG2	1:A:340:ASN:OD1	0.40	2.69	5	1
1:A:273:ILE:O	1:A:297:GLU:CD	0.40	2.60	9	1
1:A:267:ASN:HB3	1:A:298:ILE:CG2	0.40	2.46	10	1
1:A:272:ILE:O	1:A:273:ILE:C	0.40	2.59	12	2
1:A:298:ILE:CD1	1:A:304:LYS:HD3	0.40	2.47	14	1
1:A:267:ASN:O	1:A:267:ASN:OD1	0.40	2.39	18	1
1:A:343:THR:O	1:A:343:THR:OG1	0.40	2.40	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:275:GLY:C	1:A:276:ASN:CG	0.40	2.81	4	1
1:A:267:ASN:HB3	1:A:273:ILE:CD1	0.40	2.47	9	1
1:A:269:THR:C	1:A:270:ASN:CG	0.40	2.80	11	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	95/107 (89%)	68±2 (71±3%)	21±4 (23±4%)	6±2 (6±2%)	3	19
All	All	1900/2140 (89%)	1355 (71%)	428 (23%)	117 (6%)	3	19

All 27 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	346	SER	17
1	A	347	PRO	15
1	A	298	ILE	9
1	A	311	SER	9
1	A	321	MET	8
1	A	336	CYS	8
1	A	271	ILE	5
1	A	300	ILE	5
1	A	310	PRO	4
1	A	280	GLU	4
1	A	262	HIS	3
1	A	279	PHE	3
1	A	303	GLN	3
1	A	344	LEU	3
1	A	318	ASN	3
1	A	269	THR	2
1	A	270	ASN	2
1	A	288	VAL	2
1	A	330	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	294	GLY	2
1	A	267	ASN	2
1	A	309	PHE	1
1	A	296	HIS	1
1	A	299	GLY	1
1	A	302	GLY	1
1	A	337	ALA	1
1	A	333	VAL	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	89/99 (90%)	72±2 (81±3%)	17±2 (19±3%)	4	36
All	All	1780/1980 (90%)	1442 (81%)	338 (19%)	4	36

All 52 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	249	LEU	20
1	A	250	LEU	20
1	A	265	LEU	20
1	A	335	LYS	20
1	A	314	THR	19
1	A	309	PHE	16
1	A	336	CYS	16
1	A	333	VAL	14
1	A	301	LYS	13
1	A	292	LYS	12
1	A	325	ASN	12
1	A	345	LYS	11
1	A	271	ILE	9
1	A	279	PHE	9
1	A	268	LYS	8
1	A	338	ASP	8
1	A	307	TRP	7

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Mol	Chain	Res	Type	Models (Total)
1	A	348	LEU	7
1	A	255	SER	7
1	A	321	MET	6
1	A	266	TYR	6
1	A	318	ASN	6
1	A	312	LEU	6
1	A	317	SER	5
1	A	329	GLU	5
1	A	262	HIS	4
1	A	327	ASP	4
1	A	256	ASN	4
1	A	283	SER	3
1	A	297	GLU	3
1	A	258	ASP	3
1	A	303	GLN	3
1	A	341	GLU	3
1	A	320	THR	3
1	A	346	SER	3
1	A	260	SER	3
1	A	282	SER	2
1	A	339	SER	2
1	A	273	ILE	2
1	A	324	VAL	2
1	A	259	ASN	1
1	A	300	ILE	1
1	A	276	ASN	1
1	A	251	HIS	1
1	A	281	PHE	1
1	A	305	GLU	1
1	A	331	ILE	1
1	A	269	THR	1
1	A	311	SER	1
1	A	277	CYS	1
1	A	278	THR	1
1	A	296	HIS	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

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 94% 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

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	1303
Number of shifts mapped to atoms	1303
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	102	-0.13 ± 0.20	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	97	-0.09 ± 0.19	None needed (< 0.5 ppm)
$^{13}C'$	92	0.37 ± 0.11	None needed (< 0.5 ppm)
^{15}N	95	0.64 ± 0.90	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 1221 atoms were assigned a chemical shift out of a possible 1303. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	461/474 (97%)	190/192 (99%)	181/192 (94%)	90/90 (100%)
Sidechain	693/718 (97%)	466/470 (99%)	218/231 (94%)	9/17 (53%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	67/111 (60%)	40/56 (71%)	27/51 (53%)	0/4 (0%)
Overall	1221/1303 (94%)	696/718 (97%)	426/474 (90%)	99/111 (89%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 94%, i.e. 1302 atoms were assigned a chemical shift out of a possible 1389. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	491/507 (97%)	202/205 (99%)	194/206 (94%)	95/96 (99%)
Sidechain	744/771 (96%)	499/503 (99%)	234/249 (94%)	11/19 (58%)
Aromatic	67/111 (60%)	40/56 (71%)	27/51 (53%)	0/4 (0%)
Overall	1302/1389 (94%)	741/764 (97%)	455/506 (90%)	106/119 (89%)

7.1.4 Statistically unusual chemical shifts (i)

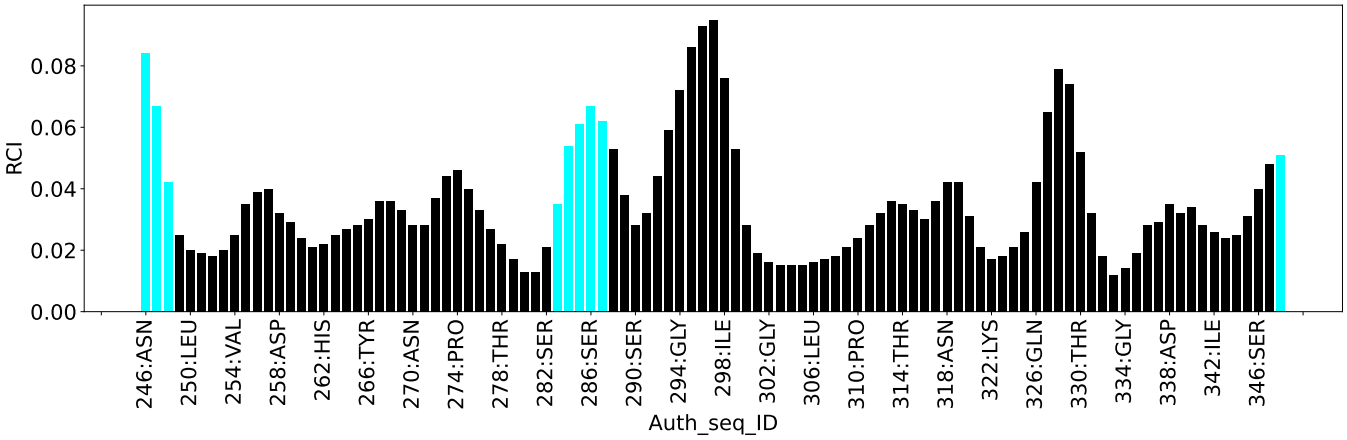
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	269	THR	HG1	6.05	0.08 – 2.19	23.3
1	A	289	PHE	HB2	1.00	1.20 – 4.80	-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
246:ASN
250:LEU
254:VAL
258:ASP
262:HIS
266:TYR
270:ASN
274:PRO
278:THR
282:SER
286:SER
290:SER
294:GLY
298:ILE
302:GLY
306:LEU
310:PRO
314:THR
318:ASN
322:LYS
326:GLN
330:THR
334:GLY
338:ASP
342:ILE
346:SER
Auth_seq_ID

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	2090
Intra-residue (|i-j|=0)	556
Sequential (|i-j|=1)	628
Medium range (|i-j|>1 and |i-j|<5)	159
Long range (|i-j|≥5)	747
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	19.5
Number of long range restraints per residue[1]	7.0

[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

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	4.2	0.2
0.2-0.5 (Medium)	2.4	0.5
>0.5 (Large)	3.6	1.28

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)

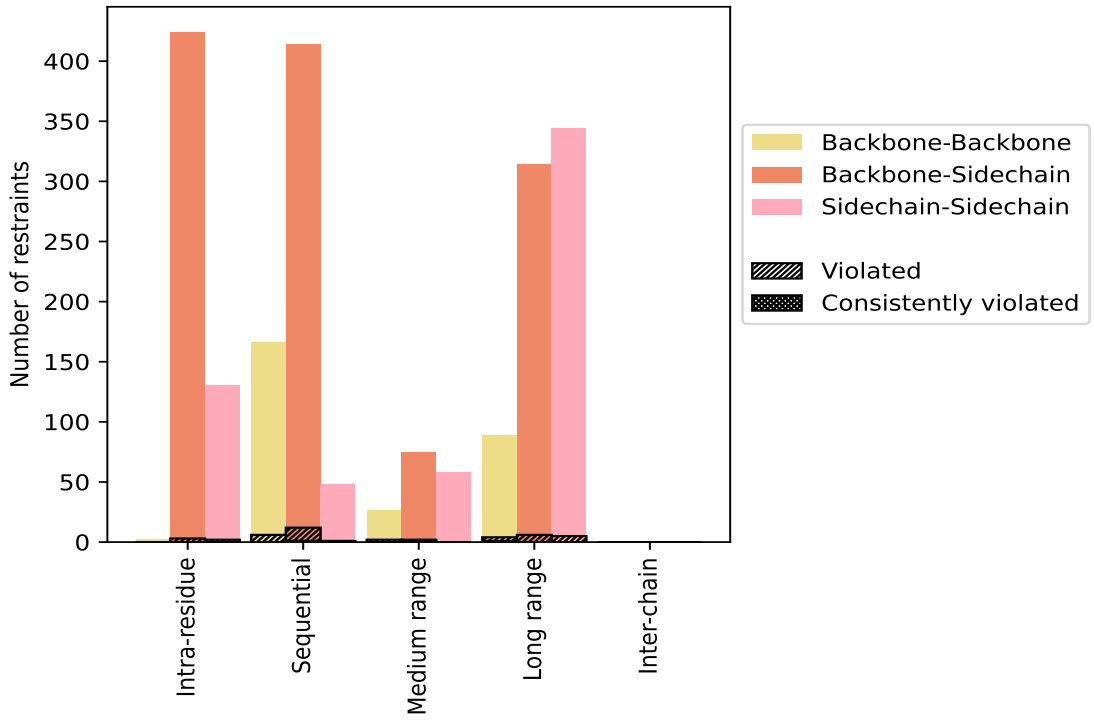
9.1 Summary of distance violations (i)

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)	556	26.6	5	0.9	0.2	0	0.0	0.0
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	424	20.3	3	0.7	0.1	0	0.0	0.0
Sidechain-Sidechain	130	6.2	2	1.5	0.1	0	0.0	0.0
Sequential (|i-j|=1)	628	30.0	19	3.0	0.9	1	0.2	0.0
Backbone-Backbone	166	7.9	6	3.6	0.3	0	0.0	0.0
Backbone-Sidechain	414	19.8	12	2.9	0.6	1	0.2	0.0
Sidechain-Sidechain	48	2.3	1	2.1	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	159	7.6	4	2.5	0.2	1	0.6	0.0
Backbone-Backbone	26	1.2	2	7.7	0.1	0	0.0	0.0
Backbone-Sidechain	75	3.6	2	2.7	0.1	1	1.3	0.0
Sidechain-Sidechain	58	2.8	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	747	35.7	15	2.0	0.7	1	0.1	0.0
Backbone-Backbone	89	4.3	4	4.5	0.2	1	1.1	0.0
Backbone-Sidechain	314	15.0	6	1.9	0.3	0	0.0	0.0
Sidechain-Sidechain	344	16.5	5	1.5	0.2	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2090	100.0	43	2.1	2.1	3	0.1	0.1
Backbone-Backbone	283	13.5	12	4.2	0.6	1	0.4	0.0
Backbone-Sidechain	1227	58.7	23	1.9	1.1	2	0.2	0.1
Sidechain-Sidechain	580	27.8	8	1.4	0.4	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



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

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	1	4	2	4	0	11	0.42	0.89	0.31	0.2
2	0	5	3	2	0	10	0.49	1.01	0.31	0.45
3	0	3	2	2	0	7	0.59	1.01	0.31	0.47
4	1	4	3	3	0	11	0.41	0.96	0.28	0.3
5	0	6	4	5	0	15	0.38	1.07	0.33	0.21
6	0	4	3	2	0	9	0.47	1.16	0.38	0.23
7	0	4	2	2	0	8	0.5	0.86	0.31	0.55
8	0	4	3	3	0	10	0.38	1.05	0.35	0.16
9	0	3	2	3	0	8	0.48	0.91	0.3	0.38
10	0	4	2	4	0	10	0.45	1.18	0.38	0.22
11	0	5	2	2	0	9	0.42	1.01	0.39	0.17

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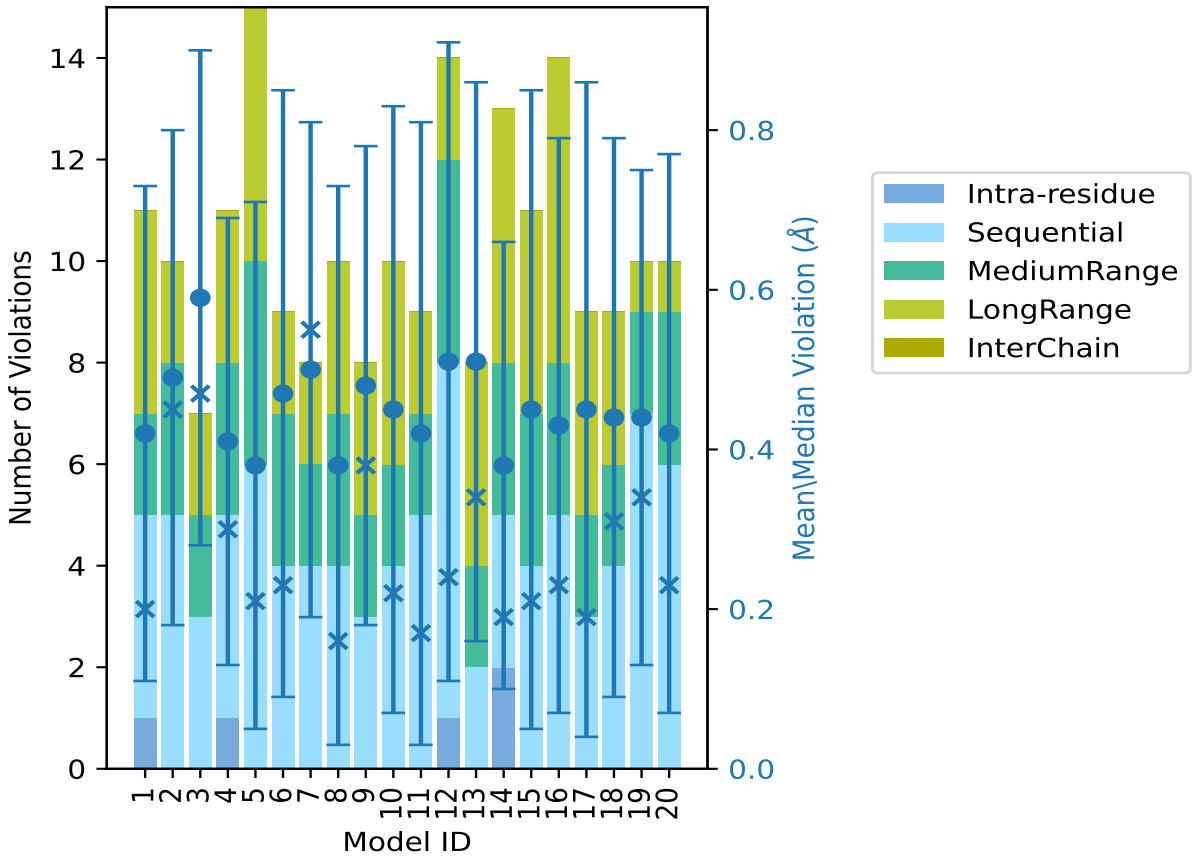
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	7	4	2	0	14	0.51	1.14	0.4	0.24
13	0	2	2	4	0	8	0.51	1.2	0.35	0.34
14	2	3	3	5	0	13	0.38	0.84	0.28	0.19
15	0	4	3	4	0	11	0.45	1.28	0.4	0.21
16	0	5	3	6	0	14	0.43	1.24	0.36	0.23
17	0	3	2	4	0	9	0.45	1.21	0.41	0.19
18	0	4	2	3	0	9	0.44	0.98	0.35	0.31
19	0	7	2	1	0	10	0.44	0.98	0.31	0.34
20	0	6	3	1	0	10	0.42	1.01	0.35	0.23

[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



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

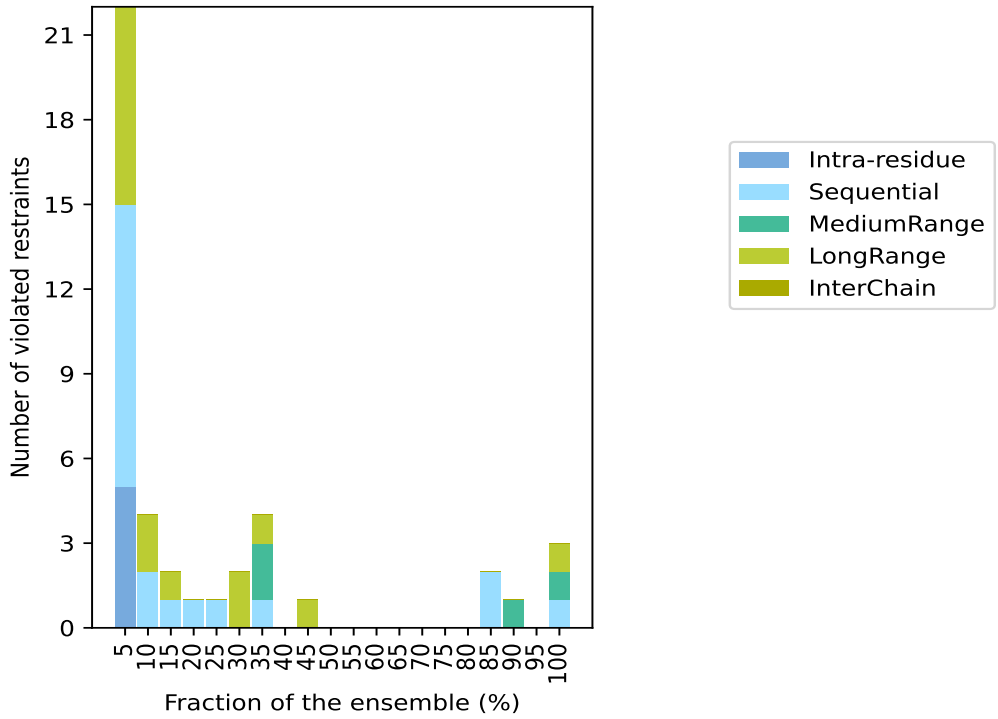
9.3 Distance violation statistics for the ensemble (i)

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, 2047(IR:551, SQ:609, MR:155, LR:732, 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	10	0	7	0	22	1	5.0
0	2	0	2	0	4	2	10.0
0	1	0	1	0	2	3	15.0
0	1	0	0	0	1	4	20.0
0	1	0	0	0	1	5	25.0
0	0	0	2	0	2	6	30.0
0	1	2	1	0	4	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	1	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	2	0	0	0	2	17	85.0
0	0	1	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
0	1	1	1	0	3	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

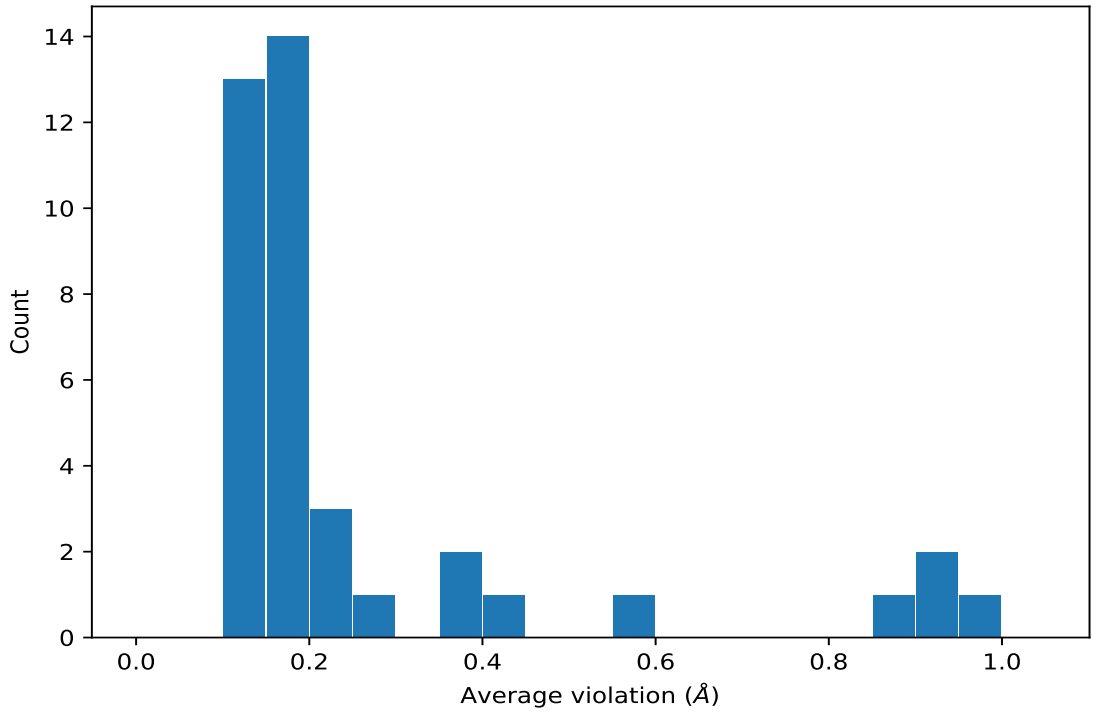
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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

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)
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	20	0.96	0.18	0.92
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	20	0.93	0.11	0.96
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	20	0.93	0.11	0.96
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	20	0.89	0.05	0.9
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	18	0.38	0.21	0.34
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	17	0.25	0.05	0.28
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	17	0.18	0.05	0.17
(1,318)	1:A:275:GLY:HA3	1:A:298:ILE:H	9	0.55	0.21	0.55
(1,1218)	1:A:275:GLY:HA2	1:A:295:PRO:HA	7	0.4	0.18	0.39
(1,91)	1:A:275:GLY:HA3	1:A:277:CYS:H	7	0.37	0.34	0.23
(1,567)	1:A:249:LEU:HA	1:A:251:HIS:H	7	0.16	0.02	0.15
(1,1465)	1:A:250:LEU:HD11	1:A:251:HIS:H	7	0.12	0.02	0.11
(1,1465)	1:A:250:LEU:HD12	1:A:251:HIS:H	7	0.12	0.02	0.11
(1,1465)	1:A:250:LEU:HD13	1:A:251:HIS:H	7	0.12	0.02	0.11
(1,1465)	1:A:250:LEU:HD21	1:A:251:HIS:H	7	0.12	0.02	0.11
(1,1465)	1:A:250:LEU:HD22	1:A:251:HIS:H	7	0.12	0.02	0.11

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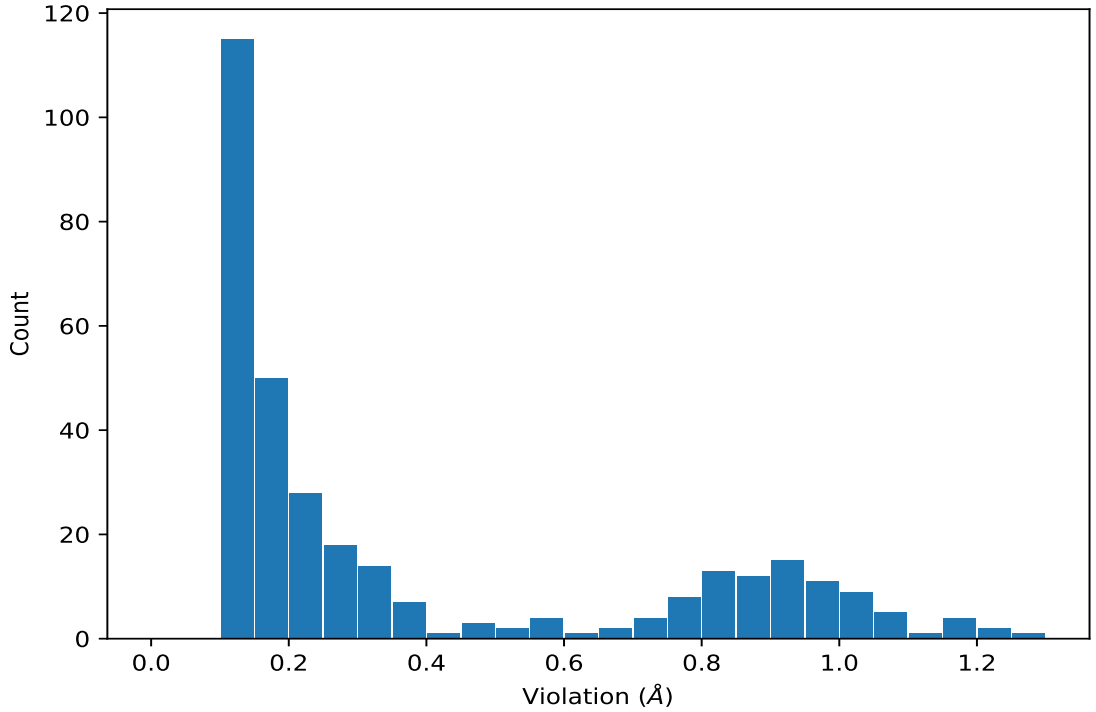
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1465)	1:A:250:LEU:HD23	1:A:251:HIS:H	7	0.12	0.02	0.11
(1,2030)	1:A:335:LYS:HB3	1:A:345:LYS:HG2	6	0.22	0.02	0.22
(1,2030)	1:A:335:LYS:HB3	1:A:345:LYS:HG3	6	0.22	0.02	0.22
(1,2026)	1:A:335:LYS:HB2	1:A:345:LYS:HD2	6	0.16	0.03	0.17
(1,2026)	1:A:335:LYS:HB2	1:A:345:LYS:HD3	6	0.16	0.03	0.17
(1,1307)	1:A:250:LEU:HG	1:A:251:HIS:HA	5	0.12	0.01	0.12
(1,1001)	1:A:250:LEU:HD21	1:A:251:HIS:H	4	0.12	0.01	0.12
(1,1001)	1:A:250:LEU:HD22	1:A:251:HIS:H	4	0.12	0.01	0.12
(1,1001)	1:A:250:LEU:HD23	1:A:251:HIS:H	4	0.12	0.01	0.12
(1,1042)	1:A:335:LYS:HA	1:A:336:CYS:HB2	3	0.24	0.06	0.27
(1,524)	1:A:316:LEU:HB3	1:A:321:MET:H	3	0.13	0.02	0.12
(1,340)	1:A:250:LEU:H	1:A:251:HIS:H	2	0.18	0.02	0.18
(1,936)	1:A:334:GLY:HA3	1:A:344:LEU:HD21	2	0.18	0.02	0.18
(1,936)	1:A:334:GLY:HA3	1:A:344:LEU:HD22	2	0.18	0.02	0.18
(1,936)	1:A:334:GLY:HA3	1:A:344:LEU:HD23	2	0.18	0.02	0.18
(1,1492)	1:A:252:VAL:HG11	1:A:265:LEU:HG	2	0.17	0.01	0.17
(1,1492)	1:A:252:VAL:HG12	1:A:265:LEU:HG	2	0.17	0.01	0.17
(1,1492)	1:A:252:VAL:HG13	1:A:265:LEU:HG	2	0.17	0.01	0.17
(1,1492)	1:A:252:VAL:HG21	1:A:265:LEU:HG	2	0.17	0.01	0.17
(1,1492)	1:A:252:VAL:HG22	1:A:265:LEU:HG	2	0.17	0.01	0.17
(1,1492)	1:A:252:VAL:HG23	1:A:265:LEU:HG	2	0.17	0.01	0.17
(1,2084)	1:A:347:PRO:HA	1:A:348:LEU:HB2	2	0.15	0.0	0.15
(1,2084)	1:A:347:PRO:HA	1:A:348:LEU:HB3	2	0.15	0.0	0.15

[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)
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	15	1.28
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	16	1.24
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	17	1.21
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	13	1.2
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	10	1.18
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	6	1.16
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	6	1.16
(1,91)	1:A:275:GLY:HA3	1:A:277:CYS:H	12	1.14
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	5	1.07
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	8	1.05
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	8	1.05
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	15	1.05
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	15	1.05
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	17	1.02
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	17	1.02
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	2	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	2	1.01
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	11	1.01
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	11	1.01
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	20	1.01
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	20	1.01
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	3	1.01
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	12	0.99
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	12	0.99
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	18	0.98
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	18	0.98
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	19	0.98
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	16	0.97
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	16	0.97
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	5	0.96
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	5	0.96
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	11	0.96
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	4	0.96
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	6	0.95
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	20	0.95
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	18	0.95
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	12	0.94
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	11	0.94
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	12	0.93
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	3	0.92
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	2	0.91
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	9	0.91
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	16	0.91
(1,318)	1:A:275:GLY:HA3	1:A:298:ILE:H	12	0.9
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	10	0.9
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	10	0.9
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	6	0.9
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	8	0.9
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	1	0.89
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	1	0.89
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	3	0.89
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	3	0.89
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	9	0.89
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	1	0.88
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	15	0.88
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	5	0.87
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	13	0.87
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	7	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	7	0.86
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	19	0.86
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	12	0.85
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	14	0.84
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	14	0.84
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	20	0.84
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	19	0.83
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	19	0.83
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	7	0.83
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	18	0.83
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	10	0.82
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	17	0.82
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	4	0.81
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	4	0.81
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	4	0.81
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	9	0.77
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	9	0.77
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	14	0.77
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	14	0.77
(1,1110)	1:A:334:GLY:HA3	1:A:335:LYS:HB2	7	0.77
(1,1218)	1:A:275:GLY:HA2	1:A:295:PRO:HA	7	0.76
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	1	0.75
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	8	0.75
(1,318)	1:A:275:GLY:HA3	1:A:298:ILE:H	16	0.74
(1,318)	1:A:275:GLY:HA3	1:A:298:ILE:H	2	0.73
(1,1688)	1:A:273:ILE:HG12	1:A:275:GLY:HA3	13	0.72
(1,1688)	1:A:273:ILE:HG13	1:A:275:GLY:HA3	13	0.72
(1,141)	1:A:334:GLY:HA3	1:A:345:LYS:H	2	0.68
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	1	0.65
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	14	0.61
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	10	0.6
(1,318)	1:A:275:GLY:HA3	1:A:298:ILE:H	5	0.59
(1,91)	1:A:275:GLY:HA3	1:A:277:CYS:H	2	0.55
(1,318)	1:A:275:GLY:HA3	1:A:298:ILE:H	1	0.55
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	5	0.53
(1,318)	1:A:275:GLY:HA3	1:A:298:ILE:H	14	0.5
(1,318)	1:A:275:GLY:HA3	1:A:298:ILE:H	3	0.47
(1,1218)	1:A:275:GLY:HA2	1:A:295:PRO:HA	15	0.46
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	16	0.45
(1,1218)	1:A:275:GLY:HA2	1:A:295:PRO:HA	9	0.41
(1,1218)	1:A:275:GLY:HA2	1:A:295:PRO:HA	4	0.39
(1,376)	1:A:271:ILE:HB	1:A:272:ILE:H	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	13	0.38
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	19	0.38
(1,1218)	1:A:275:GLY:HA2	1:A:295:PRO:HA	18	0.38
(1,2021)	1:A:335:LYS:HA	1:A:336:CYS:HB2	20	0.36
(1,2021)	1:A:335:LYS:HA	1:A:336:CYS:HB3	20	0.36
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	2	0.35
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	7	0.34
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	9	0.34
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	3	0.33
(1,640)	1:A:298:ILE:HG21	1:A:298:ILE:HD11	4	0.31
(1,640)	1:A:298:ILE:HG21	1:A:298:ILE:HD12	4	0.31
(1,640)	1:A:298:ILE:HG21	1:A:298:ILE:HD13	4	0.31
(1,640)	1:A:298:ILE:HG22	1:A:298:ILE:HD11	4	0.31
(1,640)	1:A:298:ILE:HG22	1:A:298:ILE:HD12	4	0.31
(1,640)	1:A:298:ILE:HG22	1:A:298:ILE:HD13	4	0.31
(1,640)	1:A:298:ILE:HG23	1:A:298:ILE:HD11	4	0.31
(1,640)	1:A:298:ILE:HG23	1:A:298:ILE:HD12	4	0.31
(1,640)	1:A:298:ILE:HG23	1:A:298:ILE:HD13	4	0.31
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	18	0.31
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	4	0.3
(1,1218)	1:A:275:GLY:HA2	1:A:295:PRO:HA	13	0.3
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	2	0.29
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	3	0.29
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	8	0.29
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	9	0.29
(1,1042)	1:A:335:LYS:HA	1:A:336:CYS:HB2	19	0.29
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	12	0.28
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	13	0.28
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	16	0.28
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	19	0.27
(1,1042)	1:A:335:LYS:HA	1:A:336:CYS:HB2	20	0.27
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	11	0.26
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	15	0.26
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	4	0.26
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	6	0.26
(1,318)	1:A:275:GLY:HA3	1:A:298:ILE:H	4	0.25
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	5	0.25
(1,91)	1:A:275:GLY:HA3	1:A:277:CYS:H	16	0.24
(1,2030)	1:A:335:LYS:HB3	1:A:345:LYS:HG2	10	0.24
(1,2030)	1:A:335:LYS:HB3	1:A:345:LYS:HG3	10	0.24
(1,2030)	1:A:335:LYS:HB3	1:A:345:LYS:HG2	17	0.24
(1,2030)	1:A:335:LYS:HB3	1:A:345:LYS:HG3	17	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:A:275:GLY:HA3	1:A:277:CYS:H	6	0.23
(1,2030)	1:A:335:LYS:HB3	1:A:345:LYS:HG2	5	0.23
(1,2030)	1:A:335:LYS:HB3	1:A:345:LYS:HG3	5	0.23
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	3	0.23
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	6	0.23
(1,2030)	1:A:335:LYS:HB3	1:A:345:LYS:HG2	16	0.22
(1,2030)	1:A:335:LYS:HB3	1:A:345:LYS:HG3	16	0.22
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	16	0.22
(1,340)	1:A:250:LEU:H	1:A:251:HIS:H	5	0.21
(1,318)	1:A:275:GLY:HA3	1:A:298:ILE:H	10	0.21
(1,2030)	1:A:335:LYS:HB3	1:A:345:LYS:HG2	15	0.21
(1,2030)	1:A:335:LYS:HB3	1:A:345:LYS:HG3	15	0.21
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	7	0.21
(1,936)	1:A:334:GLY:HA3	1:A:344:LEU:HD21	1	0.2
(1,936)	1:A:334:GLY:HA3	1:A:344:LEU:HD22	1	0.2
(1,936)	1:A:334:GLY:HA3	1:A:344:LEU:HD23	1	0.2
(1,91)	1:A:275:GLY:HA3	1:A:277:CYS:H	15	0.2
(1,1875)	1:A:312:LEU:HA	1:A:312:LEU:HD11	14	0.2
(1,1875)	1:A:312:LEU:HA	1:A:312:LEU:HD12	14	0.2
(1,1875)	1:A:312:LEU:HA	1:A:312:LEU:HD13	14	0.2
(1,1875)	1:A:312:LEU:HA	1:A:312:LEU:HD21	14	0.2
(1,1875)	1:A:312:LEU:HA	1:A:312:LEU:HD22	14	0.2
(1,1875)	1:A:312:LEU:HA	1:A:312:LEU:HD23	14	0.2
(1,642)	1:A:298:ILE:HB	1:A:298:ILE:HD11	14	0.19
(1,642)	1:A:298:ILE:HB	1:A:298:ILE:HD12	14	0.19
(1,642)	1:A:298:ILE:HB	1:A:298:ILE:HD13	14	0.19
(1,567)	1:A:249:LEU:HA	1:A:251:HIS:H	12	0.19
(1,2026)	1:A:335:LYS:HB2	1:A:345:LYS:HD2	17	0.19
(1,2026)	1:A:335:LYS:HB2	1:A:345:LYS:HD3	17	0.19
(1,1819)	1:A:298:ILE:HG12	1:A:305:GLU:H	14	0.19
(1,1819)	1:A:298:ILE:HG13	1:A:305:GLU:H	14	0.19
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	20	0.19
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	15	0.19
(1,983)	1:A:312:LEU:HG	1:A:313:PRO:HD3	14	0.18
(1,2030)	1:A:335:LYS:HB3	1:A:345:LYS:HG2	13	0.18
(1,2030)	1:A:335:LYS:HB3	1:A:345:LYS:HG3	13	0.18
(1,2026)	1:A:335:LYS:HB2	1:A:345:LYS:HD2	13	0.18
(1,2026)	1:A:335:LYS:HB2	1:A:345:LYS:HD3	13	0.18
(1,2026)	1:A:335:LYS:HB2	1:A:345:LYS:HD2	16	0.18
(1,2026)	1:A:335:LYS:HB2	1:A:345:LYS:HD3	16	0.18
(1,1492)	1:A:252:VAL:HG11	1:A:265:LEU:HG	6	0.18
(1,1492)	1:A:252:VAL:HG12	1:A:265:LEU:HG	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1492)	1:A:252:VAL:HG13	1:A:265:LEU:HG	6	0.18
(1,1492)	1:A:252:VAL:HG21	1:A:265:LEU:HG	6	0.18
(1,1492)	1:A:252:VAL:HG22	1:A:265:LEU:HG	6	0.18
(1,1492)	1:A:252:VAL:HG23	1:A:265:LEU:HG	6	0.18
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	6	0.18
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	8	0.18
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	20	0.18
(1,936)	1:A:334:GLY:HA3	1:A:344:LEU:HD21	14	0.17
(1,936)	1:A:334:GLY:HA3	1:A:344:LEU:HD22	14	0.17
(1,936)	1:A:334:GLY:HA3	1:A:344:LEU:HD23	14	0.17
(1,646)	1:A:298:ILE:HD11	1:A:299:GLY:H	4	0.17
(1,646)	1:A:298:ILE:HD12	1:A:299:GLY:H	4	0.17
(1,646)	1:A:298:ILE:HD13	1:A:299:GLY:H	4	0.17
(1,567)	1:A:249:LEU:HA	1:A:251:HIS:H	2	0.17
(1,567)	1:A:249:LEU:HA	1:A:251:HIS:H	14	0.17
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	1	0.17
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	4	0.17
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	11	0.17
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	17	0.17
(1,340)	1:A:250:LEU:H	1:A:251:HIS:H	12	0.16
(1,2026)	1:A:335:LYS:HB2	1:A:345:LYS:HD2	15	0.16
(1,2026)	1:A:335:LYS:HB2	1:A:345:LYS:HD3	15	0.16
(1,1492)	1:A:252:VAL:HG11	1:A:265:LEU:HG	9	0.16
(1,1492)	1:A:252:VAL:HG12	1:A:265:LEU:HG	9	0.16
(1,1492)	1:A:252:VAL:HG13	1:A:265:LEU:HG	9	0.16
(1,1492)	1:A:252:VAL:HG21	1:A:265:LEU:HG	9	0.16
(1,1492)	1:A:252:VAL:HG22	1:A:265:LEU:HG	9	0.16
(1,1492)	1:A:252:VAL:HG23	1:A:265:LEU:HG	9	0.16
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	17	0.16
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	5	0.16
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	18	0.16
(1,567)	1:A:249:LEU:HA	1:A:251:HIS:H	20	0.15
(1,524)	1:A:316:LEU:HB3	1:A:321:MET:H	16	0.15
(1,474)	1:A:250:LEU:HG	1:A:344:LEU:H	16	0.15
(1,421)	1:A:324:VAL:HB	1:A:330:THR:H	17	0.15
(1,2084)	1:A:347:PRO:HA	1:A:348:LEU:HB2	10	0.15
(1,2084)	1:A:347:PRO:HA	1:A:348:LEU:HB3	10	0.15
(1,2084)	1:A:347:PRO:HA	1:A:348:LEU:HB2	12	0.15
(1,2084)	1:A:347:PRO:HA	1:A:348:LEU:HB3	12	0.15
(1,1728)	1:A:281:PHE:H	1:A:321:MET:HB2	18	0.15
(1,1728)	1:A:281:PHE:H	1:A:321:MET:HB3	18	0.15
(1,1465)	1:A:250:LEU:HD11	1:A:251:HIS:H	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1465)	1:A:250:LEU:HD12	1:A:251:HIS:H	12	0.15
(1,1465)	1:A:250:LEU:HD13	1:A:251:HIS:H	12	0.15
(1,1465)	1:A:250:LEU:HD21	1:A:251:HIS:H	12	0.15
(1,1465)	1:A:250:LEU:HD22	1:A:251:HIS:H	12	0.15
(1,1465)	1:A:250:LEU:HD23	1:A:251:HIS:H	12	0.15
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	15	0.15
(1,1042)	1:A:335:LYS:HA	1:A:336:CYS:HB2	6	0.15
(1,567)	1:A:249:LEU:HA	1:A:251:HIS:H	5	0.14
(1,567)	1:A:249:LEU:HA	1:A:251:HIS:H	8	0.14
(1,2069)	1:A:345:LYS:HA	1:A:345:LYS:HE2	1	0.14
(1,2069)	1:A:345:LYS:HA	1:A:345:LYS:HE3	1	0.14
(1,1760)	1:A:287:GLU:H	1:A:288:VAL:HG11	16	0.14
(1,1760)	1:A:287:GLU:H	1:A:288:VAL:HG12	16	0.14
(1,1760)	1:A:287:GLU:H	1:A:288:VAL:HG13	16	0.14
(1,1760)	1:A:287:GLU:H	1:A:288:VAL:HG21	16	0.14
(1,1760)	1:A:287:GLU:H	1:A:288:VAL:HG22	16	0.14
(1,1760)	1:A:287:GLU:H	1:A:288:VAL:HG23	16	0.14
(1,1465)	1:A:250:LEU:HD11	1:A:251:HIS:H	5	0.14
(1,1465)	1:A:250:LEU:HD12	1:A:251:HIS:H	5	0.14
(1,1465)	1:A:250:LEU:HD13	1:A:251:HIS:H	5	0.14
(1,1465)	1:A:250:LEU:HD21	1:A:251:HIS:H	5	0.14
(1,1465)	1:A:250:LEU:HD22	1:A:251:HIS:H	5	0.14
(1,1465)	1:A:250:LEU:HD23	1:A:251:HIS:H	5	0.14
(1,1307)	1:A:250:LEU:HG	1:A:251:HIS:HA	7	0.14
(1,1291)	1:A:275:GLY:HA3	1:A:276:ASN:HA	12	0.14
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	8	0.14
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	11	0.14
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	10	0.14
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	19	0.14
(1,88)	1:A:277:CYS:H	1:A:277:CYS:HB2	12	0.13
(1,567)	1:A:249:LEU:HA	1:A:251:HIS:H	4	0.13
(1,1465)	1:A:250:LEU:HD11	1:A:251:HIS:H	2	0.13
(1,1465)	1:A:250:LEU:HD12	1:A:251:HIS:H	2	0.13
(1,1465)	1:A:250:LEU:HD13	1:A:251:HIS:H	2	0.13
(1,1465)	1:A:250:LEU:HD21	1:A:251:HIS:H	2	0.13
(1,1465)	1:A:250:LEU:HD22	1:A:251:HIS:H	2	0.13
(1,1465)	1:A:250:LEU:HD23	1:A:251:HIS:H	2	0.13
(1,1307)	1:A:250:LEU:HG	1:A:251:HIS:HA	18	0.13
(1,1001)	1:A:250:LEU:HD21	1:A:251:HIS:H	12	0.13
(1,1001)	1:A:250:LEU:HD22	1:A:251:HIS:H	12	0.13
(1,1001)	1:A:250:LEU:HD23	1:A:251:HIS:H	12	0.13
(1,91)	1:A:275:GLY:HA3	1:A:277:CYS:H	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,91)	1:A:275:GLY:HA3	1:A:277:CYS:H	20	0.12
(1,64)	1:A:275:GLY:HA2	1:A:276:ASN:H	7	0.12
(1,524)	1:A:316:LEU:HB3	1:A:321:MET:H	5	0.12
(1,512)	1:A:278:THR:H	1:A:279:PHE:H	16	0.12
(1,2026)	1:A:335:LYS:HB2	1:A:345:LYS:HD2	5	0.12
(1,2026)	1:A:335:LYS:HB2	1:A:345:LYS:HD3	5	0.12
(1,1383)	1:A:271:ILE:H	1:A:272:ILE:HA	19	0.12
(1,1307)	1:A:250:LEU:HG	1:A:251:HIS:HA	11	0.12
(1,1307)	1:A:250:LEU:HG	1:A:251:HIS:HA	15	0.12
(1,1300)	1:A:334:GLY:HA3	1:A:335:LYS:HA	14	0.12
(1,1218)	1:A:275:GLY:HA2	1:A:295:PRO:HA	8	0.12
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	1	0.12
(1,1094)	1:A:278:THR:HG21	1:A:324:VAL:HB	8	0.12
(1,1094)	1:A:278:THR:HG22	1:A:324:VAL:HB	8	0.12
(1,1094)	1:A:278:THR:HG23	1:A:324:VAL:HB	8	0.12
(1,1001)	1:A:250:LEU:HD21	1:A:251:HIS:H	5	0.12
(1,1001)	1:A:250:LEU:HD22	1:A:251:HIS:H	5	0.12
(1,1001)	1:A:250:LEU:HD23	1:A:251:HIS:H	5	0.12
(1,524)	1:A:316:LEU:HB3	1:A:321:MET:H	1	0.11
(1,2026)	1:A:335:LYS:HB2	1:A:345:LYS:HD2	10	0.11
(1,2026)	1:A:335:LYS:HB2	1:A:345:LYS:HD3	10	0.11
(1,1956)	1:A:324:VAL:HG11	1:A:325:ASN:HA	17	0.11
(1,1956)	1:A:324:VAL:HG12	1:A:325:ASN:HA	17	0.11
(1,1956)	1:A:324:VAL:HG13	1:A:325:ASN:HA	17	0.11
(1,1956)	1:A:324:VAL:HG21	1:A:325:ASN:HA	17	0.11
(1,1956)	1:A:324:VAL:HG22	1:A:325:ASN:HA	17	0.11
(1,1956)	1:A:324:VAL:HG23	1:A:325:ASN:HA	17	0.11
(1,1465)	1:A:250:LEU:HD11	1:A:251:HIS:H	1	0.11
(1,1465)	1:A:250:LEU:HD12	1:A:251:HIS:H	1	0.11
(1,1465)	1:A:250:LEU:HD13	1:A:251:HIS:H	1	0.11
(1,1465)	1:A:250:LEU:HD21	1:A:251:HIS:H	1	0.11
(1,1465)	1:A:250:LEU:HD22	1:A:251:HIS:H	1	0.11
(1,1465)	1:A:250:LEU:HD23	1:A:251:HIS:H	1	0.11
(1,1465)	1:A:250:LEU:HD11	1:A:251:HIS:H	8	0.11
(1,1465)	1:A:250:LEU:HD12	1:A:251:HIS:H	8	0.11
(1,1465)	1:A:250:LEU:HD13	1:A:251:HIS:H	8	0.11
(1,1465)	1:A:250:LEU:HD21	1:A:251:HIS:H	8	0.11
(1,1465)	1:A:250:LEU:HD22	1:A:251:HIS:H	8	0.11
(1,1465)	1:A:250:LEU:HD23	1:A:251:HIS:H	8	0.11
(1,1465)	1:A:250:LEU:HD11	1:A:251:HIS:H	19	0.11
(1,1465)	1:A:250:LEU:HD12	1:A:251:HIS:H	19	0.11
(1,1465)	1:A:250:LEU:HD13	1:A:251:HIS:H	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1465)	1:A:250:LEU:HD21	1:A:251:HIS:H	19	0.11
(1,1465)	1:A:250:LEU:HD22	1:A:251:HIS:H	19	0.11
(1,1465)	1:A:250:LEU:HD23	1:A:251:HIS:H	19	0.11
(1,1465)	1:A:250:LEU:HD11	1:A:251:HIS:H	20	0.11
(1,1465)	1:A:250:LEU:HD12	1:A:251:HIS:H	20	0.11
(1,1465)	1:A:250:LEU:HD13	1:A:251:HIS:H	20	0.11
(1,1465)	1:A:250:LEU:HD21	1:A:251:HIS:H	20	0.11
(1,1465)	1:A:250:LEU:HD22	1:A:251:HIS:H	20	0.11
(1,1465)	1:A:250:LEU:HD23	1:A:251:HIS:H	20	0.11
(1,1380)	1:A:298:ILE:HA	1:A:303:GLN:H	14	0.11
(1,1307)	1:A:250:LEU:HG	1:A:251:HIS:HA	10	0.11
(1,1224)	1:A:273:ILE:HB	1:A:275:GLY:HA3	18	0.11
(1,1215)	1:A:274:PRO:HB2	1:A:275:GLY:HA2	9	0.11
(1,1118)	1:A:316:LEU:HB3	1:A:321:MET:HB2	11	0.11
(1,1001)	1:A:250:LEU:HD21	1:A:251:HIS:H	2	0.11
(1,1001)	1:A:250:LEU:HD22	1:A:251:HIS:H	2	0.11
(1,1001)	1:A:250:LEU:HD23	1:A:251:HIS:H	2	0.11
(1,1001)	1:A:250:LEU:HD21	1:A:251:HIS:H	11	0.11
(1,1001)	1:A:250:LEU:HD22	1:A:251:HIS:H	11	0.11
(1,1001)	1:A:250:LEU:HD23	1:A:251:HIS:H	11	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found