



Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 12:29 AM UTC

PDB ID : 2LOU / pdb_00002lou
BMRB ID : 18225
Title : AR55 solubilised in DPC micelles
Authors : Langelaan, D.N.; Rainey, J.K.
Deposited on : 2012-01-27

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

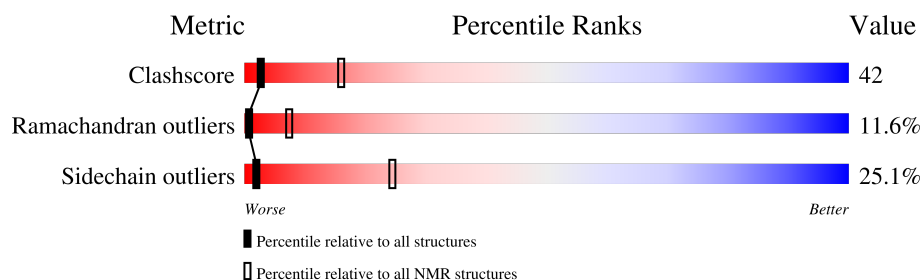
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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	64	

2 Ensemble composition and analysis ⓘ

This entry contains 40 models. Model 28 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *extended conformation*.

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:5-A:29 (25)	3.86	15
2	A:30-A:56 (27)	2.75	28

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 6 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 12, 14, 18, 22, 23, 30, 32, 34, 39, 40
2	2, 8, 10, 11, 13, 21, 28, 33, 37
3	3, 4, 7, 24, 27, 35, 36, 38
4	16, 19, 20, 25, 29, 31
5	6, 15, 17, 26
6	5, 9

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 988 atoms, of which 472 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apelin receptor.

Mol	Chain	Residues	Atoms						Trace
1	A	64	Total	C	H	N	O	S	0
			988	329	472	88	96	3	

There are 9 discrepancies between the modelled and reference sequences:

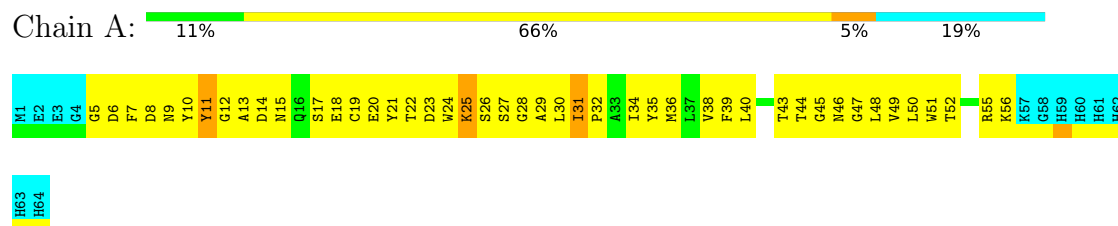
Chain	Residue	Modelled	Actual	Comment	Reference
A	56	LYS	-	expression tag	UNP P35414
A	57	LYS	-	expression tag	UNP P35414
A	58	GLY	-	expression tag	UNP P35414
A	59	HIS	-	expression tag	UNP P35414
A	60	HIS	-	expression tag	UNP P35414
A	61	HIS	-	expression tag	UNP P35414
A	62	HIS	-	expression tag	UNP P35414
A	63	HIS	-	expression tag	UNP P35414
A	64	HIS	-	expression tag	UNP P35414

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: Apelin receptor

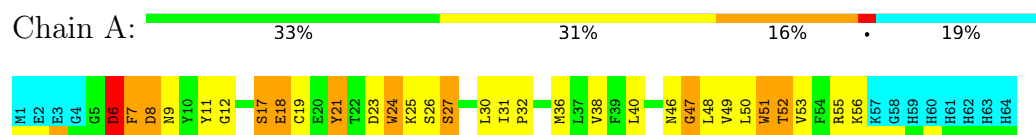


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

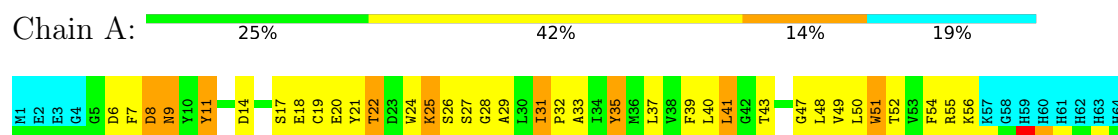
4.2.1 Score per residue for model 1

- Molecule 1: Apelin receptor



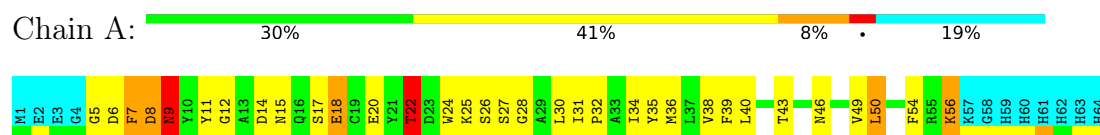
4.2.2 Score per residue for model 2

- Molecule 1: Apelin receptor



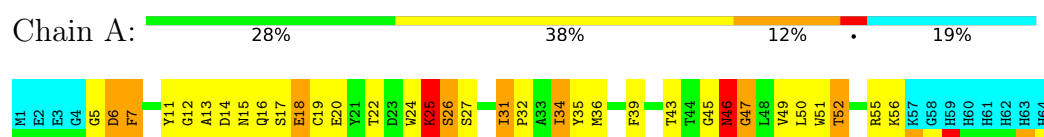
4.2.3 Score per residue for model 3

- Molecule 1: Apelin receptor



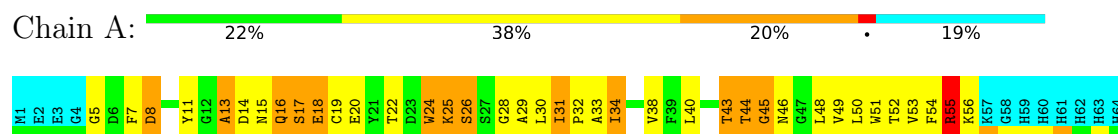
4.2.4 Score per residue for model 4

- Molecule 1: Apelin receptor



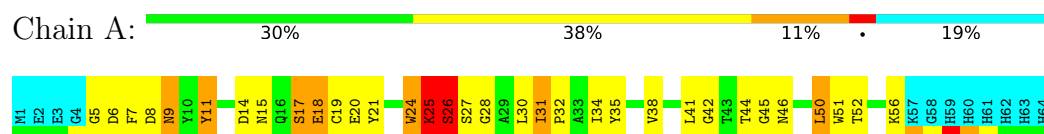
4.2.5 Score per residue for model 5

- Molecule 1: Apelin receptor



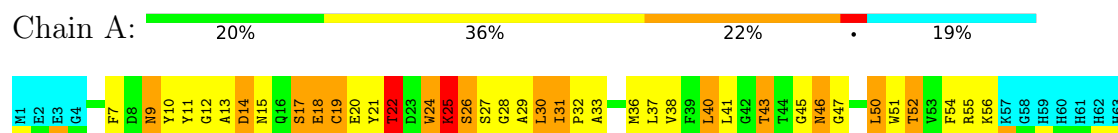
4.2.6 Score per residue for model 6

- Molecule 1: Apelin receptor



4.2.7 Score per residue for model 7

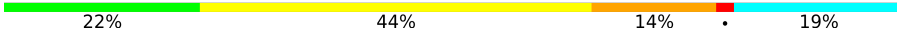
- Molecule 1: Apelin receptor

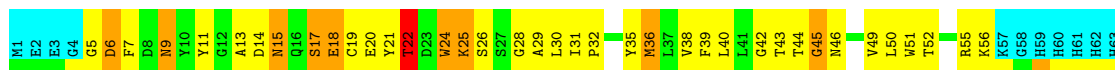


H64

4.2.8 Score per residue for model 8

- Molecule 1: Apelin receptor

Chain A:  22% 44% 14% • 19%



H64

4.2.9 Score per residue for model 9

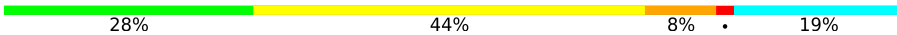
- Molecule 1: Apelin receptor

Chain A:  27% 36% 16% • 19%



4.2.10 Score per residue for model 10

- Molecule 1: Apelin receptor

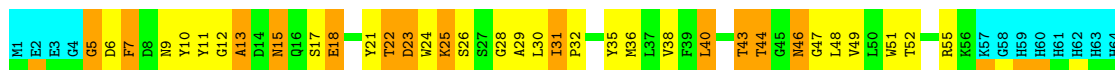
Chain A:  28% 44% 8% • 19%



4.2.11 Score per residue for model 11

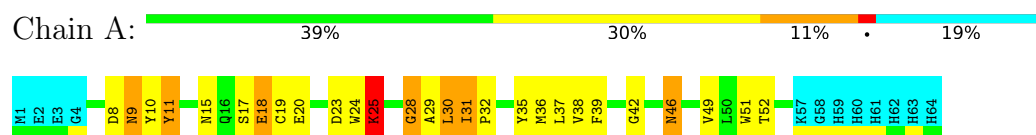
- Molecule 1: Apelin receptor

Chain A:  27% 34% 20% 19%



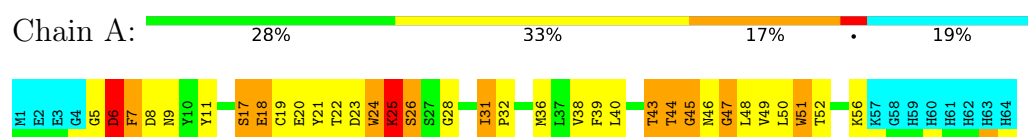
4.2.12 Score per residue for model 12

- Molecule 1: Apelin receptor



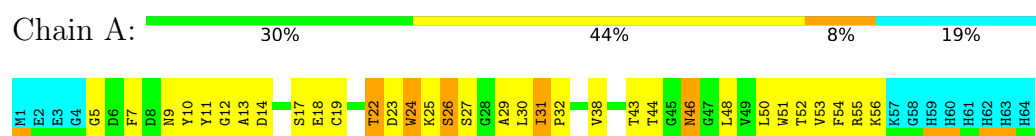
4.2.13 Score per residue for model 13

- Molecule 1: Apelin receptor



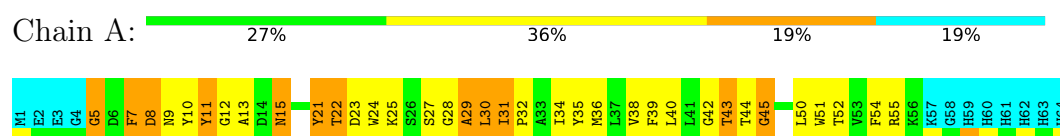
4.2.14 Score per residue for model 14

- Molecule 1: Apelin receptor



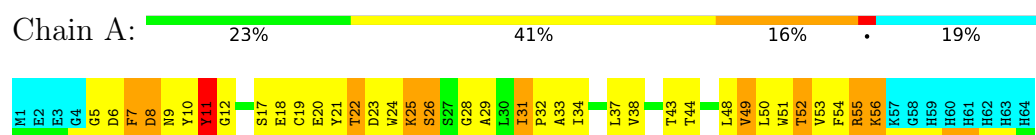
4.2.15 Score per residue for model 15

- Molecule 1: Apelin receptor



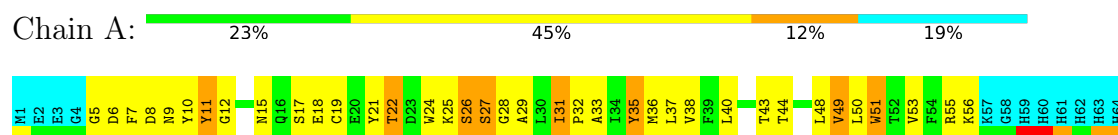
4.2.16 Score per residue for model 16

- Molecule 1: Apelin receptor



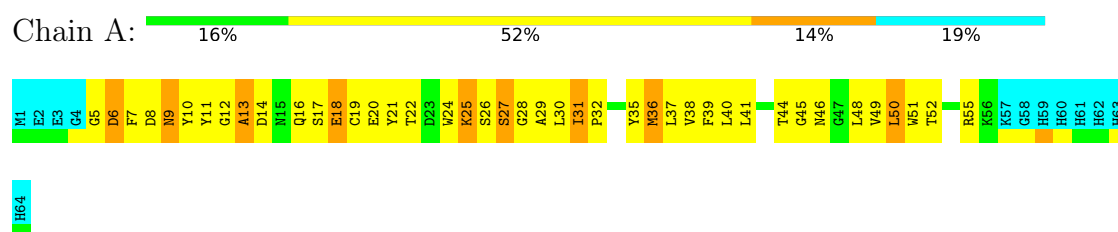
4.2.17 Score per residue for model 17

- Molecule 1: Apelin receptor



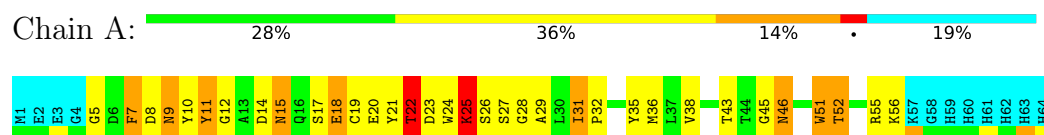
4.2.18 Score per residue for model 18

- Molecule 1: Apelin receptor



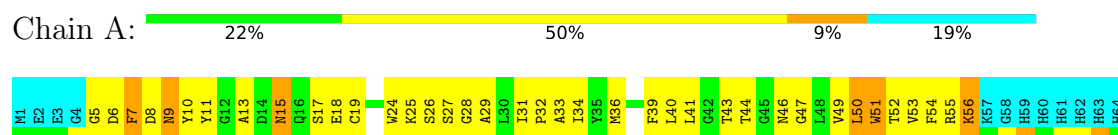
4.2.19 Score per residue for model 19

- Molecule 1: Apelin receptor



4.2.20 Score per residue for model 20

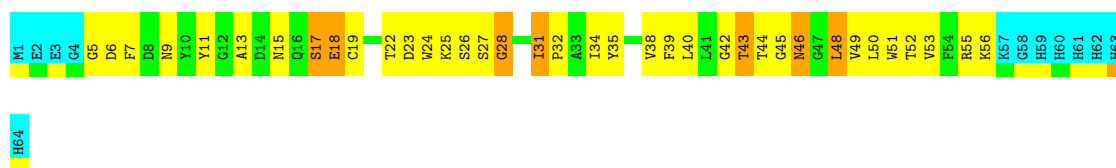
- Molecule 1: Apelin receptor



4.2.21 Score per residue for model 21

- Molecule 1: Apelin receptor

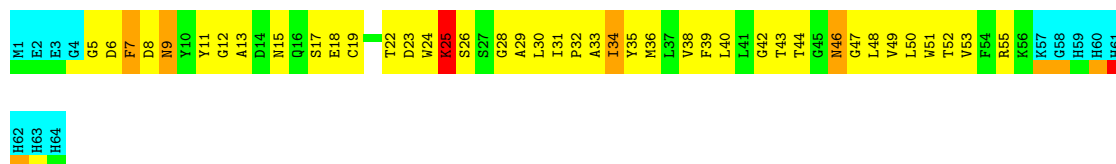




4.2.22 Score per residue for model 22

- Molecule 1: Apelin receptor

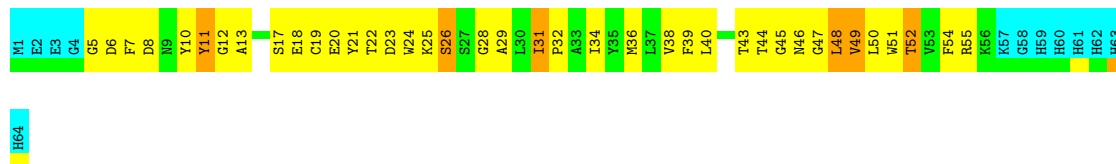
Chain A: 17% 56% 6% 19%



4.2.23 Score per residue for model 23

- Molecule 1: Apelin receptor

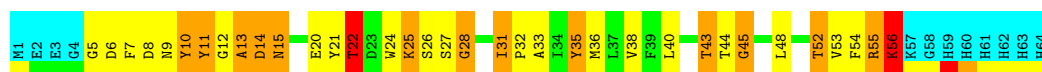
Chain A: 20% 52% 9% 19%



4.2.24 Score per residue for model 24

- Molecule 1: Apelin receptor

Chain A: 27% 31% 20% 19%



4.2.25 Score per residue for model 25

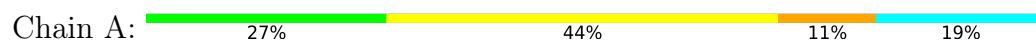
- Molecule 1: Apelin receptor

Chain A: 25% 36% 17% 19%



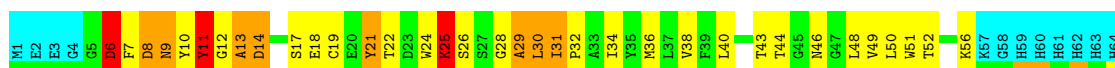
4.2.26 Score per residue for model 26

- Molecule 1: Apelin receptor



4.2.27 Score per residue for model 27

- Molecule 1: Apelin receptor



4.2.28 Score per residue for model 28 (medoid)

- Molecule 1: Apelin receptor



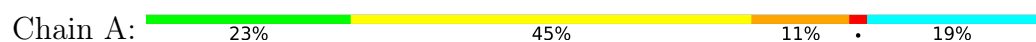
4.2.29 Score per residue for model 29

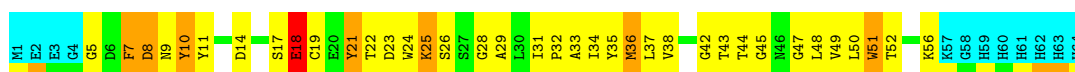
- Molecule 1: Apelin receptor



4.2.30 Score per residue for model 30

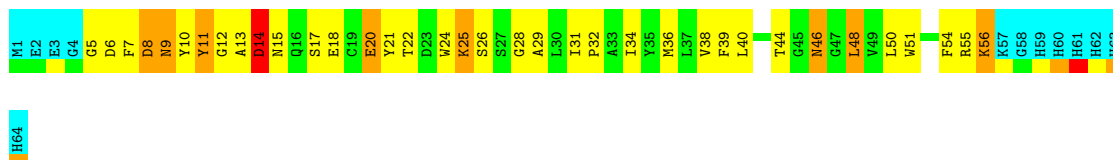
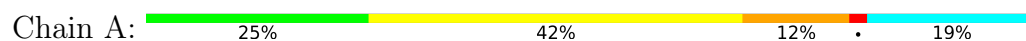
- Molecule 1: Apelin receptor





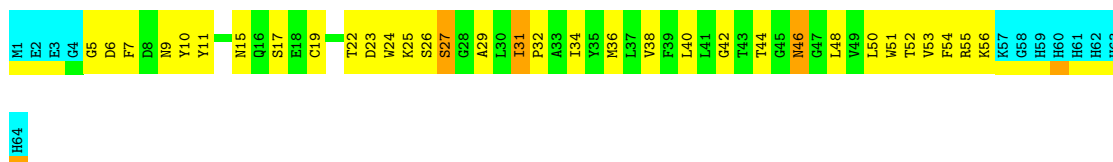
4.2.31 Score per residue for model 31

- Molecule 1: Apelin receptor



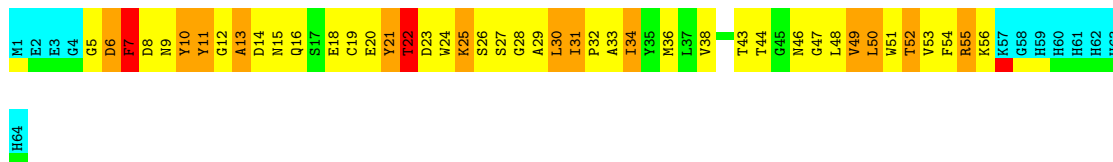
4.2.32 Score per residue for model 32

- Molecule 1: Apelin receptor



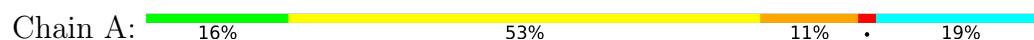
4.2.33 Score per residue for model 33

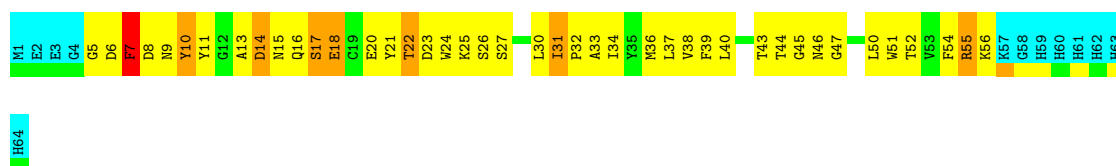
- Molecule 1: Apelin receptor



4.2.34 Score per residue for model 34

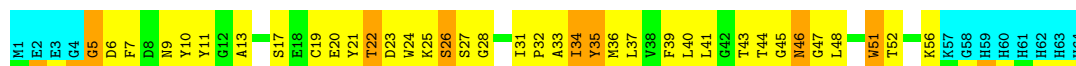
- Molecule 1: Apelin receptor





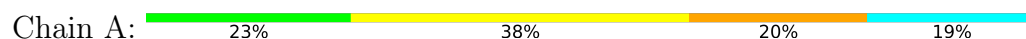
4.2.35 Score per residue for model 35

- Molecule 1: Apelin receptor



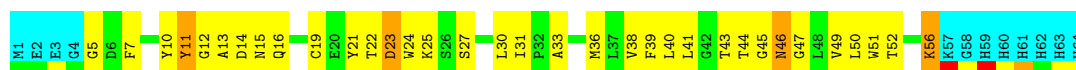
4.2.36 Score per residue for model 36

- Molecule 1: Apelin receptor



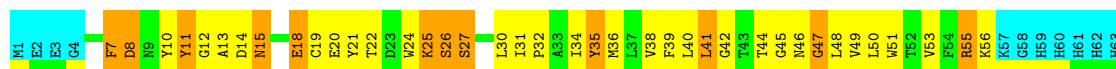
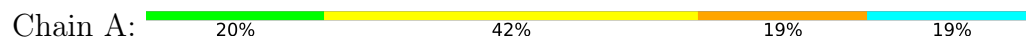
4.2.37 Score per residue for model 37

- Molecule 1: Apelin receptor



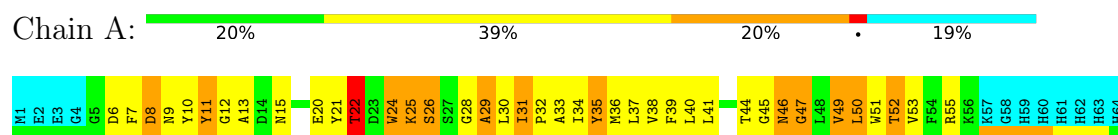
4.2.38 Score per residue for model 38

- Molecule 1: Apelin receptor



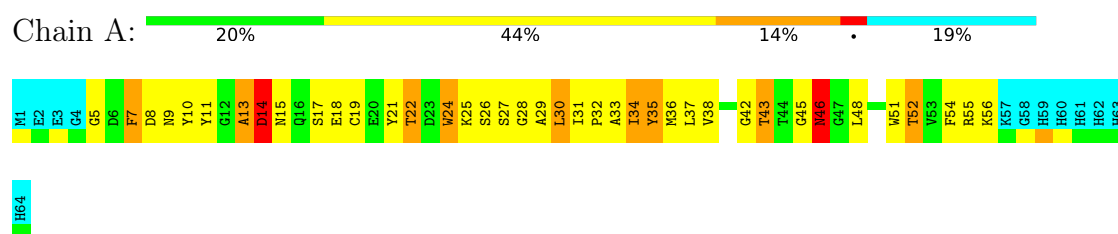
4.2.39 Score per residue for model 39

- Molecule 1: Apelin receptor



4.2.40 Score per residue for model 40

- Molecule 1: Apelin receptor



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 40 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
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	755
Number of shifts mapped to atoms	755
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	412	388	388	33±7
All	All	16480	15520	15520	1329

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 42.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:HD22	1:A:48:LEU:N	0.79	1.92	21	3
1:A:30:LEU:N	1:A:30:LEU:HD23	0.77	1.95	28	9
1:A:34:ILE:N	1:A:34:ILE:HD13	0.71	2.00	28	1
1:A:50:LEU:H	1:A:50:LEU:HD12	0.67	1.49	36	1
1:A:49:VAL:HG22	1:A:49:VAL:O	0.67	1.89	17	8
1:A:38:VAL:HG12	1:A:38:VAL:O	0.66	1.91	19	13
1:A:50:LEU:HD12	1:A:50:LEU:N	0.66	2.04	36	1
1:A:24:TRP:H	1:A:24:TRP:CD1	0.65	2.10	23	3
1:A:49:VAL:HG12	1:A:49:VAL:O	0.64	1.92	13	7
1:A:31:ILE:N	1:A:32:PRO:CD	0.63	2.61	8	38
1:A:33:ALA:O	1:A:37:LEU:HD12	0.63	1.93	39	6
1:A:31:ILE:HD13	1:A:31:ILE:N	0.63	2.08	18	5
1:A:24:TRP:CG	1:A:25:LYS:N	0.63	2.67	22	21
1:A:44:THR:HG23	1:A:48:LEU:HD12	0.62	1.71	32	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:TRP:CG	1:A:52:THR:N	0.62	2.67	13	26
1:A:11:TYR:CG	1:A:12:GLY:N	0.62	2.68	38	5
1:A:46:ASN:ND2	1:A:47:GLY:N	0.62	2.48	11	2
1:A:9:ASN:ND2	1:A:10:TYR:CE2	0.61	2.68	11	2
1:A:34:ILE:O	1:A:38:VAL:HG23	0.61	1.94	9	9
1:A:7:PHE:CG	1:A:8:ASP:N	0.61	2.68	38	3
1:A:53:VAL:HG12	1:A:53:VAL:O	0.61	1.94	1	2
1:A:21:TYR:CD1	1:A:21:TYR:N	0.61	2.68	33	2
1:A:51:TRP:NE1	1:A:55:ARG:NH1	0.61	2.48	18	2
1:A:11:TYR:CD1	1:A:12:GLY:N	0.60	2.68	16	4
1:A:28:GLY:O	1:A:29:ALA:HB3	0.60	1.97	8	23
1:A:51:TRP:HE1	1:A:55:ARG:NH2	0.60	1.95	15	2
1:A:31:ILE:N	1:A:31:ILE:HD13	0.60	2.11	15	3
1:A:35:TYR:CD1	1:A:36:MET:N	0.60	2.70	35	5
1:A:48:LEU:N	1:A:48:LEU:CD2	0.60	2.65	21	11
1:A:54:PHE:CD2	1:A:55:ARG:N	0.60	2.70	29	1
1:A:10:TYR:CB	1:A:13:ALA:HB3	0.59	2.26	35	1
1:A:24:TRP:CD1	1:A:25:LYS:N	0.59	2.69	6	4
1:A:24:TRP:CG	1:A:25:LYS:H	0.59	2.16	9	15
1:A:51:TRP:HE1	1:A:55:ARG:NE	0.58	1.95	4	3
1:A:9:ASN:ND2	1:A:10:TYR:CD2	0.58	2.71	15	1
1:A:30:LEU:HD23	1:A:30:LEU:H	0.58	1.56	15	9
1:A:51:TRP:NE1	1:A:55:ARG:NH2	0.58	2.51	15	1
1:A:27:SER:H	1:A:31:ILE:HD13	0.57	1.57	19	1
1:A:24:TRP:CD1	1:A:24:TRP:N	0.57	2.73	23	5
1:A:24:TRP:CD1	1:A:25:LYS:H	0.57	2.16	24	6
1:A:9:ASN:HD21	1:A:16:GLN:NE2	0.57	1.97	18	1
1:A:30:LEU:N	1:A:30:LEU:CD2	0.57	2.67	27	9
1:A:7:PHE:N	1:A:7:PHE:CD1	0.57	2.68	11	4
1:A:47:GLY:O	1:A:49:VAL:HG12	0.56	1.99	39	1
1:A:24:TRP:CG	1:A:24:TRP:O	0.56	2.58	37	2
1:A:34:ILE:H	1:A:34:ILE:CD1	0.56	2.13	28	1
1:A:51:TRP:HE1	1:A:55:ARG:NH1	0.56	1.99	38	2
1:A:11:TYR:CD2	1:A:12:GLY:N	0.56	2.73	10	6
1:A:11:TYR:O	1:A:13:ALA:N	0.56	2.39	39	2
1:A:55:ARG:N	1:A:55:ARG:CD	0.56	2.69	16	6
1:A:24:TRP:N	1:A:24:TRP:CD1	0.55	2.74	28	4
1:A:34:ILE:HD13	1:A:34:ILE:H	0.55	1.60	28	1
1:A:48:LEU:O	1:A:50:LEU:N	0.55	2.40	17	4
1:A:10:TYR:HB2	1:A:13:ALA:HB3	0.55	1.78	35	1
1:A:51:TRP:NE1	1:A:55:ARG:CZ	0.54	2.70	40	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:PHE:CD2	1:A:8:ASP:N	0.54	2.75	38	2
1:A:21:TYR:CE2	1:A:25:LYS:NZ	0.54	2.75	37	1
1:A:7:PHE:O	1:A:7:PHE:CG	0.53	2.60	1	3
1:A:24:TRP:O	1:A:26:SER:N	0.53	2.41	27	9
1:A:45:GLY:O	1:A:47:GLY:N	0.53	2.41	35	2
1:A:16:GLN:H	1:A:16:GLN:CD	0.53	2.11	5	1
1:A:43:THR:HG23	1:A:44:THR:N	0.53	2.18	26	11
1:A:55:ARG:CD	1:A:55:ARG:H	0.53	2.14	16	1
1:A:12:GLY:O	1:A:14:ASP:N	0.53	2.42	36	7
1:A:51:TRP:CD1	1:A:51:TRP:C	0.53	2.86	10	8
1:A:46:ASN:ND2	1:A:47:GLY:H	0.53	2.01	11	1
1:A:47:GLY:O	1:A:49:VAL:N	0.53	2.42	33	3
1:A:48:LEU:C	1:A:50:LEU:N	0.53	2.67	17	7
1:A:13:ALA:C	1:A:15:ASN:N	0.53	2.66	5	18
1:A:5:GLY:O	1:A:7:PHE:CG	0.53	2.62	20	1
1:A:50:LEU:O	1:A:54:PHE:CD1	0.53	2.62	34	2
1:A:19:CYS:O	1:A:21:TYR:CD2	0.53	2.62	35	6
1:A:32:PRO:O	1:A:36:MET:N	0.53	2.42	34	1
1:A:10:TYR:O	1:A:12:GLY:N	0.53	2.42	27	9
1:A:54:PHE:O	1:A:54:PHE:CG	0.53	2.62	33	2
1:A:51:TRP:CD1	1:A:51:TRP:O	0.53	2.62	30	3
1:A:17:SER:O	1:A:19:CYS:N	0.52	2.43	17	18
1:A:24:TRP:CD2	1:A:24:TRP:O	0.52	2.62	30	6
1:A:37:LEU:O	1:A:41:LEU:N	0.52	2.42	2	1
1:A:20:GLU:O	1:A:24:TRP:CD1	0.52	2.62	31	8
1:A:52:THR:O	1:A:55:ARG:N	0.52	2.43	14	4
1:A:43:THR:O	1:A:47:GLY:N	0.52	2.43	11	3
1:A:9:ASN:O	1:A:10:TYR:CG	0.52	2.62	31	3
1:A:51:TRP:HE1	1:A:55:ARG:CZ	0.52	2.17	18	4
1:A:24:TRP:O	1:A:24:TRP:CE3	0.52	2.63	25	5
1:A:5:GLY:O	1:A:7:PHE:CD1	0.52	2.62	20	1
1:A:39:PHE:CD1	1:A:39:PHE:O	0.52	2.62	18	10
1:A:20:GLU:O	1:A:24:TRP:NE1	0.52	2.42	23	10
1:A:21:TYR:CD2	1:A:21:TYR:O	0.52	2.63	11	5
1:A:38:VAL:O	1:A:42:GLY:N	0.52	2.43	6	6
1:A:47:GLY:C	1:A:49:VAL:N	0.52	2.65	23	3
1:A:22:THR:O	1:A:24:TRP:N	0.52	2.43	23	5
1:A:21:TYR:O	1:A:21:TYR:CG	0.52	2.63	15	6
1:A:5:GLY:C	1:A:7:PHE:N	0.52	2.68	20	21
1:A:5:GLY:O	1:A:7:PHE:N	0.52	2.43	34	10
1:A:24:TRP:O	1:A:24:TRP:CG	0.52	2.63	32	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:PHE:O	1:A:54:PHE:CD2	0.52	2.63	5	1
1:A:10:TYR:O	1:A:13:ALA:N	0.52	2.42	18	1
1:A:9:ASN:O	1:A:11:TYR:N	0.52	2.42	34	15
1:A:22:THR:C	1:A:24:TRP:N	0.52	2.67	37	7
1:A:7:PHE:O	1:A:9:ASN:N	0.52	2.43	27	5
1:A:44:THR:O	1:A:44:THR:HG22	0.52	2.04	24	9
1:A:19:CYS:O	1:A:21:TYR:CE1	0.52	2.63	7	1
1:A:46:ASN:O	1:A:48:LEU:N	0.52	2.42	1	3
1:A:51:TRP:C	1:A:51:TRP:CD1	0.52	2.85	33	5
1:A:46:ASN:ND2	1:A:46:ASN:O	0.52	2.43	18	4
1:A:9:ASN:O	1:A:10:TYR:CD1	0.52	2.62	31	2
1:A:8:ASP:OD1	1:A:8:ASP:N	0.52	2.42	5	3
1:A:7:PHE:CD2	1:A:7:PHE:O	0.52	2.63	7	1
1:A:9:ASN:C	1:A:10:TYR:CG	0.52	2.88	17	14
1:A:52:THR:HG23	1:A:53:VAL:N	0.52	2.20	20	1
1:A:21:TYR:CD2	1:A:25:LYS:NZ	0.52	2.78	37	1
1:A:46:ASN:C	1:A:46:ASN:HD22	0.52	2.12	7	2
1:A:19:CYS:O	1:A:21:TYR:CZ	0.52	2.63	7	1
1:A:35:TYR:CD1	1:A:35:TYR:O	0.52	2.63	8	1
1:A:44:THR:C	1:A:46:ASN:N	0.52	2.67	38	4
1:A:45:GLY:O	1:A:46:ASN:ND2	0.52	2.42	23	2
1:A:11:TYR:CZ	1:A:16:GLN:OE1	0.52	2.63	37	1
1:A:43:THR:C	1:A:45:GLY:N	0.51	2.68	13	10
1:A:51:TRP:NE1	1:A:55:ARG:NE	0.51	2.58	4	3
1:A:51:TRP:C	1:A:53:VAL:N	0.51	2.68	16	5
1:A:7:PHE:CG	1:A:7:PHE:O	0.51	2.62	31	2
1:A:48:LEU:N	1:A:48:LEU:HD22	0.51	2.20	23	7
1:A:51:TRP:CZ3	1:A:52:THR:OG1	0.51	2.63	16	1
1:A:39:PHE:CD1	1:A:39:PHE:C	0.51	2.88	36	7
1:A:19:CYS:O	1:A:21:TYR:CE2	0.51	2.62	17	2
1:A:54:PHE:C	1:A:56:LYS:N	0.51	2.67	20	2
1:A:8:ASP:O	1:A:10:TYR:CE1	0.51	2.63	16	1
1:A:33:ALA:O	1:A:36:MET:N	0.51	2.43	22	3
1:A:26:SER:OG	1:A:27:SER:N	0.51	2.42	32	2
1:A:52:THR:OG1	1:A:56:LYS:NZ	0.51	2.43	1	1
1:A:45:GLY:C	1:A:47:GLY:N	0.51	2.68	4	1
1:A:7:PHE:C	1:A:7:PHE:CD1	0.51	2.88	14	1
1:A:9:ASN:ND2	1:A:16:GLN:NE2	0.51	2.58	18	1
1:A:33:ALA:C	1:A:35:TYR:N	0.51	2.68	22	2
1:A:9:ASN:C	1:A:9:ASN:ND2	0.51	2.68	22	3
1:A:16:GLN:CD	1:A:16:GLN:N	0.51	2.68	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ASN:C	1:A:46:ASN:ND2	0.51	2.68	7	1
1:A:51:TRP:NE1	1:A:55:ARG:HE	0.51	2.04	7	2
1:A:33:ALA:O	1:A:35:TYR:N	0.51	2.43	22	2
1:A:7:PHE:O	1:A:7:PHE:CD1	0.50	2.65	1	2
1:A:51:TRP:CD2	1:A:52:THR:N	0.50	2.80	2	6
1:A:46:ASN:CG	1:A:47:GLY:N	0.50	2.68	11	3
1:A:6:ASP:C	1:A:7:PHE:CG	0.50	2.88	11	3
1:A:6:ASP:O	1:A:8:ASP:N	0.50	2.43	27	2
1:A:31:ILE:N	1:A:31:ILE:CD1	0.50	2.73	18	7
1:A:21:TYR:O	1:A:24:TRP:CD1	0.50	2.65	28	1
1:A:9:ASN:ND2	1:A:9:ASN:C	0.50	2.70	18	2
1:A:21:TYR:C	1:A:22:THR:HG22	0.50	2.32	19	4
1:A:8:ASP:C	1:A:10:TYR:N	0.50	2.67	31	1
1:A:7:PHE:C	1:A:9:ASN:N	0.50	2.69	13	2
1:A:36:MET:C	1:A:36:MET:SD	0.50	2.95	30	2
1:A:21:TYR:N	1:A:23:ASP:OD2	0.50	2.44	35	1
1:A:32:PRO:O	1:A:36:MET:SD	0.49	2.70	27	3
1:A:12:GLY:O	1:A:13:ALA:HB3	0.49	2.06	15	2
1:A:34:ILE:HD12	1:A:34:ILE:N	0.49	2.22	6	1
1:A:9:ASN:OD1	1:A:10:TYR:N	0.49	2.45	40	1
1:A:21:TYR:O	1:A:21:TYR:CD2	0.49	2.64	30	2
1:A:19:CYS:SG	1:A:21:TYR:CD1	0.49	3.04	6	1
1:A:28:GLY:O	1:A:29:ALA:CB	0.49	2.61	39	20
1:A:7:PHE:CD1	1:A:7:PHE:C	0.49	2.88	4	2
1:A:51:TRP:HE1	1:A:55:ARG:HH21	0.49	1.48	32	1
1:A:6:ASP:C	1:A:8:ASP:H	0.49	2.14	25	2
1:A:46:ASN:C	1:A:48:LEU:N	0.49	2.68	1	2
1:A:35:TYR:O	1:A:35:TYR:CG	0.49	2.65	40	2
1:A:35:TYR:O	1:A:39:PHE:N	0.49	2.45	21	2
1:A:29:ALA:C	1:A:30:LEU:HD22	0.49	2.32	22	1
1:A:19:CYS:O	1:A:21:TYR:CD1	0.49	2.66	7	1
1:A:35:TYR:C	1:A:35:TYR:CD1	0.49	2.90	19	1
1:A:39:PHE:CG	1:A:40:LEU:N	0.49	2.80	38	1
1:A:35:TYR:CD1	1:A:35:TYR:C	0.48	2.88	17	6
1:A:19:CYS:SG	1:A:19:CYS:O	0.48	2.71	38	1
1:A:24:TRP:C	1:A:26:SER:N	0.48	2.68	13	3
1:A:21:TYR:CA	1:A:24:TRP:HE1	0.48	2.22	23	1
1:A:6:ASP:C	1:A:8:ASP:N	0.48	2.70	17	4
1:A:23:ASP:OD1	1:A:23:ASP:N	0.48	2.43	13	1
1:A:18:GLU:N	1:A:18:GLU:CD	0.48	2.71	38	1
1:A:51:TRP:CD1	1:A:55:ARG:HE	0.48	2.27	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:TYR:CD1	1:A:10:TYR:N	0.48	2.80	19	6
1:A:17:SER:OG	1:A:18:GLU:N	0.48	2.47	30	1
1:A:21:TYR:C	1:A:21:TYR:CD1	0.48	2.88	27	2
1:A:49:VAL:O	1:A:49:VAL:CG2	0.48	2.62	20	4
1:A:20:GLU:C	1:A:21:TYR:CD1	0.48	2.92	39	3
1:A:13:ALA:O	1:A:15:ASN:N	0.48	2.47	37	7
1:A:49:VAL:O	1:A:49:VAL:CG1	0.48	2.62	13	7
1:A:48:LEU:C	1:A:50:LEU:H	0.48	2.17	30	9
1:A:10:TYR:O	1:A:11:TYR:CB	0.48	2.62	9	7
1:A:6:ASP:O	1:A:7:PHE:CG	0.48	2.66	13	1
1:A:38:VAL:O	1:A:38:VAL:CG1	0.47	2.62	19	7
1:A:24:TRP:CD2	1:A:24:TRP:C	0.47	2.92	34	3
1:A:44:THR:O	1:A:46:ASN:N	0.47	2.48	38	2
1:A:5:GLY:O	1:A:7:PHE:CD2	0.47	2.68	20	1
1:A:17:SER:O	1:A:18:GLU:C	0.47	2.58	34	11
1:A:19:CYS:SG	1:A:20:GLU:N	0.47	2.87	4	4
1:A:25:LYS:O	1:A:26:SER:CB	0.47	2.62	23	7
1:A:8:ASP:O	1:A:10:TYR:CD1	0.47	2.68	16	1
1:A:51:TRP:O	1:A:54:PHE:N	0.47	2.48	32	3
1:A:9:ASN:C	1:A:11:TYR:H	0.47	2.17	36	7
1:A:34:ILE:O	1:A:38:VAL:CG2	0.47	2.62	27	10
1:A:20:GLU:O	1:A:22:THR:N	0.47	2.47	16	2
1:A:45:GLY:C	1:A:46:ASN:HD22	0.47	2.17	10	1
1:A:54:PHE:O	1:A:56:LYS:N	0.47	2.48	20	1
1:A:24:TRP:CD2	1:A:25:LYS:N	0.47	2.82	14	6
1:A:43:THR:C	1:A:45:GLY:H	0.47	2.17	24	6
1:A:44:THR:C	1:A:46:ASN:H	0.47	2.18	38	1
1:A:5:GLY:O	1:A:7:PHE:CE1	0.47	2.68	20	1
1:A:7:PHE:O	1:A:7:PHE:CD2	0.47	2.68	30	1
1:A:14:ASP:C	1:A:16:GLN:N	0.47	2.72	34	1
1:A:51:TRP:O	1:A:53:VAL:N	0.47	2.48	16	2
1:A:8:ASP:O	1:A:10:TYR:N	0.47	2.48	31	1
1:A:33:ALA:O	1:A:37:LEU:CD1	0.46	2.63	39	4
1:A:47:GLY:C	1:A:49:VAL:H	0.46	2.17	38	3
1:A:40:LEU:O	1:A:45:GLY:N	0.46	2.48	38	1
1:A:53:VAL:O	1:A:53:VAL:CG1	0.46	2.63	1	1
1:A:18:GLU:O	1:A:18:GLU:CG	0.46	2.63	33	3
1:A:26:SER:O	1:A:27:SER:CB	0.46	2.63	34	5
1:A:5:GLY:C	1:A:7:PHE:H	0.46	2.19	20	19
1:A:11:TYR:CD1	1:A:11:TYR:C	0.46	2.91	26	2
1:A:31:ILE:C	1:A:33:ALA:N	0.46	2.73	37	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:ASN:C	1:A:9:ASN:HD22	0.46	2.18	10	2
1:A:35:TYR:C	1:A:37:LEU:N	0.46	2.72	30	2
1:A:21:TYR:C	1:A:24:TRP:HE1	0.46	2.19	18	3
1:A:14:ASP:C	1:A:16:GLN:H	0.46	2.19	34	1
1:A:50:LEU:HD12	1:A:50:LEU:C	0.46	2.36	39	7
1:A:31:ILE:HD12	1:A:31:ILE:N	0.46	2.25	36	1
1:A:10:TYR:O	1:A:11:TYR:C	0.46	2.59	18	1
1:A:52:THR:HG22	1:A:52:THR:O	0.46	2.11	22	1
1:A:54:PHE:C	1:A:56:LYS:H	0.46	2.19	20	2
1:A:27:SER:OG	1:A:28:GLY:N	0.46	2.48	25	1
1:A:52:THR:C	1:A:54:PHE:N	0.46	2.73	24	4
1:A:22:THR:H	1:A:24:TRP:HE1	0.46	1.54	35	1
1:A:43:THR:CG2	1:A:44:THR:N	0.45	2.79	37	9
1:A:20:GLU:C	1:A:24:TRP:HE1	0.45	2.19	23	1
1:A:36:MET:C	1:A:38:VAL:N	0.45	2.74	15	2
1:A:22:THR:N	1:A:24:TRP:HE1	0.45	2.09	40	1
1:A:24:TRP:O	1:A:24:TRP:CD2	0.45	2.70	4	4
1:A:11:TYR:C	1:A:13:ALA:N	0.45	2.73	26	3
1:A:30:LEU:O	1:A:33:ALA:HB3	0.45	2.09	37	1
1:A:41:LEU:HD21	1:A:48:LEU:CD1	0.45	2.42	38	1
1:A:51:TRP:C	1:A:53:VAL:H	0.45	2.19	22	2
1:A:53:VAL:C	1:A:55:ARG:N	0.45	2.74	22	2
1:A:18:GLU:CD	1:A:18:GLU:H	0.45	2.20	38	1
1:A:30:LEU:HD12	1:A:34:ILE:HD11	0.45	1.87	40	1
1:A:34:ILE:HG22	1:A:35:TYR:N	0.45	2.25	4	1
1:A:24:TRP:C	1:A:26:SER:H	0.45	2.20	20	3
1:A:22:THR:HG23	1:A:23:ASP:N	0.45	2.26	14	1
1:A:8:ASP:C	1:A:10:TYR:H	0.45	2.19	31	2
1:A:49:VAL:O	1:A:49:VAL:HG12	0.45	2.10	36	1
1:A:24:TRP:CZ3	1:A:25:LYS:O	0.45	2.70	27	1
1:A:44:THR:O	1:A:44:THR:CG2	0.45	2.64	24	9
1:A:30:LEU:H	1:A:30:LEU:HD23	0.45	1.71	38	1
1:A:36:MET:C	1:A:38:VAL:H	0.45	2.20	34	21
1:A:43:THR:O	1:A:45:GLY:N	0.45	2.50	10	3
1:A:9:ASN:C	1:A:11:TYR:N	0.45	2.74	18	2
1:A:31:ILE:C	1:A:33:ALA:H	0.45	2.20	2	5
1:A:26:SER:HB3	1:A:29:ALA:HB3	0.45	1.88	17	1
1:A:26:SER:OG	1:A:29:ALA:HB3	0.45	2.12	22	1
1:A:21:TYR:CE1	1:A:22:THR:CG2	0.45	3.00	37	1
1:A:21:TYR:C	1:A:23:ASP:H	0.45	2.20	35	1
1:A:33:ALA:C	1:A:34:ILE:HD12	0.45	2.37	39	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:THR:C	1:A:24:TRP:H	0.44	2.20	30	6
1:A:26:SER:C	1:A:28:GLY:H	0.44	2.21	30	9
1:A:7:PHE:CD1	1:A:8:ASP:N	0.44	2.85	34	2
1:A:50:LEU:HD12	1:A:51:TRP:N	0.44	2.27	39	4
1:A:35:TYR:O	1:A:35:TYR:CD2	0.44	2.70	15	1
1:A:35:TYR:O	1:A:37:LEU:N	0.44	2.51	30	1
1:A:31:ILE:O	1:A:33:ALA:N	0.44	2.49	37	1
1:A:26:SER:C	1:A:28:GLY:N	0.44	2.75	31	5
1:A:19:CYS:C	1:A:21:TYR:H	0.44	2.21	7	1
1:A:39:PHE:O	1:A:39:PHE:CG	0.44	2.68	8	1
1:A:55:ARG:HH11	1:A:55:ARG:CG	0.44	2.26	14	1
1:A:49:VAL:O	1:A:49:VAL:HG22	0.44	2.13	2	1
1:A:53:VAL:C	1:A:55:ARG:H	0.44	2.19	32	6
1:A:29:ALA:O	1:A:30:LEU:HD12	0.44	2.13	18	1
1:A:46:ASN:ND2	1:A:46:ASN:C	0.44	2.76	22	1
1:A:8:ASP:CG	1:A:9:ASN:N	0.44	2.76	3	1
1:A:13:ALA:C	1:A:15:ASN:H	0.44	2.18	5	6
1:A:44:THR:O	1:A:45:GLY:C	0.44	2.61	5	11
1:A:52:THR:C	1:A:54:PHE:H	0.44	2.21	24	1
1:A:39:PHE:O	1:A:43:THR:CG2	0.44	2.66	26	1
1:A:10:TYR:O	1:A:11:TYR:O	0.44	2.36	26	4
1:A:26:SER:HB2	1:A:29:ALA:HB3	0.44	1.90	32	1
1:A:24:TRP:O	1:A:25:LYS:C	0.43	2.61	16	25
1:A:19:CYS:O	1:A:21:TYR:CG	0.43	2.70	7	1
1:A:51:TRP:O	1:A:52:THR:C	0.43	2.61	34	4
1:A:9:ASN:N	1:A:9:ASN:OD1	0.43	2.49	21	1
1:A:46:ASN:C	1:A:48:LEU:H	0.43	2.21	5	2
1:A:40:LEU:C	1:A:40:LEU:HD12	0.43	2.38	7	1
1:A:55:ARG:CG	1:A:55:ARG:NH1	0.43	2.80	14	1
1:A:54:PHE:CG	1:A:55:ARG:N	0.43	2.80	29	1
1:A:50:LEU:C	1:A:50:LEU:CD1	0.43	2.91	26	8
1:A:45:GLY:O	1:A:46:ASN:C	0.43	2.62	21	8
1:A:50:LEU:C	1:A:50:LEU:HD12	0.43	2.38	18	1
1:A:51:TRP:CD1	1:A:55:ARG:CZ	0.43	3.01	40	1
1:A:17:SER:O	1:A:18:GLU:O	0.43	2.36	11	1
1:A:46:ASN:O	1:A:47:GLY:C	0.43	2.62	1	3
1:A:17:SER:C	1:A:19:CYS:H	0.43	2.21	26	1
1:A:11:TYR:O	1:A:12:GLY:C	0.43	2.62	33	12
1:A:7:PHE:C	1:A:9:ASN:H	0.43	2.21	21	2
1:A:45:GLY:O	1:A:46:ASN:O	0.43	2.36	40	1
1:A:12:GLY:C	1:A:14:ASP:N	0.43	2.76	29	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:THR:O	1:A:45:GLY:O	0.43	2.37	5	2
1:A:24:TRP:O	1:A:25:LYS:O	0.43	2.37	9	6
1:A:52:THR:CG2	1:A:53:VAL:N	0.43	2.81	20	1
1:A:49:VAL:O	1:A:49:VAL:HG23	0.43	2.12	21	1
1:A:6:ASP:O	1:A:6:ASP:OD1	0.43	2.37	6	2
1:A:34:ILE:N	1:A:34:ILE:CD1	0.43	2.81	6	2
1:A:19:CYS:C	1:A:21:TYR:N	0.43	2.77	7	1
1:A:7:PHE:O	1:A:8:ASP:O	0.43	2.37	16	3
1:A:25:LYS:O	1:A:26:SER:OG	0.43	2.37	16	2
1:A:47:GLY:C	1:A:48:LEU:HD22	0.43	2.39	26	1
1:A:33:ALA:O	1:A:34:ILE:C	0.43	2.62	22	5
1:A:9:ASN:O	1:A:9:ASN:CG	0.43	2.62	34	2
1:A:22:THR:O	1:A:23:ASP:C	0.43	2.62	28	3
1:A:19:CYS:O	1:A:19:CYS:SG	0.43	2.76	16	1
1:A:40:LEU:C	1:A:40:LEU:CD1	0.42	2.92	7	1
1:A:13:ALA:O	1:A:14:ASP:OD1	0.42	2.37	31	2
1:A:46:ASN:O	1:A:47:GLY:O	0.42	2.37	38	1
1:A:20:GLU:C	1:A:21:TYR:CG	0.42	2.97	34	1
1:A:50:LEU:N	1:A:50:LEU:CD1	0.42	2.69	36	1
1:A:14:ASP:O	1:A:14:ASP:CG	0.42	2.63	40	1
1:A:8:ASP:OD1	1:A:11:TYR:CD1	0.42	2.73	18	1
1:A:52:THR:O	1:A:53:VAL:C	0.42	2.62	10	1
1:A:40:LEU:O	1:A:44:THR:OG1	0.42	2.37	11	1
1:A:12:GLY:O	1:A:13:ALA:C	0.42	2.62	25	4
1:A:19:CYS:O	1:A:20:GLU:OE2	0.42	2.37	18	1
1:A:11:TYR:C	1:A:13:ALA:H	0.42	2.23	5	3
1:A:40:LEU:C	1:A:44:THR:OG1	0.42	2.63	11	1
1:A:48:LEU:O	1:A:51:TRP:N	0.42	2.49	2	1
1:A:5:GLY:O	1:A:6:ASP:C	0.42	2.63	8	4
1:A:19:CYS:O	1:A:23:ASP:OD2	0.42	2.38	33	2
1:A:7:PHE:O	1:A:8:ASP:C	0.42	2.63	16	4
1:A:40:LEU:HD12	1:A:41:LEU:N	0.42	2.30	7	1
1:A:12:GLY:O	1:A:13:ALA:O	0.42	2.37	11	1
1:A:37:LEU:O	1:A:41:LEU:O	0.42	2.37	18	2
1:A:24:TRP:CZ3	1:A:26:SER:OG	0.42	2.72	19	2
1:A:5:GLY:O	1:A:6:ASP:O	0.42	2.37	25	1
1:A:46:ASN:CG	1:A:47:GLY:H	0.42	2.22	7	1
1:A:14:ASP:O	1:A:17:SER:N	0.42	2.53	9	1
1:A:14:ASP:O	1:A:14:ASP:OD2	0.42	2.37	31	2
1:A:6:ASP:O	1:A:7:PHE:C	0.41	2.63	18	1
1:A:5:GLY:O	1:A:7:PHE:CZ	0.41	2.73	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ASN:O	1:A:46:ASN:CG	0.41	2.63	29	2
1:A:46:ASN:OD1	1:A:46:ASN:C	0.41	2.62	35	1
1:A:16:GLN:N	1:A:16:GLN:OE1	0.41	2.49	5	1
1:A:35:TYR:O	1:A:38:VAL:N	0.41	2.53	12	1
1:A:12:GLY:O	1:A:15:ASN:OD1	0.41	2.37	22	1
1:A:18:GLU:O	1:A:18:GLU:CD	0.41	2.63	6	1
1:A:14:ASP:O	1:A:15:ASN:C	0.41	2.64	19	2
1:A:26:SER:CB	1:A:29:ALA:HB3	0.41	2.44	14	1
1:A:48:LEU:HD22	1:A:48:LEU:H	0.41	1.74	23	1
1:A:51:TRP:CG	1:A:52:THR:H	0.41	2.33	34	1
1:A:19:CYS:SG	1:A:23:ASP:OD1	0.41	2.71	9	1
1:A:48:LEU:O	1:A:49:VAL:C	0.41	2.62	17	1
1:A:27:SER:OG	1:A:31:ILE:HD13	0.41	2.16	21	1
1:A:34:ILE:O	1:A:35:TYR:C	0.41	2.62	4	3
1:A:8:ASP:OD1	1:A:8:ASP:O	0.41	2.39	6	1
1:A:18:GLU:OE2	1:A:23:ASP:CG	0.41	2.63	11	1
1:A:35:TYR:O	1:A:36:MET:C	0.41	2.63	30	1
1:A:12:GLY:C	1:A:14:ASP:H	0.41	2.23	14	1
1:A:24:TRP:O	1:A:27:SER:OG	0.41	2.37	24	2
1:A:23:ASP:O	1:A:24:TRP:C	0.41	2.63	22	1
1:A:22:THR:N	1:A:24:TRP:NE1	0.41	2.68	40	1
1:A:5:GLY:O	1:A:7:PHE:CE2	0.41	2.73	20	1
1:A:6:ASP:O	1:A:7:PHE:O	0.41	2.39	33	1
1:A:34:ILE:C	1:A:36:MET:N	0.41	2.76	40	1
1:A:9:ASN:O	1:A:10:TYR:C	0.41	2.63	24	2
1:A:52:THR:O	1:A:52:THR:CG2	0.41	2.69	22	1
1:A:55:ARG:CG	1:A:55:ARG:O	0.41	2.67	24	1
1:A:26:SER:C	1:A:27:SER:OG	0.41	2.63	1	1
1:A:19:CYS:O	1:A:20:GLU:C	0.41	2.64	6	1
1:A:9:ASN:O	1:A:10:TYR:CD2	0.41	2.74	14	1
1:A:43:THR:O	1:A:44:THR:C	0.41	2.63	15	2
1:A:49:VAL:O	1:A:53:VAL:CG2	0.41	2.69	38	1
1:A:41:LEU:O	1:A:42:GLY:C	0.41	2.64	38	1
1:A:27:SER:H	1:A:31:ILE:HD11	0.40	1.76	2	1
1:A:9:ASN:OD1	1:A:9:ASN:N	0.40	2.51	15	1
1:A:9:ASN:HD22	1:A:9:ASN:C	0.40	2.25	8	1
1:A:24:TRP:C	1:A:24:TRP:CE3	0.40	3.00	14	1
1:A:7:PHE:O	1:A:9:ASN:OD1	0.40	2.40	35	1
1:A:25:LYS:C	1:A:26:SER:OG	0.40	2.62	39	1
1:A:42:GLY:O	1:A:43:THR:OG1	0.40	2.37	40	1
1:A:11:TYR:O	1:A:14:ASP:OD2	0.40	2.39	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:MET:O	1:A:39:PHE:N	0.40	2.48	4	1
1:A:18:GLU:H	1:A:18:GLU:CD	0.40	2.24	9	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	52/64 (81%)	26±3 (50±6%)	20±3 (39±6%)	6±2 (12±4%)	1	7
All	All	2080/2560 (81%)	1032 (50%)	807 (39%)	241 (12%)	1	7

All 38 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	18	GLU	26
1	A	22	THR	26
1	A	11	TYR	22
1	A	25	LYS	18
1	A	8	ASP	13
1	A	6	ASP	12
1	A	13	ALA	12
1	A	47	GLY	11
1	A	24	TRP	8
1	A	7	PHE	8
1	A	46	ASN	7
1	A	45	GLY	7
1	A	43	THR	6
1	A	14	ASP	6
1	A	49	VAL	5
1	A	26	SER	5
1	A	42	GLY	5
1	A	28	GLY	5
1	A	23	ASP	4
1	A	5	GLY	4

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Mol	Chain	Res	Type	Models (Total)
1	A	29	ALA	4
1	A	34	ILE	3
1	A	10	TYR	3
1	A	30	LEU	2
1	A	41	LEU	2
1	A	9	ASN	2
1	A	55	ARG	2
1	A	20	GLU	2
1	A	50	LEU	2
1	A	51	TRP	1
1	A	44	THR	1
1	A	21	TYR	1
1	A	52	THR	1
1	A	48	LEU	1
1	A	56	LYS	1
1	A	27	SER	1
1	A	36	MET	1
1	A	12	GLY	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	43/53 (81%)	32±2 (75±6%)	11±2 (25±6%)	2	24
All	All	1720/2120 (81%)	1288 (75%)	432 (25%)	2	24

All 40 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	40	LEU	28
1	A	31	ILE	25
1	A	25	LYS	23
1	A	50	LEU	21
1	A	56	LYS	18
1	A	46	ASN	18
1	A	6	ASP	17

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Mol	Chain	Res	Type	Models (Total)
1	A	27	SER	17
1	A	52	THR	16
1	A	15	ASN	16
1	A	30	LEU	16
1	A	9	ASN	15
1	A	23	ASP	14
1	A	14	ASP	14
1	A	22	THR	14
1	A	26	SER	14
1	A	17	SER	13
1	A	18	GLU	13
1	A	51	TRP	12
1	A	7	PHE	11
1	A	35	TYR	11
1	A	43	THR	11
1	A	8	ASP	10
1	A	55	ARG	9
1	A	21	TYR	5
1	A	36	MET	5
1	A	11	TYR	5
1	A	54	PHE	5
1	A	34	ILE	5
1	A	44	THR	4
1	A	41	LEU	4
1	A	19	CYS	4
1	A	49	VAL	4
1	A	16	GLN	3
1	A	20	GLU	3
1	A	10	TYR	3
1	A	48	LEU	2
1	A	39	PHE	2
1	A	24	TRP	1
1	A	53	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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	755
Number of shifts mapped to atoms	755
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	64	-0.58 ± 0.12	Should be checked
$^{13}\text{C}_\beta$	56	0.44 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	61	-0.10 ± 0.05	None needed (< 0.5 ppm)
^{15}N	62	0.96 ± 0.23	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 628 atoms were assigned a chemical shift out of a possible 687. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	259/264 (98%)	106/109 (97%)	102/104 (98%)	51/51 (100%)
Sidechain	298/333 (89%)	197/218 (90%)	95/106 (90%)	6/9 (67%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	71/90 (79%)	37/43 (86%)	32/45 (71%)	2/2 (100%)
Overall	628/687 (91%)	340/370 (92%)	229/255 (90%)	59/62 (95%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 755 atoms were assigned a chemical shift out of a possible 846. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	318/326 (98%)	131/135 (97%)	125/128 (98%)	62/63 (98%)
Sidechain	342/388 (88%)	224/253 (89%)	112/125 (90%)	6/10 (60%)
Aromatic	95/132 (72%)	49/67 (73%)	44/57 (77%)	2/8 (25%)
Overall	755/846 (89%)	404/455 (89%)	281/310 (91%)	70/81 (86%)

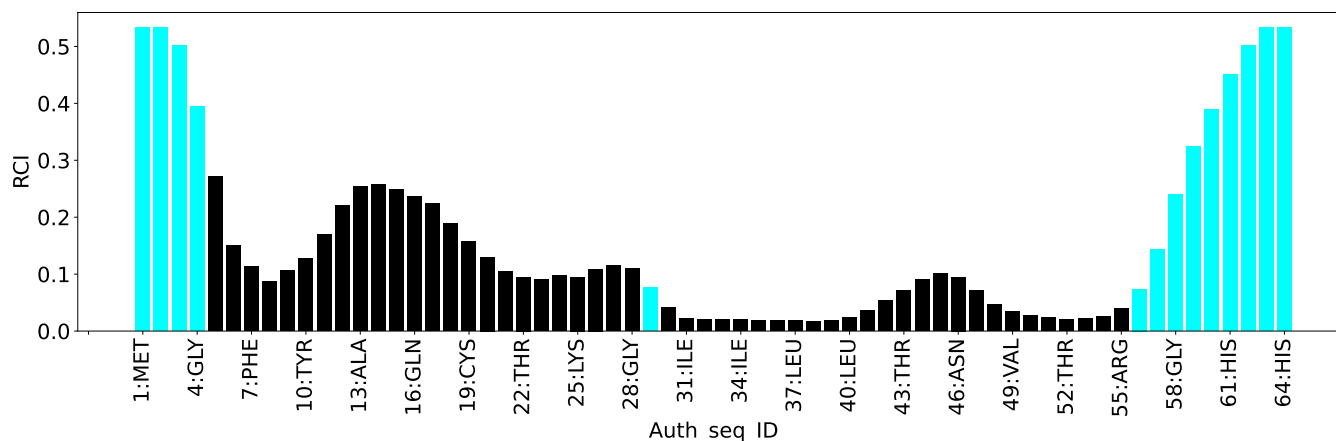
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain 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	1535
Intra-residue ($ i-j =0$)	975
Sequential ($ i-j =1$)	331
Medium range ($ i-j >1$ and $ i-j <5$)	228
Long range ($ i-j \geq 5$)	1
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	24.0
Number of long range restraints per residue ¹	0.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	2.5	0.2
0.2-0.5 (Medium)	5.0	0.5
>0.5 (Large)	7.7	2.1

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

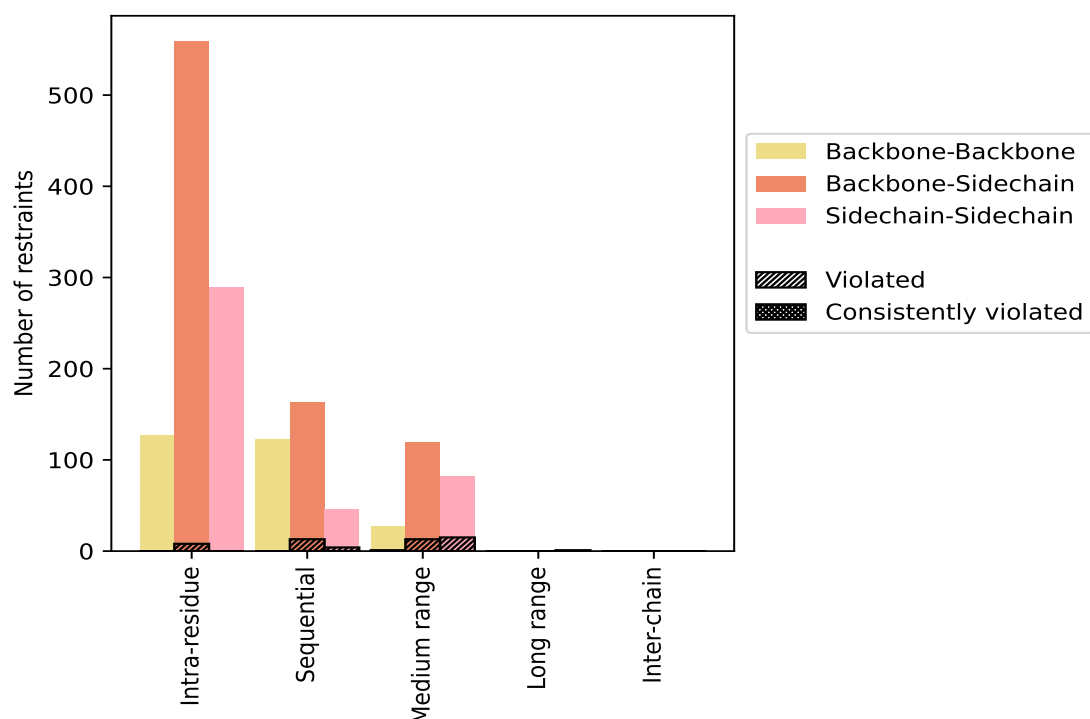
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	975	63.5	8	0.8	0.5	0	0.0	0.0
Backbone-Backbone	127	8.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	559	36.4	8	1.4	0.5	0	0.0	0.0
Sidechain-Sidechain	289	18.8	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	331	21.6	17	5.1	1.1	0	0.0	0.0
Backbone-Backbone	122	7.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	163	10.6	13	8.0	0.8	0	0.0	0.0
Sidechain-Sidechain	46	3.0	4	8.7	0.3	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	228	14.9	29	12.7	1.9	0	0.0	0.0
Backbone-Backbone	27	1.8	1	3.7	0.1	0	0.0	0.0
Backbone-Sidechain	119	7.8	13	10.9	0.8	0	0.0	0.0
Sidechain-Sidechain	82	5.3	15	18.3	1.0	0	0.0	0.0
Long range ($i-j \geq 5$)	1	0.1	1	100.0	0.1	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	1	0.1	1	100.0	0.1	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	1535	100.0	55	3.6	3.6	0	0.0	0.0
Backbone-Backbone	276	18.0	1	0.4	0.1	0	0.0	0.0
Backbone-Sidechain	841	54.8	34	4.0	2.2	0	0.0	0.0
Sidechain-Sidechain	418	27.2	20	4.8	1.3	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model [i](#)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	7	6	1	0	14	0.7	1.35	0.37	0.56
2	1	6	4	1	0	12	0.62	1.59	0.41	0.54
3	0	6	6	1	0	13	0.67	1.35	0.36	0.52
4	0	8	5	0	0	13	0.87	1.93	0.51	0.57
5	0	9	5	0	0	14	0.66	1.63	0.39	0.66
6	1	7	4	1	0	13	0.75	1.34	0.4	0.74
7	0	7	8	1	0	16	0.61	1.31	0.39	0.61
8	0	9	5	0	0	14	0.6	1.35	0.4	0.48
9	0	7	5	0	0	12	0.71	1.19	0.36	0.62
10	0	7	6	0	0	13	0.6	1.3	0.36	0.46

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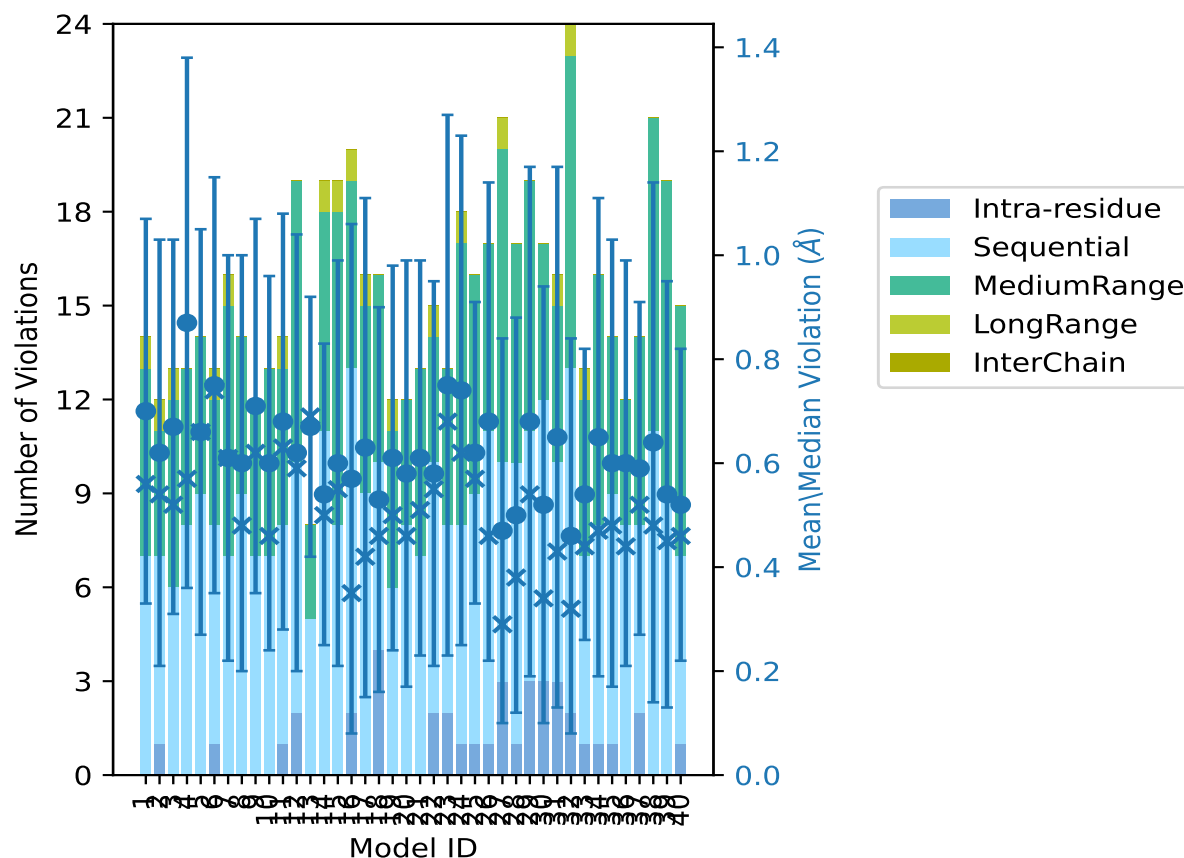
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	7	5	1	0	14	0.68	1.68	0.4	0.63
12	2	8	9	0	0	19	0.62	1.36	0.42	0.59
13	0	5	3	0	0	8	0.67	1.03	0.25	0.69
14	0	11	7	1	0	19	0.54	1.19	0.29	0.5
15	0	8	10	1	0	19	0.6	1.85	0.39	0.55
16	2	11	6	1	0	20	0.57	1.89	0.49	0.35
17	0	9	6	1	0	16	0.63	1.5	0.48	0.42
18	4	6	6	0	0	16	0.53	1.21	0.37	0.46
19	0	6	5	1	0	12	0.61	1.27	0.37	0.5
20	0	8	4	0	0	12	0.58	1.54	0.41	0.46
21	0	7	6	0	0	13	0.61	1.47	0.38	0.51
22	2	8	4	1	0	15	0.58	1.32	0.37	0.55
23	2	6	5	0	0	13	0.75	2.02	0.52	0.68
24	1	7	9	1	0	18	0.74	2.03	0.49	0.62
25	1	8	7	0	0	16	0.62	1.12	0.29	0.57
26	1	10	6	0	0	17	0.68	1.6	0.46	0.46
27	3	7	10	1	0	21	0.47	1.27	0.37	0.29
28	1	9	7	0	0	17	0.5	1.38	0.38	0.38
29	3	8	8	0	0	19	0.68	1.6	0.49	0.54
30	3	9	5	0	0	17	0.52	1.53	0.42	0.34
31	3	7	5	1	0	16	0.65	1.94	0.52	0.43
32	2	11	10	1	0	24	0.46	1.61	0.38	0.32
33	1	6	5	1	0	13	0.54	1.15	0.28	0.44
34	1	7	8	0	0	16	0.65	1.82	0.46	0.47
35	1	8	5	0	0	14	0.6	1.51	0.43	0.48
36	0	8	4	0	0	12	0.6	1.25	0.39	0.44
37	2	6	6	0	0	14	0.59	1.18	0.32	0.52
38	0	11	10	0	0	21	0.64	2.1	0.5	0.48
39	0	9	10	0	0	19	0.54	1.61	0.41	0.45
40	1	6	8	0	0	15	0.52	1.18	0.3	0.46

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1480(IR:967, SQ:314, MR:199, LR:0, 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	3	6	0	0	14	1	2.5
1	5	0	0	0	6	2	5.0
0	1	4	0	0	5	3	7.5
0	0	1	0	0	1	4	10.0
2	0	0	0	0	2	5	12.5
0	0	2	0	0	2	6	15.0

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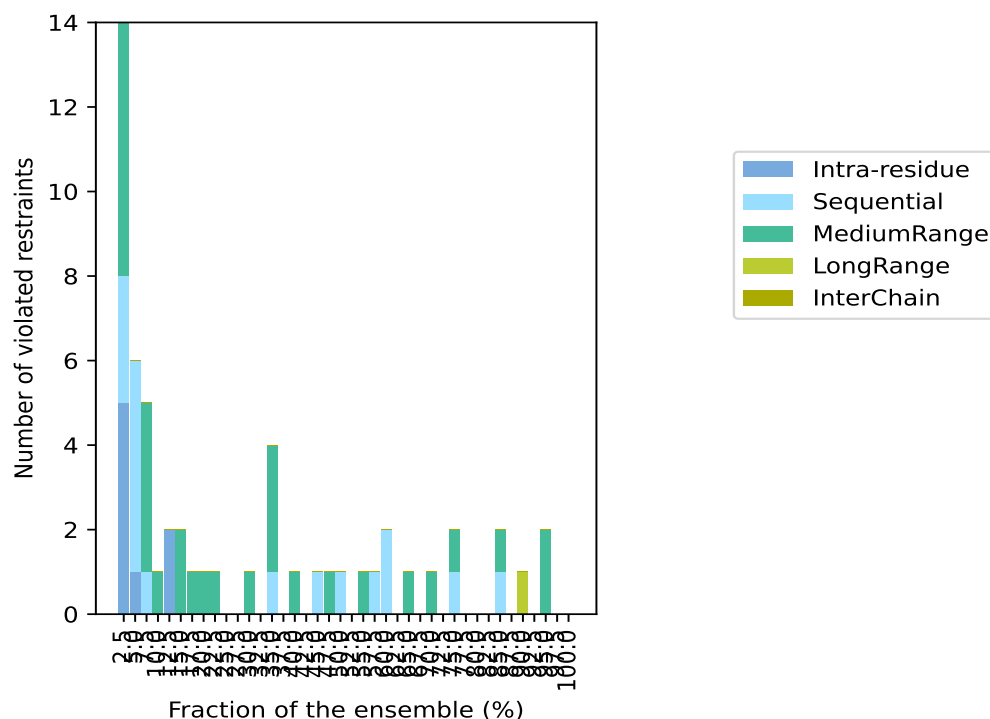
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	1	0	0	1	7	17.5
0	0	1	0	0	1	8	20.0
0	0	1	0	0	1	9	22.5
0	0	0	0	0	0	10	25.0
0	0	0	0	0	0	11	27.5
0	0	1	0	0	1	12	30.0
0	0	0	0	0	0	13	32.5
0	1	3	0	0	4	14	35.0
0	0	0	0	0	0	15	37.5
0	0	1	0	0	1	16	40.0
0	0	0	0	0	0	17	42.5
0	1	0	0	0	1	18	45.0
0	0	1	0	0	1	19	47.5
0	1	0	0	0	1	20	50.0
0	0	0	0	0	0	21	52.5
0	0	1	0	0	1	22	55.0
0	1	0	0	0	1	23	57.5
0	2	0	0	0	2	24	60.0
0	0	0	0	0	0	25	62.5
0	0	1	0	0	1	26	65.0
0	0	0	0	0	0	27	67.5
0	0	1	0	0	1	28	70.0
0	0	0	0	0	0	29	72.5
0	1	1	0	0	2	30	75.0
0	0	0	0	0	0	31	77.5
0	0	0	0	0	0	32	80.0
0	0	0	0	0	0	33	82.5
0	1	1	0	0	2	34	85.0
0	0	0	0	0	0	35	87.5
0	0	0	1	0	1	36	90.0
0	0	0	0	0	0	37	92.5
0	0	2	0	0	2	38	95.0
0	0	0	0	0	0	39	97.5
0	0	0	0	0	0	40	100.0

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

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

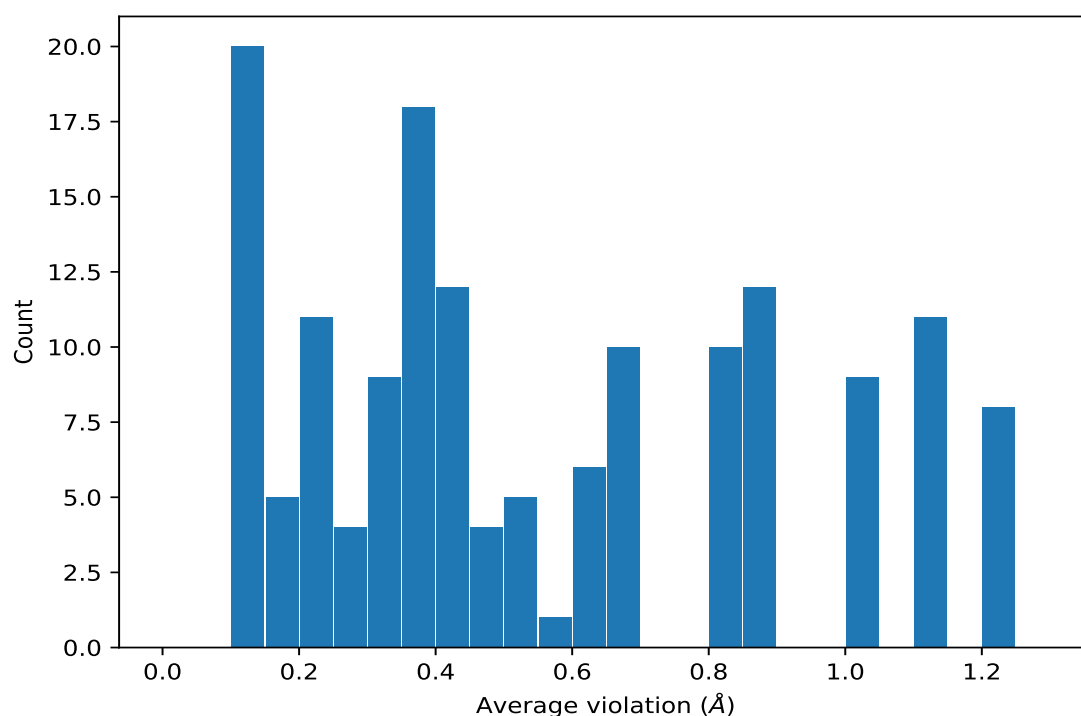
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,78)	1:13:A:ALA:HB2	1:9:A:ASN:HD22	38	1.15	0.57	1.16
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD21	38	1.15	0.57	1.16
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD22	38	1.15	0.57	1.16
(1,78)	1:13:A:ALA:HB2	1:9:A:ASN:HD21	38	1.15	0.57	1.16
(1,78)	1:13:A:ALA:HB1	1:9:A:ASN:HD21	38	1.15	0.57	1.16
(1,78)	1:13:A:ALA:HB2	1:11:A:TYR:HE2	38	1.15	0.57	1.16
(1,78)	1:13:A:ALA:HB3	1:11:A:TYR:HE2	38	1.15	0.57	1.16
(1,78)	1:13:A:ALA:HB2	1:11:A:TYR:HE1	38	1.15	0.57	1.16
(1,1165)	1:48:A:LEU:HD22	1:51:A:TRP:HE1	38	0.89	0.22	0.88
(1,1165)	1:48:A:LEU:HD23	1:51:A:TRP:HE1	38	0.89	0.22	0.88
(1,1165)	1:48:A:LEU:HD21	1:51:A:TRP:HE1	38	0.89	0.22	0.88
(1,1165)	1:48:A:LEU:HD13	1:51:A:TRP:HE1	38	0.89	0.22	0.88
(1,1165)	1:48:A:LEU:HD11	1:51:A:TRP:HE1	38	0.89	0.22	0.88
(1,1165)	1:48:A:LEU:HD12	1:51:A:TRP:HE1	38	0.89	0.22	0.88
(1,250)	1:44:A:THR:HG22	1:39:A:PHE:HE2	36	1.01	0.29	1.08
(1,250)	1:44:A:THR:HG22	1:39:A:PHE:HE1	36	1.01	0.29	1.08

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,250)	1:44:A:THR:HG21	1:39:A:PHE:HE1	36	1.01	0.29	1.08
(1,250)	1:52:A:THR:HG22	1:51:A:TRP:HD1	36	1.01	0.29	1.08
(1,250)	1:52:A:THR:HG21	1:51:A:TRP:HD1	36	1.01	0.29	1.08
(1,250)	1:44:A:THR:HG21	1:39:A:PHE:HE2	36	1.01	0.29	1.08
(1,250)	1:44:A:THR:HG23	1:39:A:PHE:HE2	36	1.01	0.29	1.08
(1,250)	1:52:A:THR:HG23	1:51:A:TRP:HD1	36	1.01	0.29	1.08
(1,250)	1:44:A:THR:HG23	1:39:A:PHE:HE1	36	1.01	0.29	1.08
(1,199)	1:34:A:ILE:HG22	1:33:A:ALA:HB2	34	1.22	0.22	1.26
(1,199)	1:34:A:ILE:HG22	1:33:A:ALA:HB3	34	1.22	0.22	1.26
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB3	34	1.22	0.22	1.26
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB2	34	1.22	0.22	1.26
(1,199)	1:34:A:ILE:HG23	1:33:A:ALA:HB2	34	1.22	0.22	1.26
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB1	34	1.22	0.22	1.26
(1,199)	1:34:A:ILE:HG23	1:33:A:ALA:HB1	34	1.22	0.22	1.26
(1,199)	1:34:A:ILE:HG23	1:33:A:ALA:HB3	34	1.22	0.22	1.26
(1,170)	1:36:A:MET:HE1	1:39:A:PHE:H	34	0.88	0.31	0.9
(1,170)	1:36:A:MET:HE3	1:39:A:PHE:H	34	0.88	0.31	0.9
(1,170)	1:36:A:MET:HE1	1:35:A:TYR:H	34	0.88	0.31	0.9
(1,170)	1:36:A:MET:HE2	1:39:A:PHE:H	34	0.88	0.31	0.9
(1,170)	1:36:A:MET:HE3	1:35:A:TYR:H	34	0.88	0.31	0.9
(1,170)	1:36:A:MET:HE2	1:35:A:TYR:H	34	0.88	0.31	0.9
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG21	30	0.53	0.07	0.57
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG22	30	0.53	0.07	0.57
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG23	30	0.53	0.07	0.57
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	30	0.32	0.12	0.34
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	28	0.41	0.21	0.34
(1,205)	1:37:A:LEU:HB2	1:33:A:ALA:HB3	28	0.41	0.21	0.34
(1,205)	1:37:A:LEU:HB2	1:33:A:ALA:HB2	28	0.41	0.21	0.34
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG13	28	0.41	0.21	0.34
(1,205)	1:37:A:LEU:HB2	1:33:A:ALA:HB1	28	0.41	0.21	0.34
(1,618)	1:37:A:LEU:HD23	1:36:A:MET:HE1	26	0.83	0.42	0.93
(1,618)	1:37:A:LEU:HD21	1:36:A:MET:HE1	26	0.83	0.42	0.93
(1,618)	1:37:A:LEU:HD23	1:36:A:MET:HE3	26	0.83	0.42	0.93
(1,618)	1:37:A:LEU:HD11	1:36:A:MET:HE1	26	0.83	0.42	0.93
(1,618)	1:37:A:LEU:HD21	1:36:A:MET:HE2	26	0.83	0.42	0.93
(1,618)	1:37:A:LEU:HD22	1:36:A:MET:HE1	26	0.83	0.42	0.93
(1,618)	1:37:A:LEU:HD22	1:36:A:MET:HE2	26	0.83	0.42	0.93
(1,618)	1:37:A:LEU:HD12	1:36:A:MET:HE2	26	0.83	0.42	0.93
(1,618)	1:37:A:LEU:HD23	1:36:A:MET:HE2	26	0.83	0.42	0.93
(1,618)	1:37:A:LEU:HD21	1:36:A:MET:HE3	26	0.83	0.42	0.93
(1,1360)	1:30:A:LEU:HB2	1:31:A:ILE:H	24	0.37	0.09	0.39
(1,1360)	1:30:A:LEU:HB3	1:31:A:ILE:H	24	0.37	0.09	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,922)	1:30:A:LEU:HB2	1:29:A:ALA:HA	24	0.28	0.12	0.24
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	24	0.28	0.12	0.24
(1,922)	1:32:A:PRO:HB2	1:29:A:ALA:HA	24	0.28	0.12	0.24
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB2	23	0.33	0.12	0.29
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HG	23	0.33	0.12	0.29
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB3	23	0.33	0.12	0.29
(1,251)	1:52:A:THR:HG22	1:56:A:LYS:HE2	22	0.66	0.34	0.61
(1,251)	1:52:A:THR:HG23	1:56:A:LYS:HE2	22	0.66	0.34	0.61
(1,251)	1:52:A:THR:HG21	1:56:A:LYS:HE2	22	0.66	0.34	0.61
(1,251)	1:52:A:THR:HG22	1:56:A:LYS:HE3	22	0.66	0.34	0.61
(1,251)	1:52:A:THR:HG23	1:56:A:LYS:HE3	22	0.66	0.34	0.61
(1,251)	1:52:A:THR:HG21	1:56:A:LYS:HE3	22	0.66	0.34	0.61
(1,8)	1:10:A:TYR:HE2	1:9:A:ASN:H	20	0.35	0.12	0.34
(1,8)	1:10:A:TYR:HE1	1:9:A:ASN:H	20	0.35	0.12	0.34
(1,525)	1:38:A:VAL:HG11	1:39:A:PHE:H	19	0.41	0.16	0.46
(1,525)	1:38:A:VAL:HG23	1:39:A:PHE:H	19	0.41	0.16	0.46
(1,525)	1:38:A:VAL:HG13	1:39:A:PHE:H	19	0.41	0.16	0.46
(1,525)	1:38:A:VAL:HG12	1:39:A:PHE:H	19	0.41	0.16	0.46
(1,525)	1:38:A:VAL:HG22	1:39:A:PHE:H	19	0.41	0.16	0.46
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	18	0.39	0.24	0.36
(1,442)	1:24:A:TRP:HZ3	1:24:A:TRP:HA	18	0.39	0.24	0.36
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD12	16	0.63	0.18	0.66
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD13	16	0.63	0.18	0.66
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD11	16	0.63	0.18	0.66
(1,132)	1:31:A:ILE:HD12	1:30:A:LEU:HA	14	1.12	0.18	1.17
(1,132)	1:31:A:ILE:HD13	1:30:A:LEU:HA	14	1.12	0.18	1.17
(1,132)	1:31:A:ILE:HD11	1:30:A:LEU:HA	14	1.12	0.18	1.17
(1,995)	1:29:A:ALA:HB1	1:32:A:PRO:HG2	14	0.48	0.19	0.46
(1,995)	1:29:A:ALA:HB2	1:32:A:PRO:HG2	14	0.48	0.19	0.46
(1,995)	1:29:A:ALA:HB3	1:32:A:PRO:HG2	14	0.48	0.19	0.46
(1,995)	1:29:A:ALA:HB2	1:32:A:PRO:HG3	14	0.48	0.19	0.46
(1,1223)	1:41:A:LEU:HG	1:41:A:LEU:H	14	0.42	0.18	0.52
(1,1223)	1:41:A:LEU:HG	1:37:A:LEU:HB3	14	0.42	0.18	0.52
(1,42)	1:38:A:VAL:HG13	1:35:A:TYR:HE2	14	0.39	0.32	0.22
(1,42)	1:38:A:VAL:HG11	1:35:A:TYR:HE2	14	0.39	0.32	0.22
(1,42)	1:31:A:ILE:HG22	1:35:A:TYR:HE1	14	0.39	0.32	0.22
(1,42)	1:31:A:ILE:HG21	1:35:A:TYR:HE1	14	0.39	0.32	0.22
(1,42)	1:38:A:VAL:HG12	1:35:A:TYR:HE1	14	0.39	0.32	0.22
(1,42)	1:38:A:VAL:HG22	1:35:A:TYR:HE2	14	0.39	0.32	0.22
(1,42)	1:31:A:ILE:HG21	1:35:A:TYR:HE2	14	0.39	0.32	0.22
(1,42)	1:31:A:ILE:HG23	1:35:A:TYR:HE1	14	0.39	0.32	0.22
(1,42)	1:38:A:VAL:HG11	1:35:A:TYR:HE1	14	0.39	0.32	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,64)	1:33:A:ALA:HA	1:36:A:MET:HG2	12	0.22	0.09	0.19
(1,64)	1:33:A:ALA:HA	1:36:A:MET:HG3	12	0.22	0.09	0.19
(1,64)	1:35:A:TYR:HA	1:36:A:MET:HG3	12	0.22	0.09	0.19
(1,439)	1:32:A:PRO:HG2	1:29:A:ALA:HA	9	0.51	0.14	0.51
(1,439)	1:32:A:PRO:HG3	1:29:A:ALA:HA	9	0.51	0.14	0.51
(1,1022)	1:48:A:LEU:HB2	1:45:A:GLY:HA2	8	0.7	0.37	0.65
(1,1022)	1:30:A:LEU:HB3	1:28:A:GLY:HA2	8	0.7	0.37	0.65
(1,1022)	1:48:A:LEU:HB2	1:45:A:GLY:HA3	8	0.7	0.37	0.65
(1,1022)	1:30:A:LEU:HB2	1:28:A:GLY:HA2	8	0.7	0.37	0.65
(1,354)	1:35:A:TYR:HE1	1:38:A:VAL:HB	7	0.56	0.21	0.58
(1,1379)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	6	0.37	0.19	0.34
(1,1379)	1:25:A:LYS:HG2	1:24:A:TRP:HE1	6	0.37	0.19	0.34
(1,1379)	1:22:A:THR:HG22	1:24:A:TRP:HE1	6	0.37	0.19	0.34
(1,1379)	1:22:A:THR:HG21	1:24:A:TRP:HE1	6	0.37	0.19	0.34
(1,1379)	1:22:A:THR:HG23	1:24:A:TRP:HE1	6	0.37	0.19	0.34
(1,875)	1:25:A:LYS:HE3	1:22:A:THR:HB	6	0.32	0.11	0.33
(1,497)	1:25:A:LYS:HG2	1:25:A:LYS:H	5	0.12	0.01	0.12
(1,497)	1:25:A:LYS:HG3	1:25:A:LYS:H	5	0.12	0.01	0.12
(1,1449)	1:25:A:LYS:HG2	1:25:A:LYS:H	5	0.12	0.01	0.12
(1,1449)	1:25:A:LYS:HG3	1:25:A:LYS:H	5	0.12	0.01	0.12
(1,766)	1:51:A:TRP:HE3	1:52:A:THR:HG22	4	0.62	0.45	0.5
(1,766)	1:51:A:TRP:HE3	1:52:A:THR:HG23	4	0.62	0.45	0.5
(1,766)	1:51:A:TRP:HE1	1:52:A:THR:HG21	4	0.62	0.45	0.5
(1,1073)	1:35:A:TYR:HE2	1:36:A:MET:HA	3	0.31	0.23	0.19
(1,1073)	1:35:A:TYR:HE2	1:32:A:PRO:HA	3	0.31	0.23	0.19
(1,32)	1:16:A:GLN:HA	1:19:A:CYS:HB3	3	0.23	0.1	0.17
(1,32)	1:18:A:GLU:HA	1:19:A:CYS:HB3	3	0.23	0.1	0.17
(1,32)	1:16:A:GLN:HA	1:19:A:CYS:HB2	3	0.23	0.1	0.17
(1,457)	1:16:A:GLN:HA	1:19:A:CYS:HB3	3	0.23	0.1	0.17
(1,457)	1:18:A:GLU:HA	1:19:A:CYS:HB3	3	0.23	0.1	0.17
(1,457)	1:16:A:GLN:HA	1:19:A:CYS:HB2	3	0.23	0.1	0.17
(1,713)	1:53:A:VAL:HA	1:56:A:LYS:HB2	3	0.23	0.07	0.18
(1,713)	1:53:A:VAL:HA	1:56:A:LYS:HB3	3	0.23	0.07	0.18
(1,1207)	1:3:A:GLU:H	1:3:A:GLU:HG3	3	0.16	0.03	0.15
(1,1207)	1:3:A:GLU:H	1:3:A:GLU:HG2	3	0.16	0.03	0.15
(1,503)	1:38:A:VAL:HA	1:41:A:LEU:HB3	2	0.28	0.08	0.28
(1,428)	1:48:A:LEU:HG	1:48:A:LEU:H	2	0.16	0.02	0.16
(1,1312)	1:3:A:GLU:HB3	1:3:A:GLU:H	2	0.16	0.01	0.16
(1,1515)	1:3:A:GLU:HB3	1:3:A:GLU:H	2	0.16	0.01	0.16
(1,663)	1:46:A:ASN:HB2	1:45:A:GLY:HA2	2	0.14	0.02	0.14
(1,663)	1:46:A:ASN:HB2	1:45:A:GLY:HA3	2	0.14	0.02	0.14
(1,663)	1:46:A:ASN:HB3	1:45:A:GLY:HA2	2	0.14	0.02	0.14

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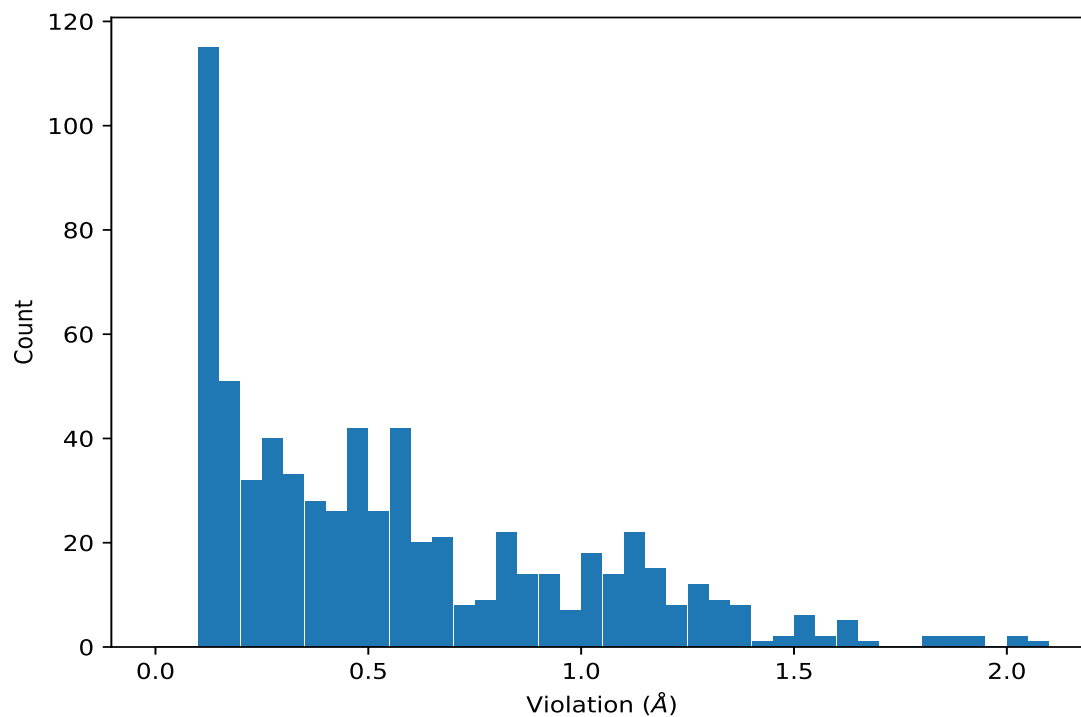
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,663)	1:46:A:ASN:HB3	1:45:A:GLY:HA3	2	0.14	0.02	0.14
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG11	2	0.12	0.0	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG12	2	0.12	0.0	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG13	2	0.12	0.0	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG21	2	0.12	0.0	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG22	2	0.12	0.0	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG23	2	0.12	0.0	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG11	2	0.12	0.0	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG12	2	0.12	0.0	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG13	2	0.12	0.0	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG21	2	0.12	0.0	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG22	2	0.12	0.0	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG23	2	0.12	0.0	0.12

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:13:A:ALA:HB2	1:11:A:TYR:HE1	38	2.1
(1,78)	1:13:A:ALA:HB3	1:11:A:TYR:HE2	24	2.03
(1,78)	1:13:A:ALA:HB2	1:9:A:ASN:HD21	23	2.02
(1,78)	1:13:A:ALA:HB2	1:9:A:ASN:HD21	31	1.94
(1,618)	1:37:A:LEU:HD21	1:36:A:MET:HE1	4	1.93
(1,78)	1:13:A:ALA:HB2	1:11:A:TYR:HE2	16	1.89
(1,78)	1:13:A:ALA:HB2	1:9:A:ASN:HD21	15	1.85
(1,78)	1:13:A:ALA:HB2	1:9:A:ASN:HD22	34	1.82
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD21	4	1.81
(1,78)	1:13:A:ALA:HB2	1:9:A:ASN:HD21	11	1.68
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD21	5	1.63
(1,199)	1:34:A:ILE:HG22	1:33:A:ALA:HB3	39	1.61
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD21	32	1.61
(1,618)	1:37:A:LEU:HD12	1:36:A:MET:HE2	26	1.6
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD22	29	1.6
(1,250)	1:52:A:THR:HG23	1:51:A:TRP:HD1	29	1.59
(1,199)	1:34:A:ILE:HG22	1:33:A:ALA:HB3	2	1.59
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB1	20	1.54
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB1	31	1.54
(1,199)	1:34:A:ILE:HG22	1:33:A:ALA:HB3	29	1.53
(1,78)	1:13:A:ALA:HB2	1:9:A:ASN:HD22	30	1.53
(1,78)	1:13:A:ALA:HB2	1:9:A:ASN:HD21	35	1.51
(1,170)	1:36:A:MET:HE2	1:39:A:PHE:H	17	1.5
(1,250)	1:52:A:THR:HG23	1:51:A:TRP:HD1	21	1.47
(1,199)	1:34:A:ILE:HG23	1:33:A:ALA:HB2	26	1.46
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB1	17	1.44
(1,250)	1:52:A:THR:HG22	1:51:A:TRP:HD1	28	1.38
(1,199)	1:34:A:ILE:HG22	1:33:A:ALA:HB2	23	1.37
(1,132)	1:31:A:ILE:HD13	1:30:A:LEU:HA	24	1.37
(1,250)	1:52:A:THR:HG23	1:51:A:TRP:HD1	12	1.36
(1,251)	1:52:A:THR:HG22	1:56:A:LYS:HE2	1	1.35
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB3	3	1.35
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB2	8	1.35
(1,199)	1:34:A:ILE:HG23	1:33:A:ALA:HB2	16	1.35
(1,170)	1:36:A:MET:HE3	1:35:A:TYR:H	35	1.34
(1,132)	1:31:A:ILE:HD13	1:30:A:LEU:HA	6	1.34
(1,766)	1:51:A:TRP:HE1	1:52:A:THR:HG21	22	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD21	26	1.32
(1,1165)	1:48:A:LEU:HD11	1:51:A:TRP:HE1	16	1.31
(1,170)	1:36:A:MET:HE3	1:39:A:PHE:H	7	1.31
(1,199)	1:34:A:ILE:HG23	1:33:A:ALA:HB2	10	1.3
(1,199)	1:34:A:ILE:HG22	1:33:A:ALA:HB2	12	1.3
(1,78)	1:13:A:ALA:HB2	1:9:A:ASN:HD22	1	1.3
(1,1165)	1:48:A:LEU:HD11	1:51:A:TRP:HE1	26	1.28
(1,199)	1:34:A:ILE:HG23	1:33:A:ALA:HB2	7	1.28
(1,250)	1:52:A:THR:HG23	1:51:A:TRP:HD1	20	1.27
(1,199)	1:34:A:ILE:HG23	1:33:A:ALA:HB3	19	1.27
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB3	27	1.27
(1,199)	1:34:A:ILE:HG22	1:33:A:ALA:HB3	30	1.27
(1,132)	1:31:A:ILE:HD11	1:30:A:LEU:HA	17	1.26
(1,132)	1:31:A:ILE:HD12	1:30:A:LEU:HA	38	1.26
(1,250)	1:52:A:THR:HG23	1:51:A:TRP:HD1	36	1.25
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB3	4	1.25
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB2	6	1.25
(1,132)	1:31:A:ILE:HD11	1:30:A:LEU:HA	23	1.25
(1,1022)	1:48:A:LEU:HB2	1:45:A:GLY:HA3	38	1.24
(1,250)	1:52:A:THR:HG22	1:51:A:TRP:HD1	4	1.24
(1,132)	1:31:A:ILE:HD12	1:30:A:LEU:HA	32	1.24
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD22	12	1.23
(1,250)	1:44:A:THR:HG21	1:39:A:PHE:HE2	17	1.22
(1,250)	1:52:A:THR:HG23	1:51:A:TRP:HD1	18	1.21
(1,132)	1:31:A:ILE:HD12	1:30:A:LEU:HA	16	1.21
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD21	3	1.21
(1,250)	1:52:A:THR:HG22	1:51:A:TRP:HD1	39	1.2
(1,1165)	1:48:A:LEU:HD12	1:51:A:TRP:HE1	30	1.19
(1,618)	1:37:A:LEU:HD21	1:36:A:MET:HE1	19	1.19
(1,199)	1:34:A:ILE:HG22	1:33:A:ALA:HB3	14	1.19
(1,170)	1:36:A:MET:HE3	1:39:A:PHE:H	9	1.19
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD21	6	1.19
(1,251)	1:52:A:THR:HG21	1:56:A:LYS:HE3	37	1.18
(1,250)	1:52:A:THR:HG22	1:51:A:TRP:HD1	40	1.18
(1,170)	1:36:A:MET:HE1	1:39:A:PHE:H	31	1.18
(1,199)	1:34:A:ILE:HG23	1:33:A:ALA:HB3	34	1.17
(1,170)	1:36:A:MET:HE3	1:39:A:PHE:H	3	1.17
(1,170)	1:36:A:MET:HE1	1:35:A:TYR:H	8	1.17
(1,1165)	1:48:A:LEU:HD13	1:51:A:TRP:HE1	10	1.16
(1,251)	1:52:A:THR:HG21	1:56:A:LYS:HE2	34	1.16
(1,170)	1:36:A:MET:HE1	1:39:A:PHE:H	27	1.16
(1,618)	1:37:A:LEU:HD23	1:36:A:MET:HE1	1	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,618)	1:37:A:LEU:HD23	1:36:A:MET:HE3	9	1.15
(1,250)	1:44:A:THR:HG22	1:39:A:PHE:HE2	19	1.15
(1,250)	1:44:A:THR:HG22	1:39:A:PHE:HE2	24	1.15
(1,205)	1:37:A:LEU:HB2	1:33:A:ALA:HB2	33	1.15
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB1	15	1.15
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB2	11	1.14
(1,170)	1:36:A:MET:HE2	1:35:A:TYR:H	39	1.14
(1,132)	1:31:A:ILE:HD12	1:30:A:LEU:HA	5	1.14
(1,78)	1:13:A:ALA:HB2	1:9:A:ASN:HD21	27	1.14
(1,1165)	1:48:A:LEU:HD21	1:51:A:TRP:HE1	8	1.13
(1,1165)	1:48:A:LEU:HD23	1:51:A:TRP:HE1	28	1.13
(1,250)	1:52:A:THR:HG22	1:51:A:TRP:HD1	34	1.13
(1,170)	1:36:A:MET:HE3	1:39:A:PHE:H	12	1.13
(1,1165)	1:48:A:LEU:HD22	1:51:A:TRP:HE1	6	1.12
(1,250)	1:44:A:THR:HG23	1:39:A:PHE:HE2	7	1.12
(1,250)	1:44:A:THR:HG21	1:39:A:PHE:HE1	31	1.12
(1,170)	1:36:A:MET:HE2	1:35:A:TYR:H	25	1.12
(1,170)	1:36:A:MET:HE1	1:39:A:PHE:H	38	1.12
(1,1022)	1:30:A:LEU:HB3	1:28:A:GLY:HA2	1	1.11
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB1	22	1.11
(1,199)	1:34:A:ILE:HG22	1:33:A:ALA:HB2	25	1.11
(1,1165)	1:48:A:LEU:HD11	1:51:A:TRP:HE1	35	1.09
(1,250)	1:44:A:THR:HG22	1:39:A:PHE:HE1	2	1.09
(1,42)	1:31:A:ILE:HG22	1:35:A:TYR:HE1	38	1.09
(1,1165)	1:48:A:LEU:HD13	1:51:A:TRP:HE1	17	1.08
(1,1165)	1:48:A:LEU:HD11	1:51:A:TRP:HE1	24	1.08
(1,250)	1:52:A:THR:HG22	1:51:A:TRP:HD1	9	1.08
(1,250)	1:52:A:THR:HG22	1:51:A:TRP:HD1	8	1.07
(1,170)	1:36:A:MET:HE1	1:35:A:TYR:H	6	1.07
(1,199)	1:34:A:ILE:HG22	1:33:A:ALA:HB2	9	1.06
(1,618)	1:37:A:LEU:HD21	1:36:A:MET:HE1	15	1.05
(1,618)	1:37:A:LEU:HD22	1:36:A:MET:HE1	40	1.05
(1,251)	1:52:A:THR:HG22	1:56:A:LYS:HE2	24	1.05
(1,199)	1:34:A:ILE:HG23	1:33:A:ALA:HB1	36	1.05
(1,78)	1:13:A:ALA:HB2	1:9:A:ASN:HD21	36	1.05
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD21	22	1.04
(1,1022)	1:30:A:LEU:HB2	1:28:A:GLY:HA2	18	1.03
(1,250)	1:52:A:THR:HG23	1:51:A:TRP:HD1	13	1.03
(1,199)	1:34:A:ILE:HG23	1:33:A:ALA:HB1	32	1.03
(1,170)	1:36:A:MET:HE3	1:39:A:PHE:H	24	1.03
(1,132)	1:31:A:ILE:HD13	1:30:A:LEU:HA	29	1.03
(1,250)	1:52:A:THR:HG23	1:51:A:TRP:HD1	26	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1165)	1:48:A:LEU:HD23	1:51:A:TRP:HE1	14	1.01
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	36	1.01
(1,251)	1:52:A:THR:HG22	1:56:A:LYS:HE2	29	1.01
(1,250)	1:52:A:THR:HG22	1:51:A:TRP:HD1	23	1.01
(1,199)	1:34:A:ILE:HG23	1:33:A:ALA:HB1	21	1.01
(1,170)	1:36:A:MET:HE2	1:35:A:TYR:H	18	1.01
(1,170)	1:36:A:MET:HE2	1:39:A:PHE:H	29	1.01
(1,132)	1:31:A:ILE:HD13	1:30:A:LEU:HA	7	1.01
(1,132)	1:31:A:ILE:HD13	1:30:A:LEU:HA	12	1.01
(1,618)	1:37:A:LEU:HD21	1:36:A:MET:HE2	10	1.0
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD11	24	1.0
(1,1165)	1:48:A:LEU:HD22	1:51:A:TRP:HE1	9	0.99
(1,132)	1:31:A:ILE:HD13	1:30:A:LEU:HA	39	0.99
(1,1165)	1:48:A:LEU:HD11	1:51:A:TRP:HE1	21	0.98
(1,618)	1:37:A:LEU:HD21	1:36:A:MET:HE2	33	0.98
(1,1165)	1:48:A:LEU:HD21	1:51:A:TRP:HE1	4	0.96
(1,618)	1:37:A:LEU:HD23	1:36:A:MET:HE2	28	0.96
(1,618)	1:37:A:LEU:HD21	1:36:A:MET:HE2	37	0.96
(1,618)	1:37:A:LEU:HD23	1:36:A:MET:HE3	25	0.95
(1,250)	1:52:A:THR:HG21	1:51:A:TRP:HD1	25	0.95
(1,1165)	1:48:A:LEU:HD23	1:51:A:TRP:HE1	2	0.94
(1,618)	1:37:A:LEU:HD21	1:36:A:MET:HE2	29	0.94
(1,250)	1:44:A:THR:HG23	1:39:A:PHE:HE2	11	0.94
(1,618)	1:37:A:LEU:HD21	1:36:A:MET:HE2	34	0.92
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB2	13	0.92
(1,199)	1:34:A:ILE:HG21	1:33:A:ALA:HB1	38	0.92
(1,250)	1:44:A:THR:HG23	1:39:A:PHE:HE2	16	0.91
(1,199)	1:34:A:ILE:HG23	1:33:A:ALA:HB1	18	0.91
(1,170)	1:36:A:MET:HE1	1:39:A:PHE:H	21	0.91
(1,1165)	1:48:A:LEU:HD23	1:51:A:TRP:HE1	5	0.9
(1,1165)	1:48:A:LEU:HD21	1:51:A:TRP:HE1	22	0.9
(1,251)	1:52:A:THR:HG23	1:56:A:LYS:HE2	5	0.9
(1,1165)	1:48:A:LEU:HD11	1:51:A:TRP:HE1	18	0.89
(1,1165)	1:48:A:LEU:HD21	1:51:A:TRP:HE1	37	0.89
(1,1165)	1:48:A:LEU:HD23	1:51:A:TRP:HE1	11	0.88
(1,170)	1:36:A:MET:HE2	1:39:A:PHE:H	28	0.88
(1,250)	1:44:A:THR:HG21	1:39:A:PHE:HE2	14	0.87
(1,199)	1:34:A:ILE:HG22	1:33:A:ALA:HB3	37	0.87
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD22	13	0.87
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD21	37	0.87
(1,42)	1:38:A:VAL:HG11	1:35:A:TYR:HE2	6	0.87
(1,1165)	1:48:A:LEU:HD23	1:51:A:TRP:HE1	32	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1165)	1:48:A:LEU:HD23	1:51:A:TRP:HE1	36	0.86
(1,618)	1:37:A:LEU:HD21	1:36:A:MET:HE3	30	0.86
(1,170)	1:36:A:MET:HE2	1:35:A:TYR:H	26	0.86
(1,42)	1:31:A:ILE:HG21	1:35:A:TYR:HE1	24	0.86
(1,618)	1:37:A:LEU:HD21	1:36:A:MET:HE1	12	0.85
(1,250)	1:44:A:THR:HG22	1:39:A:PHE:HE2	1	0.85
(1,1165)	1:48:A:LEU:HD22	1:51:A:TRP:HE1	38	0.84
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD21	2	0.84
(1,1165)	1:48:A:LEU:HD23	1:51:A:TRP:HE1	12	0.83
(1,1165)	1:48:A:LEU:HD22	1:51:A:TRP:HE1	20	0.83
(1,618)	1:37:A:LEU:HD23	1:36:A:MET:HE3	14	0.83
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD11	3	0.83
(1,251)	1:52:A:THR:HG22	1:56:A:LYS:HE2	31	0.83
(1,170)	1:36:A:MET:HE1	1:35:A:TYR:H	11	0.83
(1,354)	1:35:A:TYR:HE1	1:38:A:VAL:HB	27	0.82
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD13	11	0.82
(1,250)	1:44:A:THR:HG21	1:39:A:PHE:HE1	3	0.82
(1,132)	1:31:A:ILE:HD13	1:30:A:LEU:HA	33	0.82
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD22	21	0.82
(1,1165)	1:48:A:LEU:HD12	1:51:A:TRP:HE1	27	0.81
(1,995)	1:29:A:ALA:HB3	1:32:A:PRO:HG2	38	0.81
(1,354)	1:35:A:TYR:HE1	1:38:A:VAL:HB	25	0.81
(1,250)	1:52:A:THR:HG22	1:51:A:TRP:HD1	35	0.81
(1,170)	1:36:A:MET:HE1	1:39:A:PHE:H	40	0.81
(1,1165)	1:48:A:LEU:HD22	1:51:A:TRP:HE1	7	0.8
(1,78)	1:13:A:ALA:HB1	1:9:A:ASN:HD21	10	0.8
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	28	0.79
(1,250)	1:52:A:THR:HG21	1:51:A:TRP:HD1	5	0.79
(1,250)	1:44:A:THR:HG21	1:39:A:PHE:HE2	22	0.79
(1,1165)	1:48:A:LEU:HD13	1:51:A:TRP:HE1	23	0.77
(1,251)	1:52:A:THR:HG22	1:56:A:LYS:HE2	13	0.77
(1,1165)	1:48:A:LEU:HD13	1:51:A:TRP:HE1	31	0.76
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD11	10	0.75
(1,170)	1:36:A:MET:HE1	1:35:A:TYR:H	5	0.75
(1,132)	1:31:A:ILE:HD11	1:30:A:LEU:HA	37	0.75
(1,250)	1:44:A:THR:HG21	1:39:A:PHE:HE2	6	0.74
(1,1165)	1:48:A:LEU:HD23	1:51:A:TRP:HE1	39	0.73
(1,251)	1:52:A:THR:HG23	1:56:A:LYS:HE3	23	0.73
(1,250)	1:44:A:THR:HG21	1:39:A:PHE:HE2	32	0.72
(1,1379)	1:22:A:THR:HG21	1:24:A:TRP:HE1	25	0.71
(1,1165)	1:48:A:LEU:HD22	1:51:A:TRP:HE1	34	0.71
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD12	5	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,170)	1:36:A:MET:HE2	1:35:A:TYR:H	22	0.71
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	4	0.69
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD11	35	0.69
(1,1022)	1:48:A:LEU:HB2	1:45:A:GLY:HA3	24	0.68
(1,995)	1:29:A:ALA:HB2	1:32:A:PRO:HG2	7	0.68
(1,766)	1:51:A:TRP:HE3	1:52:A:THR:HG23	14	0.68
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG13	23	0.68
(1,1165)	1:48:A:LEU:HD12	1:51:A:TRP:HE1	19	0.67
(1,525)	1:38:A:VAL:HG13	1:39:A:PHE:H	14	0.67
(1,439)	1:32:A:PRO:HG3	1:29:A:ALA:HA	15	0.67
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD13	33	0.67
(1,199)	1:34:A:ILE:HG22	1:33:A:ALA:HB2	1	0.67
(1,1165)	1:48:A:LEU:HD23	1:51:A:TRP:HE1	33	0.66
(1,1165)	1:48:A:LEU:HD12	1:51:A:TRP:HE1	40	0.66
(1,995)	1:29:A:ALA:HB2	1:32:A:PRO:HG2	35	0.66
(1,439)	1:32:A:PRO:HG3	1:29:A:ALA:HA	27	0.66
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD12	12	0.66
(1,170)	1:36:A:MET:HE3	1:35:A:TYR:H	32	0.66
(1,78)	1:13:A:ALA:HB2	1:9:A:ASN:HD21	8	0.66
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD13	14	0.65
(1,251)	1:52:A:THR:HG22	1:56:A:LYS:HE3	12	0.65
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	18	0.65
(1,1073)	1:35:A:TYR:HE2	1:32:A:PRO:HA	14	0.64
(1,354)	1:35:A:TYR:HE1	1:38:A:VAL:HB	7	0.64
(1,42)	1:38:A:VAL:HG12	1:35:A:TYR:HE1	11	0.64
(1,1165)	1:48:A:LEU:HD23	1:51:A:TRP:HE1	15	0.63
(1,1165)	1:48:A:LEU:HD21	1:51:A:TRP:HE1	25	0.63
(1,439)	1:32:A:PRO:HG3	1:29:A:ALA:HA	28	0.63
(1,251)	1:52:A:THR:HG21	1:56:A:LYS:HE2	15	0.63
(1,170)	1:36:A:MET:HE2	1:39:A:PHE:H	30	0.63
(1,78)	1:13:A:ALA:HB2	1:9:A:ASN:HD21	19	0.63
(1,1022)	1:48:A:LEU:HB2	1:45:A:GLY:HA2	22	0.62
(1,995)	1:29:A:ALA:HB1	1:32:A:PRO:HG2	29	0.62
(1,525)	1:38:A:VAL:HG11	1:39:A:PHE:H	38	0.62
(1,170)	1:36:A:MET:HE1	1:39:A:PHE:H	15	0.62
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD22	7	0.62
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD21	9	0.62
(1,8)	1:10:A:TYR:HE2	1:9:A:ASN:H	11	0.62
(1,995)	1:29:A:ALA:HB1	1:32:A:PRO:HG2	39	0.61
(1,525)	1:38:A:VAL:HG23	1:39:A:PHE:H	11	0.61
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	9	0.61
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD12	13	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,995)	1:29:A:ALA:HB1	1:32:A:PRO:HG2	25	0.6
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD12	1	0.6
(1,170)	1:36:A:MET:HE2	1:39:A:PHE:H	34	0.6
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG22	5	0.6
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG21	6	0.6
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG23	7	0.6
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG23	16	0.6
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG21	29	0.6
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG21	39	0.6
(1,1165)	1:48:A:LEU:HD22	1:51:A:TRP:HE1	3	0.59
(1,251)	1:52:A:THR:HG23	1:56:A:LYS:HE3	40	0.59
(1,205)	1:37:A:LEU:HB2	1:33:A:ALA:HB3	40	0.59
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG22	12	0.59
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG21	17	0.59
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG22	23	0.59
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG22	26	0.59
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG23	32	0.59
(1,525)	1:38:A:VAL:HG13	1:39:A:PHE:H	19	0.58
(1,439)	1:32:A:PRO:HG3	1:29:A:ALA:HA	39	0.58
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	8	0.58
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	20	0.58
(1,354)	1:35:A:TYR:HE1	1:38:A:VAL:HB	15	0.58
(1,251)	1:52:A:THR:HG21	1:56:A:LYS:HE2	9	0.58
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	10	0.58
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	21	0.58
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG23	9	0.58
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG22	18	0.58
(1,1223)	1:41:A:LEU:HG	1:41:A:LEU:H	37	0.57
(1,251)	1:52:A:THR:HG23	1:56:A:LYS:HE2	27	0.57
(1,170)	1:36:A:MET:HE2	1:35:A:TYR:H	36	0.57
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG21	2	0.57
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG22	4	0.57
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG21	15	0.57
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG23	27	0.57
(1,170)	1:36:A:MET:HE1	1:35:A:TYR:H	16	0.56
(1,8)	1:10:A:TYR:HE1	1:9:A:ASN:H	14	0.56
(1,1223)	1:41:A:LEU:HG	1:41:A:LEU:H	2	0.55
(1,618)	1:37:A:LEU:HD22	1:36:A:MET:HE2	20	0.55
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB2	22	0.55
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	15	0.55
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	16	0.55
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG21	24	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1223)	1:41:A:LEU:HG	1:41:A:LEU:H	25	0.54
(1,1223)	1:41:A:LEU:HG	1:41:A:LEU:H	29	0.54
(1,525)	1:38:A:VAL:HG23	1:39:A:PHE:H	4	0.54
(1,250)	1:44:A:THR:HG23	1:39:A:PHE:HE1	15	0.54
(1,170)	1:36:A:MET:HE3	1:39:A:PHE:H	4	0.54
(1,1223)	1:41:A:LEU:HG	1:41:A:LEU:H	18	0.53
(1,1223)	1:41:A:LEU:HG	1:37:A:LEU:HB3	20	0.53
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	4	0.53
(1,1223)	1:41:A:LEU:HG	1:41:A:LEU:H	35	0.52
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	3	0.52
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	1	0.52
(1,170)	1:36:A:MET:HE1	1:39:A:PHE:H	2	0.52
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG23	25	0.52
(1,1223)	1:41:A:LEU:HG	1:41:A:LEU:H	31	0.51
(1,525)	1:38:A:VAL:HG22	1:39:A:PHE:H	16	0.51
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	21	0.51
(1,439)	1:32:A:PRO:HG3	1:29:A:ALA:HA	29	0.51
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD11	8	0.51
(1,251)	1:52:A:THR:HG23	1:56:A:LYS:HE3	30	0.51
(1,1360)	1:30:A:LEU:HB2	1:31:A:ILE:H	39	0.5
(1,1223)	1:41:A:LEU:HG	1:41:A:LEU:H	27	0.5
(1,439)	1:32:A:PRO:HG3	1:29:A:ALA:HA	7	0.5
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB3	24	0.5
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD21	14	0.5
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG23	30	0.5
(1,8)	1:10:A:TYR:HE2	1:9:A:ASN:H	1	0.5
(1,875)	1:25:A:LYS:HE3	1:22:A:THR:HB	4	0.49
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	15	0.49
(1,354)	1:35:A:TYR:HE1	1:38:A:VAL:HB	29	0.49
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG22	38	0.49
(1,1360)	1:30:A:LEU:HB3	1:31:A:ILE:H	25	0.48
(1,1223)	1:41:A:LEU:HG	1:41:A:LEU:H	23	0.48
(1,995)	1:29:A:ALA:HB2	1:32:A:PRO:HG2	34	0.48
(1,618)	1:37:A:LEU:HD11	1:36:A:MET:HE1	6	0.48
(1,618)	1:37:A:LEU:HD22	1:36:A:MET:HE1	38	0.48
(1,525)	1:38:A:VAL:HG11	1:39:A:PHE:H	1	0.48
(1,1379)	1:25:A:LYS:HG2	1:24:A:TRP:HE1	37	0.47
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	38	0.47
(1,78)	1:13:A:ALA:HB2	1:9:A:ASN:HD22	40	0.47
(1,64)	1:33:A:ALA:HA	1:36:A:MET:HG3	26	0.47
(1,1360)	1:30:A:LEU:HB3	1:31:A:ILE:H	7	0.46
(1,1360)	1:30:A:LEU:HB3	1:31:A:ILE:H	29	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	14	0.46
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	32	0.46
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	34	0.46
(1,525)	1:38:A:VAL:HG23	1:39:A:PHE:H	10	0.46
(1,525)	1:38:A:VAL:HG13	1:39:A:PHE:H	22	0.46
(1,525)	1:38:A:VAL:HG22	1:39:A:PHE:H	26	0.46
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD11	40	0.46
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB3	14	0.46
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HG	32	0.46
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB3	34	0.46
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG21	1	0.46
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG21	3	0.46
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG22	8	0.46
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG22	10	0.46
(1,8)	1:10:A:TYR:HE2	1:9:A:ASN:H	31	0.46
(1,1360)	1:30:A:LEU:HB3	1:31:A:ILE:H	12	0.45
(1,1360)	1:30:A:LEU:HB2	1:31:A:ILE:H	27	0.45
(1,1360)	1:30:A:LEU:HB3	1:31:A:ILE:H	33	0.45
(1,995)	1:29:A:ALA:HB2	1:32:A:PRO:HG2	3	0.45
(1,618)	1:37:A:LEU:HD23	1:36:A:MET:HE3	5	0.45
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	24	0.45
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD13	25	0.45
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG13	37	0.45
(1,78)	1:13:A:ALA:HB1	1:9:A:ASN:HD21	39	0.45
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG21	28	0.45
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG21	40	0.45
(1,1360)	1:30:A:LEU:HB2	1:31:A:ILE:H	15	0.44
(1,995)	1:29:A:ALA:HB2	1:32:A:PRO:HG2	33	0.44
(1,922)	1:32:A:PRO:HB2	1:29:A:ALA:HA	24	0.44
(1,439)	1:32:A:PRO:HG3	1:29:A:ALA:HA	25	0.44
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HG	3	0.44
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG23	35	0.44
(1,1360)	1:30:A:LEU:HB2	1:31:A:ILE:H	28	0.43
(1,1022)	1:48:A:LEU:HB2	1:45:A:GLY:HA3	34	0.43
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	17	0.43
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB2	4	0.43
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB2	13	0.43
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB3	17	0.43
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB2	26	0.43
(1,1360)	1:30:A:LEU:HB2	1:31:A:ILE:H	10	0.42
(1,995)	1:29:A:ALA:HB1	1:32:A:PRO:HG2	12	0.42
(1,525)	1:38:A:VAL:HG13	1:39:A:PHE:H	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	19	0.42
(1,170)	1:36:A:MET:HE3	1:35:A:TYR:H	13	0.42
(1,1360)	1:30:A:LEU:HB2	1:31:A:ILE:H	8	0.41
(1,922)	1:30:A:LEU:HB2	1:29:A:ALA:HA	30	0.41
(1,251)	1:52:A:THR:HG22	1:56:A:LYS:HE2	6	0.41
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	8	0.41
(1,8)	1:10:A:TYR:HE1	1:9:A:ASN:H	26	0.41
(1,1360)	1:30:A:LEU:HB2	1:31:A:ILE:H	3	0.4
(1,525)	1:38:A:VAL:HG23	1:39:A:PHE:H	17	0.4
(1,78)	1:13:A:ALA:HB1	1:9:A:ASN:HD21	18	0.4
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	31	0.39
(1,8)	1:10:A:TYR:HE2	1:9:A:ASN:H	20	0.39
(1,8)	1:10:A:TYR:HE1	1:9:A:ASN:H	33	0.39
(1,1379)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	1	0.38
(1,1360)	1:30:A:LEU:HB2	1:31:A:ILE:H	40	0.38
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	5	0.38
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	2	0.38
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	33	0.38
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	38	0.38
(1,251)	1:52:A:THR:HG23	1:56:A:LYS:HE2	38	0.38
(1,170)	1:36:A:MET:HE2	1:39:A:PHE:H	37	0.38
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD21	25	0.38
(1,8)	1:10:A:TYR:HE2	1:9:A:ASN:H	28	0.38
(1,995)	1:29:A:ALA:HB1	1:32:A:PRO:HG2	32	0.37
(1,457)	1:16:A:GLN:HA	1:19:A:CYS:HB3	26	0.37
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	16	0.37
(1,32)	1:16:A:GLN:HA	1:19:A:CYS:HB3	26	0.37
(1,1360)	1:30:A:LEU:HB2	1:31:A:ILE:H	5	0.36
(1,875)	1:25:A:LYS:HE3	1:22:A:THR:HB	37	0.36
(1,618)	1:37:A:LEU:HD23	1:36:A:MET:HE1	23	0.36
(1,503)	1:38:A:VAL:HA	1:41:A:LEU:HB3	19	0.36
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	1	0.36
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	19	0.36
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	22	0.36
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	26	0.36
(1,251)	1:52:A:THR:HG22	1:56:A:LYS:HE2	14	0.36
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG22	31	0.36
(1,8)	1:10:A:TYR:HE2	1:9:A:ASN:H	21	0.36
(1,1360)	1:30:A:LEU:HB2	1:31:A:ILE:H	11	0.35
(1,525)	1:38:A:VAL:HG12	1:39:A:PHE:H	21	0.35
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	6	0.35
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	17	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:37:A:LEU:HB2	1:33:A:ALA:HB3	32	0.35
(1,42)	1:31:A:ILE:HG22	1:35:A:TYR:HE1	26	0.35
(1,31)	1:32:A:PRO:HD3	1:31:A:ILE:HG21	20	0.35
(1,8)	1:10:A:TYR:HE2	1:9:A:ASN:H	32	0.35
(1,875)	1:25:A:LYS:HE3	1:22:A:THR:HB	15	0.34
(1,525)	1:38:A:VAL:HG22	1:39:A:PHE:H	33	0.34
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	4	0.34
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	30	0.34
(1,205)	1:37:A:LEU:HB2	1:33:A:ALA:HB3	3	0.34
(1,8)	1:10:A:TYR:HE2	1:9:A:ASN:H	10	0.34
(1,1360)	1:30:A:LEU:HB2	1:31:A:ILE:H	34	0.33
(1,1360)	1:30:A:LEU:HB2	1:31:A:ILE:H	35	0.33
(1,766)	1:51:A:TRP:HE3	1:52:A:THR:HG22	16	0.33
(1,713)	1:53:A:VAL:HA	1:56:A:LYS:HB2	40	0.33
(1,713)	1:53:A:VAL:HA	1:56:A:LYS:HB3	40	0.33
(1,442)	1:24:A:TRP:HZ3	1:24:A:TRP:HA	33	0.33
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	39	0.33
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD11	15	0.33
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	2	0.33
(1,1360)	1:30:A:LEU:HB2	1:31:A:ILE:H	14	0.32
(1,875)	1:25:A:LYS:HE3	1:22:A:THR:HB	10	0.32
(1,354)	1:35:A:TYR:HE1	1:38:A:VAL:HB	28	0.32
(1,42)	1:31:A:ILE:HG21	1:35:A:TYR:HE1	39	0.32
(1,1360)	1:30:A:LEU:HB3	1:31:A:ILE:H	16	0.31
(1,439)	1:32:A:PRO:HG2	1:29:A:ALA:HA	12	0.31
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	24	0.31
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	17	0.31
(1,8)	1:10:A:TYR:HE2	1:9:A:ASN:H	13	0.31
(1,8)	1:10:A:TYR:HE1	1:9:A:ASN:H	36	0.31
(1,1379)	1:25:A:LYS:HG3	1:24:A:TRP:HE1	11	0.3
(1,922)	1:30:A:LEU:HB2	1:29:A:ALA:HA	19	0.3
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB2	19	0.3
(1,205)	1:37:A:LEU:HB2	1:33:A:ALA:HB2	9	0.3
(1,8)	1:10:A:TYR:HE2	1:9:A:ASN:H	30	0.3
(1,1360)	1:30:A:LEU:HB2	1:31:A:ILE:H	32	0.29
(1,922)	1:30:A:LEU:HB2	1:29:A:ALA:HA	36	0.29
(1,875)	1:25:A:LYS:HE3	1:22:A:THR:HB	27	0.29
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	22	0.29
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	12	0.29
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	21	0.29
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	35	0.29
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB2	18	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HG	30	0.29
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB2	36	0.29
(1,205)	1:37:A:LEU:HB2	1:33:A:ALA:HB1	24	0.29
(1,8)	1:10:A:TYR:HE2	1:9:A:ASN:H	40	0.29
(1,1360)	1:30:A:LEU:HB3	1:31:A:ILE:H	38	0.28
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	32	0.28
(1,251)	1:52:A:THR:HG21	1:56:A:LYS:HE3	32	0.28
(1,1524)	1:48:A:LEU:HB2	1:49:A:VAL:H	31	0.27
(1,995)	1:29:A:ALA:HB3	1:32:A:PRO:HG2	17	0.27
(1,922)	1:30:A:LEU:HB2	1:29:A:ALA:HA	31	0.27
(1,312)	1:30:A:LEU:HA	1:34:A:ILE:HD11	21	0.27
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB2	21	0.27
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB2	31	0.27
(1,1360)	1:30:A:LEU:HB3	1:31:A:ILE:H	17	0.26
(1,922)	1:30:A:LEU:HB2	1:29:A:ALA:HA	20	0.26
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	37	0.26
(1,439)	1:32:A:PRO:HG2	1:29:A:ALA:HA	33	0.26
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB2	20	0.26
(1,64)	1:33:A:ALA:HA	1:36:A:MET:HG2	16	0.26
(1,1022)	1:48:A:LEU:HB2	1:45:A:GLY:HA2	14	0.25
(1,525)	1:38:A:VAL:HG11	1:39:A:PHE:H	8	0.25
(1,354)	1:35:A:TYR:HE1	1:38:A:VAL:HB	16	0.25
(1,250)	1:44:A:THR:HG21	1:39:A:PHE:HE2	27	0.25
(1,64)	1:33:A:ALA:HA	1:36:A:MET:HG3	11	0.25
(1,64)	1:33:A:ALA:HA	1:36:A:MET:HG2	14	0.25
(1,64)	1:33:A:ALA:HA	1:36:A:MET:HG2	39	0.25
(1,8)	1:10:A:TYR:HE2	1:9:A:ASN:H	6	0.25
(1,1240)	1:30:A:LEU:HB3	1:29:A:ALA:H	38	0.24
(1,525)	1:38:A:VAL:HG12	1:39:A:PHE:H	15	0.24
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	14	0.24
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	27	0.24
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG13	29	0.24
(1,205)	1:37:A:LEU:HB2	1:33:A:ALA:HB1	31	0.24
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	40	0.23
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	30	0.23
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	29	0.23
(1,78)	1:13:A:ALA:HB1	1:9:A:ASN:HD21	20	0.23
(1,42)	1:31:A:ILE:HG21	1:35:A:TYR:HE2	15	0.23
(1,1379)	1:22:A:THR:HG23	1:24:A:TRP:HE1	30	0.22
(1,1223)	1:41:A:LEU:HG	1:37:A:LEU:HB3	12	0.22
(1,618)	1:37:A:LEU:HD22	1:36:A:MET:HE1	16	0.22
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,442)	1:24:A:TRP:HZ3	1:24:A:TRP:HA	11	0.22
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	22	0.22
(1,205)	1:37:A:LEU:HB2	1:33:A:ALA:HB1	35	0.22
(1,42)	1:38:A:VAL:HG11	1:35:A:TYR:HE1	29	0.22
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	15	0.21
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	28	0.21
(1,618)	1:37:A:LEU:HD22	1:36:A:MET:HE2	39	0.21
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	28	0.21
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB3	15	0.21
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB3	28	0.21
(1,251)	1:52:A:THR:HG22	1:56:A:LYS:HE3	36	0.21
(1,250)	1:44:A:THR:HG21	1:39:A:PHE:HE2	33	0.21
(1,1207)	1:3:A:GLU:H	1:3:A:GLU:HG3	24	0.2
(1,1022)	1:48:A:LEU:HB2	1:45:A:GLY:HA2	32	0.2
(1,922)	1:30:A:LEU:HB2	1:29:A:ALA:HA	2	0.2
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB2	2	0.2
(1,205)	1:37:A:LEU:HB2	1:33:A:ALA:HB3	38	0.2
(1,1360)	1:30:A:LEU:HB3	1:31:A:ILE:H	23	0.19
(1,1073)	1:35:A:TYR:HE2	1:36:A:MET:HA	25	0.19
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	11	0.19
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	35	0.19
(1,503)	1:38:A:VAL:HA	1:41:A:LEU:HB3	28	0.19
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	7	0.19
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB3	35	0.19
(1,64)	1:33:A:ALA:HA	1:36:A:MET:HG2	17	0.19
(1,64)	1:33:A:ALA:HA	1:36:A:MET:HG2	18	0.19
(1,64)	1:33:A:ALA:HA	1:36:A:MET:HG2	34	0.19
(1,8)	1:10:A:TYR:HE1	1:9:A:ASN:H	7	0.19
(1,8)	1:10:A:TYR:HE2	1:9:A:ASN:H	38	0.19
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	8	0.18
(1,713)	1:53:A:VAL:HA	1:56:A:LYS:HB2	32	0.18
(1,713)	1:53:A:VAL:HA	1:56:A:LYS:HB3	32	0.18
(1,618)	1:37:A:LEU:HD21	1:36:A:MET:HE2	32	0.18
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	39	0.18
(1,428)	1:48:A:LEU:HG	1:48:A:LEU:H	23	0.18
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	3	0.18
(1,288)	1:29:A:ALA:HB1	1:28:A:GLY:HA3	38	0.18
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	27	0.18
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	36	0.18
(1,42)	1:31:A:ILE:HG23	1:35:A:TYR:HE1	16	0.18
(1,922)	1:30:A:LEU:HB2	1:29:A:ALA:HA	9	0.17
(1,713)	1:53:A:VAL:HA	1:56:A:LYS:HB2	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,713)	1:53:A:VAL:HA	1:56:A:LYS:HB3	20	0.17
(1,457)	1:16:A:GLN:HA	1:19:A:CYS:HB2	39	0.17
(1,456)	1:56:A:LYS:HA	1:56:A:LYS:HD2	32	0.17
(1,456)	1:56:A:LYS:HA	1:56:A:LYS:HD3	32	0.17
(1,442)	1:24:A:TRP:HZ3	1:24:A:TRP:HA	34	0.17
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	36	0.17
(1,337)	1:56:A:LYS:HA	1:56:A:LYS:HD2	32	0.17
(1,337)	1:56:A:LYS:HA	1:56:A:LYS:HD3	32	0.17
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB2	9	0.17
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG13	34	0.17
(1,42)	1:38:A:VAL:HG11	1:35:A:TYR:HE2	23	0.17
(1,32)	1:16:A:GLN:HA	1:19:A:CYS:HB2	39	0.17
(1,8)	1:10:A:TYR:HE1	1:9:A:ASN:H	29	0.17
(1,1515)	1:3:A:GLU:HB3	1:3:A:GLU:H	30	0.16
(1,1312)	1:3:A:GLU:HB3	1:3:A:GLU:H	30	0.16
(1,995)	1:29:A:ALA:HB2	1:32:A:PRO:HG3	28	0.16
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	16	0.16
(1,663)	1:46:A:ASN:HB2	1:45:A:GLY:HA2	35	0.16
(1,663)	1:46:A:ASN:HB2	1:45:A:GLY:HA3	35	0.16
(1,663)	1:46:A:ASN:HB3	1:45:A:GLY:HA2	35	0.16
(1,663)	1:46:A:ASN:HB3	1:45:A:GLY:HA3	35	0.16
(1,618)	1:37:A:LEU:HD22	1:36:A:MET:HE2	22	0.16
(1,525)	1:38:A:VAL:HG13	1:39:A:PHE:H	18	0.16
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	32	0.16
(1,64)	1:33:A:ALA:HA	1:36:A:MET:HG2	40	0.16
(1,8)	1:10:A:TYR:HE2	1:9:A:ASN:H	8	0.16
(1,1515)	1:3:A:GLU:HB3	1:3:A:GLU:H	18	0.15
(1,1312)	1:3:A:GLU:HB3	1:3:A:GLU:H	18	0.15
(1,1207)	1:3:A:GLU:H	1:3:A:GLU:HG2	30	0.15
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	5	0.15
(1,251)	1:52:A:THR:HG23	1:56:A:LYS:HE3	39	0.15
(1,205)	1:37:A:LEU:HB2	1:34:A:ILE:HG12	7	0.15
(1,64)	1:33:A:ALA:HA	1:36:A:MET:HG3	7	0.15
(1,64)	1:35:A:TYR:HA	1:36:A:MET:HG3	27	0.15
(1,922)	1:32:A:PRO:HB2	1:29:A:ALA:HA	18	0.14
(1,922)	1:30:A:LEU:HB3	1:29:A:ALA:HA	27	0.14
(1,842)	1:55:A:ARG:HG2	1:54:A:PHE:HD1	34	0.14
(1,842)	1:55:A:ARG:HG2	1:54:A:PHE:HD2	34	0.14
(1,842)	1:55:A:ARG:HG3	1:54:A:PHE:HD1	34	0.14
(1,842)	1:55:A:ARG:HG3	1:54:A:PHE:HD2	34	0.14
(1,766)	1:51:A:TRP:HE3	1:52:A:THR:HG23	17	0.14
(1,525)	1:38:A:VAL:HG13	1:39:A:PHE:H	24	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,457)	1:18:A:GLU:HA	1:19:A:CYS:HB3	14	0.14
(1,255)	1:29:A:ALA:HA	1:30:A:LEU:HB3	27	0.14
(1,251)	1:52:A:THR:HG23	1:56:A:LYS:HE3	28	0.14
(1,170)	1:36:A:MET:HE2	1:39:A:PHE:H	10	0.14
(1,78)	1:13:A:ALA:HB3	1:9:A:ASN:HD21	17	0.14
(1,42)	1:38:A:VAL:HG22	1:35:A:TYR:HE2	12	0.14
(1,32)	1:18:A:GLU:HA	1:19:A:CYS:HB3	14	0.14
(1,1449)	1:25:A:LYS:HG2	1:25:A:LYS:H	27	0.13
(1,1449)	1:25:A:LYS:HG3	1:25:A:LYS:H	27	0.13
(1,1449)	1:25:A:LYS:HG2	1:25:A:LYS:H	31	0.13
(1,1449)	1:25:A:LYS:HG3	1:25:A:LYS:H	31	0.13
(1,1379)	1:22:A:THR:HG22	1:24:A:TRP:HE1	21	0.13
(1,1360)	1:30:A:LEU:HB3	1:31:A:ILE:H	24	0.13
(1,1223)	1:41:A:LEU:HG	1:41:A:LEU:H	40	0.13
(1,1207)	1:3:A:GLU:H	1:3:A:GLU:HG2	18	0.13
(1,497)	1:25:A:LYS:HG2	1:25:A:LYS:H	27	0.13
(1,497)	1:25:A:LYS:HG3	1:25:A:LYS:H	27	0.13
(1,497)	1:25:A:LYS:HG2	1:25:A:LYS:H	31	0.13
(1,497)	1:25:A:LYS:HG3	1:25:A:LYS:H	31	0.13
(1,428)	1:48:A:LEU:HG	1:48:A:LEU:H	26	0.13
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	37	0.13
(1,1502)	1:48:A:LEU:HB2	1:51:A:TRP:H	39	0.12
(1,1502)	1:48:A:LEU:HB3	1:51:A:TRP:H	39	0.12
(1,1449)	1:25:A:LYS:HG2	1:25:A:LYS:H	12	0.12
(1,1449)	1:25:A:LYS:HG3	1:25:A:LYS:H	12	0.12
(1,1449)	1:25:A:LYS:HG2	1:25:A:LYS:H	22	0.12
(1,1449)	1:25:A:LYS:HG3	1:25:A:LYS:H	22	0.12
(1,1223)	1:41:A:LEU:HG	1:41:A:LEU:H	6	0.12
(1,995)	1:29:A:ALA:HB1	1:32:A:PRO:HG2	27	0.12
(1,663)	1:46:A:ASN:HB2	1:45:A:GLY:HA2	26	0.12
(1,663)	1:46:A:ASN:HB2	1:45:A:GLY:HA3	26	0.12
(1,663)	1:46:A:ASN:HB3	1:45:A:GLY:HA2	26	0.12
(1,663)	1:46:A:ASN:HB3	1:45:A:GLY:HA3	26	0.12
(1,497)	1:25:A:LYS:HG2	1:25:A:LYS:H	12	0.12
(1,497)	1:25:A:LYS:HG3	1:25:A:LYS:H	12	0.12
(1,497)	1:25:A:LYS:HG2	1:25:A:LYS:H	22	0.12
(1,497)	1:25:A:LYS:HG3	1:25:A:LYS:H	22	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG11	10	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG12	10	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG13	10	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG21	10	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG22	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG23	10	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG11	10	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG12	10	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG13	10	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG21	10	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG22	10	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG23	10	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG11	30	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG12	30	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG13	30	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG21	30	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG22	30	0.12
(1,63)	1:48:A:LEU:HB2	1:49:A:VAL:HG23	30	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG11	30	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG12	30	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG13	30	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG21	30	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG22	30	0.12
(1,63)	1:48:A:LEU:HB3	1:49:A:VAL:HG23	30	0.12
(1,42)	1:38:A:VAL:HG13	1:35:A:TYR:HE2	5	0.12
(1,42)	1:38:A:VAL:HG11	1:35:A:TYR:HE2	8	0.12
(1,42)	1:31:A:ILE:HG23	1:35:A:TYR:HE1	27	0.12
(1,1449)	1:25:A:LYS:HG2	1:25:A:LYS:H	16	0.11
(1,1449)	1:25:A:LYS:HG3	1:25:A:LYS:H	16	0.11
(1,1223)	1:41:A:LEU:HG	1:41:A:LEU:H	28	0.11
(1,1165)	1:48:A:LEU:HD22	1:51:A:TRP:HE1	1	0.11
(1,1073)	1:35:A:TYR:HE2	1:36:A:MET:HA	16	0.11
(1,875)	1:25:A:LYS:HE3	1:22:A:THR:HB	32	0.11
(1,525)	1:38:A:VAL:HG11	1:39:A:PHE:H	7	0.11
(1,497)	1:25:A:LYS:HG2	1:25:A:LYS:H	16	0.11
(1,497)	1:25:A:LYS:HG3	1:25:A:LYS:H	16	0.11
(1,459)	1:34:A:ILE:HD11	1:30:A:LEU:HG	32	0.11
(1,459)	1:34:A:ILE:HD12	1:30:A:LEU:HG	32	0.11
(1,459)	1:34:A:ILE:HD13	1:30:A:LEU:HG	32	0.11
(1,1447)	1:57:A:LYS:HD2	1:57:A:LYS:H	29	0.1
(1,1447)	1:57:A:LYS:HD3	1:57:A:LYS:H	29	0.1
(1,1069)	1:38:A:VAL:HA	1:41:A:LEU:HB2	19	0.1
(1,1069)	1:38:A:VAL:HA	1:41:A:LEU:HB3	19	0.1
(1,884)	1:57:A:LYS:HD2	1:57:A:LYS:H	29	0.1
(1,884)	1:57:A:LYS:HD3	1:57:A:LYS:H	29	0.1
(1,495)	1:49:A:VAL:HG11	1:46:A:ASN:HA	38	0.1
(1,495)	1:49:A:VAL:HG12	1:46:A:ASN:HA	38	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,495)	1:49:A:VAL:HG13	1:46:A:ASN:HA	38	0.1
(1,495)	1:49:A:VAL:HG21	1:46:A:ASN:HA	38	0.1
(1,495)	1:49:A:VAL:HG22	1:46:A:ASN:HA	38	0.1
(1,495)	1:49:A:VAL:HG23	1:46:A:ASN:HA	38	0.1
(1,442)	1:10:A:TYR:HD2	1:11:A:TYR:HA	12	0.1
(1,407)	1:12:A:GLY:H	1:13:A:ALA:HA	25	0.1
(1,232)	1:49:A:VAL:HG11	1:46:A:ASN:HA	38	0.1
(1,232)	1:49:A:VAL:HG12	1:46:A:ASN:HA	38	0.1
(1,232)	1:49:A:VAL:HG13	1:46:A:ASN:HA	38	0.1
(1,232)	1:49:A:VAL:HG21	1:46:A:ASN:HA	38	0.1
(1,232)	1:49:A:VAL:HG22	1:46:A:ASN:HA	38	0.1
(1,232)	1:49:A:VAL:HG23	1:46:A:ASN:HA	38	0.1
(1,152)	1:57:A:LYS:HE2	1:57:A:LYS:HA	37	0.1
(1,152)	1:57:A:LYS:HE3	1:57:A:LYS:HA	37	0.1
(1,64)	1:33:A:ALA:HA	1:36:A:MET:HG2	32	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found