



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 09:57 PM UTC

PDB ID : 2KZK / pdb_00002kzk
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

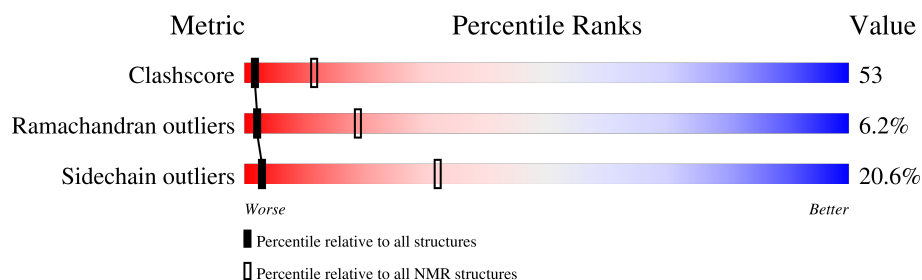
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	107	20% 59% 11% 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

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
1	A	103	Total	C	H	N	O	S	0
			1617	520	807	129	157	4	

There are 4 discrepancies between the modelled and reference sequences:

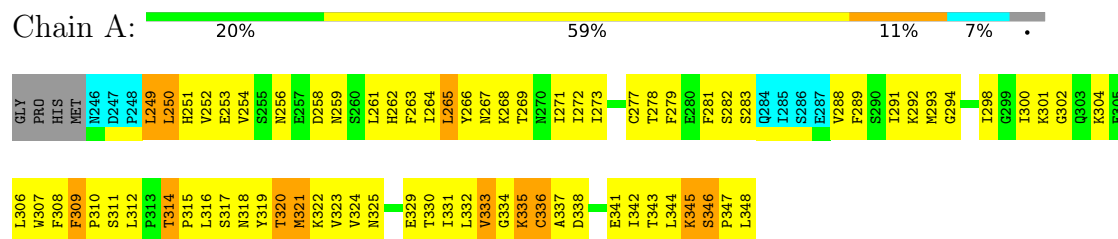
Chain	Residue	Modelled	Actual	Comment	Reference
A	242	GLY	-	expression tag	UNP Q12292
A	243	PRO	-	expression tag	UNP Q12292
A	244	HIS	-	expression tag	UNP Q12292
A	245	MET	-	expression tag	UNP Q12292

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

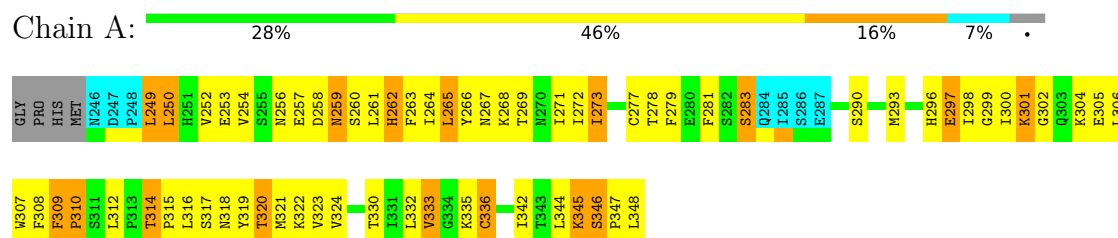


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

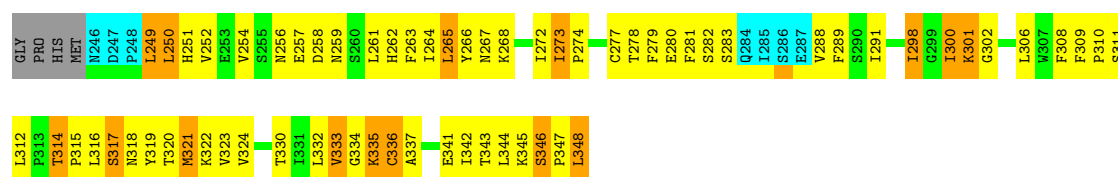
- Molecule 1: Uncharacterized protein YOL083W



4.2.2 Score per residue for model 2

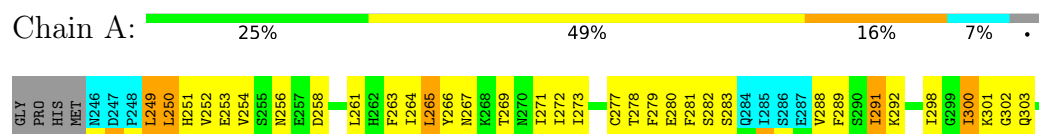
- Molecule 1: Uncharacterized protein YOL083W





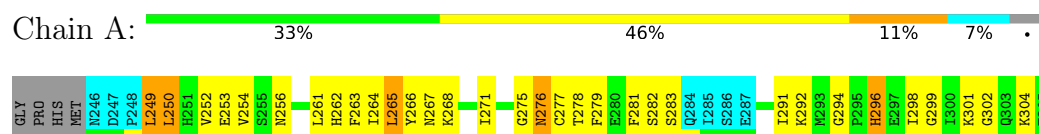
4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein YOL083W



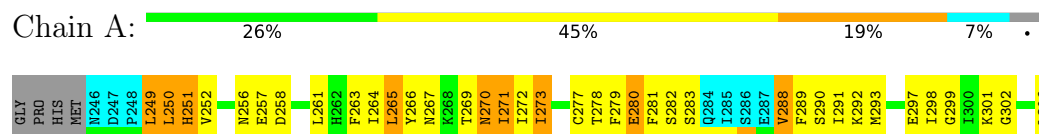
4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein YOL083W



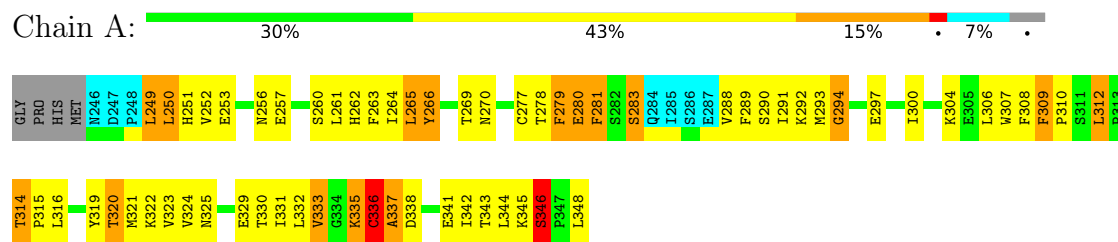
4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein YOL083W



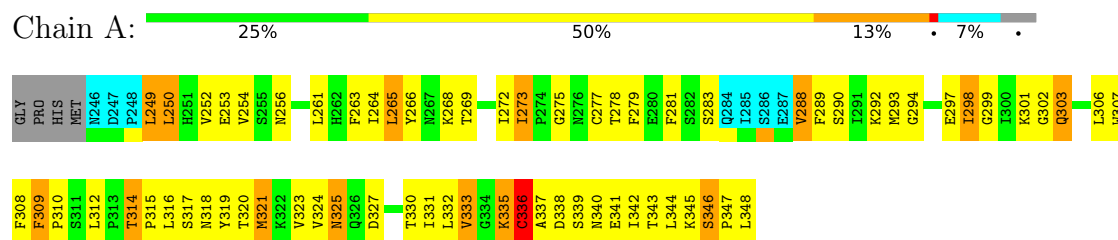
4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein YOL083W



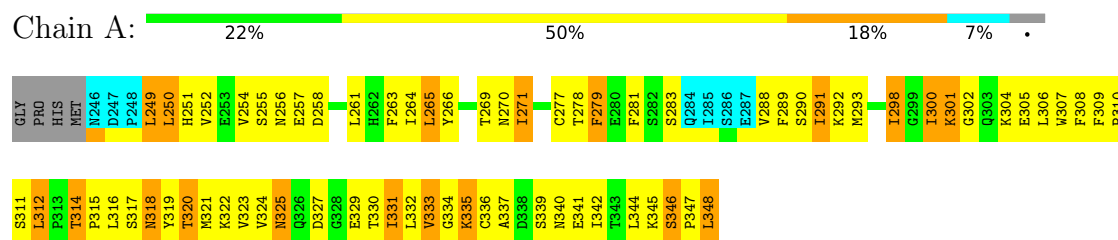
4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein YOL083W



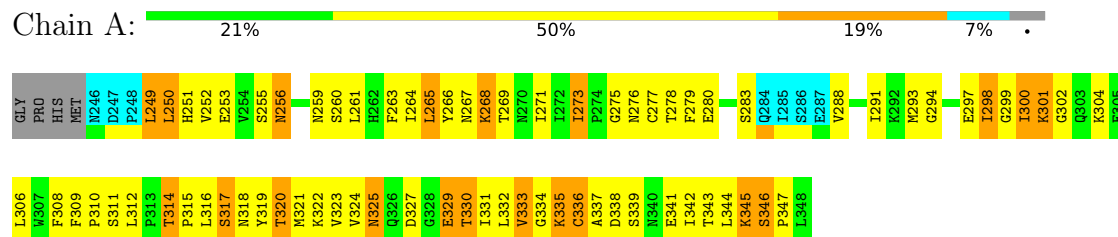
4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein YOL083W



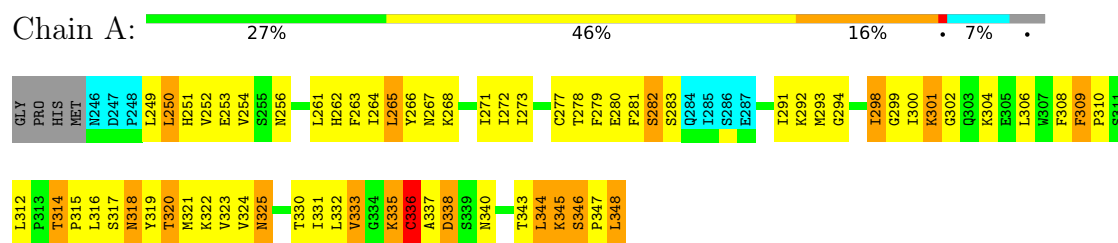
4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein YOL083W



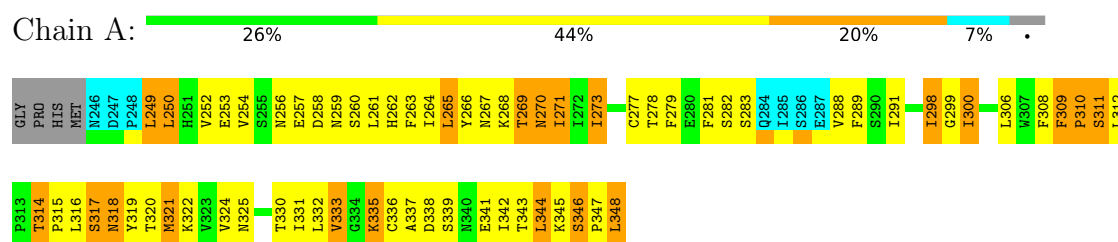
4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein YOL083W



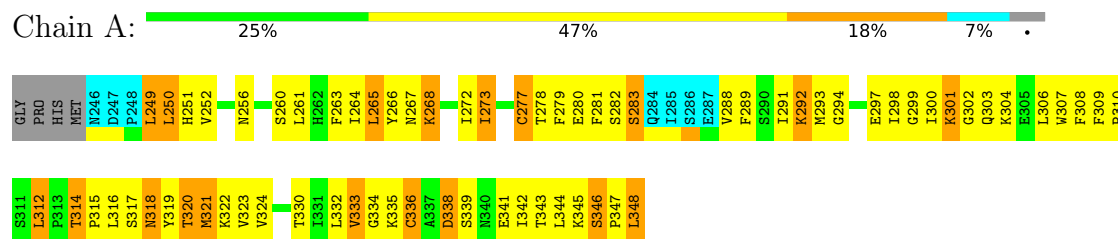
4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein YOL083W



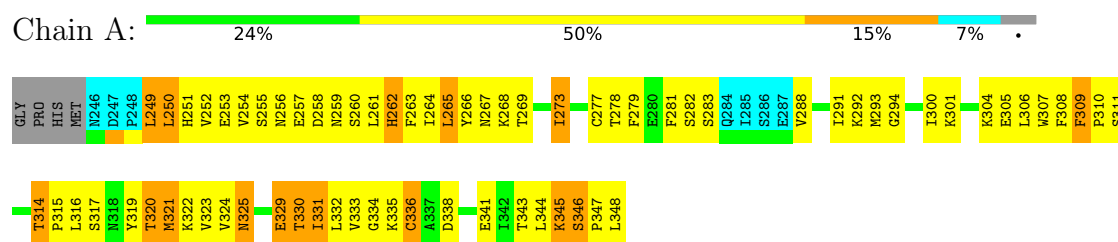
4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein YOL083W



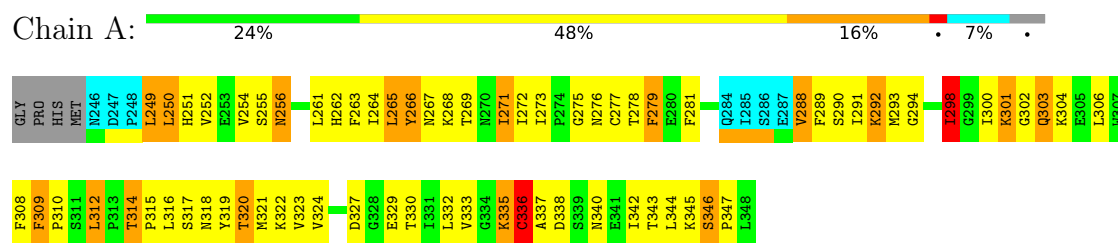
4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein YOL083W



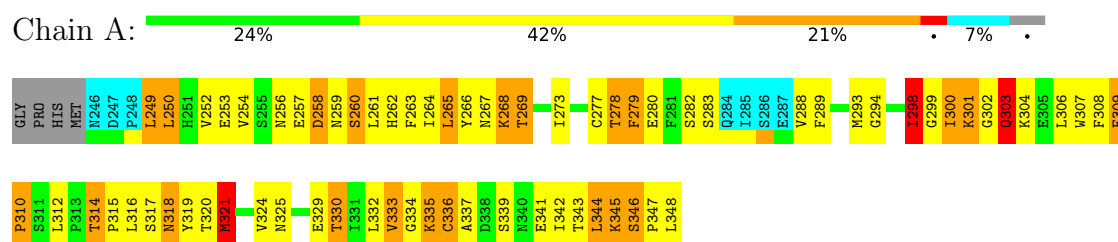
4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein YOL083W



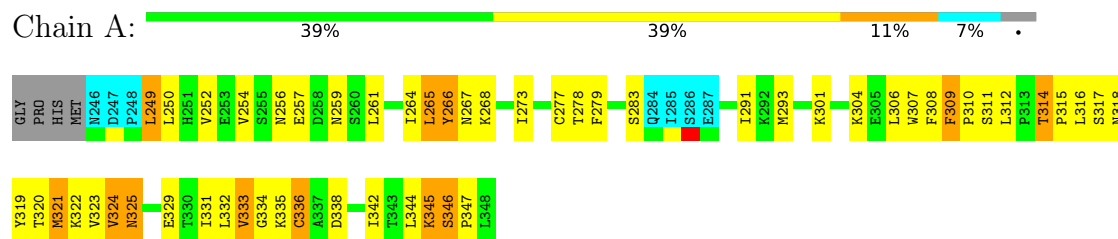
4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein YOL083W



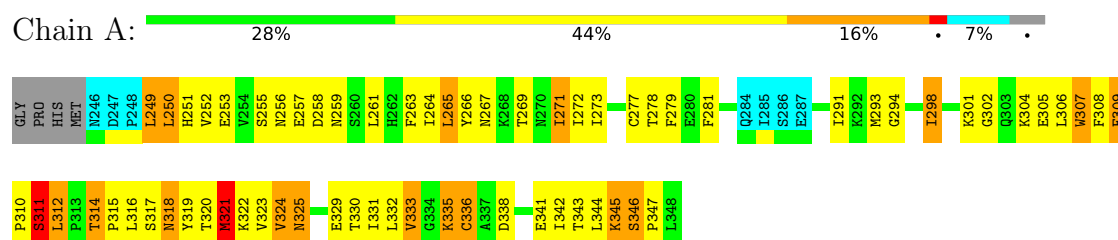
4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein YOL083W



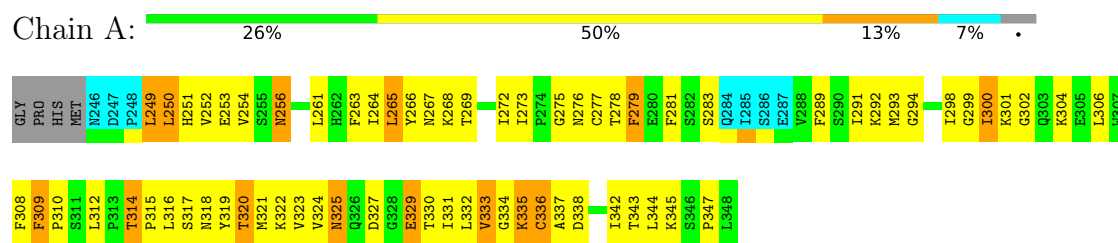
4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized protein YOL083W



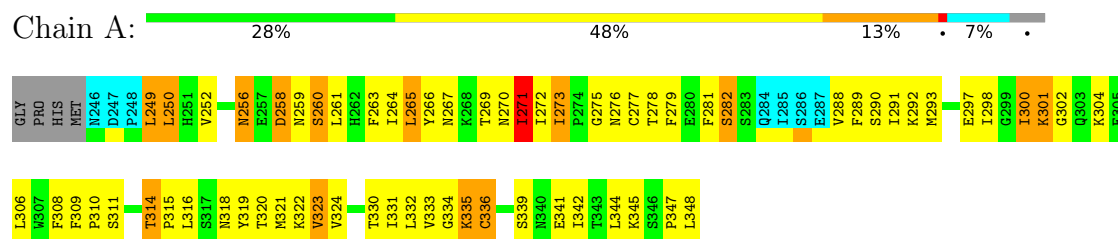
4.2.18 Score per residue for model 18

- Molecule 1: Uncharacterized protein YOL083W



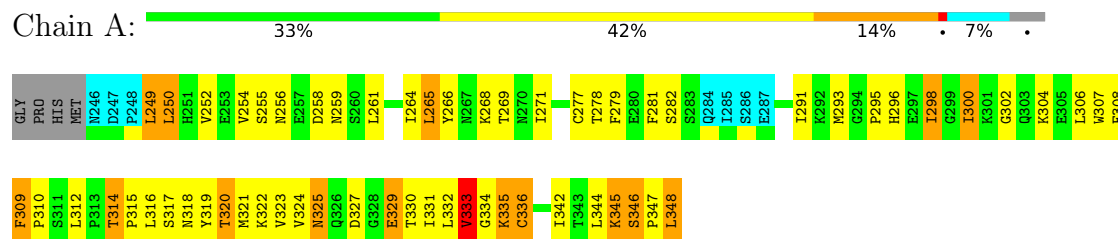
4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein YOL083W



4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: Uncharacterized protein YOL083W



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	80±9
All	All	15100	15160	15100	1594

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 53.

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:321:MET:HE2	1:A:336:CYS:SG	0.87	2.09	16	2
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	0.86	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:316:LEU:HD13	1:A:321:MET:HE2	0.82	1.51	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:316:LEU:HD12	1:A:321:MET:HE2	0.79	1.54	4	3
1:A:281:PHE:CE2	1:A:308:PHE:CD2	0.79	2.70	11	5
1:A:335:LYS:HZ2	1:A:337:ALA:HB2	0.79	1.38	9	7
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:271:ILE:C	1:A:271:ILE:HD13	0.78	2.03	19	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:321:MET:HE1	1:A:342:ILE:CD1	0.76	2.11	3	7
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:308:PHE:CE2	1:A:312:LEU:HD11	0.74	2.17	16	2
1:A:249:LEU:C	1:A:249:LEU:HD22	0.74	2.07	11	5
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: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:250:LEU:HD12	1:A:250:LEU:C	0.72	2.10	11	6
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:348:LEU:C	1:A:348:LEU:HD22	0.71	2.11	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:HD23	1:A:249:LEU:C	0.70	2.11	3	2
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
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: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:316:LEU:HD22	1:A:321:MET:HE2	0.67	1.66	13	3
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:316:LEU:HD13	1:A:321:MET:CE	0.66	2.18	18	6
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:266:TYR:N	1:A:266:TYR:CD1	0.65	2.64	14	6
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:335:LYS:HZ2	1:A:337:ALA:CB	0.65	2.04	2	7
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:316:LEU:HD22	1:A:321:MET:HE3	0.65	1.68	17	1
1:A:298:ILE:HG23	1:A:302:GLY:C	0.64	2.16	15	8
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: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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:271:ILE:C	1:A:272:ILE:HD12	0.63	2.17	14	1
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
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: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:316:LEU:HD12	1:A:321:MET:CE	0.61	2.25	4	2
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:320:THR:O	1:A:321:MET:C	0.61	2.44	11	20
1:A:321:MET:CE	1:A:342:ILE:CD1	0.61	2.79	1	9
1:A:250:LEU:C	1:A:250:LEU:CD1	0.61	2.73	11	10
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: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:293:MET:HE2	1:A:304:LYS:HE3	0.60	1.74	6	1
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	1
1:A:261:LEU:HD13	1:A:263:PHE:CZ	0.60	2.32	18	4
1:A:267:ASN:CG	1:A:273:ILE:HD13	0.60	2.22	13	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:335:LYS:HZ3	1:A:337:ALA:N	0.59	1.88	18	1
1:A:282:SER:O	1:A:319:TYR:CE2	0.59	2.55	11	4
1:A:250:LEU:C	1:A:250:LEU:HD12	0.59	2.21	17	4
1:A:267:ASN:HB3	1:A:298:ILE:HG22	0.59	1.73	4	1
1:A:308:PHE:C	1:A:309:PHE:CD1	0.59	2.81	10	4
1:A:254:VAL:HG11	1:A:314:THR:CG2	0.59	2.27	1	4
1:A:261:LEU:HD12	1:A:308:PHE:CD1	0.59	2.32	7	1
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:335:LYS:C	1:A:336:CYS:SG	0.58	2.86	20	1
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: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:325:ASN:CG	1:A:331:ILE:HD13	0.57	2.25	16	2
1:A:252:VAL:HG13	1:A:265:LEU:CD2	0.57	2.24	11	2
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	2
1:A:254:VAL:HG11	1:A:314:THR:HG21	0.56	1.75	1	7
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:332:LEU:C	1:A:333:VAL:HG12	0.56	2.26	20	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: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	1
1:A:294:GLY:CA	1:A:304:LYS:NZ	0.55	2.70	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:271:ILE:C	1:A:271:ILE:CD1	0.55	2.74	19	1
1:A:279:PHE:CE1	1:A:323:VAL:HG22	0.55	2.36	3	3
1:A:316:LEU:C	1:A:319:TYR:CD1	0.55	2.85	17	3
1:A:332:LEU:HD23	1:A:346:SER:HA	0.55	1.78	4	5
1:A:308:PHE:CZ	1:A:309:PHE:O	0.55	2.59	16	3
1:A:321:MET:HE3	1:A:336:CYS:SG	0.54	2.41	4	1
1:A:308:PHE:C	1:A:309:PHE:CG	0.54	2.86	10	1
1:A:332:LEU:CD2	1:A:345:LYS:C	0.54	2.80	20	1
1:A:267:ASN:CG	1:A:298:ILE:CG2	0.54	2.79	18	1
1:A:316:LEU:HD13	1:A:321:MET:HE1	0.54	1.79	8	1
1:A:324:VAL:HG23	1:A:329:GLU:H	0.54	1.61	16	1
1:A:293:MET:HE2	1:A:304:LYS:HE2	0.54	1.79	18	5
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:256:ASN:CG	1:A:314:THR:HG1	0.53	2.11	9	2
1:A:324:VAL:HG12	1:A:329:GLU:C	0.53	2.28	20	5
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:249:LEU:CD1	1:A:249:LEU:C	0.52	2.82	9	1
1:A:251:HIS:CE1	1:A:341:GLU:CD	0.52	2.87	9	1
1:A:298:ILE:CG2	1:A:302:GLY:C	0.52	2.82	1	6
1:A:325:ASN:ND2	1:A:325:ASN:N	0.52	2.57	3	4
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:348:LEU:C	1:A:348:LEU:CD2	0.52	2.83	3	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:283:SER:CB	1:A:312:LEU:HD23	0.52	2.35	9	5
1:A:332:LEU:C	1:A:333:VAL:CG1	0.52	2.82	3	14
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:267:ASN:CG	1:A:267:ASN:O	0.51	2.51	15	3
1:A:316:LEU:HD23	1:A:319:TYR:HD2	0.51	1.65	15	2
1:A:249:LEU:C	1:A:249:LEU:CD2	0.51	2.84	3	5
1:A:316:LEU:HD22	1:A:319:TYR:CE2	0.51	2.40	2	2
1:A:329:GLU:O	1:A:329:GLU:CG	0.51	2.59	8	4
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:270:ASN:C	1:A:271:ILE:CG2	0.51	2.83	11	1
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:316:LEU:HD13	1:A:321:MET:HE3	0.51	1.81	7	4
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:314:THR:HA	1:A:315:PRO:C	0.51	2.31	8	20
1:A:258:ASP:O	1:A:259:ASN:CB	0.51	2.59	11	2
1:A:348:LEU:HD13	1:A:348:LEU:C	0.51	2.30	13	1
1:A:312:LEU:HD12	1:A:312:LEU:O	0.51	2.04	14	1
1:A:249:LEU:HD13	1:A:249:LEU:C	0.51	2.31	7	2
1:A:316:LEU:CD2	1:A:319:TYR:CD2	0.51	2.94	7	3
1:A:277:CYS:SG	1:A:293:MET:HE2	0.51	2.46	12	1
1:A:280:GLU:CG	1:A:288:VAL:HG21	0.51	2.36	2	2
1:A:312:LEU:C	1:A:312:LEU:CD1	0.51	2.83	14	1
1:A:294:GLY:CA	1:A:304:LYS:HZ2	0.51	2.18	18	1
1:A:267:ASN:CG	1:A:273:ILE:CD1	0.50	2.85	19	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: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:HG22	1:A:322:LYS:HG3	0.50	1.83	2	5
1:A:251:HIS:CD2	1:A:341:GLU:CD	0.50	2.89	5	1
1:A:256:ASN:OD1	1:A:314:THR:CG2	0.50	2.60	9	3
1:A:335:LYS:NZ	1:A:337:ALA:HB2	0.49	2.18	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:269:THR:C	1:A:270:ASN:CG	0.49	2.80	11	1
1:A:275:GLY:O	1:A:276:ASN:CB	0.49	2.60	18	3
1:A:268:LYS:CE	1:A:300:ILE:O	0.49	2.60	1	2
1:A:309:PHE:HA	1:A:310:PRO:C	0.49	2.31	12	20
1:A:261:LEU:HD13	1:A:263:PHE:HZ	0.49	1.67	5	2
1:A:282:SER:HB3	1:A:288:VAL:HG23	0.49	1.84	15	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:300:ILE:C	1:A:302:GLY:N	0.49	2.70	8	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
1:A:275:GLY:C	1:A:276:ASN:CG	0.49	2.81	4	1
1:A:294:GLY:H	1:A:304:LYS:NZ	0.49	2.06	4	2
1:A:293:MET:HB3	1:A:304:LYS:HZ1	0.49	1.68	6	1
1:A:322:LYS:C	1:A:323:VAL:CG2	0.49	2.86	6	7
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	4
1:A:316:LEU:C	1:A:336:CYS:HG	0.48	2.16	11	1
1:A:281:PHE:CE1	1:A:291:ILE:HD12	0.48	2.43	3	1
1:A:283:SER:O	1:A:319:TYR:CE2	0.48	2.66	9	1
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:275:GLY:C	1:A:277:CYS:N	0.48	2.71	4	2
1:A:299:GLY:O	1:A:300:ILE:C	0.48	2.57	15	5
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:293:MET:O	1:A:294:GLY:C	0.48	2.57	18	6
1:A:333:VAL:HG22	1:A:346:SER:C	0.48	2.34	14	1
1:A:271:ILE:HD13	1:A:271:ILE:O	0.48	2.09	19	1
1:A:335:LYS:O	1:A:336:CYS:C	0.47	2.57	17	6
1:A:298:ILE:HG22	1:A:299:GLY:H	0.47	1.63	15	2
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:268:LYS:HZ1	1:A:301:LYS:HA	0.47	1.68	13	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:314:THR:CB	1:A:315:PRO:HA	0.47	2.39	14	10
1:A:343:THR:O	1:A:344:LEU:C	0.47	2.58	13	12
1:A:321:MET:CE	1:A:336:CYS:SG	0.47	3.02	4	1
1:A:252:VAL:N	1:A:342:ILE:O	0.47	2.48	14	2
1:A:322:LYS:CG	1:A:333:VAL:HG12	0.47	2.40	19	2
1:A:320:THR:HG23	1:A:322:LYS:HZ3	0.47	1.70	20	1
1:A:323:VAL:HG21	1:A:344:LEU:HD21	0.47	1.83	1	1
1:A:321:MET:HE1	1:A:342:ILE:HD11	0.47	1.87	15	2
1:A:330:THR:HG22	1:A:347:PRO:HG3	0.47	1.86	12	1
1:A:316:LEU:CD1	1:A:321:MET:CE	0.47	2.93	12	1
1:A:338:ASP:CG	1:A:338:ASP:O	0.47	2.57	14	2
1:A:277:CYS:SG	1:A:331:ILE:CD1	0.47	3.03	19	1
1:A:256:ASN:O	1:A:256:ASN:CG	0.47	2.58	12	11
1:A:306:LEU:HB3	1:A:308:PHE:CZ	0.47	2.45	17	8
1:A:277:CYS:C	1:A:278:THR:OG1	0.46	2.59	13	18
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:321:MET:HE1	1:A:342:ILE:HD13	0.46	1.85	14	1
1:A:348:LEU:C	1:A:348:LEU:HD12	0.46	2.34	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:272:ILE:HD12	1:A:272:ILE:N	0.46	2.25	18	3
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: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:334:GLY:C	1:A:336:CYS:N	0.46	2.72	2	11
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:347:PRO:O	1:A:348:LEU:C	0.46	2.58	12	2
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:320:THR:C	1:A:322:LYS:N	0.46	2.73	17	2
1:A:348:LEU:C	1:A:348:LEU:HD13	0.46	2.36	2	4
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:298:ILE:HG21	0.46	2.34	18	1
1:A:299:GLY:C	1:A:301:LYS:N	0.46	2.70	12	3
1:A:251:HIS:CE1	1:A:341:GLU:HG2	0.46	2.46	2	2
1:A:270:ASN:O	1:A:271:ILE:C	0.46	2.58	19	1
1:A:258:ASP:O	1:A:259:ASN:C	0.45	2.59	17	4
1:A:275:GLY:O	1:A:276:ASN:C	0.45	2.59	4	2
1:A:336:CYS:SG	1:A:337:ALA:N	0.45	2.88	6	1
1:A:319:TYR:O	1:A:320:THR:C	0.45	2.59	18	2
1:A:266:TYR:CD1	1:A:266:TYR:N	0.45	2.85	5	4
1:A:261:LEU:HD22	1:A:263:PHE:CZ	0.45	2.46	18	1
1:A:257:GLU:O	1:A:258:ASP:C	0.45	2.60	13	5
1:A:339:SER:C	1:A:341:GLU:N	0.45	2.72	19	7
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:C	1:A:252:VAL:HG23	0.45	2.36	14	3
1:A:281:PHE:CE2	1:A:312:LEU:HD11	0.45	2.47	8	2
1:A:317:SER:OG	1:A:337:ALA:C	0.45	2.60	5	1
1:A:251:HIS:C	1:A:252:VAL:CG2	0.45	2.90	8	1
1:A:249:LEU:O	1:A:269:THR:CG2	0.45	2.64	11	1
1:A:298:ILE:N	1:A:298:ILE:HD13	0.45	2.25	14	1
1:A:272:ILE:O	1:A:273:ILE:C	0.45	2.60	10	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:279:PHE:CZ	1:A:321:MET:HG2	0.45	2.47	4	2
1:A:273:ILE:O	1:A:297:GLU:CD	0.45	2.60	9	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:259:ASN:C	1:A:260:SER:OG	0.45	2.60	19	1
1:A:308:PHE:O	1:A:309:PHE:C	0.45	2.58	12	2
1:A:333:VAL:O	1:A:333:VAL:CG2	0.45	2.64	17	3
1:A:256:ASN:CG	1:A:314:THR:OG1	0.45	2.60	9	3
1:A:283:SER:CB	1:A:319:TYR:OH	0.45	2.65	6	1
1:A:249:LEU:N	1:A:249:LEU:CD1	0.45	2.70	5	2
1:A:300:ILE:O	1:A:301:LYS:C	0.45	2.60	8	1
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:258:ASP:C	1:A:259:ASN:CG	0.45	2.81	15	1
1:A:258:ASP:C	1:A:259:ASN:OD1	0.44	2.60	1	2
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:332:LEU:C	1:A:333:VAL:HG13	0.44	2.37	14	1
1:A:329:GLU:O	1:A:330:THR:C	0.44	2.60	17	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: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:337:ALA:O	1:A:338:ASP:C	0.44	2.59	14	3
1:A:267:ASN:OD1	1:A:267:ASN:C	0.44	2.60	2	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:262:HIS:CD2	1:A:262:HIS:C	0.44	2.96	13	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:257:GLU:C	1:A:259:ASN:N	0.44	2.76	16	1
1:A:325:ASN:ND2	1:A:331:ILE:CG2	0.43	2.76	3	1
1:A:339:SER:O	1:A:340:ASN:C	0.43	2.61	7	1
1:A:250:LEU:HD12	1:A:267:ASN:HA	0.43	1.90	2	2
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: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: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: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: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:316:LEU:CD1	1:A:321:MET:HE2	0.43	2.37	2	1
1:A:283:SER:CB	1:A:312:LEU:HD21	0.43	2.43	5	1
1:A:280:GLU:O	1:A:322:LYS:N	0.43	2.52	6	1
1:A:261:LEU:HD11	1:A:312:LEU:CB	0.43	2.37	7	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:267:ASN:OD1	1:A:299:GLY:C	0.43	2.62	10	1
1:A:288:VAL:HG22	1:A:289:PHE:H	0.43	1.74	14	1
1:A:341:GLU:C	1:A:342:ILE:CG1	0.43	2.92	4	3
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: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:321:MET:HE3	1:A:342:ILE:CD1	0.42	2.43	8	3
1:A:294:GLY:HA3	1:A:304:LYS:HZ3	0.42	1.74	12	1
1:A:269:THR:OG1	1:A:270:ASN:N	0.42	2.52	5	1
1:A:300:ILE:C	1:A:301:LYS:CD	0.42	2.92	8	1
1:A:269:THR:O	1:A:270:ASN:CG	0.42	2.62	11	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:306:LEU:O	1:A:307:TRP:C	0.42	2.61	5	1
1:A:252:VAL:CG2	1:A:265:LEU:CD2	0.42	2.98	10	2
1:A:294:GLY:H	1:A:304:LYS:HZ1	0.42	1.57	12	1
1:A:312:LEU:HD12	1:A:312:LEU:C	0.42	2.40	14	1
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: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: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: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:277:CYS:C	1:A:278:THR:HG1	0.41	2.23	5	2
1:A:302:GLY:O	1:A:303:GLN:C	0.41	2.61	15	2
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:301:LYS:C	1:A:301:LYS:HD2	0.41	2.40	15	1
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:327:ASP:C	1:A:329:GLU:N	0.41	2.75	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:301:LYS:N	1:A:301:LYS:HD3	0.41	2.30	7	1
1:A:267:ASN:O	1:A:267:ASN:CG	0.41	2.60	10	2
1:A:335:LYS:HB3	1:A:345:LYS:CE	0.41	2.46	5	2
1:A:256:ASN:ND2	1:A:312:LEU:O	0.41	2.53	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:322:LYS:C	1:A:323:VAL:HG23	0.41	2.41	9	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: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:267:ASN:C	1:A:269:THR:N	0.41	2.79	15	1
1:A:338:ASP:O	1:A:338:ASP:CG	0.41	2.61	16	1
1:A:256:ASN:OD1	1:A:312:LEU:O	0.41	2.39	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: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:338:ASP:OD2	0.40	2.39	12	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:270:ASN:C	1:A:271:ILE:O	0.40	2.65	8	1
1:A:334:GLY:O	1:A:335:LYS:C	0.40	2.63	18	1
1:A:320:THR:C	1:A:321:MET:CG	0.40	2.94	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:267:ASN:HB3	1:A:298:ILE:CG2	0.40	2.46	10	1
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:315:PRO:C	1:A:316:LEU:HD23	0.40	2.42	2	1
1:A:267:ASN:HB3	1:A:273:ILE:CD1	0.40	2.47	9	1
1:A:300:ILE:CG2	1:A:301:LYS:N	0.40	2.84	15	1
1:A:295:PRO:O	1:A:296:HIS:C	0.40	2.64	20	1

6.3 Torsion angles

6.3.1 Protein backbone

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

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

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%)	71±3 (79±3%)	18±3 (21±3%)	3	32
All	All	1780/1980 (90%)	1413 (79%)	367 (21%)	3	32

All 59 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	314	THR	20
1	A	335	LYS	20
1	A	333	VAL	18
1	A	301	LYS	15
1	A	336	CYS	15
1	A	309	PHE	13
1	A	345	LYS	13
1	A	320	THR	12
1	A	325	ASN	12
1	A	348	LEU	11
1	A	292	LYS	11
1	A	273	ILE	10
1	A	268	LYS	10
1	A	271	ILE	9
1	A	338	ASP	8
1	A	318	ASN	6
1	A	255	SER	6
1	A	262	HIS	5
1	A	317	SER	5
1	A	307	TRP	5
1	A	312	LEU	5
1	A	297	GLU	4
1	A	300	ILE	4
1	A	341	GLU	4
1	A	327	ASP	4
1	A	256	ASN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	329	GLU	4
1	A	283	SER	3
1	A	258	ASP	3
1	A	303	GLN	3
1	A	321	MET	3
1	A	330	THR	3
1	A	266	TYR	3
1	A	331	ILE	3
1	A	298	ILE	3
1	A	282	SER	3
1	A	260	SER	3
1	A	291	ILE	2
1	A	253	GLU	2
1	A	311	SER	2
1	A	279	PHE	2
1	A	324	VAL	2
1	A	259	ASN	1
1	A	276	ASN	1
1	A	251	HIS	1
1	A	281	PHE	1
1	A	346	SER	1
1	A	272	ILE	1
1	A	288	VAL	1
1	A	305	GLU	1
1	A	269	THR	1
1	A	339	SER	1
1	A	277	CYS	1
1	A	278	THR	1
1	A	290	SER	1
1	A	323	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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

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 $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	102	-0.14 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	97	-0.08 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	92	0.36 ± 0.15	None needed (< 0.5 ppm)
^{15}N	95	0.67 ± 0.54	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	^1H	^{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	¹H	¹³C	¹⁵N
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	¹H	¹³C	¹⁵N
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 ⓘ

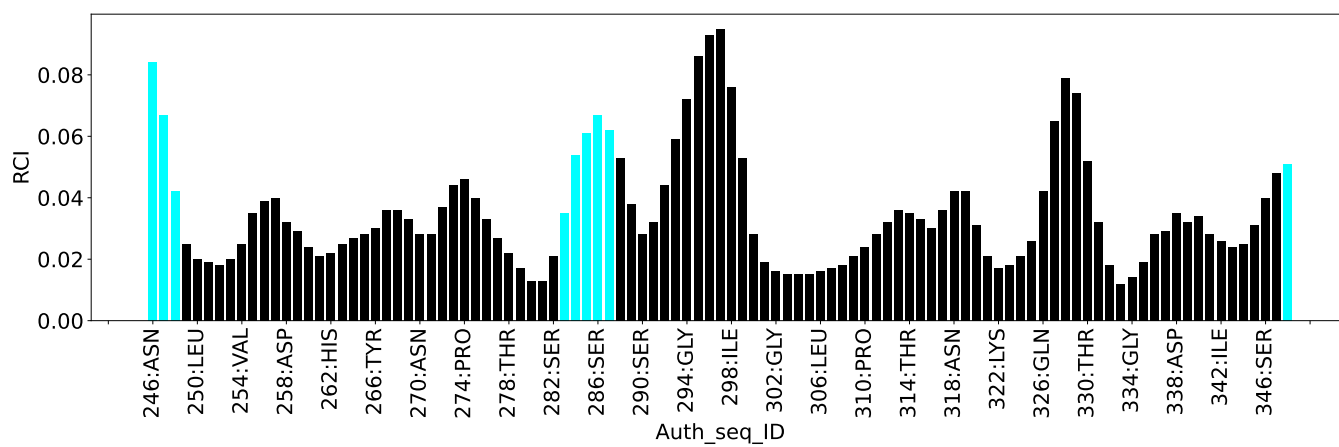
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

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 ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	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 \geq 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

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	4.2	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 ⓘ

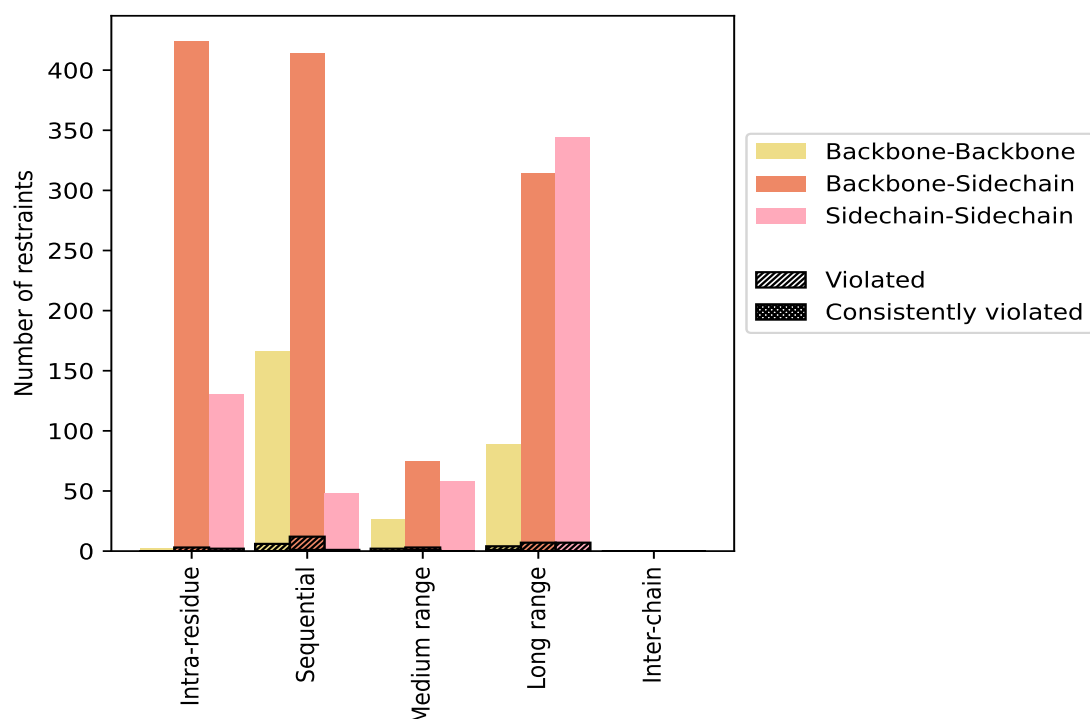
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

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	5	3.1	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	3	4.0	0.1	1	1.3	0.0
Sidechain-Sidechain	58	2.8	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	747	35.7	18	2.4	0.9	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	7	2.2	0.3	0	0.0	0.0
Sidechain-Sidechain	344	16.5	7	2.0	0.3	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	47	2.2	2.2	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	25	2.0	1.2	2	0.2	0.1
Sidechain-Sidechain	580	27.8	10	1.7	0.5	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	1	4	2	4	0	11	0.42	0.89	0.31	0.2
2	0	7	4	3	0	14	0.38	1.01	0.32	0.23
3	0	3	2	2	0	7	0.59	1.01	0.31	0.47
4	1	5	3	3	0	12	0.39	0.96	0.29	0.28
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	4	2	3	0	9	0.44	0.91	0.31	0.34
10	0	4	2	4	0	10	0.45	1.18	0.38	0.22

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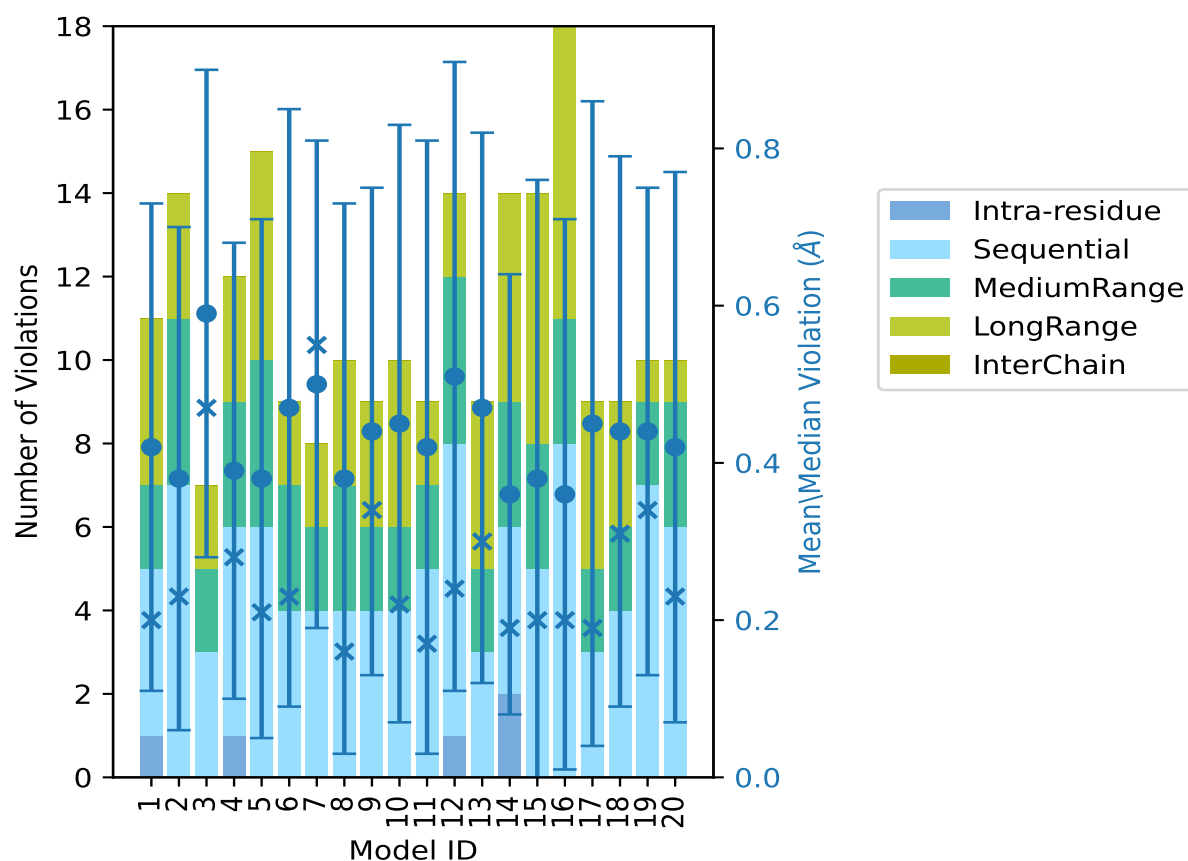
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	5	2	2	0	9	0.42	1.01	0.39	0.17
12	1	7	4	2	0	14	0.51	1.14	0.4	0.24
13	0	3	2	4	0	9	0.47	1.2	0.35	0.3
14	2	4	3	5	0	14	0.36	0.84	0.28	0.19
15	0	5	3	6	0	14	0.38	1.28	0.38	0.2
16	0	8	3	7	0	18	0.36	1.24	0.35	0.2
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

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

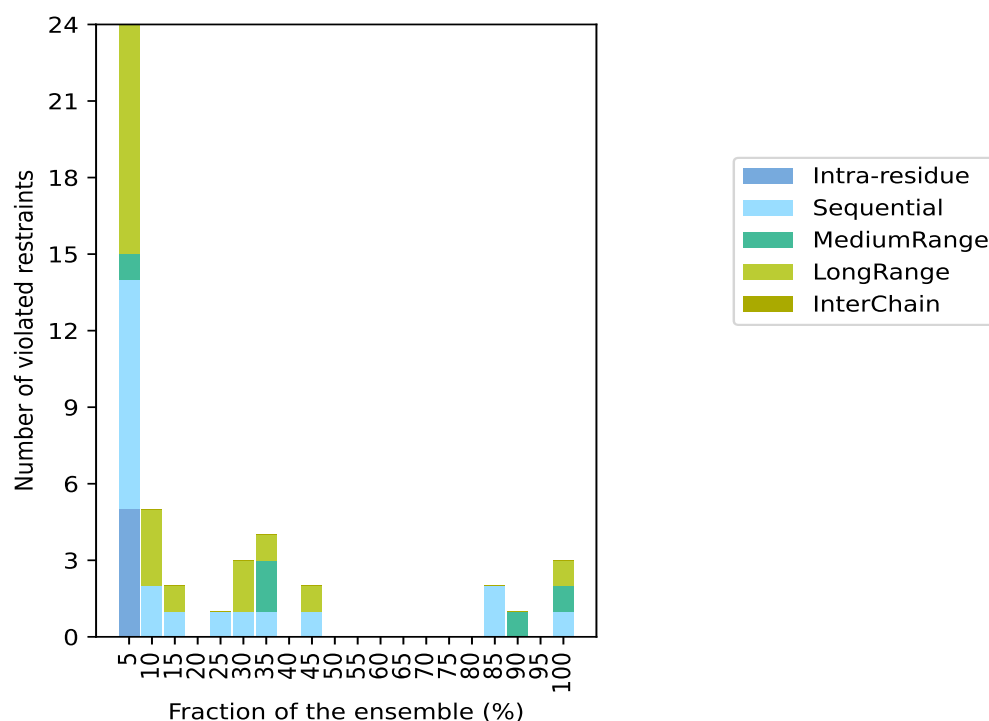
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2043(IR:551, SQ:609, MR:154, LR:729, IC:0) restraints are 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	9	1	9	0	24	1	5.0
0	2	0	3	0	5	2	10.0
0	1	0	1	0	2	3	15.0
0	0	0	0	0	0	4	20.0
0	1	0	0	0	1	5	25.0
0	1	0	2	0	3	6	30.0
0	1	2	1	0	4	7	35.0
0	0	0	0	0	0	8	40.0
0	1	0	1	0	2	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

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

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

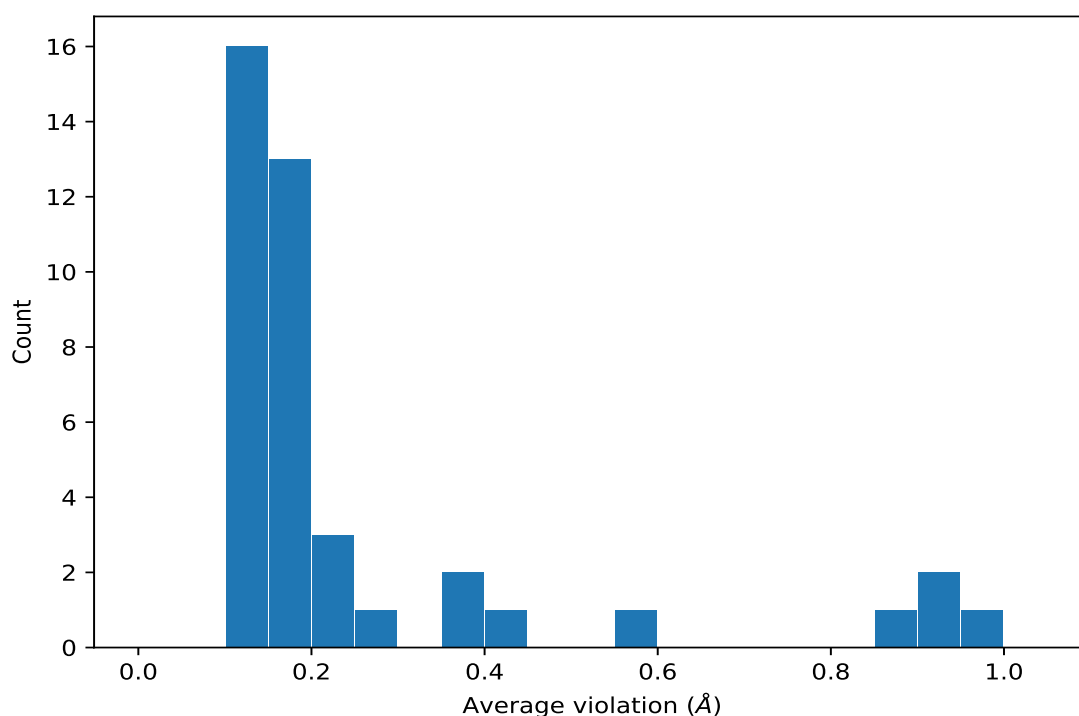
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

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

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,141)	1:334:A:GLY:HA3	1:345:A:LYS:H	20	0.96	0.18	0.92
(1,1688)	1:273:A:ILE:HG12	1:275:A:GLY:HA3	20	0.93	0.11	0.96
(1,1688)	1:273:A:ILE:HG13	1:275:A:GLY:HA3	20	0.93	0.11	0.96
(1,1110)	1:334:A:GLY:HA3	1:335:A:LYS:HB2	20	0.89	0.05	0.9
(1,1224)	1:273:A:ILE:HB	1:275:A:GLY:HA3	18	0.38	0.21	0.34
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	17	0.25	0.05	0.28
(1,1215)	1:274:A:PRO:HB2	1:275:A:GLY:HA2	17	0.18	0.05	0.17
(1,318)	1:275:A:GLY:HA3	1:298:A:ILE:H	9	0.55	0.21	0.55
(1,1465)	1:250:A:LEU:HD11	1:251:A:HIS:H	9	0.12	0.02	0.11
(1,1465)	1:250:A:LEU:HD12	1:251:A:HIS:H	9	0.12	0.02	0.11
(1,1465)	1:250:A:LEU:HD13	1:251:A:HIS:H	9	0.12	0.02	0.11
(1,1465)	1:250:A:LEU:HD21	1:251:A:HIS:H	9	0.12	0.02	0.11
(1,1465)	1:250:A:LEU:HD22	1:251:A:HIS:H	9	0.12	0.02	0.11
(1,1465)	1:250:A:LEU:HD23	1:251:A:HIS:H	9	0.12	0.02	0.11
(1,1218)	1:275:A:GLY:HA2	1:295:A:PRO:HA	7	0.4	0.18	0.39
(1,91)	1:275:A:GLY:HA3	1:277:A:CYS:H	7	0.37	0.34	0.23

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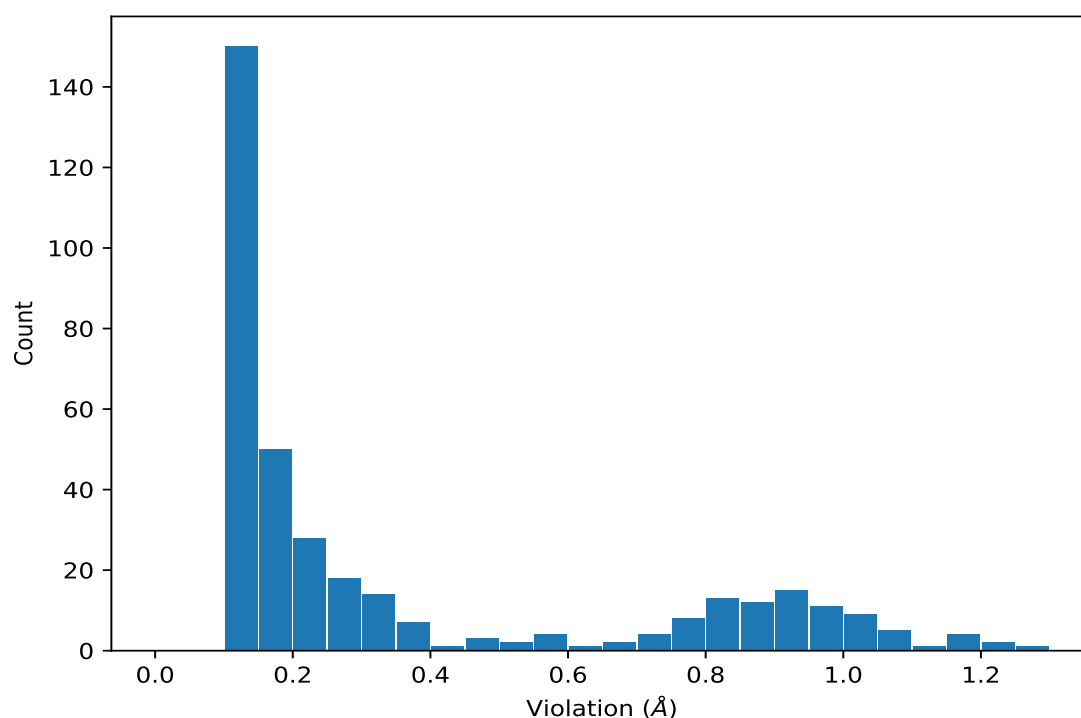
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,567)	1:249:A:LEU:HA	1:251:A:HIS:H	7	0.16	0.02	0.15
(1,1307)	1:250:A:LEU:HG	1:251:A:HIS:HA	7	0.12	0.01	0.12
(1,2030)	1:335:A:LYS:HB3	1:345:A:LYS:HG2	6	0.22	0.02	0.22
(1,2030)	1:335:A:LYS:HB3	1:345:A:LYS:HG3	6	0.22	0.02	0.22
(1,2026)	1:335:A:LYS:HB2	1:345:A:LYS:HD2	6	0.16	0.03	0.17
(1,2026)	1:335:A:LYS:HB2	1:345:A:LYS:HD3	6	0.16	0.03	0.17
(1,1001)	1:250:A:LEU:HD21	1:251:A:HIS:H	6	0.11	0.01	0.11
(1,1001)	1:250:A:LEU:HD22	1:251:A:HIS:H	6	0.11	0.01	0.11
(1,1001)	1:250:A:LEU:HD23	1:251:A:HIS:H	6	0.11	0.01	0.11
(1,340)	1:250:A:LEU:H	1:251:A:HIS:H	5	0.13	0.04	0.1
(1,1042)	1:335:A:LYS:HA	1:336:A:CYS:HB2	3	0.24	0.06	0.27
(1,524)	1:316:A:LEU:HB3	1:321:A:MET:H	3	0.13	0.02	0.12
(1,936)	1:334:A:GLY:HA3	1:344:A:LEU:HD21	2	0.18	0.02	0.18
(1,936)	1:334:A:GLY:HA3	1:344:A:LEU:HD22	2	0.18	0.02	0.18
(1,936)	1:334:A:GLY:HA3	1:344:A:LEU:HD23	2	0.18	0.02	0.18
(1,1492)	1:252:A:VAL:HG11	1:265:A:LEU:HG	2	0.17	0.01	0.17
(1,1492)	1:252:A:VAL:HG12	1:265:A:LEU:HG	2	0.17	0.01	0.17
(1,1492)	1:252:A:VAL:HG13	1:265:A:LEU:HG	2	0.17	0.01	0.17
(1,1492)	1:252:A:VAL:HG21	1:265:A:LEU:HG	2	0.17	0.01	0.17
(1,1492)	1:252:A:VAL:HG22	1:265:A:LEU:HG	2	0.17	0.01	0.17
(1,1492)	1:252:A:VAL:HG23	1:265:A:LEU:HG	2	0.17	0.01	0.17
(1,2084)	1:347:A:PRO:HA	1:348:A:LEU:HB2	2	0.15	0.0	0.15
(1,2084)	1:347:A:PRO:HA	1:348:A:LEU:HB3	2	0.15	0.0	0.15
(1,1291)	1:275:A:GLY:HA3	1:276:A:ASN:HA	2	0.12	0.02	0.12
(1,1380)	1:298:A:ILE:HA	1:303:A:GLN:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

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

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

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

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	1:273:A:ILE:HB	1:275:A:GLY:HA3	19	0.38
(1,1218)	1:275:A:GLY:HA2	1:295:A:PRO:HA	18	0.38
(1,376)	1:271:A:ILE:HB	1:272:A:ILE:H	19	0.38
(1,2021)	1:335:A:LYS:HA	1:336:A:CYS:HB2	20	0.36
(1,2021)	1:335:A:LYS:HA	1:336:A:CYS:HB3	20	0.36
(1,1215)	1:274:A:PRO:HB2	1:275:A:GLY:HA2	2	0.35
(1,1224)	1:273:A:ILE:HB	1:275:A:GLY:HA3	7	0.34
(1,1224)	1:273:A:ILE:HB	1:275:A:GLY:HA3	9	0.34
(1,1224)	1:273:A:ILE:HB	1:275:A:GLY:HA3	3	0.33
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	18	0.31
(1,640)	1:298:A:ILE:HG21	1:298:A:ILE:HD11	4	0.31
(1,640)	1:298:A:ILE:HG21	1:298:A:ILE:HD12	4	0.31
(1,640)	1:298:A:ILE:HG21	1:298:A:ILE:HD13	4	0.31
(1,640)	1:298:A:ILE:HG22	1:298:A:ILE:HD11	4	0.31
(1,640)	1:298:A:ILE:HG22	1:298:A:ILE:HD12	4	0.31
(1,640)	1:298:A:ILE:HG22	1:298:A:ILE:HD13	4	0.31
(1,640)	1:298:A:ILE:HG23	1:298:A:ILE:HD11	4	0.31
(1,640)	1:298:A:ILE:HG23	1:298:A:ILE:HD12	4	0.31
(1,640)	1:298:A:ILE:HG23	1:298:A:ILE:HD13	4	0.31
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	4	0.3
(1,1218)	1:275:A:GLY:HA2	1:295:A:PRO:HA	13	0.3
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	2	0.29
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	3	0.29
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	8	0.29
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	9	0.29
(1,1042)	1:335:A:LYS:HA	1:336:A:CYS:HB2	19	0.29
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	12	0.28
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	13	0.28
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	16	0.28
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	19	0.27
(1,1042)	1:335:A:LYS:HA	1:336:A:CYS:HB2	20	0.27
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	11	0.26
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	15	0.26
(1,1224)	1:273:A:ILE:HB	1:275:A:GLY:HA3	4	0.26
(1,1224)	1:273:A:ILE:HB	1:275:A:GLY:HA3	6	0.26
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	5	0.25
(1,318)	1:275:A:GLY:HA3	1:298:A:ILE:H	4	0.25
(1,2030)	1:335:A:LYS:HB3	1:345:A:LYS:HG2	10	0.24
(1,2030)	1:335:A:LYS:HB3	1:345:A:LYS:HG3	10	0.24
(1,2030)	1:335:A:LYS:HB3	1:345:A:LYS:HG2	17	0.24
(1,2030)	1:335:A:LYS:HB3	1:345:A:LYS:HG3	17	0.24
(1,91)	1:275:A:GLY:HA3	1:277:A:CYS:H	16	0.24

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

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1492)	1:252:A:VAL:HG21	1:265:A:LEU:HG	6	0.18
(1,1492)	1:252:A:VAL:HG22	1:265:A:LEU:HG	6	0.18
(1,1492)	1:252:A:VAL:HG23	1:265:A:LEU:HG	6	0.18
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	6	0.18
(1,1215)	1:274:A:PRO:HB2	1:275:A:GLY:HA2	8	0.18
(1,1215)	1:274:A:PRO:HB2	1:275:A:GLY:HA2	20	0.18
(1,983)	1:312:A:LEU:HG	1:313:A:PRO:HD3	14	0.18
(1,1300)	1:334:A:GLY:HA3	1:335:A:LYS:HA	1	0.17
(1,1215)	1:274:A:PRO:HB2	1:275:A:GLY:HA2	4	0.17
(1,1215)	1:274:A:PRO:HB2	1:275:A:GLY:HA2	11	0.17
(1,1215)	1:274:A:PRO:HB2	1:275:A:GLY:HA2	17	0.17
(1,936)	1:334:A:GLY:HA3	1:344:A:LEU:HD21	14	0.17
(1,936)	1:334:A:GLY:HA3	1:344:A:LEU:HD22	14	0.17
(1,936)	1:334:A:GLY:HA3	1:344:A:LEU:HD23	14	0.17
(1,646)	1:298:A:ILE:HD11	1:299:A:GLY:H	4	0.17
(1,646)	1:298:A:ILE:HD12	1:299:A:GLY:H	4	0.17
(1,646)	1:298:A:ILE:HD13	1:299:A:GLY:H	4	0.17
(1,567)	1:249:A:LEU:HA	1:251:A:HIS:H	2	0.17
(1,567)	1:249:A:LEU:HA	1:251:A:HIS:H	14	0.17
(1,2026)	1:335:A:LYS:HB2	1:345:A:LYS:HD2	15	0.16
(1,2026)	1:335:A:LYS:HB2	1:345:A:LYS:HD3	15	0.16
(1,1492)	1:252:A:VAL:HG11	1:265:A:LEU:HG	9	0.16
(1,1492)	1:252:A:VAL:HG12	1:265:A:LEU:HG	9	0.16
(1,1492)	1:252:A:VAL:HG13	1:265:A:LEU:HG	9	0.16
(1,1492)	1:252:A:VAL:HG21	1:265:A:LEU:HG	9	0.16
(1,1492)	1:252:A:VAL:HG22	1:265:A:LEU:HG	9	0.16
(1,1492)	1:252:A:VAL:HG23	1:265:A:LEU:HG	9	0.16
(1,1224)	1:273:A:ILE:HB	1:275:A:GLY:HA3	17	0.16
(1,1215)	1:274:A:PRO:HB2	1:275:A:GLY:HA2	5	0.16
(1,1215)	1:274:A:PRO:HB2	1:275:A:GLY:HA2	18	0.16
(1,340)	1:250:A:LEU:H	1:251:A:HIS:H	12	0.16
(1,2084)	1:347:A:PRO:HA	1:348:A:LEU:HB2	10	0.15
(1,2084)	1:347:A:PRO:HA	1:348:A:LEU:HB3	10	0.15
(1,2084)	1:347:A:PRO:HA	1:348:A:LEU:HB2	12	0.15
(1,2084)	1:347:A:PRO:HA	1:348:A:LEU:HB3	12	0.15
(1,1728)	1:281:A:PHE:H	1:321:A:MET:HB2	18	0.15
(1,1728)	1:281:A:PHE:H	1:321:A:MET:HB3	18	0.15
(1,1465)	1:250:A:LEU:HD11	1:251:A:HIS:H	12	0.15
(1,1465)	1:250:A:LEU:HD12	1:251:A:HIS:H	12	0.15
(1,1465)	1:250:A:LEU:HD13	1:251:A:HIS:H	12	0.15
(1,1465)	1:250:A:LEU:HD21	1:251:A:HIS:H	12	0.15
(1,1465)	1:250:A:LEU:HD22	1:251:A:HIS:H	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1465)	1:250:A:LEU:HD23	1:251:A:HIS:H	12	0.15
(1,1215)	1:274:A:PRO:HB2	1:275:A:GLY:HA2	15	0.15
(1,1042)	1:335:A:LYS:HA	1:336:A:CYS:HB2	6	0.15
(1,567)	1:249:A:LEU:HA	1:251:A:HIS:H	20	0.15
(1,524)	1:316:A:LEU:HB3	1:321:A:MET:H	16	0.15
(1,474)	1:250:A:LEU:HG	1:344:A:LEU:H	16	0.15
(1,421)	1:324:A:VAL:HB	1:330:A:THR:H	17	0.15
(1,2069)	1:345:A:LYS:HA	1:345:A:LYS:HE2	1	0.14
(1,2069)	1:345:A:LYS:HA	1:345:A:LYS:HE3	1	0.14
(1,1760)	1:287:A:GLU:H	1:288:A:VAL:HG11	16	0.14
(1,1760)	1:287:A:GLU:H	1:288:A:VAL:HG12	16	0.14
(1,1760)	1:287:A:GLU:H	1:288:A:VAL:HG13	16	0.14
(1,1760)	1:287:A:GLU:H	1:288:A:VAL:HG21	16	0.14
(1,1760)	1:287:A:GLU:H	1:288:A:VAL:HG22	16	0.14
(1,1760)	1:287:A:GLU:H	1:288:A:VAL:HG23	16	0.14
(1,1465)	1:250:A:LEU:HD11	1:251:A:HIS:H	5	0.14
(1,1465)	1:250:A:LEU:HD12	1:251:A:HIS:H	5	0.14
(1,1465)	1:250:A:LEU:HD13	1:251:A:HIS:H	5	0.14
(1,1465)	1:250:A:LEU:HD21	1:251:A:HIS:H	5	0.14
(1,1465)	1:250:A:LEU:HD22	1:251:A:HIS:H	5	0.14
(1,1465)	1:250:A:LEU:HD23	1:251:A:HIS:H	5	0.14
(1,1307)	1:250:A:LEU:HG	1:251:A:HIS:HA	7	0.14
(1,1291)	1:275:A:GLY:HA3	1:276:A:ASN:HA	12	0.14
(1,1224)	1:273:A:ILE:HB	1:275:A:GLY:HA3	8	0.14
(1,1224)	1:273:A:ILE:HB	1:275:A:GLY:HA3	11	0.14
(1,1215)	1:274:A:PRO:HB2	1:275:A:GLY:HA2	10	0.14
(1,1215)	1:274:A:PRO:HB2	1:275:A:GLY:HA2	19	0.14
(1,567)	1:249:A:LEU:HA	1:251:A:HIS:H	5	0.14
(1,567)	1:249:A:LEU:HA	1:251:A:HIS:H	8	0.14
(1,1465)	1:250:A:LEU:HD11	1:251:A:HIS:H	2	0.13
(1,1465)	1:250:A:LEU:HD12	1:251:A:HIS:H	2	0.13
(1,1465)	1:250:A:LEU:HD13	1:251:A:HIS:H	2	0.13
(1,1465)	1:250:A:LEU:HD21	1:251:A:HIS:H	2	0.13
(1,1465)	1:250:A:LEU:HD22	1:251:A:HIS:H	2	0.13
(1,1465)	1:250:A:LEU:HD23	1:251:A:HIS:H	2	0.13
(1,1307)	1:250:A:LEU:HG	1:251:A:HIS:HA	18	0.13
(1,1001)	1:250:A:LEU:HD21	1:251:A:HIS:H	12	0.13
(1,1001)	1:250:A:LEU:HD22	1:251:A:HIS:H	12	0.13
(1,1001)	1:250:A:LEU:HD23	1:251:A:HIS:H	12	0.13
(1,567)	1:249:A:LEU:HA	1:251:A:HIS:H	4	0.13
(1,88)	1:277:A:CYS:H	1:277:A:CYS:HB2	12	0.13
(1,2026)	1:335:A:LYS:HB2	1:345:A:LYS:HD2	5	0.12

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

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1465)	1:250:A:LEU:HD22	1:251:A:HIS:H	19	0.11
(1,1465)	1:250:A:LEU:HD23	1:251:A:HIS:H	19	0.11
(1,1465)	1:250:A:LEU:HD11	1:251:A:HIS:H	20	0.11
(1,1465)	1:250:A:LEU:HD12	1:251:A:HIS:H	20	0.11
(1,1465)	1:250:A:LEU:HD13	1:251:A:HIS:H	20	0.11
(1,1465)	1:250:A:LEU:HD21	1:251:A:HIS:H	20	0.11
(1,1465)	1:250:A:LEU:HD22	1:251:A:HIS:H	20	0.11
(1,1465)	1:250:A:LEU:HD23	1:251:A:HIS:H	20	0.11
(1,1380)	1:298:A:ILE:HA	1:303:A:GLN:H	14	0.11
(1,1307)	1:250:A:LEU:HG	1:251:A:HIS:HA	10	0.11
(1,1224)	1:273:A:ILE:HB	1:275:A:GLY:HA3	18	0.11
(1,1215)	1:274:A:PRO:HB2	1:275:A:GLY:HA2	9	0.11
(1,1118)	1:316:A:LEU:HB3	1:321:A:MET:HB2	11	0.11
(1,1001)	1:250:A:LEU:HD21	1:251:A:HIS:H	2	0.11
(1,1001)	1:250:A:LEU:HD22	1:251:A:HIS:H	2	0.11
(1,1001)	1:250:A:LEU:HD23	1:251:A:HIS:H	2	0.11
(1,1001)	1:250:A:LEU:HD21	1:251:A:HIS:H	11	0.11
(1,1001)	1:250:A:LEU:HD22	1:251:A:HIS:H	11	0.11
(1,1001)	1:250:A:LEU:HD23	1:251:A:HIS:H	11	0.11
(1,524)	1:316:A:LEU:HB3	1:321:A:MET:H	1	0.11
(1,1465)	1:250:A:LEU:HD11	1:251:A:HIS:H	4	0.1
(1,1465)	1:250:A:LEU:HD12	1:251:A:HIS:H	4	0.1
(1,1465)	1:250:A:LEU:HD13	1:251:A:HIS:H	4	0.1
(1,1465)	1:250:A:LEU:HD21	1:251:A:HIS:H	4	0.1
(1,1465)	1:250:A:LEU:HD22	1:251:A:HIS:H	4	0.1
(1,1465)	1:250:A:LEU:HD23	1:251:A:HIS:H	4	0.1
(1,1465)	1:250:A:LEU:HD11	1:251:A:HIS:H	16	0.1
(1,1465)	1:250:A:LEU:HD12	1:251:A:HIS:H	16	0.1
(1,1465)	1:250:A:LEU:HD13	1:251:A:HIS:H	16	0.1
(1,1465)	1:250:A:LEU:HD21	1:251:A:HIS:H	16	0.1
(1,1465)	1:250:A:LEU:HD22	1:251:A:HIS:H	16	0.1
(1,1465)	1:250:A:LEU:HD23	1:251:A:HIS:H	16	0.1
(1,1380)	1:298:A:ILE:HA	1:303:A:GLN:H	15	0.1
(1,1307)	1:250:A:LEU:HG	1:251:A:HIS:HA	9	0.1
(1,1307)	1:250:A:LEU:HG	1:251:A:HIS:HA	13	0.1
(1,1291)	1:275:A:GLY:HA3	1:276:A:ASN:HA	2	0.1
(1,1221)	1:273:A:ILE:HG21	1:275:A:GLY:HA3	2	0.1
(1,1221)	1:273:A:ILE:HG22	1:275:A:GLY:HA3	2	0.1
(1,1221)	1:273:A:ILE:HG23	1:275:A:GLY:HA3	2	0.1
(1,1151)	1:274:A:PRO:HG3	1:325:A:ASN:HB3	15	0.1
(1,1001)	1:250:A:LEU:HD21	1:251:A:HIS:H	14	0.1
(1,1001)	1:250:A:LEU:HD22	1:251:A:HIS:H	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:250:A:LEU:HD23	1:251:A:HIS:H	14	0.1
(1,1001)	1:250:A:LEU:HD21	1:251:A:HIS:H	16	0.1
(1,1001)	1:250:A:LEU:HD22	1:251:A:HIS:H	16	0.1
(1,1001)	1:250:A:LEU:HD23	1:251:A:HIS:H	16	0.1
(1,934)	1:250:A:LEU:HA	1:344:A:LEU:HD21	2	0.1
(1,934)	1:250:A:LEU:HA	1:344:A:LEU:HD22	2	0.1
(1,934)	1:250:A:LEU:HA	1:344:A:LEU:HD23	2	0.1
(1,683)	1:321:A:MET:HG2	1:342:A:ILE:HD11	16	0.1
(1,683)	1:321:A:MET:HG2	1:342:A:ILE:HD12	16	0.1
(1,683)	1:321:A:MET:HG2	1:342:A:ILE:HD13	16	0.1
(1,340)	1:250:A:LEU:H	1:251:A:HIS:H	2	0.1
(1,340)	1:250:A:LEU:H	1:251:A:HIS:H	15	0.1
(1,340)	1:250:A:LEU:H	1:251:A:HIS:H	16	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found