Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 05:50 PM EDT

PDB ID	:	2MOT
BMRB ID	:	17278
Title	:	Backbone Structure of Actin Depolymerizing Factor (ADF) of Toxoplasma gondii Based on Prot3DNMR Approach
Authors	:	Kumar, D.; Raikwal, N.; Raval, I.; Jaiswal, N.; Shukla, V.; Arora, A.
Deposited on	:	2014-05-05

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

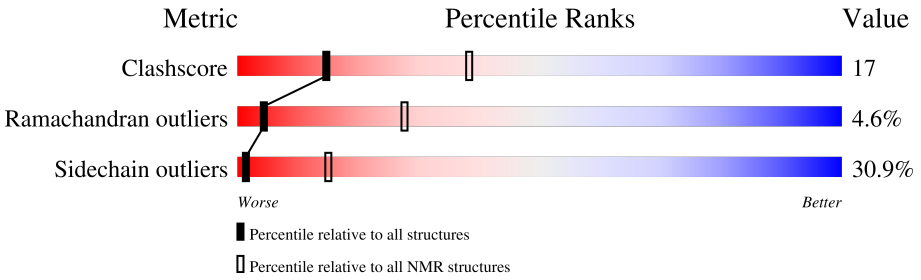
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 83%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	118	53% 36% 6% •

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:114 (113)	0.63	14

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

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

The models can be grouped into 3 clusters and 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1819 atoms, of which 914 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Actin depolymerizing factor ADF.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	118	1819	573	914	157	167	8	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Actin depolymerizing factor ADF

Chain A: 53% 36% 6% •

M1 A2 S3 G4 M5 G6 V7 R14 F15 L18 R21 K22 T23 V24 K25 W26 I27 V28 F29 K30 I31 E32 N33 T34 K35 I36 K40 D41 G42 K43 R50 L53 D57 C58 R59 F60 G61 V62 Y63 K68 L73 W74 C75 K82 P83 R84 M85 T86 Y87 A88

S89 S90 K91 L94 L95 K96 K97 L98 L106 E107 L114 A115 P116 L117 A118

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: Actin depolymerizing factor ADF

Chain A: 47% 36% 13% •

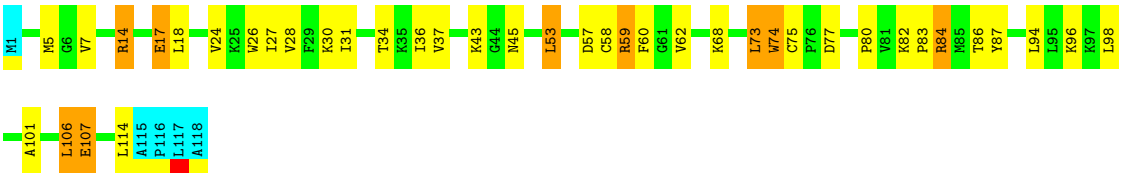
M1 A2 S3 V7 N10 R14 F15 N16 E17 L18 K19 K22 T23 V24 K25 W26 I27 V28 F29 K30 I31 E32 N33 T34 K35 I36 V37 V38 E39 K40 D41 G42 K43 G44 D47 E48 F49 R50 L53 D57 C58 R59 F60 G61 V62 N67 K68 I69 L73 K82

P83 R84 M85 T86 Y87 A88 S89 S90 K91 D92 A93 L94 L95 K96 K97 L98 D99 T102 L106 E107 D113 L114 A115 P116 L117 A118

4.2.2 Score per residue for model 2

• Molecule 1: Actin depolymerizing factor ADF

Chain A: 62% 26% 8% •



4.2.3 Score per residue for model 3

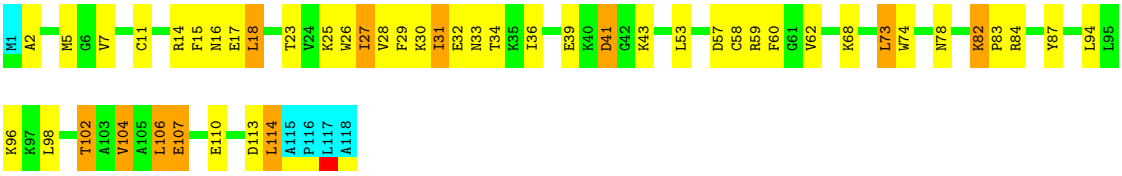
- Molecule 1: Actin depolymerizing factor ADF

Chain A: 58% 31% 7% •

4.2.4 Score per residue for model 4

- Molecule 1: Actin depolymerizing factor ADF

Chain A: 55% 31% 9% •



4.2.5 Score per residue for model 5

- Molecule 1: Actin depolymerizing factor ADF

Chain A: 53% 30% 13% •

4.2.6 Score per residue for model 6

- Molecule 1: Actin depolymerizing factor ADF

Chain A: 51% 40% 5% •

M1 A2 S3 G4 M5 G6 V7 R14 F15 N16 E17 L18 K19 T20 R21 K22 T23 V24 K25 W26 I27 K30 I31 T34 K35 I36 D41 G42 K43 G44 N45 A46 D47 R50 D57 C58 R59 V62 Y63 D64 N67 K68 I69 Q70 L73 W74 D77 K82 P83

R84 M85 T86 Y87 A88 K91 D92 A93 L94 L95 K96 K97 L98 A101 L106 E107 L114 A115 P116 L117 A118

4.2.7 Score per residue for model 7

- Molecule 1: Actin depolymerizing factor ADF

Chain A: 47% 36% 14% •

M1 A2 S3 G4 M5 G6 V7 D8 E9 N10 R14 F15 N16 E17 L18 T23 V24 K25 W26 I27 V28 F29 K30 I31 E32 N33 T34 K35 I36 V37 V38 E39 K40 D41 G42 K43 A46 F49 R50 D57 C58 R59 F60 G61 V62 Y63 D64 K68 I69 Q70 F71 V72 L73 W74

C75 N78 A79 K82 P83 R84 Y87 A88 S89 D92 A93 L94 L95 K96 K97 L98 A101 L106 E107 E110 L114 A115 P116 L117 A118

4.2.8 Score per residue for model 8

- Molecule 1: Actin depolymerizing factor ADF

Chain A: 44% 45% 7% •

M1 A2 M5 G6 V7 C11 R14 F15 V24 K25 W26 I27 V28 F29 K30 I31 E32 N33 T34 K35 I36 V37 V38 E39 K40 D41 G42 K43 G44 N45 A46 D47 E48 F49 R50 G51 A52 L53 D57 C58 R59 F60 G61 V62 Y63 N67 K68 I69 Q70 F71 V72 L73 W74 C75

K82 P83 R84 M85 T86 Y87 A88 S89 S90 K91 D92 A93 L94 L95 K96 K97 L98 D99 G100 A101 T102 A105 L106 E110 D113 L114 A115 P116 L117 A118

4.2.9 Score per residue for model 9

- Molecule 1: Actin depolymerizing factor ADF

Chain A: 51% 34% 11% •

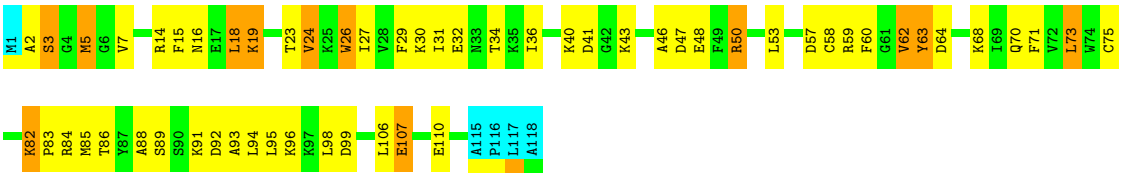
M1 A2 S3 V7 C11 V12 A13 R14 F15 L18 R21 K22 T23 V24 K25 W26 I27 V28 F29 K30 I31 T34 K35 I36 V37 V38 E39 K40 D41 G42 K43 G44 D47 E48 L53 P54 D57 C58 R59 F60 G61 V62 Y63 K68 F71 V72 L73 K82 P83

R84 Y87 A88 S89 S90 L94 L95 L98 D99 T102 A103 V104 A105 L106 D113 L114 A115 P116 L117 A118

4.2.10 Score per residue for model 10

- Molecule 1: Actin depolymerizing factor ADF

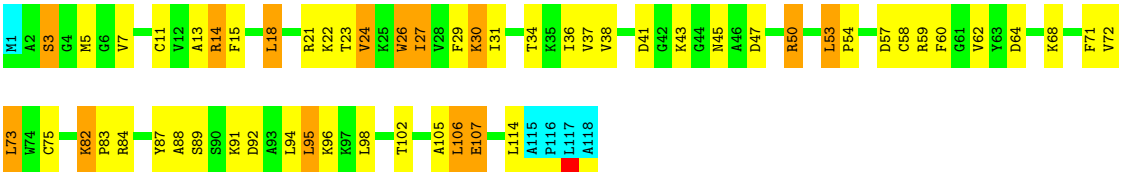
Chain A: 47% 38% 10% •



4.2.11 Score per residue for model 11

- Molecule 1: Actin depolymerizing factor ADF

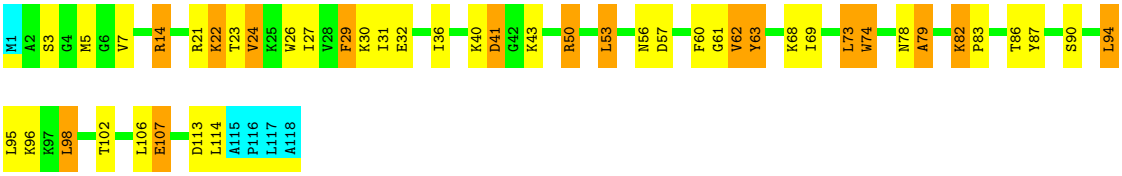
Chain A: 48% 36% 12% •



4.2.12 Score per residue for model 12

- Molecule 1: Actin depolymerizing factor ADF

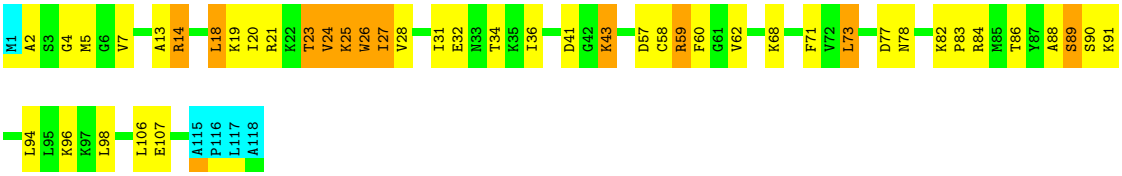
Chain A: 57% 25% 14% •



4.2.13 Score per residue for model 13

- Molecule 1: Actin depolymerizing factor ADF

Chain A: 58% 29% 9% •



4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Actin depolymerizing factor ADF

Chain A: 57% 31% 7%

M1 A2 S3 G4 M5 G6 V7 F15 N16 E17 L18 R21 V24 K25 W26 I27 K30 I31 E32 N33 T34 K35 I36 D41 R50 L53 D57 C58 R59 F60 Y63 D64 C65 K68 L73 D77 K82 P83 T86 Y87 K91 D92 L95 K96

K97 L98 A101 V104 A105 L106 E107 E110 D113 L114 A115 P116 L117 A118

4.2.15 Score per residue for model 15

- Molecule 1: Actin depolymerizing factor ADF

Chain A: 56% 31% 8%

M1 A2 S3 G4 M5 G6 V7 R14 F15 L18 R21 V24 K25 W26 I27 V28 F29 K30 I31 E32 N33 T34 K35 I36 D41 G42 K43 G44 D57 C58 R59 F60 G61 V62 Y63 K68 I69 Q70 L73 W74 C75 K82 P83 R84 M85 T86 Y87 A88 K91 D92

A93 L94 L95 K96 K97 L98 D99 V104 A105 L106 E107 A115 P116 L117 A118

4.2.16 Score per residue for model 16

- Molecule 1: Actin depolymerizing factor ADF

Chain A: 46% 39% 11%

M1 A2 S3 G4 M5 G6 V7 D8 E9 R14 F15 N16 E17 L18 R21 K22 T23 V24 K25 W26 I27 V28 F29 K30 I31 T34 K35 I36 K40 D41 G42 K43 G44 N45 A46 D47 E48 F49 A52 L53 D57 C58 R59 F60 G61 V62 K68 I69 L73 W74 C75 P76

D77 N78 A79 K82 P83 T86 Y87 A88 S89 S90 K91 D92 A93 L94 L95 K96 K97 L98 A101 L106 E107 M111 L114 A115 P116 L117 A118

4.2.17 Score per residue for model 17

- Molecule 1: Actin depolymerizing factor ADF

Chain A: 54% 34% 7%

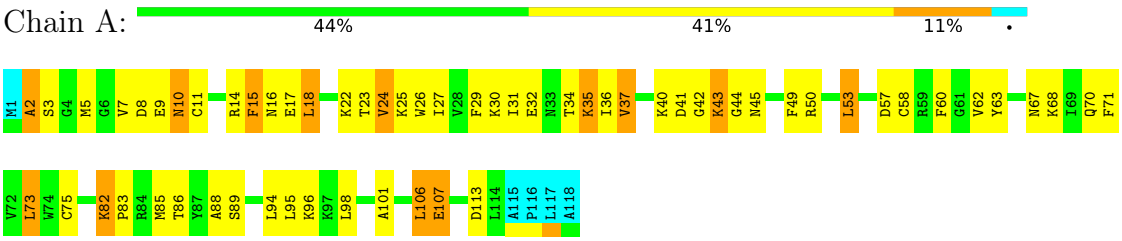
M1 M5 G6 V7 F15 N16 E17 L18 K22 T23 V24 K25 W26 I27 V28 F29 K30 I31 E32 N33 T34 K35 I36 K40 D41 G42 K43 A46 D47 E48 F49 R50 L53 C58 R59 F60 G61 V62 Y63 K68 I69 Q70 F71 V72 L73 W74 A79 K82 P83 R84

M85 T86 Y87 A88 A93 L94 L95 K96 K97 L98 T102 E107 M111 L114 A115 P116 L117 A118

4.2.18 Score per residue for model 18

- Molecule 1: Actin depolymerizing factor ADF

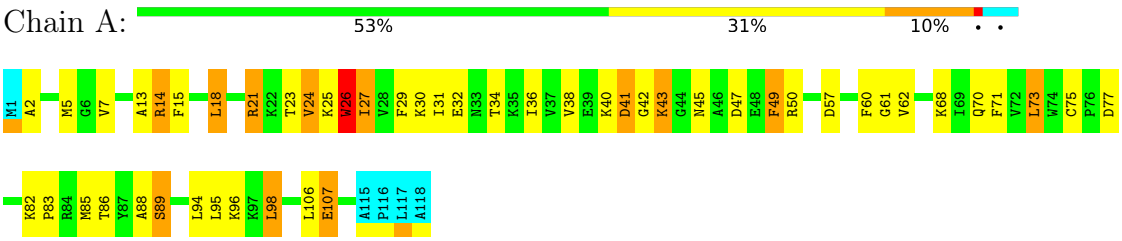
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Actin depolymerizing factor ADF

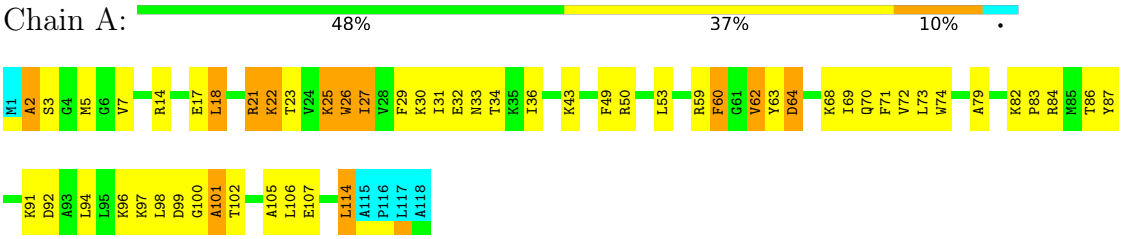
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Actin depolymerizing factor ADF

Chain A:



5 Refinement protocol and experimental data overview (i)

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

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

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

Software name	**Classification**	**Version**
CYANA	structure solution	2.1
CYANA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1308
Number of shifts mapped to atoms	1308
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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	872	877	877	30±5
All	All	17440	17540	17540	596

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ILE:HG21	1:A:94:LEU:HD21	0.92	1.40	20	12
1:A:24:VAL:HG13	1:A:24:VAL:O	0.86	1.69	19	1
1:A:62:VAL:HG11	1:A:98:LEU:HD22	0.85	1.45	15	8
1:A:23:THR:O	1:A:24:VAL:HG12	0.84	1.72	19	1
1:A:26:TRP:O	1:A:26:TRP:CG	0.76	2.38	13	10
1:A:73:LEU:N	1:A:73:LEU:HD13	0.75	1.95	11	10
1:A:23:THR:O	1:A:24:VAL:CG1	0.73	2.36	19	1
1:A:18:LEU:HD23	1:A:27:ILE:CD1	0.73	2.14	20	7
1:A:29:PHE:CE2	1:A:31:ILE:HG23	0.72	2.19	12	1
1:A:62:VAL:HG12	1:A:69:ILE:HG21	0.72	1.58	8	2
1:A:73:LEU:C	1:A:73:LEU:HD22	0.70	2.06	6	5
1:A:90:SER:O	1:A:94:LEU:HD22	0.69	1.88	12	5
1:A:95:LEU:HA	1:A:98:LEU:HD12	0.69	1.64	8	9
1:A:2:ALA:HB1	1:A:89:SER:CB	0.68	2.19	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:VAL:HG11	1:A:98:LEU:CD2	0.67	2.19	20	6
1:A:72:VAL:C	1:A:73:LEU:HD13	0.67	2.09	11	1
1:A:31:ILE:HD11	1:A:87:TYR:CG	0.67	2.24	12	2
1:A:23:THR:O	1:A:24:VAL:CB	0.66	2.43	19	7
1:A:15:PHE:CE1	1:A:98:LEU:HD23	0.66	2.24	5	4
1:A:53:LEU:HD11	1:A:114:LEU:HD22	0.66	1.67	20	1
1:A:60:PHE:CD2	1:A:73:LEU:HD11	0.66	2.26	8	2
1:A:40:LYS:HD3	1:A:52:ALA:HB1	0.65	1.68	16	1
1:A:98:LEU:HD12	1:A:101:ALA:CB	0.64	2.23	3	1
1:A:18:LEU:HD12	1:A:64:ASP:N	0.64	2.06	10	1
1:A:18:LEU:HD23	1:A:27:ILE:HD13	0.64	1.68	20	8
1:A:4:GLY:O	1:A:34:THR:HG23	0.64	1.93	6	2
1:A:24:VAL:HG13	1:A:63:TYR:HB3	0.64	1.68	15	3
1:A:73:LEU:HD11	1:A:87:TYR:CD1	0.64	2.27	9	1
1:A:28:VAL:HG13	1:A:60:PHE:O	0.63	1.94	8	7
1:A:53:LEU:HD22	1:A:53:LEU:C	0.63	2.14	14	1
1:A:2:ALA:HB1	1:A:89:SER:HB2	0.62	1.71	7	3
1:A:60:PHE:CE2	1:A:73:LEU:HD11	0.62	2.28	8	1
1:A:31:ILE:HD11	1:A:87:TYR:CD1	0.62	2.29	4	5
1:A:21:ARG:HB3	1:A:23:THR:HG22	0.62	1.71	19	2
1:A:73:LEU:HD22	1:A:73:LEU:H	0.62	1.55	11	1
1:A:7:VAL:HA	1:A:36:ILE:HD12	0.61	1.72	4	18
1:A:2:ALA:HB2	1:A:86:THR:HA	0.61	1.72	16	4
1:A:31:ILE:HG22	1:A:36:ILE:HG12	0.60	1.72	8	15
1:A:53:LEU:HD13	1:A:54:PRO:HD2	0.60	1.73	5	3
1:A:53:LEU:HD21	1:A:59:ARG:HB3	0.60	1.72	9	1
1:A:23:THR:C	1:A:24:VAL:HG13	0.60	2.18	17	1
1:A:29:PHE:CE1	1:A:94:LEU:HD12	0.59	2.33	19	2
1:A:14:ARG:CB	1:A:27:ILE:HG21	0.59	2.28	7	3
1:A:68:LYS:C	1:A:69:ILE:HD12	0.59	2.18	5	1
1:A:60:PHE:HB3	1:A:73:LEU:HD12	0.58	1.74	12	1
1:A:71:PHE:CE1	1:A:95:LEU:HD21	0.58	2.33	9	6
1:A:2:ALA:HB1	1:A:89:SER:HB3	0.58	1.74	16	3
1:A:72:VAL:HG13	1:A:74:TRP:CZ2	0.58	2.33	20	1
1:A:71:PHE:CE1	1:A:105:ALA:HB2	0.58	2.33	11	2
1:A:69:ILE:HD13	1:A:99:ASP:O	0.58	1.99	5	2
1:A:95:LEU:HA	1:A:98:LEU:HD11	0.58	1.76	7	1
1:A:98:LEU:HD22	1:A:101:ALA:HB2	0.57	1.75	7	1
1:A:25:LYS:O	1:A:26:TRP:C	0.57	2.43	1	4
1:A:31:ILE:CG2	1:A:94:LEU:HD11	0.57	2.29	4	6
1:A:27:ILE:HD12	1:A:62:VAL:HG23	0.57	1.76	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:VAL:O	1:A:24:VAL:CG1	0.57	2.43	19	1
1:A:29:PHE:CD1	1:A:29:PHE:C	0.57	2.78	12	1
1:A:82:LYS:CB	1:A:83:PRO:CD	0.56	2.83	9	20
1:A:62:VAL:CG1	1:A:69:ILE:HG21	0.56	2.30	8	3
1:A:14:ARG:HA	1:A:27:ILE:HG21	0.56	1.77	1	3
1:A:73:LEU:HD22	1:A:73:LEU:O	0.56	2.00	7	14
1:A:18:LEU:HD23	1:A:19:LYS:N	0.56	2.15	10	1
1:A:24:VAL:HG22	1:A:63:TYR:HB2	0.56	1.76	14	2
1:A:73:LEU:CD2	1:A:73:LEU:N	0.56	2.69	9	1
1:A:95:LEU:HD23	1:A:101:ALA:HB1	0.56	1.77	18	1
1:A:49:PHE:O	1:A:53:LEU:HD12	0.55	2.01	18	1
1:A:62:VAL:HG13	1:A:98:LEU:HD22	0.55	1.76	16	4
1:A:82:LYS:O	1:A:86:THR:HG22	0.55	2.01	12	2
1:A:2:ALA:N	1:A:86:THR:HG23	0.55	2.16	16	2
1:A:5:MET:CG	1:A:93:ALA:HB2	0.55	2.31	15	2
1:A:53:LEU:HD11	1:A:114:LEU:CD2	0.55	2.32	20	1
1:A:14:ARG:HD3	1:A:27:ILE:HG21	0.55	1.78	4	4
1:A:29:PHE:CE2	1:A:94:LEU:HD12	0.55	2.37	3	5
1:A:102:THR:OG1	1:A:104:VAL:HG12	0.55	2.02	9	2
1:A:62:VAL:HG13	1:A:71:PHE:CZ	0.54	2.38	17	1
1:A:60:PHE:C	1:A:60:PHE:CD1	0.54	2.80	12	2
1:A:27:ILE:HD12	1:A:62:VAL:O	0.54	2.03	13	8
1:A:74:TRP:CZ3	1:A:114:LEU:HD22	0.54	2.38	4	1
1:A:18:LEU:HD11	1:A:64:ASP:HB2	0.54	1.79	6	1
1:A:24:VAL:HG13	1:A:63:TYR:HB2	0.54	1.79	8	1
1:A:28:VAL:HG11	1:A:53:LEU:CD2	0.54	2.33	9	1
1:A:24:VAL:HG22	1:A:63:TYR:CB	0.54	2.33	10	1
1:A:24:VAL:HG13	1:A:63:TYR:CB	0.54	2.32	15	1
1:A:5:MET:CE	1:A:93:ALA:HB2	0.53	2.34	10	1
1:A:53:LEU:HD22	1:A:53:LEU:O	0.53	2.02	14	1
1:A:50:ARG:O	1:A:114:LEU:HD13	0.53	2.04	8	1
1:A:24:VAL:HG22	1:A:24:VAL:O	0.53	2.02	18	1
1:A:21:ARG:O	1:A:22:LYS:CB	0.53	2.57	20	1
1:A:73:LEU:N	1:A:73:LEU:CD1	0.53	2.66	11	10
1:A:84:ARG:O	1:A:88:ALA:HB2	0.53	2.03	11	4
1:A:18:LEU:HD21	1:A:64:ASP:CB	0.52	2.34	6	1
1:A:18:LEU:O	1:A:18:LEU:HD13	0.52	2.05	6	1
1:A:73:LEU:C	1:A:73:LEU:CD2	0.52	2.79	6	4
1:A:13:ALA:HB3	1:A:14:ARG:NH1	0.52	2.20	13	1
1:A:85:MET:O	1:A:88:ALA:HB3	0.52	2.05	15	8
1:A:62:VAL:HG11	1:A:98:LEU:HG	0.52	1.80	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:THR:O	1:A:24:VAL:HB	0.51	2.05	18	8
1:A:50:ARG:HA	1:A:114:LEU:HD22	0.51	1.82	17	1
1:A:31:ILE:HD12	1:A:86:THR:HG22	0.51	1.81	18	2
1:A:23:THR:HG23	1:A:43:LYS:HD2	0.51	1.83	19	1
1:A:14:ARG:CD	1:A:27:ILE:HG21	0.51	2.36	9	3
1:A:53:LEU:HD12	1:A:74:TRP:CD1	0.51	2.40	16	1
1:A:2:ALA:H	1:A:86:THR:HG23	0.51	1.64	19	3
1:A:104:VAL:HG13	1:A:104:VAL:O	0.51	2.06	9	2
1:A:29:PHE:CZ	1:A:31:ILE:HG23	0.51	2.41	12	1
1:A:26:TRP:O	1:A:26:TRP:CD1	0.51	2.63	15	2
1:A:63:TYR:CG	1:A:63:TYR:O	0.50	2.65	8	1
1:A:106:LEU:HD13	1:A:107:GLU:N	0.50	2.22	4	10
1:A:106:LEU:HD12	1:A:107:GLU:N	0.50	2.22	12	5
1:A:27:ILE:HG23	1:A:41:ASP:HB3	0.50	1.82	1	2
1:A:98:LEU:HD12	1:A:101:ALA:HB2	0.50	1.83	3	1
1:A:14:ARG:CZ	1:A:38:VAL:HG11	0.50	2.37	8	4
1:A:15:PHE:CD1	1:A:15:PHE:N	0.49	2.78	1	4
1:A:49:PHE:O	1:A:53:LEU:HD23	0.49	2.07	16	2
1:A:27:ILE:HG23	1:A:41:ASP:HB2	0.49	1.84	17	2
1:A:31:ILE:HG22	1:A:36:ILE:CG1	0.49	2.37	6	2
1:A:52:ALA:O	1:A:53:LEU:HD23	0.49	2.08	8	1
1:A:62:VAL:CG1	1:A:98:LEU:HD22	0.49	2.37	10	3
1:A:53:LEU:HD12	1:A:74:TRP:NE1	0.49	2.23	12	1
1:A:111:MET:HA	1:A:114:LEU:HD12	0.49	1.85	16	1
1:A:25:LYS:HB3	1:A:27:ILE:HD11	0.48	1.84	17	2
1:A:27:ILE:HG23	1:A:41:ASP:CB	0.48	2.39	9	1
1:A:62:VAL:CG1	1:A:98:LEU:HD23	0.48	2.38	7	1
1:A:24:VAL:HG12	1:A:24:VAL:O	0.48	2.08	10	3
1:A:60:PHE:CD1	1:A:73:LEU:HD12	0.48	2.44	4	1
1:A:31:ILE:HG22	1:A:94:LEU:HD11	0.48	1.85	20	1
1:A:83:PRO:O	1:A:87:TYR:N	0.48	2.47	16	3
1:A:7:VAL:O	1:A:7:VAL:HG23	0.48	2.09	5	5
1:A:73:LEU:HD22	1:A:87:TYR:CE2	0.47	2.44	17	1
1:A:18:LEU:HD23	1:A:27:ILE:HD11	0.47	1.84	5	1
1:A:73:LEU:N	1:A:73:LEU:HD22	0.47	2.24	11	1
1:A:73:LEU:HD21	1:A:107:GLU:HB3	0.47	1.84	10	3
1:A:62:VAL:CG1	1:A:98:LEU:HD13	0.47	2.39	11	1
1:A:53:LEU:HD22	1:A:74:TRP:CE2	0.47	2.44	20	1
1:A:5:MET:HG2	1:A:93:ALA:HB2	0.47	1.86	6	1
1:A:29:PHE:CD1	1:A:60:PHE:CE2	0.47	3.02	12	1
1:A:21:ARG:O	1:A:22:LYS:HB2	0.47	2.10	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:LEU:HD22	1:A:94:LEU:H	0.47	1.70	20	2
1:A:49:PHE:CE1	1:A:53:LEU:HD13	0.47	2.44	17	1
1:A:29:PHE:CE2	1:A:60:PHE:CD1	0.46	3.03	20	2
1:A:24:VAL:HG23	1:A:63:TYR:HB3	0.46	1.86	12	1
1:A:23:THR:HG22	1:A:24:VAL:HG12	0.46	1.88	3	2
1:A:11:CYS:HB3	1:A:36:ILE:HG21	0.46	1.88	8	3
1:A:23:THR:O	1:A:24:VAL:HG22	0.46	2.09	17	1
1:A:62:VAL:HG11	1:A:98:LEU:CG	0.46	2.41	19	1
1:A:106:LEU:HD13	1:A:107:GLU:H	0.46	1.70	3	8
1:A:30:LYS:CG	1:A:37:VAL:HG23	0.46	2.41	5	1
1:A:25:LYS:O	1:A:26:TRP:O	0.46	2.34	13	1
1:A:5:MET:SD	1:A:93:ALA:HB2	0.46	2.51	17	4
1:A:10:ASN:OD1	1:A:38:VAL:HG12	0.45	2.11	7	2
1:A:24:VAL:O	1:A:24:VAL:HG22	0.45	2.12	13	4
1:A:60:PHE:CD1	1:A:60:PHE:N	0.45	2.83	8	1
1:A:73:LEU:H	1:A:73:LEU:HD13	0.45	1.71	7	3
1:A:58:CYS:SG	1:A:73:LEU:HD23	0.45	2.51	7	1
1:A:73:LEU:N	1:A:73:LEU:HD23	0.45	2.26	9	1
1:A:28:VAL:HG12	1:A:59:ARG:HG2	0.45	1.88	2	2
1:A:53:LEU:CD1	1:A:53:LEU:N	0.45	2.80	14	1
1:A:30:LYS:HG3	1:A:37:VAL:HG23	0.45	1.88	2	2
1:A:62:VAL:HG11	1:A:98:LEU:HD13	0.45	1.87	11	1
1:A:71:PHE:O	1:A:71:PHE:CG	0.45	2.70	13	1
1:A:59:ARG:O	1:A:73:LEU:HD12	0.45	2.12	16	1
1:A:27:ILE:CD1	1:A:62:VAL:HG23	0.45	2.42	1	2
1:A:73:LEU:HD22	1:A:106:LEU:O	0.45	2.11	11	1
1:A:13:ALA:HB3	1:A:14:ARG:CZ	0.44	2.42	13	2
1:A:82:LYS:CB	1:A:83:PRO:HD3	0.44	2.42	9	18
1:A:100:GLY:O	1:A:102:THR:HG23	0.44	2.12	20	2
1:A:22:LYS:O	1:A:22:LYS:CG	0.44	2.66	1	4
1:A:60:PHE:CB	1:A:73:LEU:HD12	0.44	2.42	12	1
1:A:74:TRP:CZ2	1:A:114:LEU:HD11	0.44	2.48	12	1
1:A:53:LEU:C	1:A:53:LEU:CD2	0.44	2.86	14	1
1:A:62:VAL:HG12	1:A:69:ILE:CG2	0.44	2.42	20	1
1:A:24:VAL:O	1:A:24:VAL:CG2	0.44	2.63	17	1
1:A:14:ARG:HB3	1:A:27:ILE:HG21	0.44	1.88	15	1
1:A:98:LEU:HD13	1:A:101:ALA:HB3	0.44	1.90	7	1
1:A:71:PHE:CZ	1:A:105:ALA:HB2	0.43	2.48	9	1
1:A:23:THR:C	1:A:24:VAL:CG1	0.43	2.86	17	1
1:A:15:PHE:HA	1:A:18:LEU:HD22	0.43	1.89	10	1
1:A:74:TRP:CE2	1:A:114:LEU:HD11	0.43	2.48	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:THR:HG23	1:A:87:TYR:N	0.43	2.28	14	2
1:A:40:LYS:CD	1:A:52:ALA:HB1	0.43	2.40	16	1
1:A:104:VAL:O	1:A:104:VAL:HG22	0.43	2.14	9	2
1:A:53:LEU:HD12	1:A:74:TRP:HE1	0.43	1.74	12	1
1:A:68:LYS:HD3	1:A:104:VAL:HG11	0.43	1.91	14	1
1:A:14:ARG:HD2	1:A:29:PHE:CD1	0.43	2.49	16	1
1:A:69:ILE:HB	1:A:101:ALA:HB2	0.43	1.90	20	1
1:A:15:PHE:O	1:A:18:LEU:HD23	0.43	2.14	10	1
1:A:69:ILE:HD12	1:A:69:ILE:N	0.43	2.29	1	1
1:A:17:GLU:CB	1:A:25:LYS:HG2	0.43	2.43	6	1
1:A:71:PHE:O	1:A:105:ALA:HB1	0.43	2.14	20	1
1:A:17:GLU:HB3	1:A:25:LYS:HG2	0.43	1.90	6	1
1:A:95:LEU:HD23	1:A:101:ALA:CB	0.43	2.43	18	1
1:A:24:VAL:HG22	1:A:63:TYR:HB3	0.42	1.90	10	1
1:A:24:VAL:O	1:A:24:VAL:HG12	0.42	2.14	8	1
1:A:74:TRP:CZ3	1:A:114:LEU:HD11	0.42	2.49	8	1
1:A:13:ALA:HB3	1:A:14:ARG:NH2	0.42	2.29	9	3
1:A:71:PHE:CE2	1:A:98:LEU:HD13	0.42	2.49	17	1
1:A:106:LEU:HD12	1:A:107:GLU:H	0.42	1.74	19	1
1:A:24:VAL:HG22	1:A:26:TRP:CE3	0.42	2.48	19	1
1:A:69:ILE:O	1:A:69:ILE:HG22	0.42	2.15	5	1
1:A:18:LEU:HD21	1:A:64:ASP:HB3	0.42	1.91	6	1
1:A:78:ASN:O	1:A:79:ALA:HB2	0.42	2.14	7	2
1:A:10:ASN:CG	1:A:37:VAL:HA	0.42	2.34	18	1
1:A:72:VAL:HG22	1:A:106:LEU:CB	0.42	2.45	3	2
1:A:62:VAL:HG13	1:A:69:ILE:HG21	0.42	1.89	16	1
1:A:36:ILE:CG2	1:A:37:VAL:N	0.42	2.82	18	1
1:A:29:PHE:HE1	1:A:62:VAL:HG13	0.42	1.74	1	1
1:A:52:ALA:O	1:A:53:LEU:HD22	0.42	2.15	16	1
1:A:7:VAL:HG23	1:A:7:VAL:O	0.42	2.15	1	4
1:A:73:LEU:HD23	1:A:73:LEU:H	0.42	1.73	9	1
1:A:17:GLU:CB	1:A:27:ILE:HG12	0.42	2.45	1	2
1:A:71:PHE:HE1	1:A:95:LEU:HD21	0.42	1.75	7	2
1:A:91:LYS:HA	1:A:91:LYS:CE	0.41	2.45	15	1
1:A:15:PHE:HA	1:A:18:LEU:HD23	0.41	1.90	18	1
1:A:7:VAL:HG12	1:A:97:LYS:HD3	0.41	1.91	5	1
1:A:21:ARG:CB	1:A:25:LYS:HB2	0.41	2.44	20	1
1:A:26:TRP:O	1:A:26:TRP:CD2	0.41	2.71	13	2
1:A:14:ARG:O	1:A:27:ILE:HD13	0.41	2.15	6	1
1:A:62:VAL:HG11	1:A:98:LEU:HD23	0.41	1.92	7	1
1:A:32:GLU:CG	1:A:35:LYS:HB3	0.41	2.45	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:PHE:CE1	1:A:53:LEU:HD11	0.41	2.51	8	1
1:A:73:LEU:HD11	1:A:87:TYR:OH	0.41	2.15	14	1
1:A:36:ILE:O	1:A:37:VAL:HG13	0.41	2.15	1	1
1:A:98:LEU:HD13	1:A:101:ALA:CB	0.41	2.45	6	2
1:A:82:LYS:HB3	1:A:83:PRO:CD	0.41	2.46	13	2
1:A:10:ASN:HD22	1:A:11:CYS:N	0.41	2.14	18	1
1:A:27:ILE:O	1:A:61:GLY:HA2	0.41	2.16	19	2
1:A:62:VAL:HG13	1:A:71:PHE:CE2	0.41	2.50	17	1
1:A:49:PHE:CD1	1:A:49:PHE:C	0.41	2.92	19	1
1:A:28:VAL:HG22	1:A:49:PHE:CE1	0.41	2.51	7	1
1:A:73:LEU:CD1	1:A:73:LEU:N	0.41	2.84	13	1
1:A:32:GLU:N	1:A:35:LYS:O	0.41	2.54	18	1
1:A:6:GLY:O	1:A:36:ILE:HD12	0.41	2.16	6	1
1:A:29:PHE:CE1	1:A:62:VAL:HG22	0.41	2.50	18	1
1:A:94:LEU:H	1:A:94:LEU:HD22	0.41	1.76	7	1
1:A:21:ARG:O	1:A:22:LYS:CG	0.41	2.69	11	1
1:A:94:LEU:N	1:A:94:LEU:HD13	0.41	2.31	16	2
1:A:82:LYS:HB3	1:A:83:PRO:HD3	0.41	1.93	13	1
1:A:49:PHE:CZ	1:A:53:LEU:HD11	0.41	2.50	1	1
1:A:62:VAL:CG1	1:A:98:LEU:CD2	0.41	2.99	1	1
1:A:53:LEU:HD11	1:A:74:TRP:HD1	0.40	1.75	2	1
1:A:38:VAL:HG21	1:A:41:ASP:OD2	0.40	2.16	19	1
1:A:73:LEU:HD13	1:A:73:LEU:H	0.40	1.75	1	1
1:A:74:TRP:CE3	1:A:114:LEU:HD22	0.40	2.52	4	1
1:A:104:VAL:HG22	1:A:104:VAL:O	0.40	2.17	15	1
1:A:80:PRO:O	1:A:84:ARG:N	0.40	2.55	2	1
1:A:53:LEU:N	1:A:53:LEU:HD13	0.40	2.31	14	1
1:A:73:LEU:HD13	1:A:87:TYR:CZ	0.40	2.52	17	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	113/118 (96%)	89±2 (79±2%)	19±2 (17±2%)	5±2 (5±2%)	4 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2260/2360 (96%)	1783 (79%)	373 (17%)	104 (5%)	4 27

All 18 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	24	VAL	18
1	A	26	TRP	17
1	A	43	LYS	10
1	A	41	ASP	9
1	A	2	ALA	6
1	A	44	GLY	6
1	A	3	SER	5
1	A	42	GLY	5
1	A	98	LEU	5
1	A	102	THR	5
1	A	79	ALA	5
1	A	101	ALA	3
1	A	64	ASP	3
1	A	45	ASN	3
1	A	4	GLY	1
1	A	104	VAL	1
1	A	22	LYS	1
1	A	33	ASN	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	92/95 (97%)	64±4 (69±4%)	28±4 (31±4%)	1 15
All	All	1840/1900 (97%)	1272 (69%)	568 (31%)	1 15

All 73 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	68	LYS	20

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Mol	Chain	Res	Type	Models (Total)
1	A	73	LEU	19
1	A	57	ASP	18
1	A	96	LYS	18
1	A	34	THR	17
1	A	5	MET	17
1	A	43	LYS	16
1	A	107	GLU	16
1	A	30	LYS	15
1	A	58	CYS	14
1	A	106	LEU	14
1	A	27	ILE	14
1	A	32	GLU	13
1	A	59	ARG	13
1	A	82	LYS	12
1	A	18	LEU	12
1	A	3	SER	11
1	A	14	ARG	11
1	A	25	LYS	11
1	A	40	LYS	11
1	A	114	LEU	11
1	A	75	CYS	11
1	A	91	LYS	11
1	A	15	PHE	10
1	A	50	ARG	10
1	A	60	PHE	10
1	A	87	TYR	10
1	A	53	LEU	10
1	A	63	TYR	10
1	A	92	ASP	9
1	A	41	ASP	9
1	A	99	ASP	8
1	A	62	VAL	8
1	A	21	ARG	8
1	A	70	GLN	8
1	A	22	LYS	7
1	A	17	GLU	7
1	A	77	ASP	7
1	A	89	SER	7
1	A	16	ASN	7
1	A	47	ASP	6
1	A	113	ASP	6
1	A	74	TRP	6

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Mol	Chain	Res	Type	Models (Total)
1	A	84	ARG	6
1	A	23	THR	6
1	A	67	ASN	5
1	A	94	LEU	5
1	A	45	ASN	5
1	A	98	LEU	5
1	A	110	GLU	5
1	A	19	LYS	4
1	A	9	GLU	4
1	A	97	LYS	4
1	A	111	MET	3
1	A	78	ASN	3
1	A	64	ASP	3
1	A	39	GLU	2
1	A	31	ILE	2
1	A	26	TRP	2
1	A	35	LYS	2
1	A	48	GLU	2
1	A	11	CYS	1
1	A	33	ASN	1
1	A	95	LEU	1
1	A	29	PHE	1
1	A	56	ASN	1
1	A	20	ILE	1
1	A	65	CYS	1
1	A	24	VAL	1
1	A	8	ASP	1
1	A	10	ASN	1
1	A	37	VAL	1
1	A	49	PHE	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	1308
Number of shifts mapped to atoms	1308
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	116	-0.26 ± 0.21	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	107	0.10 ± 0.16	None needed (< 0.5 ppm)
$^{13}C'$	116	0.35 ± 0.19	None needed (< 0.5 ppm)
^{15}N	107	0.79 ± 0.61	None needed (imprecise)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 83%, i.e. 1257 atoms were assigned a chemical shift out of a possible 1513. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	539/566 (95%)	214/231 (93%)	222/226 (98%)	103/109 (94%)
Sidechain	665/848 (78%)	450/549 (82%)	213/264 (81%)	2/35 (6%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	53/99 (54%)	31/49 (63%)	22/47 (47%)	0/3 (0%)
Overall	1257/1513 (83%)	695/829 (84%)	457/537 (85%)	105/147 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1307 atoms were assigned a chemical shift out of a possible 1576. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	559/589 (95%)	220/240 (92%)	232/236 (98%)	107/113 (95%)
Sidechain	695/888 (78%)	469/577 (81%)	224/276 (81%)	2/35 (6%)
Aromatic	53/99 (54%)	31/49 (63%)	22/47 (47%)	0/3 (0%)
Overall	1307/1576 (83%)	720/866 (83%)	478/559 (86%)	109/151 (72%)

7.1.4 Statistically unusual chemical shifts (i)

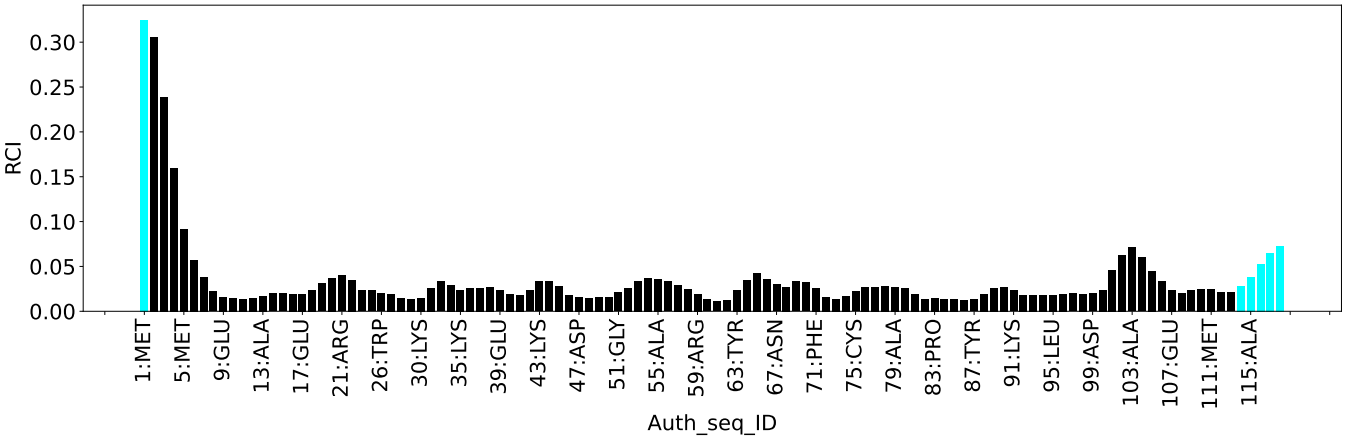
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	49	PHE	CD1	118.04	125.33 – 137.83	-10.8
1	A	61	GLY	HA2	5.96	2.15 – 5.77	5.5
1	A	59	ARG	CD	38.10	38.57 – 47.75	-5.5
1	A	49	PHE	CE1	124.05	124.17 – 137.29	-5.1

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.30
0.25
0.20
0.15
0.10
0.05
0.00
1:MET
5:MET
9:GLU
13:ALA
17:GLU
21:ARG
26:TRP
30:LYS
35:LYS
39:GLU
43:LYS
47:ASP
51:GLY
55:ALA
59:ARG
63:TYR
67:ASN
71:PHE
75:CYS
79:ALA
83:PRO
87:TYR
91:LYS
95:LEU
99:ASP
103:ALA
107:GLU
111:MET
115:ALA
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	1168
Intra-residue (|i-j|=0)	1
Sequential (|i-j|=1)	516
Medium range (|i-j|>1 and |i-j|<5)	329
Long range (|i-j|≥5)	322
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	9.9
Number of long range restraints per residue[1]	2.7

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

8.2 Residual restraint violations (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	28.4	0.2
0.2-0.5 (Medium)	6.6	0.49
>0.5 (Large)	2.6	4.04

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

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

9 Distance violation analysis (i)

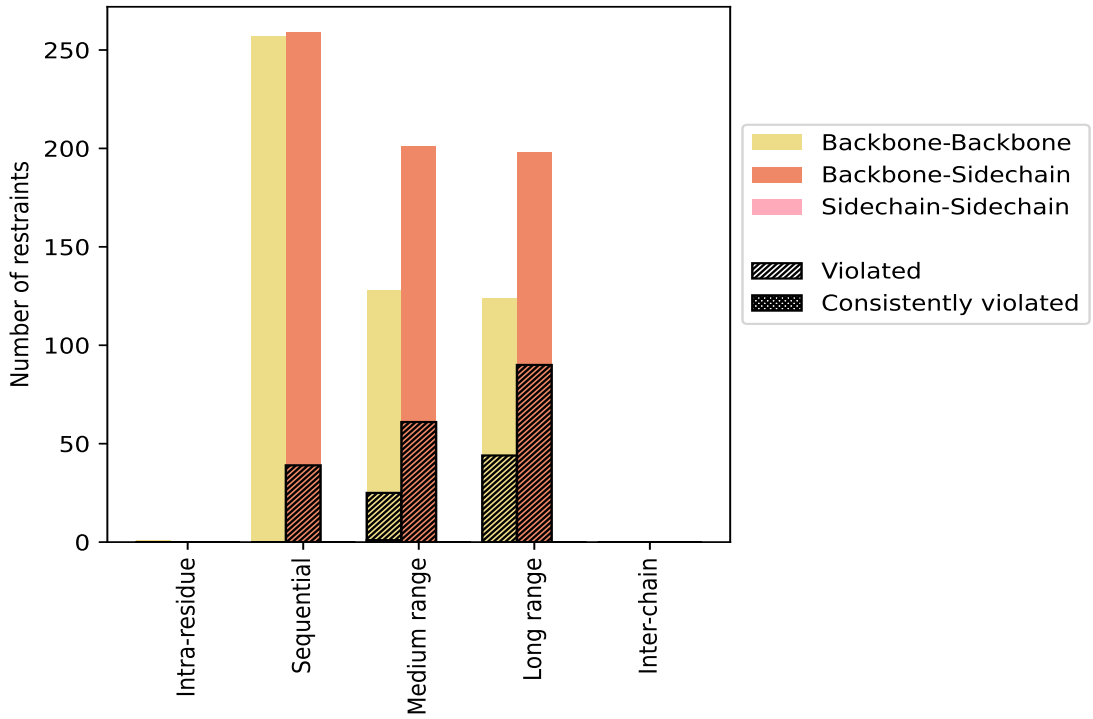
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	516	44.2	39	7.6	3.3	0	0.0	0.0
Backbone-Backbone	257	22.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	259	22.2	39	15.1	3.3	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	329	28.2	86	26.1	7.4	1	0.3	0.1
Backbone-Backbone	128	11.0	25	19.5	2.1	1	0.8	0.1
Backbone-Sidechain	201	17.2	61	30.3	5.2	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	322	27.6	134	41.6	11.5	0	0.0	0.0
Backbone-Backbone	124	10.6	44	35.5	3.8	0	0.0	0.0
Backbone-Sidechain	198	17.0	90	45.5	7.7	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	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	1168	100.0	259	22.2	22.2	1	0.1	0.1
Backbone-Backbone	510	43.7	69	13.5	5.9	1	0.2	0.1
Backbone-Sidechain	658	56.3	190	28.9	16.3	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	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	14	22	0	43	0.22	0.92	0.15	0.15
2	0	1	10	13	0	24	0.23	0.9	0.23	0.13
3	0	2	6	13	0	21	0.4	3.69	0.77	0.14
4	0	3	12	15	0	30	0.18	1.04	0.17	0.13
5	0	3	13	16	0	32	0.18	1.02	0.18	0.12
6	0	5	18	25	0	48	0.21	1.08	0.2	0.14
7	0	0	9	17	0	26	0.2	0.8	0.15	0.15
8	0	5	15	23	0	43	0.2	0.81	0.13	0.15
9	0	4	14	20	0	38	0.2	0.76	0.14	0.14
10	0	1	15	28	0	44	0.29	4.03	0.59	0.16
11	0	5	10	19	0	34	0.22	1.08	0.2	0.15

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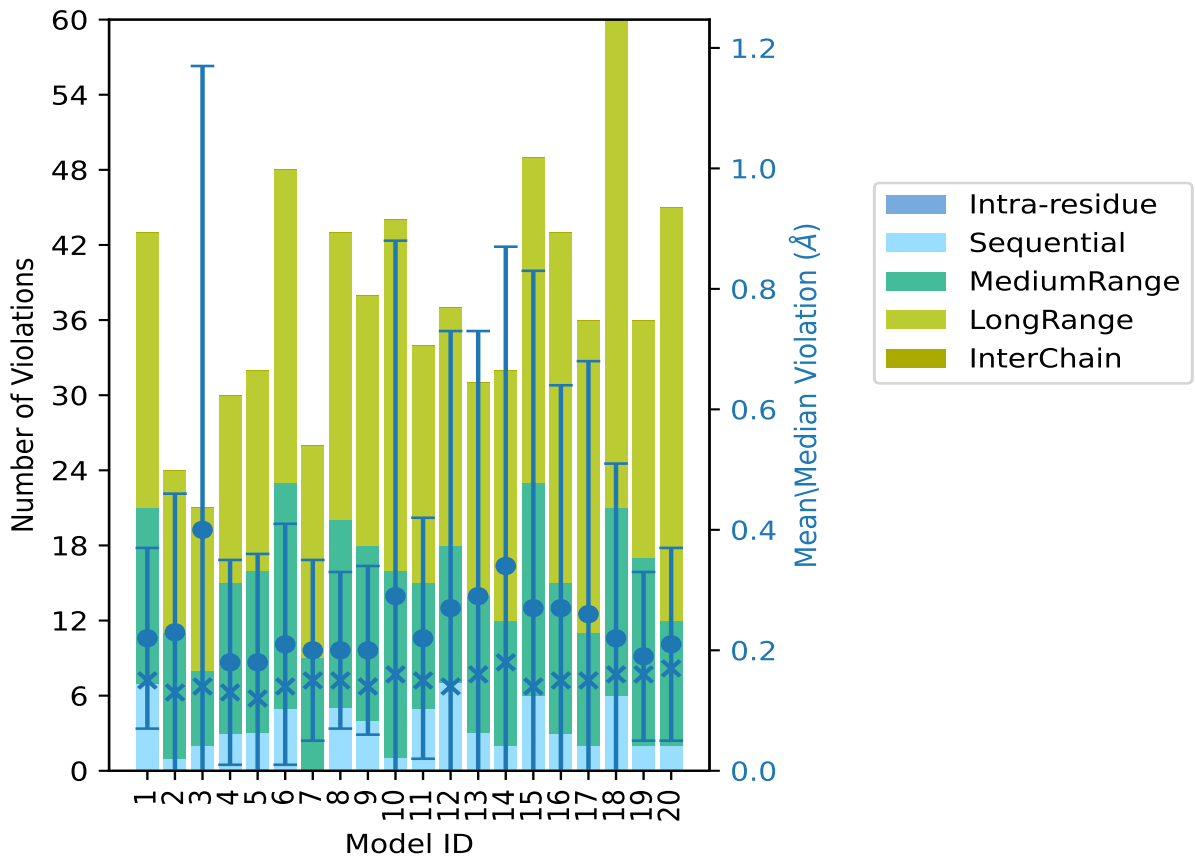
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	7	11	19	0	37	0.27	2.85	0.46	0.14
13	0	3	11	17	0	31	0.29	2.32	0.44	0.16
14	0	2	10	20	0	32	0.34	2.72	0.53	0.18
15	0	6	17	26	0	49	0.27	4.04	0.56	0.14
16	0	3	12	28	0	43	0.27	1.88	0.37	0.15
17	0	2	9	25	0	36	0.26	2.65	0.42	0.15
18	0	6	15	39	0	60	0.22	2.13	0.29	0.16
19	0	2	15	19	0	36	0.19	0.86	0.14	0.16
20	0	2	10	33	0	45	0.21	0.96	0.16	0.17

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

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



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

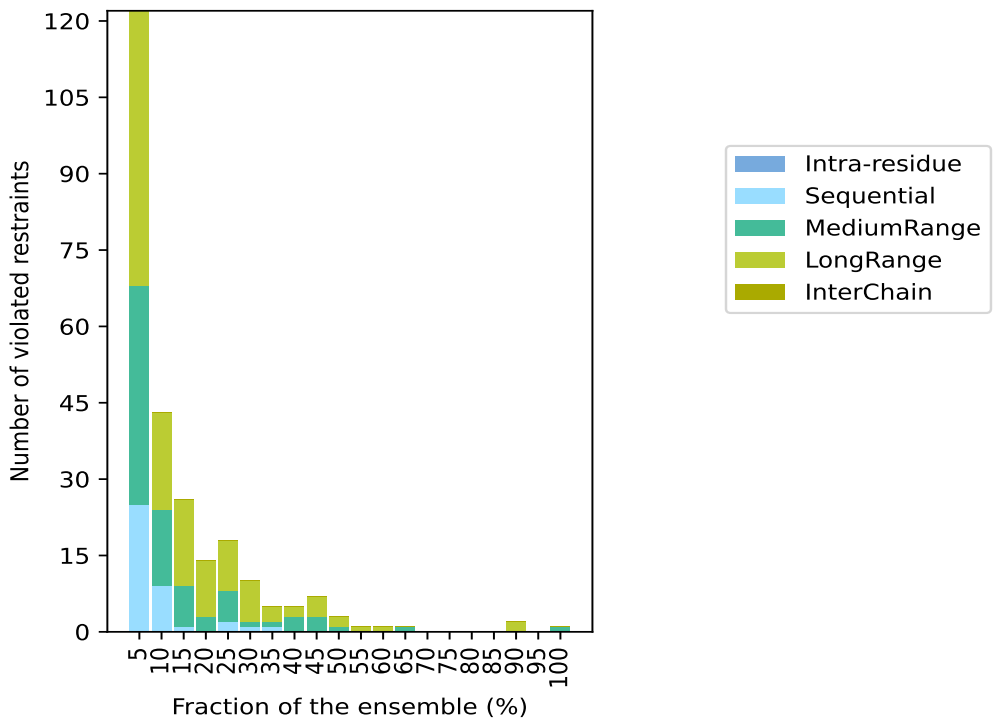
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 909(IR:1, SQ:477, MR:243, LR:188, 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]	%
0	25	43	54	0	122	1	5.0
0	9	15	19	0	43	2	10.0
0	1	8	17	0	26	3	15.0
0	0	3	11	0	14	4	20.0
0	2	6	10	0	18	5	25.0
0	1	1	8	0	10	6	30.0
0	1	1	3	0	5	7	35.0
0	0	3	2	0	5	8	40.0
0	0	3	4	0	7	9	45.0
0	0	1	2	0	3	10	50.0
0	0	0	1	0	1	11	55.0
0	0	0	1	0	1	12	60.0
0	0	1	0	0	1	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	2	0	2	18	90.0
0	0	0	0	0	0	19	95.0
0	0	1	0	0	1	20	100.0

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

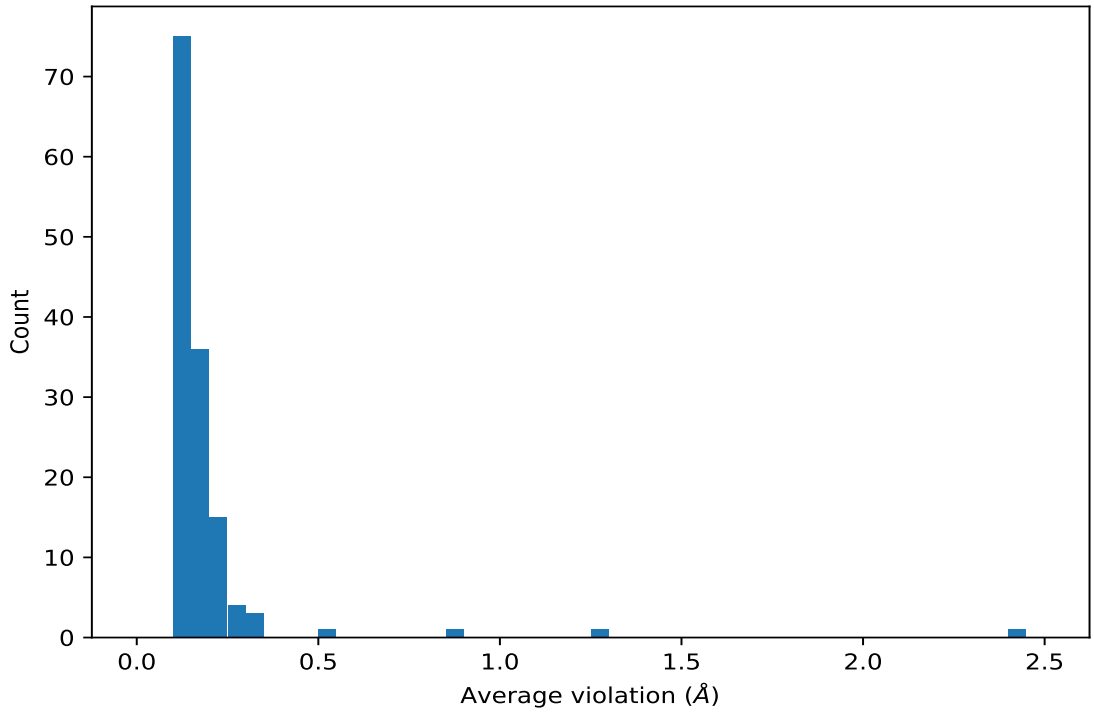
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	20	0.89	0.2	0.91
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	18	0.22	0.07	0.2
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	18	0.21	0.08	0.21
(2,34)	1:A:17:GLU:H	1:A:15:PHE:HE1	13	0.54	0.25	0.55
(1,464)	1:A:61:GLY:N	1:A:29:PHE:CA	12	0.16	0.05	0.15
(2,147)	1:A:61:GLY:H	1:A:29:PHE:HD2	11	1.28	0.69	1.0
(2,41)	1:A:25:LYS:N	1:A:17:GLU:CA	10	0.21	0.08	0.19
(2,155)	1:A:63:TYR:N	1:A:26:TRP:CB	10	0.18	0.06	0.17
(1,157)	1:A:22:LYS:N	1:A:18:LEU:CB	10	0.14	0.02	0.13
(2,60)	1:A:28:VAL:H	1:A:49:PHE:HD1	9	2.41	1.39	2.65
(1,733)	1:A:96:LYS:N	1:A:98:LEU:CG	9	0.22	0.1	0.2
(1,183)	1:A:27:ILE:N	1:A:25:LYS:CG	9	0.19	0.05	0.19
(2,253)	1:A:98:LEU:N	1:A:62:VAL:CG1	9	0.18	0.08	0.17
(1,166)	1:A:25:LYS:N	1:A:43:LYS:CB	9	0.15	0.03	0.14
(1,515)	1:A:69:ILE:N	1:A:64:ASP:CA	9	0.15	0.06	0.13
(1,809)	1:A:107:GLU:N	1:A:105:ALA:CB	9	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,172)	1:A:26:TRP:N	1:A:24:VAL:CG2	8	0.34	0.11	0.32
(2,44)	1:A:25:LYS:N	1:A:21:ARG:CA	8	0.18	0.07	0.15
(1,122)	1:A:15:PHE:N	1:A:27:ILE:CG1	8	0.17	0.05	0.16
(2,102)	1:A:41:ASP:N	1:A:25:LYS:CG	8	0.16	0.04	0.16
(1,486)	1:A:64:ASP:N	1:A:62:VAL:CB	8	0.15	0.03	0.15
(1,461)	1:A:61:GLY:H	1:A:60:PHE:HD2	7	0.34	0.21	0.38
(1,543)	1:A:72:VAL:N	1:A:60:PHE:CB	7	0.19	0.15	0.13
(1,479)	1:A:63:TYR:N	1:A:61:GLY:CA	7	0.17	0.03	0.16
(1,455)	1:A:60:PHE:N	1:A:29:PHE:CA	7	0.16	0.03	0.14
(2,148)	1:A:61:GLY:N	1:A:29:PHE:CB	7	0.16	0.03	0.16
(2,56)	1:A:27:ILE:N	1:A:14:ARG:CG	6	0.29	0.12	0.26
(2,94)	1:A:39:GLU:N	1:A:30:LYS:CD	6	0.16	0.04	0.14
(1,743)	1:A:97:LYS:N	1:A:96:LYS:CE	6	0.15	0.07	0.12
(2,108)	1:A:43:LYS:N	1:A:24:VAL:CA	6	0.15	0.04	0.15
(1,328)	1:A:43:LYS:N	1:A:41:ASP:CB	6	0.15	0.03	0.14
(1,827)	1:A:108:ALA:N	1:A:74:TRP:CB	6	0.15	0.04	0.13
(2,267)	1:A:106:LEU:N	1:A:70:GLN:CA	6	0.14	0.03	0.12
(1,62)	1:A:11:CYS:H	1:A:37:VAL:H	6	0.14	0.02	0.15
(1,268)	1:A:37:VAL:H	1:A:11:CYS:H	6	0.14	0.02	0.15
(1,217)	1:A:29:PHE:N	1:A:61:GLY:CA	6	0.13	0.01	0.12
(2,42)	1:A:25:LYS:N	1:A:17:GLU:CB	5	0.26	0.08	0.27
(2,252)	1:A:98:LEU:N	1:A:15:PHE:CA	5	0.23	0.09	0.18
(2,134)	1:A:53:LEU:N	1:A:40:LYS:CG	5	0.17	0.04	0.14
(1,281)	1:A:38:VAL:N	1:A:14:ARG:CG	5	0.17	0.01	0.17
(2,95)	1:A:39:GLU:N	1:A:30:LYS:CG	5	0.16	0.05	0.15
(1,870)	1:A:115:ALA:N	1:A:117:LEU:CB	5	0.16	0.05	0.14
(2,166)	1:A:69:ILE:N	1:A:18:LEU:CD1	5	0.15	0.02	0.15
(1,485)	1:A:64:ASP:N	1:A:62:VAL:CA	5	0.15	0.02	0.14
(2,57)	1:A:27:ILE:N	1:A:25:LYS:CD	5	0.14	0.02	0.15
(1,195)	1:A:28:VAL:N	1:A:27:ILE:CD1	5	0.14	0.03	0.12
(2,170)	1:A:71:PHE:N	1:A:101:ALA:CB	5	0.14	0.02	0.13
(1,545)	1:A:72:VAL:N	1:A:70:GLN:CA	5	0.13	0.02	0.13
(2,39)	1:A:21:ARG:N	1:A:43:LYS:CE	5	0.13	0.02	0.12
(1,299)	1:A:39:GLU:N	1:A:40:LYS:CE	5	0.13	0.02	0.12
(1,127)	1:A:16:ASN:N	1:A:14:ARG:CB	5	0.12	0.01	0.12
(1,416)	1:A:52:ALA:N	1:A:50:ARG:CB	5	0.12	0.01	0.12
(2,152)	1:A:62:VAL:N	1:A:29:PHE:CA	5	0.12	0.01	0.12
(2,183)	1:A:78:ASN:N	1:A:57:ASP:CA	5	0.12	0.01	0.12
(1,141)	1:A:17:GLU:N	1:A:25:LYS:CD	4	0.32	0.03	0.31
(2,52)	1:A:26:TRP:N	1:A:45:ASN:CA	4	0.21	0.06	0.2
(1,121)	1:A:15:PHE:N	1:A:27:ILE:CD1	4	0.2	0.07	0.2
(1,83)	1:A:12:VAL:N	1:A:97:LYS:CB	4	0.17	0.05	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,542)	1:A:72:VAL:N	1:A:106:LEU:CB	4	0.16	0.01	0.16
(2,24)	1:A:13:ALA:N	1:A:17:GLU:CG	4	0.16	0.06	0.13
(1,123)	1:A:15:PHE:N	1:A:62:VAL:CB	4	0.15	0.03	0.15
(1,7)	1:A:3:SER:N	1:A:90:SER:CA	4	0.15	0.03	0.15
(2,281)	1:A:114:LEU:N	1:A:50:ARG:CG	4	0.15	0.02	0.15
(1,120)	1:A:15:PHE:N	1:A:27:ILE:CB	4	0.14	0.03	0.13
(2,165)	1:A:66:GLY:N	1:A:69:ILE:CG1	4	0.13	0.03	0.12
(1,490)	1:A:64:ASP:N	1:A:69:ILE:CG1	4	0.12	0.01	0.12
(2,265)	1:A:104:VAL:N	1:A:70:GLN:CA	4	0.12	0.01	0.12
(1,596)	1:A:81:VAL:N	1:A:85:MET:CB	4	0.12	0.01	0.11
(1,392)	1:A:50:ARG:N	1:A:117:LEU:CB	3	0.3	0.15	0.2
(2,274)	1:A:108:ALA:N	1:A:73:LEU:CD2	3	0.23	0.08	0.28
(2,232)	1:A:92:ASP:N	1:A:96:LYS:CG	3	0.21	0.08	0.18
(2,46)	1:A:25:LYS:N	1:A:27:ILE:CA	3	0.2	0.1	0.15
(1,460)	1:A:60:PHE:N	1:A:73:LEU:CA	3	0.18	0.04	0.15
(1,140)	1:A:17:GLU:N	1:A:25:LYS:CB	3	0.18	0.05	0.16
(1,526)	1:A:70:GLN:N	1:A:68:LYS:CB	3	0.18	0.03	0.18
(2,16)	1:A:10:ASN:N	1:A:36:ILE:CA	3	0.18	0.07	0.13
(2,25)	1:A:14:ARG:N	1:A:12:VAL:CG2	3	0.18	0.04	0.15
(2,55)	1:A:27:ILE:N	1:A:14:ARG:CB	3	0.18	0.03	0.16
(2,66)	1:A:29:PHE:N	1:A:27:ILE:CG2	3	0.17	0.04	0.19
(1,363)	1:A:47:ASP:N	1:A:50:ARG:CB	3	0.17	0.02	0.16
(2,61)	1:A:28:VAL:N	1:A:26:TRP:CB	3	0.17	0.04	0.18
(2,59)	1:A:27:ILE:N	1:A:40:LYS:CA	3	0.16	0.04	0.14
(1,101)	1:A:14:ARG:N	1:A:12:VAL:CB	3	0.16	0.04	0.13
(1,304)	1:A:40:LYS:N	1:A:27:ILE:CA	3	0.15	0.04	0.14
(1,202)	1:A:28:VAL:N	1:A:40:LYS:CD	3	0.15	0.02	0.15
(1,175)	1:A:26:TRP:N	1:A:25:LYS:CD	3	0.14	0.04	0.12
(1,559)	1:A:74:TRP:N	1:A:58:CYS:CB	3	0.14	0.02	0.13
(2,48)	1:A:25:LYS:N	1:A:42:GLY:CA	3	0.14	0.02	0.13
(2,96)	1:A:39:GLU:N	1:A:59:ARG:CD	3	0.13	0.02	0.12
(2,98)	1:A:40:LYS:N	1:A:27:ILE:CB	3	0.13	0.01	0.13
(2,150)	1:A:61:GLY:N	1:A:72:VAL:CB	3	0.13	0.01	0.12
(2,233)	1:A:93:ALA:N	1:A:36:ILE:CD1	3	0.12	0.01	0.13
(2,99)	1:A:40:LYS:N	1:A:27:ILE:CG2	3	0.12	0.01	0.12
(2,186)	1:A:79:ALA:N	1:A:56:ASN:CA	3	0.11	0.0	0.11
(1,216)	1:A:29:PHE:N	1:A:60:PHE:CB	2	0.28	0.12	0.28
(2,93)	1:A:39:GLU:N	1:A:28:VAL:CG2	2	0.24	0.06	0.24
(1,342)	1:A:45:ASN:N	1:A:43:LYS:CB	2	0.23	0.05	0.23
(2,239)	1:A:94:LEU:N	1:A:31:ILE:CG2	2	0.22	0.04	0.22
(1,525)	1:A:70:GLN:N	1:A:68:LYS:CA	2	0.2	0.01	0.2
(1,544)	1:A:72:VAL:N	1:A:61:GLY:CA	2	0.2	0.06	0.2

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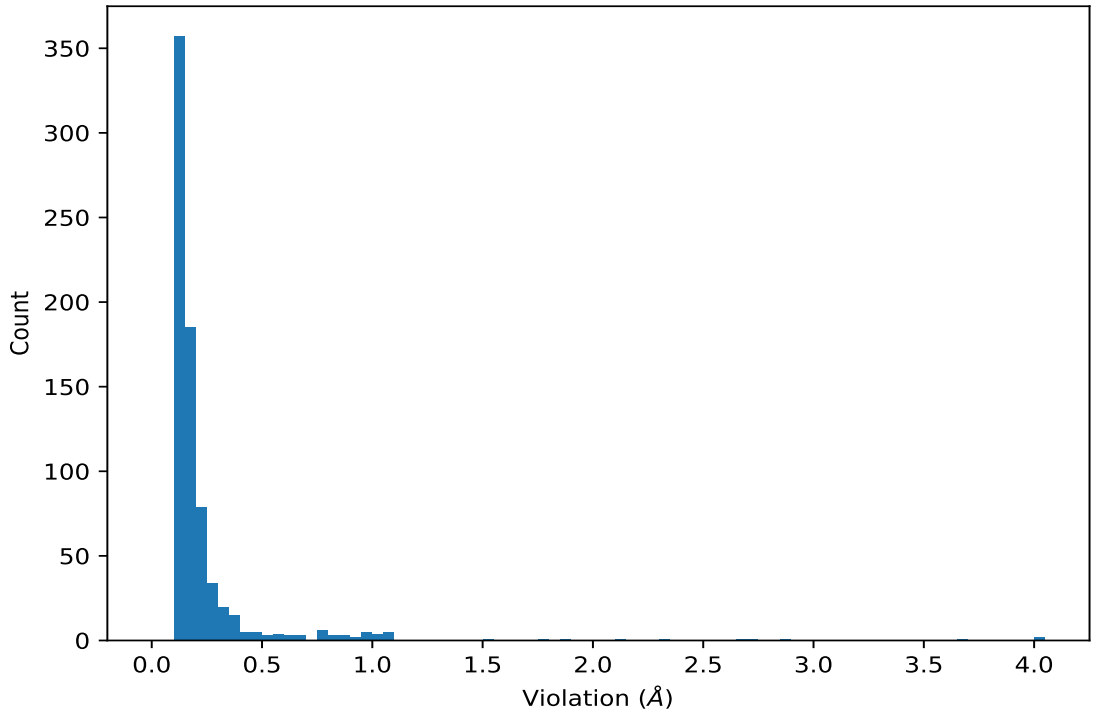
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,43)	1:A:25:LYS:N	1:A:18:LEU:CD2	2	0.19	0.08	0.19
(2,103)	1:A:41:ASP:N	1:A:26:TRP:CA	2	0.19	0.01	0.19
(1,186)	1:A:27:ILE:N	1:A:28:VAL:CG2	2	0.18	0.07	0.18
(1,93)	1:A:13:ALA:N	1:A:14:ARG:CG	2	0.16	0.04	0.16
(1,762)	1:A:99:ASP:N	1:A:69:ILE:CG2	2	0.16	0.0	0.16
(1,776)	1:A:101:ALA:N	1:A:99:ASP:CB	2	0.16	0.02	0.16
(1,524)	1:A:70:GLN:N	1:A:104:VAL:CG1	2	0.15	0.02	0.15
(1,199)	1:A:28:VAL:N	1:A:29:PHE:CB	2	0.15	0.0	0.15
(2,194)	1:A:82:LYS:N	1:A:86:THR:CA	2	0.15	0.03	0.15
(1,124)	1:A:16:ASN:N	1:A:12:VAL:CA	2	0.14	0.02	0.14
(1,223)	1:A:30:LYS:N	1:A:31:ILE:CG2	2	0.14	0.02	0.14
(2,58)	1:A:27:ILE:N	1:A:28:VAL:CG1	2	0.14	0.01	0.14
(1,325)	1:A:43:LYS:N	1:A:25:LYS:CB	2	0.14	0.01	0.14
(1,513)	1:A:68:LYS:N	1:A:69:ILE:CG1	2	0.14	0.01	0.14
(1,696)	1:A:93:ALA:N	1:A:91:LYS:CB	2	0.14	0.02	0.14
(1,774)	1:A:101:ALA:N	1:A:95:LEU:CD2	2	0.14	0.02	0.14
(2,21)	1:A:11:CYS:N	1:A:14:ARG:CA	2	0.14	0.02	0.14
(2,187)	1:A:79:ALA:N	1:A:57:ASP:CA	2	0.14	0.02	0.14
(2,222)	1:A:90:SER:N	1:A:86:THR:CG2	2	0.14	0.01	0.14
(1,125)	1:A:16:ASN:N	1:A:12:VAL:CG1	2	0.13	0.02	0.13
(1,863)	1:A:114:LEU:N	1:A:117:LEU:CA	2	0.13	0.01	0.13
(2,117)	1:A:46:ALA:N	1:A:50:ARG:CB	2	0.13	0.0	0.13
(1,34)	1:A:7:VAL:N	1:A:93:ALA:CB	2	0.12	0.02	0.12
(1,714)	1:A:95:LEU:N	1:A:93:ALA:CB	2	0.12	0.02	0.12
(2,177)	1:A:73:LEU:N	1:A:60:PHE:CB	2	0.12	0.01	0.12
(2,218)	1:A:90:SER:N	1:A:3:SER:CB	2	0.12	0.01	0.12
(2,123)	1:A:49:PHE:N	1:A:26:TRP:CB	2	0.12	0.0	0.12
(1,472)	1:A:62:VAL:N	1:A:27:ILE:CD1	2	0.12	0.0	0.12
(1,573)	1:A:75:CYS:N	1:A:76:PRO:CG	2	0.12	0.0	0.12
(1,872)	1:A:117:LEU:N	1:A:115:ALA:CB	2	0.12	0.0	0.12
(2,1)	1:A:2:ALA:N	1:A:34:THR:CG2	2	0.12	0.0	0.12
(2,110)	1:A:44:GLY:N	1:A:43:LYS:CE	2	0.12	0.0	0.12
(2,116)	1:A:46:ALA:N	1:A:50:ARG:CA	2	0.12	0.0	0.12
(2,167)	1:A:69:ILE:N	1:A:70:GLN:CG	2	0.12	0.0	0.12
(2,234)	1:A:93:ALA:N	1:A:5:MET:CA	2	0.12	0.0	0.12
(1,241)	1:A:31:ILE:N	1:A:37:VAL:CG2	2	0.11	0.0	0.11
(2,277)	1:A:109:HIS:N	1:A:107:GLU:CB	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,60)	1:A:28:VAL:H	1:A:49:PHE:HD1	15	4.04
(2,60)	1:A:28:VAL:H	1:A:49:PHE:HD1	10	4.03
(2,60)	1:A:28:VAL:H	1:A:49:PHE:HD1	3	3.69
(2,147)	1:A:61:GLY:H	1:A:29:PHE:HD2	12	2.85
(2,60)	1:A:28:VAL:H	1:A:49:PHE:HD1	14	2.72
(2,60)	1:A:28:VAL:H	1:A:49:PHE:HD1	17	2.65
(2,60)	1:A:28:VAL:H	1:A:49:PHE:HD1	13	2.32
(2,147)	1:A:61:GLY:H	1:A:29:PHE:HD2	18	2.13
(2,60)	1:A:28:VAL:H	1:A:49:PHE:HD1	16	1.88
(2,147)	1:A:61:GLY:H	1:A:29:PHE:HD2	14	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,147)	1:A:61:GLY:H	1:A:29:PHE:HD2	16	1.51
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	3	1.09
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	18	1.09
(2,147)	1:A:61:GLY:H	1:A:29:PHE:HD2	6	1.08
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	11	1.08
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	13	1.08
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	4	1.04
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	16	1.04
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	5	1.02
(2,147)	1:A:61:GLY:H	1:A:29:PHE:HD2	10	1.0
(2,147)	1:A:61:GLY:H	1:A:29:PHE:HD2	13	0.99
(2,34)	1:A:17:GLU:H	1:A:15:PHE:HE1	16	0.98
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	6	0.98
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	12	0.97
(2,147)	1:A:61:GLY:H	1:A:29:PHE:HD2	20	0.96
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	1	0.92
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	2	0.9
(2,34)	1:A:17:GLU:H	1:A:15:PHE:HE1	2	0.86
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	19	0.86
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	10	0.85
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	8	0.81
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	7	0.8
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	14	0.8
(2,34)	1:A:17:GLU:H	1:A:15:PHE:HE1	13	0.79
(2,147)	1:A:61:GLY:H	1:A:29:PHE:HD2	11	0.77
(1,461)	1:A:61:GLY:H	1:A:60:PHE:HD2	6	0.77
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	15	0.77
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	9	0.76
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	17	0.75
(1,597)	1:A:81:VAL:N	1:A:85:MET:CG	2	0.67
(2,34)	1:A:17:GLU:H	1:A:15:PHE:HE1	14	0.66
(1,417)	1:A:52:ALA:N	1:A:50:ARG:CG	18	0.65
(2,50)	1:A:25:LYS:N	1:A:64:ASP:CB	20	0.63
(1,550)	1:A:72:VAL:N	1:A:73:LEU:CD1	9	0.63
(2,34)	1:A:17:GLU:H	1:A:15:PHE:HE1	5	0.62
(2,147)	1:A:61:GLY:H	1:A:29:PHE:HD2	3	0.59
(2,34)	1:A:17:GLU:H	1:A:15:PHE:HE1	8	0.58
(2,34)	1:A:17:GLU:H	1:A:15:PHE:HE1	1	0.55
(1,172)	1:A:26:TRP:N	1:A:24:VAL:CG2	20	0.55
(1,543)	1:A:72:VAL:N	1:A:60:PHE:CB	9	0.54
(2,34)	1:A:17:GLU:H	1:A:15:PHE:HE1	3	0.51
(1,392)	1:A:50:ARG:N	1:A:117:LEU:CB	19	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:A:92:ASP:N	1:A:91:LYS:CE	15	0.49
(2,56)	1:A:27:ILE:N	1:A:14:ARG:CG	7	0.48
(1,684)	1:A:92:ASP:N	1:A:91:LYS:CD	15	0.48
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	17	0.46
(1,733)	1:A:96:LYS:N	1:A:98:LEU:CG	19	0.46
(2,34)	1:A:17:GLU:H	1:A:15:PHE:HE1	11	0.44
(1,172)	1:A:26:TRP:N	1:A:24:VAL:CG2	8	0.44
(2,56)	1:A:27:ILE:N	1:A:14:ARG:CG	6	0.42
(2,147)	1:A:61:GLY:H	1:A:29:PHE:HD2	1	0.42
(2,34)	1:A:17:GLU:H	1:A:15:PHE:HE1	4	0.4
(2,42)	1:A:25:LYS:N	1:A:17:GLU:CB	6	0.39
(1,461)	1:A:61:GLY:H	1:A:60:PHE:HD2	11	0.39
(1,461)	1:A:61:GLY:H	1:A:60:PHE:HD2	12	0.39
(1,216)	1:A:29:PHE:N	1:A:60:PHE:CB	12	0.39
(2,41)	1:A:25:LYS:N	1:A:17:GLU:CA	6	0.38
(1,461)	1:A:61:GLY:H	1:A:60:PHE:HD2	20	0.38
(1,172)	1:A:26:TRP:N	1:A:24:VAL:CG2	7	0.38
(1,878)	1:A:118:ALA:N	1:A:116:PRO:CA	17	0.37
(1,362)	1:A:47:ASP:N	1:A:48:GLU:CG	9	0.37
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	1	0.36
(1,667)	1:A:90:SER:N	1:A:91:LYS:CG	15	0.36
(1,141)	1:A:17:GLU:N	1:A:25:LYS:CD	1	0.36
(2,285)	1:A:118:ALA:N	1:A:116:PRO:CD	17	0.35
(2,253)	1:A:98:LEU:N	1:A:62:VAL:CG1	1	0.35
(1,172)	1:A:26:TRP:N	1:A:24:VAL:CG2	15	0.35
(2,46)	1:A:25:LYS:N	1:A:27:ILE:CA	20	0.34
(2,41)	1:A:25:LYS:N	1:A:17:GLU:CA	20	0.34
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	8	0.34
(2,34)	1:A:17:GLU:H	1:A:15:PHE:HE1	9	0.33
(2,252)	1:A:98:LEU:N	1:A:15:PHE:CA	1	0.33
(2,252)	1:A:98:LEU:N	1:A:15:PHE:CA	14	0.33
(1,721)	1:A:95:LEU:N	1:A:96:LYS:CE	1	0.33
(2,56)	1:A:27:ILE:N	1:A:14:ARG:CG	3	0.32
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	16	0.32
(1,141)	1:A:17:GLU:N	1:A:25:LYS:CD	6	0.32
(2,232)	1:A:92:ASP:N	1:A:96:LYS:CG	1	0.31
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	12	0.31
(2,93)	1:A:39:GLU:N	1:A:28:VAL:CG2	11	0.3
(2,52)	1:A:26:TRP:N	1:A:45:ASN:CA	8	0.3
(2,274)	1:A:108:ALA:N	1:A:73:LEU:CD2	8	0.3
(2,155)	1:A:63:TYR:N	1:A:26:TRP:CB	10	0.3
(1,743)	1:A:97:LYS:N	1:A:96:LYS:CE	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,733)	1:A:96:LYS:N	1:A:98:LEU:CG	14	0.3
(1,141)	1:A:17:GLU:N	1:A:25:LYS:CD	18	0.3
(1,121)	1:A:15:PHE:N	1:A:27:ILE:CD1	16	0.3
(2,42)	1:A:25:LYS:N	1:A:17:GLU:CB	20	0.29
(2,253)	1:A:98:LEU:N	1:A:62:VAL:CG1	14	0.29
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	7	0.29
(1,515)	1:A:69:ILE:N	1:A:64:ASP:CA	8	0.29
(1,464)	1:A:61:GLY:N	1:A:29:PHE:CA	12	0.29
(1,172)	1:A:26:TRP:N	1:A:24:VAL:CG2	10	0.29
(1,141)	1:A:17:GLU:N	1:A:25:LYS:CD	2	0.29
(2,44)	1:A:25:LYS:N	1:A:21:ARG:CA	4	0.28
(2,44)	1:A:25:LYS:N	1:A:21:ARG:CA	17	0.28
(2,274)	1:A:108:ALA:N	1:A:73:LEU:CD2	20	0.28
(2,16)	1:A:10:ASN:N	1:A:36:ILE:CA	18	0.28
(1,733)	1:A:96:LYS:N	1:A:98:LEU:CG	5	0.28
(1,342)	1:A:45:ASN:N	1:A:43:LYS:CB	8	0.28
(1,183)	1:A:27:ILE:N	1:A:25:LYS:CG	1	0.28
(2,43)	1:A:25:LYS:N	1:A:18:LEU:CD2	20	0.27
(2,42)	1:A:25:LYS:N	1:A:17:GLU:CB	1	0.27
(2,216)	1:A:89:SER:N	1:A:91:LYS:CE	15	0.27
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	11	0.27
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	9	0.27
(1,172)	1:A:26:TRP:N	1:A:24:VAL:CG2	14	0.27
(2,155)	1:A:63:TYR:N	1:A:26:TRP:CB	9	0.26
(1,870)	1:A:115:ALA:N	1:A:117:LEU:CB	10	0.26
(1,83)	1:A:12:VAL:N	1:A:97:LYS:CB	14	0.26
(1,544)	1:A:72:VAL:N	1:A:61:GLY:CA	12	0.26
(1,122)	1:A:15:PHE:N	1:A:27:ILE:CG1	12	0.26
(1,108)	1:A:14:ARG:N	1:A:27:ILE:CD1	18	0.26
(2,24)	1:A:13:ALA:N	1:A:17:GLU:CG	2	0.25
(2,239)	1:A:94:LEU:N	1:A:31:ILE:CG2	12	0.25
(1,81)	1:A:12:VAL:N	1:A:14:ARG:CG	18	0.25
(1,665)	1:A:90:SER:N	1:A:91:LYS:CD	15	0.25
(1,407)	1:A:51:GLY:N	1:A:50:ARG:CD	18	0.25
(1,251)	1:A:32:GLU:N	1:A:35:LYS:CG	18	0.25
(1,244)	1:A:32:GLU:N	1:A:30:LYS:CG	18	0.25
(1,186)	1:A:27:ILE:N	1:A:28:VAL:CG2	11	0.25
(2,95)	1:A:39:GLU:N	1:A:30:LYS:CG	14	0.24
(2,44)	1:A:25:LYS:N	1:A:21:ARG:CA	7	0.24
(2,42)	1:A:25:LYS:N	1:A:17:GLU:CB	2	0.24
(2,25)	1:A:14:ARG:N	1:A:12:VAL:CG2	10	0.24
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,134)	1:A:53:LEU:N	1:A:40:LYS:CG	8	0.24
(2,102)	1:A:41:ASP:N	1:A:25:LYS:CG	6	0.24
(1,460)	1:A:60:PHE:N	1:A:73:LEU:CA	17	0.24
(1,183)	1:A:27:ILE:N	1:A:25:LYS:CG	2	0.24
(1,140)	1:A:17:GLU:N	1:A:25:LYS:CB	4	0.24
(2,94)	1:A:39:GLU:N	1:A:30:LYS:CD	10	0.23
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	5	0.23
(1,515)	1:A:69:ILE:N	1:A:64:ASP:CA	16	0.23
(1,479)	1:A:63:TYR:N	1:A:61:GLY:CA	1	0.23
(1,228)	1:A:30:LYS:N	1:A:39:GLU:CA	18	0.23
(1,183)	1:A:27:ILE:N	1:A:25:LYS:CG	10	0.23
(1,166)	1:A:25:LYS:N	1:A:43:LYS:CB	7	0.23
(2,60)	1:A:28:VAL:H	1:A:49:PHE:HD1	11	0.22
(2,59)	1:A:27:ILE:N	1:A:40:LYS:CA	19	0.22
(2,55)	1:A:27:ILE:N	1:A:14:ARG:CB	13	0.22
(2,52)	1:A:26:TRP:N	1:A:45:ASN:CA	11	0.22
(2,41)	1:A:25:LYS:N	1:A:17:GLU:CA	11	0.22
(2,269)	1:A:106:LEU:N	1:A:72:VAL:CG1	20	0.22
(2,236)	1:A:93:ALA:N	1:A:91:LYS:CG	15	0.22
(2,212)	1:A:89:SER:N	1:A:85:MET:CB	15	0.22
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	6	0.22
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	14	0.22
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	18	0.22
(2,143)	1:A:59:ARG:N	1:A:30:LYS:CB	18	0.22
(2,112)	1:A:45:ASN:N	1:A:24:VAL:CA	19	0.22
(2,108)	1:A:43:LYS:N	1:A:24:VAL:CA	11	0.22
(1,827)	1:A:108:ALA:N	1:A:74:TRP:CB	8	0.22
(1,455)	1:A:60:PHE:N	1:A:29:PHE:CA	1	0.22
(1,183)	1:A:27:ILE:N	1:A:25:LYS:CG	6	0.22
(1,172)	1:A:26:TRP:N	1:A:24:VAL:CG2	4	0.22
(1,172)	1:A:26:TRP:N	1:A:24:VAL:CG2	9	0.22
(1,121)	1:A:15:PHE:N	1:A:27:ILE:CD1	5	0.22
(1,101)	1:A:14:ARG:N	1:A:12:VAL:CB	10	0.22
(2,66)	1:A:29:PHE:N	1:A:27:ILE:CG2	10	0.21
(2,61)	1:A:28:VAL:N	1:A:26:TRP:CB	8	0.21
(2,41)	1:A:25:LYS:N	1:A:17:GLU:CA	19	0.21
(2,267)	1:A:106:LEU:N	1:A:70:GLN:CA	9	0.21
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	9	0.21
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	14	0.21
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	4	0.21
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	10	0.21
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,526)	1:A:70:GLN:N	1:A:68:LYS:CB	17	0.21
(1,486)	1:A:64:ASP:N	1:A:62:VAL:CB	6	0.21
(1,364)	1:A:47:ASP:N	1:A:50:ARG:CG	19	0.21
(1,250)	1:A:32:GLU:N	1:A:35:LYS:CB	8	0.21
(1,122)	1:A:15:PHE:N	1:A:27:ILE:CG1	9	0.21
(1,122)	1:A:15:PHE:N	1:A:27:ILE:CG1	11	0.21
(2,94)	1:A:39:GLU:N	1:A:30:LYS:CD	8	0.2
(2,56)	1:A:27:ILE:N	1:A:14:ARG:CG	15	0.2
(2,41)	1:A:25:LYS:N	1:A:17:GLU:CA	1	0.2
(2,241)	1:A:94:LEU:N	1:A:96:LYS:CG	15	0.2
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	10	0.2
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	6	0.2
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	15	0.2
(2,155)	1:A:63:TYR:N	1:A:26:TRP:CB	11	0.2
(2,148)	1:A:61:GLY:N	1:A:29:PHE:CB	14	0.2
(2,134)	1:A:53:LEU:N	1:A:40:LYS:CG	10	0.2
(2,103)	1:A:41:ASP:N	1:A:26:TRP:CA	19	0.2
(1,93)	1:A:13:ALA:N	1:A:14:ARG:CG	18	0.2
(1,769)	1:A:100:GLY:N	1:A:98:LEU:CB	7	0.2
(1,747)	1:A:97:LYS:N	1:A:98:LEU:CD1	8	0.2
(1,733)	1:A:96:LYS:N	1:A:98:LEU:CG	12	0.2
(1,733)	1:A:96:LYS:N	1:A:98:LEU:CG	20	0.2
(1,525)	1:A:70:GLN:N	1:A:68:LYS:CA	5	0.2
(1,479)	1:A:63:TYR:N	1:A:61:GLY:CA	14	0.2
(1,464)	1:A:61:GLY:N	1:A:29:PHE:CA	16	0.2
(1,461)	1:A:61:GLY:H	1:A:60:PHE:HD2	18	0.2
(1,392)	1:A:50:ARG:N	1:A:117:LEU:CB	10	0.2
(1,363)	1:A:47:ASP:N	1:A:50:ARG:CB	16	0.2
(1,328)	1:A:43:LYS:N	1:A:41:ASP:CB	20	0.2
(1,304)	1:A:40:LYS:N	1:A:27:ILE:CA	19	0.2
(1,229)	1:A:30:LYS:N	1:A:39:GLU:CB	18	0.2
(1,123)	1:A:15:PHE:N	1:A:62:VAL:CB	18	0.2
(2,97)	1:A:39:GLU:N	1:A:59:ARG:CG	19	0.19
(2,95)	1:A:39:GLU:N	1:A:30:LYS:CG	1	0.19
(2,70)	1:A:29:PHE:N	1:A:62:VAL:CG2	18	0.19
(2,66)	1:A:29:PHE:N	1:A:27:ILE:CG2	18	0.19
(2,174)	1:A:73:LEU:H	1:A:59:ARG:H	20	0.19
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	7	0.19
(2,166)	1:A:69:ILE:N	1:A:18:LEU:CD1	17	0.19
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	1	0.19
(2,155)	1:A:63:TYR:N	1:A:26:TRP:CB	8	0.19
(2,155)	1:A:63:TYR:N	1:A:26:TRP:CB	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,148)	1:A:61:GLY:N	1:A:29:PHE:CB	9	0.19
(2,141)	1:A:59:ARG:H	1:A:73:LEU:H	20	0.19
(2,102)	1:A:41:ASP:N	1:A:25:LYS:CG	10	0.19
(2,102)	1:A:41:ASP:N	1:A:25:LYS:CG	15	0.19
(1,876)	1:A:117:LEU:N	1:A:46:ALA:CB	19	0.19
(1,7)	1:A:3:SER:N	1:A:90:SER:CA	7	0.19
(1,525)	1:A:70:GLN:N	1:A:68:LYS:CA	9	0.19
(1,473)	1:A:62:VAL:N	1:A:27:ILE:CG1	20	0.19
(1,455)	1:A:60:PHE:N	1:A:29:PHE:CA	20	0.19
(1,392)	1:A:50:ARG:N	1:A:117:LEU:CB	18	0.19
(1,320)	1:A:41:ASP:N	1:A:40:LYS:CD	16	0.19
(1,195)	1:A:28:VAL:N	1:A:27:ILE:CD1	17	0.19
(1,183)	1:A:27:ILE:N	1:A:25:LYS:CG	15	0.19
(1,175)	1:A:26:TRP:N	1:A:25:LYS:CD	16	0.19
(1,166)	1:A:25:LYS:N	1:A:43:LYS:CB	15	0.19
(1,159)	1:A:22:LYS:N	1:A:24:VAL:CA	20	0.19
(1,120)	1:A:15:PHE:N	1:A:27:ILE:CB	10	0.19
(2,93)	1:A:39:GLU:N	1:A:28:VAL:CG2	10	0.18
(2,61)	1:A:28:VAL:N	1:A:26:TRP:CB	15	0.18
(2,56)	1:A:27:ILE:N	1:A:14:ARG:CG	16	0.18
(2,52)	1:A:26:TRP:N	1:A:45:ASN:CA	20	0.18
(2,49)	1:A:25:LYS:N	1:A:63:TYR:CB	20	0.18
(2,41)	1:A:25:LYS:N	1:A:17:GLU:CA	13	0.18
(2,41)	1:A:25:LYS:N	1:A:17:GLU:CA	18	0.18
(2,281)	1:A:114:LEU:N	1:A:50:ARG:CG	10	0.18
(2,258)	1:A:101:ALA:N	1:A:95:LEU:CA	15	0.18
(2,253)	1:A:98:LEU:N	1:A:62:VAL:CG1	17	0.18
(2,252)	1:A:98:LEU:N	1:A:15:PHE:CA	16	0.18
(2,239)	1:A:94:LEU:N	1:A:31:ILE:CG2	14	0.18
(2,232)	1:A:92:ASP:N	1:A:96:LYS:CG	7	0.18
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	18	0.18
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	20	0.18
(2,165)	1:A:66:GLY:N	1:A:69:ILE:CG1	6	0.18
(2,103)	1:A:41:ASP:N	1:A:26:TRP:CA	4	0.18
(2,102)	1:A:41:ASP:N	1:A:25:LYS:CG	20	0.18
(1,776)	1:A:101:ALA:N	1:A:99:ASP:CB	18	0.18
(1,543)	1:A:72:VAL:N	1:A:60:PHE:CB	8	0.18
(1,542)	1:A:72:VAL:N	1:A:106:LEU:CB	20	0.18
(1,526)	1:A:70:GLN:N	1:A:68:LYS:CB	9	0.18
(1,485)	1:A:64:ASP:N	1:A:62:VAL:CA	4	0.18
(1,464)	1:A:61:GLY:N	1:A:29:PHE:CA	14	0.18
(1,342)	1:A:45:ASN:N	1:A:43:LYS:CB	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:A:43:LYS:N	1:A:41:ASP:CB	19	0.18
(1,281)	1:A:38:VAL:N	1:A:14:ARG:CG	6	0.18
(1,281)	1:A:38:VAL:N	1:A:14:ARG:CG	7	0.18
(1,157)	1:A:22:LYS:N	1:A:18:LEU:CB	2	0.18
(2,48)	1:A:25:LYS:N	1:A:42:GLY:CA	13	0.17
(2,253)	1:A:98:LEU:N	1:A:62:VAL:CG1	2	0.17
(2,253)	1:A:98:LEU:N	1:A:62:VAL:CG1	6	0.17
(2,252)	1:A:98:LEU:N	1:A:15:PHE:CA	5	0.17
(2,194)	1:A:82:LYS:N	1:A:86:THR:CA	12	0.17
(2,19)	1:A:10:ASN:N	1:A:38:VAL:CG1	13	0.17
(2,181)	1:A:75:CYS:N	1:A:73:LEU:CD2	9	0.17
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	5	0.17
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	13	0.17
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	17	0.17
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	19	0.17
(2,170)	1:A:71:PHE:N	1:A:101:ALA:CB	17	0.17
(1,827)	1:A:108:ALA:N	1:A:74:TRP:CB	10	0.17
(1,809)	1:A:107:GLU:N	1:A:105:ALA:CB	13	0.17
(1,7)	1:A:3:SER:N	1:A:90:SER:CA	20	0.17
(1,61)	1:A:11:CYS:H	1:A:36:ILE:H	18	0.17
(1,545)	1:A:72:VAL:N	1:A:70:GLN:CA	12	0.17
(1,524)	1:A:70:GLN:N	1:A:104:VAL:CG1	13	0.17
(1,486)	1:A:64:ASP:N	1:A:62:VAL:CB	8	0.17
(1,464)	1:A:61:GLY:N	1:A:29:PHE:CA	10	0.17
(1,455)	1:A:60:PHE:N	1:A:29:PHE:CA	3	0.17
(1,385)	1:A:49:PHE:N	1:A:50:ARG:CB	19	0.17
(1,281)	1:A:38:VAL:N	1:A:14:ARG:CG	15	0.17
(1,258)	1:A:36:ILE:H	1:A:11:CYS:H	18	0.17
(1,202)	1:A:28:VAL:N	1:A:40:LYS:CD	18	0.17
(1,195)	1:A:28:VAL:N	1:A:27:ILE:CD1	14	0.17
(1,187)	1:A:27:ILE:N	1:A:41:ASP:CB	6	0.17
(1,157)	1:A:22:LYS:N	1:A:18:LEU:CB	12	0.17
(1,157)	1:A:22:LYS:N	1:A:18:LEU:CB	18	0.17
(1,123)	1:A:15:PHE:N	1:A:62:VAL:CB	6	0.17
(1,121)	1:A:15:PHE:N	1:A:27:ILE:CD1	10	0.17
(2,78)	1:A:35:LYS:N	1:A:36:ILE:CD1	18	0.16
(2,57)	1:A:27:ILE:N	1:A:25:LYS:CD	15	0.16
(2,57)	1:A:27:ILE:N	1:A:25:LYS:CD	17	0.16
(2,55)	1:A:27:ILE:N	1:A:14:ARG:CB	12	0.16
(2,44)	1:A:25:LYS:N	1:A:21:ARG:CA	13	0.16
(2,40)	1:A:22:LYS:N	1:A:64:ASP:CA	19	0.16
(2,39)	1:A:21:ARG:N	1:A:43:LYS:CE	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,281)	1:A:114:LEU:N	1:A:50:ARG:CG	13	0.16
(2,21)	1:A:11:CYS:N	1:A:14:ARG:CA	6	0.16
(2,187)	1:A:79:ALA:N	1:A:57:ASP:CA	16	0.16
(2,166)	1:A:69:ILE:N	1:A:18:LEU:CD1	6	0.16
(2,148)	1:A:61:GLY:N	1:A:29:PHE:CB	11	0.16
(2,148)	1:A:61:GLY:N	1:A:29:PHE:CB	16	0.16
(2,108)	1:A:43:LYS:N	1:A:24:VAL:CA	8	0.16
(2,107)	1:A:41:ASP:N	1:A:43:LYS:CA	9	0.16
(1,870)	1:A:115:ALA:N	1:A:117:LEU:CB	18	0.16
(1,809)	1:A:107:GLU:N	1:A:105:ALA:CB	1	0.16
(1,774)	1:A:101:ALA:N	1:A:95:LEU:CD2	14	0.16
(1,762)	1:A:99:ASP:N	1:A:69:ILE:CG2	1	0.16
(1,762)	1:A:99:ASP:N	1:A:69:ILE:CG2	7	0.16
(1,662)	1:A:90:SER:N	1:A:88:ALA:CB	15	0.16
(1,559)	1:A:74:TRP:N	1:A:58:CYS:CB	18	0.16
(1,542)	1:A:72:VAL:N	1:A:106:LEU:CB	8	0.16
(1,486)	1:A:64:ASP:N	1:A:62:VAL:CB	4	0.16
(1,485)	1:A:64:ASP:N	1:A:62:VAL:CA	13	0.16
(1,479)	1:A:63:TYR:N	1:A:61:GLY:CA	9	0.16
(1,479)	1:A:63:TYR:N	1:A:61:GLY:CA	13	0.16
(1,479)	1:A:63:TYR:N	1:A:61:GLY:CA	18	0.16
(1,363)	1:A:47:ASP:N	1:A:50:ARG:CB	9	0.16
(1,299)	1:A:39:GLU:N	1:A:40:LYS:CE	1	0.16
(1,281)	1:A:38:VAL:N	1:A:14:ARG:CG	14	0.16
(1,270)	1:A:37:VAL:N	1:A:10:ASN:CA	18	0.16
(1,223)	1:A:30:LYS:N	1:A:31:ILE:CG2	12	0.16
(1,216)	1:A:29:PHE:N	1:A:60:PHE:CB	20	0.16
(1,183)	1:A:27:ILE:N	1:A:25:LYS:CG	17	0.16
(1,170)	1:A:26:TRP:H	1:A:42:GLY:H	6	0.16
(1,166)	1:A:25:LYS:N	1:A:43:LYS:CB	3	0.16
(1,140)	1:A:17:GLU:N	1:A:25:LYS:CB	19	0.16
(1,124)	1:A:16:ASN:N	1:A:12:VAL:CA	13	0.16
(1,122)	1:A:15:PHE:N	1:A:27:ILE:CG1	1	0.16
(1,122)	1:A:15:PHE:N	1:A:27:ILE:CG1	14	0.16
(1,1)	1:A:1:MET:N	1:A:86:THR:CB	19	0.16
(2,96)	1:A:39:GLU:N	1:A:59:ARG:CD	12	0.15
(2,95)	1:A:39:GLU:N	1:A:30:LYS:CG	10	0.15
(2,94)	1:A:39:GLU:N	1:A:30:LYS:CD	1	0.15
(2,86)	1:A:37:VAL:N	1:A:30:LYS:CG	20	0.15
(2,74)	1:A:32:GLU:N	1:A:35:LYS:CD	18	0.15
(2,58)	1:A:27:ILE:N	1:A:28:VAL:CG1	15	0.15
(2,57)	1:A:27:ILE:N	1:A:25:LYS:CD	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,56)	1:A:27:ILE:N	1:A:14:ARG:CG	17	0.15
(2,55)	1:A:27:ILE:N	1:A:14:ARG:CB	10	0.15
(2,52)	1:A:26:TRP:N	1:A:45:ASN:CA	4	0.15
(2,51)	1:A:26:TRP:N	1:A:18:LEU:CB	17	0.15
(2,46)	1:A:25:LYS:N	1:A:27:ILE:CA	19	0.15
(2,41)	1:A:25:LYS:N	1:A:17:GLU:CA	4	0.15
(2,39)	1:A:21:ARG:N	1:A:43:LYS:CE	8	0.15
(2,25)	1:A:14:ARG:N	1:A:12:VAL:CG2	7	0.15
(2,24)	1:A:13:ALA:N	1:A:17:GLU:CG	17	0.15
(2,183)	1:A:78:ASN:N	1:A:57:ASP:CA	16	0.15
(2,170)	1:A:71:PHE:N	1:A:101:ALA:CB	3	0.15
(2,166)	1:A:69:ILE:N	1:A:18:LEU:CD1	12	0.15
(2,166)	1:A:69:ILE:N	1:A:18:LEU:CD1	20	0.15
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	11	0.15
(2,155)	1:A:63:TYR:N	1:A:26:TRP:CB	5	0.15
(2,155)	1:A:63:TYR:N	1:A:26:TRP:CB	14	0.15
(2,155)	1:A:63:TYR:N	1:A:26:TRP:CB	17	0.15
(2,108)	1:A:43:LYS:N	1:A:24:VAL:CA	17	0.15
(1,83)	1:A:12:VAL:N	1:A:97:LYS:CB	5	0.15
(1,742)	1:A:97:LYS:N	1:A:96:LYS:CD	1	0.15
(1,733)	1:A:96:LYS:N	1:A:98:LEU:CG	1	0.15
(1,733)	1:A:96:LYS:N	1:A:98:LEU:CG	16	0.15
(1,696)	1:A:93:ALA:N	1:A:91:LYS:CB	1	0.15
(1,659)	1:A:90:SER:N	1:A:31:ILE:CD1	17	0.15
(1,62)	1:A:11:CYS:H	1:A:37:VAL:H	1	0.15
(1,62)	1:A:11:CYS:H	1:A:37:VAL:H	16	0.15
(1,62)	1:A:11:CYS:H	1:A:37:VAL:H	20	0.15
(1,542)	1:A:72:VAL:N	1:A:106:LEU:CB	16	0.15
(1,542)	1:A:72:VAL:N	1:A:106:LEU:CB	17	0.15
(1,486)	1:A:64:ASP:N	1:A:62:VAL:CB	17	0.15
(1,486)	1:A:64:ASP:N	1:A:62:VAL:CB	19	0.15
(1,464)	1:A:61:GLY:N	1:A:29:PHE:CA	1	0.15
(1,464)	1:A:61:GLY:N	1:A:29:PHE:CA	17	0.15
(1,460)	1:A:60:PHE:N	1:A:73:LEU:CA	8	0.15
(1,460)	1:A:60:PHE:N	1:A:73:LEU:CA	16	0.15
(1,430)	1:A:55:ALA:N	1:A:56:ASN:CB	3	0.15
(1,396)	1:A:50:ARG:N	1:A:48:GLU:CB	19	0.15
(1,328)	1:A:43:LYS:N	1:A:41:ASP:CB	18	0.15
(1,281)	1:A:38:VAL:N	1:A:14:ARG:CG	3	0.15
(1,268)	1:A:37:VAL:H	1:A:11:CYS:H	1	0.15
(1,268)	1:A:37:VAL:H	1:A:11:CYS:H	16	0.15
(1,268)	1:A:37:VAL:H	1:A:11:CYS:H	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,217)	1:A:29:PHE:N	1:A:61:GLY:CA	8	0.15
(1,202)	1:A:28:VAL:N	1:A:40:LYS:CD	7	0.15
(1,199)	1:A:28:VAL:N	1:A:29:PHE:CB	18	0.15
(1,179)	1:A:27:ILE:H	1:A:26:TRP:HD1	11	0.15
(1,127)	1:A:16:ASN:N	1:A:14:ARG:CB	15	0.15
(1,125)	1:A:16:ASN:N	1:A:12:VAL:CG1	19	0.15
(1,122)	1:A:15:PHE:N	1:A:27:ILE:CG1	17	0.15
(2,98)	1:A:40:LYS:N	1:A:27:ILE:CB	9	0.14
(2,59)	1:A:27:ILE:N	1:A:40:LYS:CA	4	0.14
(2,57)	1:A:27:ILE:N	1:A:25:LYS:CD	11	0.14
(2,44)	1:A:25:LYS:N	1:A:21:ARG:CA	1	0.14
(2,44)	1:A:25:LYS:N	1:A:21:ARG:CA	16	0.14
(2,34)	1:A:17:GLU:H	1:A:15:PHE:HE1	19	0.14
(2,267)	1:A:106:LEU:N	1:A:70:GLN:CA	5	0.14
(2,265)	1:A:104:VAL:N	1:A:70:GLN:CA	17	0.14
(2,253)	1:A:98:LEU:N	1:A:62:VAL:CG1	20	0.14
(2,25)	1:A:14:ARG:N	1:A:12:VAL:CG2	15	0.14
(2,222)	1:A:90:SER:N	1:A:86:THR:CG2	10	0.14
(2,176)	1:A:73:LEU:N	1:A:107:GLU:CG	3	0.14
(2,162)	1:A:65:CYS:N	1:A:69:ILE:CG2	1	0.14
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	8	0.14
(2,156)	1:A:63:TYR:N	1:A:65:CYS:CA	9	0.14
(2,152)	1:A:62:VAL:N	1:A:29:PHE:CA	18	0.14
(2,150)	1:A:61:GLY:N	1:A:72:VAL:CB	10	0.14
(2,148)	1:A:61:GLY:N	1:A:29:PHE:CB	10	0.14
(2,134)	1:A:53:LEU:N	1:A:40:LYS:CG	6	0.14
(2,134)	1:A:53:LEU:N	1:A:40:LYS:CG	9	0.14
(2,108)	1:A:43:LYS:N	1:A:24:VAL:CA	12	0.14
(2,106)	1:A:41:ASP:N	1:A:40:LYS:CE	8	0.14
(2,102)	1:A:41:ASP:N	1:A:25:LYS:CG	3	0.14
(1,870)	1:A:115:ALA:N	1:A:117:LEU:CB	19	0.14
(1,863)	1:A:114:LEU:N	1:A:117:LEU:CA	19	0.14
(1,83)	1:A:12:VAL:N	1:A:97:LYS:CB	16	0.14
(1,827)	1:A:108:ALA:N	1:A:74:TRP:CB	15	0.14
(1,809)	1:A:107:GLU:N	1:A:105:ALA:CB	2	0.14
(1,776)	1:A:101:ALA:N	1:A:99:ASP:CB	11	0.14
(1,761)	1:A:99:ASP:N	1:A:15:PHE:CB	15	0.14
(1,733)	1:A:96:LYS:N	1:A:98:LEU:CG	8	0.14
(1,714)	1:A:95:LEU:N	1:A:93:ALA:CB	8	0.14
(1,62)	1:A:11:CYS:H	1:A:37:VAL:H	10	0.14
(1,596)	1:A:81:VAL:N	1:A:85:MET:CB	16	0.14
(1,55)	1:A:10:ASN:N	1:A:37:VAL:CA	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,545)	1:A:72:VAL:N	1:A:70:GLN:CA	2	0.14
(1,526)	1:A:70:GLN:N	1:A:68:LYS:CB	5	0.14
(1,515)	1:A:69:ILE:N	1:A:64:ASP:CA	1	0.14
(1,515)	1:A:69:ILE:N	1:A:64:ASP:CA	7	0.14
(1,513)	1:A:68:LYS:N	1:A:69:ILE:CG1	1	0.14
(1,490)	1:A:64:ASP:N	1:A:69:ILE:CG1	10	0.14
(1,486)	1:A:64:ASP:N	1:A:62:VAL:CB	3	0.14
(1,485)	1:A:64:ASP:N	1:A:62:VAL:CA	6	0.14
(1,479)	1:A:63:TYR:N	1:A:61:GLY:CA	4	0.14
(1,464)	1:A:61:GLY:N	1:A:29:PHE:CA	5	0.14
(1,464)	1:A:61:GLY:N	1:A:29:PHE:CA	6	0.14
(1,464)	1:A:61:GLY:N	1:A:29:PHE:CA	7	0.14
(1,461)	1:A:61:GLY:H	1:A:60:PHE:HD2	13	0.14
(1,455)	1:A:60:PHE:N	1:A:29:PHE:CA	7	0.14
(1,455)	1:A:60:PHE:N	1:A:29:PHE:CA	10	0.14
(1,455)	1:A:60:PHE:N	1:A:29:PHE:CA	16	0.14
(1,363)	1:A:47:ASP:N	1:A:50:ARG:CB	18	0.14
(1,34)	1:A:7:VAL:N	1:A:93:ALA:CB	1	0.14
(1,325)	1:A:43:LYS:N	1:A:25:LYS:CB	8	0.14
(1,304)	1:A:40:LYS:N	1:A:27:ILE:CA	4	0.14
(1,299)	1:A:39:GLU:N	1:A:40:LYS:CE	18	0.14
(1,28)	1:A:6:GLY:N	1:A:93:ALA:CB	9	0.14
(1,268)	1:A:37:VAL:H	1:A:11:CYS:H	10	0.14
(1,227)	1:A:30:LYS:N	1:A:38:VAL:CB	18	0.14
(1,21)	1:A:6:GLY:N	1:A:35:LYS:CB	12	0.14
(1,199)	1:A:28:VAL:N	1:A:29:PHE:CB	12	0.14
(1,183)	1:A:27:ILE:N	1:A:25:LYS:CG	12	0.14
(1,166)	1:A:25:LYS:N	1:A:43:LYS:CB	6	0.14
(1,166)	1:A:25:LYS:N	1:A:43:LYS:CB	9	0.14
(1,157)	1:A:22:LYS:N	1:A:18:LEU:CB	15	0.14
(1,120)	1:A:15:PHE:N	1:A:27:ILE:CB	12	0.14
(2,99)	1:A:40:LYS:N	1:A:27:ILE:CG2	16	0.13
(2,98)	1:A:40:LYS:N	1:A:27:ILE:CB	17	0.13
(2,94)	1:A:39:GLU:N	1:A:30:LYS:CD	14	0.13
(2,94)	1:A:39:GLU:N	1:A:30:LYS:CD	15	0.13
(2,65)	1:A:29:PHE:H	1:A:27:ILE:H	12	0.13
(2,59)	1:A:27:ILE:N	1:A:40:LYS:CA	9	0.13
(2,58)	1:A:27:ILE:N	1:A:28:VAL:CG1	8	0.13
(2,53)	1:A:27:ILE:H	1:A:29:PHE:H	12	0.13
(2,48)	1:A:25:LYS:N	1:A:42:GLY:CA	15	0.13
(2,44)	1:A:25:LYS:N	1:A:21:ARG:CA	15	0.13
(2,42)	1:A:25:LYS:N	1:A:17:GLU:CB	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,281)	1:A:114:LEU:N	1:A:50:ARG:CG	6	0.13
(2,267)	1:A:106:LEU:N	1:A:70:GLN:CA	12	0.13
(2,265)	1:A:104:VAL:N	1:A:70:GLN:CA	3	0.13
(2,233)	1:A:93:ALA:N	1:A:36:ILE:CD1	5	0.13
(2,233)	1:A:93:ALA:N	1:A:36:ILE:CD1	18	0.13
(2,232)	1:A:92:ASP:N	1:A:96:LYS:CG	20	0.13
(2,222)	1:A:90:SER:N	1:A:86:THR:CG2	6	0.13
(2,218)	1:A:90:SER:N	1:A:3:SER:CB	19	0.13
(2,177)	1:A:73:LEU:N	1:A:60:PHE:CB	9	0.13
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	15	0.13
(2,170)	1:A:71:PHE:N	1:A:101:ALA:CB	19	0.13
(2,165)	1:A:66:GLY:N	1:A:69:ILE:CG1	11	0.13
(2,161)	1:A:65:CYS:N	1:A:68:LYS:CG	20	0.13
(2,16)	1:A:10:ASN:N	1:A:36:ILE:CA	2	0.13
(2,152)	1:A:62:VAL:N	1:A:29:PHE:CA	6	0.13
(2,148)	1:A:61:GLY:N	1:A:29:PHE:CB	19	0.13
(2,134)	1:A:53:LEU:N	1:A:40:LYS:CG	15	0.13
(2,117)	1:A:46:ALA:N	1:A:50:ARG:CB	10	0.13
(2,117)	1:A:46:ALA:N	1:A:50:ARG:CB	18	0.13
(2,102)	1:A:41:ASP:N	1:A:25:LYS:CG	2	0.13
(1,83)	1:A:12:VAL:N	1:A:97:LYS:CB	1	0.13
(1,817)	1:A:107:GLU:N	1:A:73:LEU:CD2	17	0.13
(1,809)	1:A:107:GLU:N	1:A:105:ALA:CB	11	0.13
(1,809)	1:A:107:GLU:N	1:A:105:ALA:CB	19	0.13
(1,789)	1:A:103:ALA:N	1:A:95:LEU:CD2	7	0.13
(1,743)	1:A:97:LYS:N	1:A:96:LYS:CE	8	0.13
(1,7)	1:A:3:SER:N	1:A:90:SER:CA	17	0.13
(1,627)	1:A:86:THR:N	1:A:82:LYS:CA	12	0.13
(1,586)	1:A:79:ALA:N	1:A:76:PRO:CD	19	0.13
(1,559)	1:A:74:TRP:N	1:A:58:CYS:CB	12	0.13
(1,545)	1:A:72:VAL:N	1:A:70:GLN:CA	16	0.13
(1,544)	1:A:72:VAL:N	1:A:61:GLY:CA	10	0.13
(1,543)	1:A:72:VAL:N	1:A:60:PHE:CB	4	0.13
(1,543)	1:A:72:VAL:N	1:A:60:PHE:CB	6	0.13
(1,524)	1:A:70:GLN:N	1:A:104:VAL:CG1	8	0.13
(1,515)	1:A:69:ILE:N	1:A:64:ASP:CA	20	0.13
(1,513)	1:A:68:LYS:N	1:A:69:ILE:CG1	5	0.13
(1,490)	1:A:64:ASP:N	1:A:69:ILE:CG1	20	0.13
(1,485)	1:A:64:ASP:N	1:A:62:VAL:CA	2	0.13
(1,479)	1:A:63:TYR:N	1:A:61:GLY:CA	10	0.13
(1,416)	1:A:52:ALA:N	1:A:50:ARG:CB	10	0.13
(1,416)	1:A:52:ALA:N	1:A:50:ARG:CB	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	1:A:49:PHE:N	1:A:52:ALA:CA	19	0.13
(1,345)	1:A:45:ASN:N	1:A:47:ASP:CA	6	0.13
(1,328)	1:A:43:LYS:N	1:A:41:ASP:CB	16	0.13
(1,325)	1:A:43:LYS:N	1:A:25:LYS:CB	11	0.13
(1,272)	1:A:37:VAL:N	1:A:30:LYS:CE	16	0.13
(1,267)	1:A:36:ILE:N	1:A:7:VAL:CA	18	0.13
(1,231)	1:A:30:LYS:N	1:A:59:ARG:CB	20	0.13
(1,23)	1:A:6:GLY:N	1:A:36:ILE:CA	6	0.13
(1,217)	1:A:29:PHE:N	1:A:61:GLY:CA	4	0.13
(1,217)	1:A:29:PHE:N	1:A:61:GLY:CA	6	0.13
(1,183)	1:A:27:ILE:N	1:A:25:LYS:CG	11	0.13
(1,166)	1:A:25:LYS:N	1:A:43:LYS:CB	5	0.13
(1,166)	1:A:25:LYS:N	1:A:43:LYS:CB	10	0.13
(1,166)	1:A:25:LYS:N	1:A:43:LYS:CB	17	0.13
(1,157)	1:A:22:LYS:N	1:A:18:LEU:CB	1	0.13
(1,157)	1:A:22:LYS:N	1:A:18:LEU:CB	9	0.13
(1,140)	1:A:17:GLU:N	1:A:25:LYS:CB	13	0.13
(1,127)	1:A:16:ASN:N	1:A:14:ARG:CB	1	0.13
(1,101)	1:A:14:ARG:N	1:A:12:VAL:CB	15	0.13
(2,99)	1:A:40:LYS:N	1:A:27:ILE:CG2	10	0.12
(2,96)	1:A:39:GLU:N	1:A:59:ARG:CD	6	0.12
(2,94)	1:A:39:GLU:N	1:A:30:LYS:CD	7	0.12
(2,8)	1:A:7:VAL:N	1:A:97:LYS:CD	20	0.12
(2,77)	1:A:35:LYS:N	1:A:31:ILE:CG2	20	0.12
(2,41)	1:A:25:LYS:N	1:A:17:GLU:CA	2	0.12
(2,39)	1:A:21:ARG:N	1:A:43:LYS:CE	17	0.12
(2,39)	1:A:21:ARG:N	1:A:43:LYS:CE	18	0.12
(2,34)	1:A:17:GLU:H	1:A:15:PHE:HE1	6	0.12
(2,281)	1:A:114:LEU:N	1:A:50:ARG:CG	16	0.12
(2,275)	1:A:108:ALA:N	1:A:75:CYS:CB	9	0.12
(2,274)	1:A:108:ALA:N	1:A:73:LEU:CD2	16	0.12
(2,267)	1:A:106:LEU:N	1:A:70:GLN:CA	15	0.12
(2,253)	1:A:98:LEU:N	1:A:62:VAL:CG1	5	0.12
(2,253)	1:A:98:LEU:N	1:A:62:VAL:CG1	8	0.12
(2,252)	1:A:98:LEU:N	1:A:15:PHE:CA	8	0.12
(2,234)	1:A:93:ALA:N	1:A:5:MET:CA	15	0.12
(2,218)	1:A:90:SER:N	1:A:3:SER:CB	11	0.12
(2,210)	1:A:88:ALA:N	1:A:83:PRO:CA	14	0.12
(2,204)	1:A:86:THR:N	1:A:82:LYS:CB	12	0.12
(2,194)	1:A:82:LYS:N	1:A:86:THR:CA	14	0.12
(2,186)	1:A:79:ALA:N	1:A:56:ASN:CA	16	0.12
(2,183)	1:A:78:ASN:N	1:A:57:ASP:CA	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,183)	1:A:78:ASN:N	1:A:57:ASP:CA	19	0.12
(2,177)	1:A:73:LEU:N	1:A:60:PHE:CB	17	0.12
(2,173)	1:A:71:PHE:N	1:A:95:LEU:CD2	2	0.12
(2,170)	1:A:71:PHE:N	1:A:101:ALA:CB	15	0.12
(2,170)	1:A:71:PHE:N	1:A:101:ALA:CB	20	0.12
(2,17)	1:A:10:ASN:N	1:A:36:ILE:CG2	18	0.12
(2,167)	1:A:69:ILE:N	1:A:70:GLN:CG	1	0.12
(2,166)	1:A:69:ILE:N	1:A:18:LEU:CD1	16	0.12
(2,16)	1:A:10:ASN:N	1:A:36:ILE:CA	15	0.12
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	2	0.12
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	3	0.12
(2,158)	1:A:64:ASP:N	1:A:22:LYS:CA	12	0.12
(2,152)	1:A:62:VAL:N	1:A:29:PHE:CA	11	0.12
(2,150)	1:A:61:GLY:N	1:A:72:VAL:CB	13	0.12
(2,150)	1:A:61:GLY:N	1:A:72:VAL:CB	15	0.12
(2,148)	1:A:61:GLY:N	1:A:29:PHE:CB	13	0.12
(2,123)	1:A:49:PHE:N	1:A:26:TRP:CB	4	0.12
(2,123)	1:A:49:PHE:N	1:A:26:TRP:CB	11	0.12
(2,116)	1:A:46:ALA:N	1:A:50:ARG:CA	6	0.12
(2,110)	1:A:44:GLY:N	1:A:43:LYS:CE	11	0.12
(2,108)	1:A:43:LYS:N	1:A:24:VAL:CA	4	0.12
(2,102)	1:A:41:ASP:N	1:A:25:LYS:CG	1	0.12
(2,1)	1:A:2:ALA:N	1:A:34:THR:CG2	11	0.12
(1,93)	1:A:13:ALA:N	1:A:14:ARG:CG	13	0.12
(1,872)	1:A:117:LEU:N	1:A:115:ALA:CB	16	0.12
(1,870)	1:A:115:ALA:N	1:A:117:LEU:CB	6	0.12
(1,863)	1:A:114:LEU:N	1:A:117:LEU:CA	5	0.12
(1,827)	1:A:108:ALA:N	1:A:74:TRP:CB	17	0.12
(1,827)	1:A:108:ALA:N	1:A:74:TRP:CB	20	0.12
(1,809)	1:A:107:GLU:N	1:A:105:ALA:CB	3	0.12
(1,809)	1:A:107:GLU:N	1:A:105:ALA:CB	15	0.12
(1,807)	1:A:106:LEU:N	1:A:72:VAL:CG2	9	0.12
(1,743)	1:A:97:LYS:N	1:A:96:LYS:CE	6	0.12
(1,743)	1:A:97:LYS:N	1:A:96:LYS:CE	12	0.12
(1,743)	1:A:97:LYS:N	1:A:96:LYS:CE	16	0.12
(1,7)	1:A:3:SER:N	1:A:90:SER:CA	19	0.12
(1,696)	1:A:93:ALA:N	1:A:91:LYS:CB	9	0.12
(1,573)	1:A:75:CYS:N	1:A:76:PRO:CG	9	0.12
(1,559)	1:A:74:TRP:N	1:A:58:CYS:CB	11	0.12
(1,545)	1:A:72:VAL:N	1:A:70:GLN:CA	9	0.12
(1,543)	1:A:72:VAL:N	1:A:60:PHE:CB	16	0.12
(1,490)	1:A:64:ASP:N	1:A:69:ILE:CG1	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,485)	1:A:64:ASP:N	1:A:62:VAL:CA	19	0.12
(1,472)	1:A:62:VAL:N	1:A:27:ILE:CD1	20	0.12
(1,464)	1:A:61:GLY:N	1:A:29:PHE:CA	3	0.12
(1,461)	1:A:61:GLY:H	1:A:60:PHE:HD2	4	0.12
(1,416)	1:A:52:ALA:N	1:A:50:ARG:CB	12	0.12
(1,416)	1:A:52:ALA:N	1:A:50:ARG:CB	15	0.12
(1,38)	1:A:8:ASP:N	1:A:11:CYS:CB	8	0.12
(1,332)	1:A:44:GLY:N	1:A:25:LYS:CA	15	0.12
(1,328)	1:A:43:LYS:N	1:A:41:ASP:CB	8	0.12
(1,299)	1:A:39:GLU:N	1:A:40:LYS:CE	6	0.12
(1,224)	1:A:30:LYS:N	1:A:37:VAL:CB	6	0.12
(1,223)	1:A:30:LYS:N	1:A:31:ILE:CG2	11	0.12
(1,217)	1:A:29:PHE:N	1:A:61:GLY:CA	2	0.12
(1,217)	1:A:29:PHE:N	1:A:61:GLY:CA	5	0.12
(1,202)	1:A:28:VAL:N	1:A:40:LYS:CD	4	0.12
(1,195)	1:A:28:VAL:N	1:A:27:ILE:CD1	12	0.12
(1,175)	1:A:26:TRP:N	1:A:25:LYS:CD	13	0.12
(1,166)	1:A:25:LYS:N	1:A:43:LYS:CB	1	0.12
(1,157)	1:A:22:LYS:N	1:A:18:LEU:CB	5	0.12
(1,157)	1:A:22:LYS:N	1:A:18:LEU:CB	8	0.12
(1,127)	1:A:16:ASN:N	1:A:14:ARG:CB	6	0.12
(1,124)	1:A:16:ASN:N	1:A:12:VAL:CA	5	0.12
(1,123)	1:A:15:PHE:N	1:A:62:VAL:CB	2	0.12
(1,123)	1:A:15:PHE:N	1:A:62:VAL:CB	3	0.12
(1,122)	1:A:15:PHE:N	1:A:27:ILE:CG1	13	0.12
(1,120)	1:A:15:PHE:N	1:A:27:ILE:CB	14	0.12
(1,101)	1:A:14:ARG:N	1:A:12:VAL:CB	7	0.12
(2,99)	1:A:40:LYS:N	1:A:27:ILE:CG2	5	0.11
(2,98)	1:A:40:LYS:N	1:A:27:ILE:CB	12	0.11
(2,96)	1:A:39:GLU:N	1:A:59:ARG:CD	10	0.11
(2,95)	1:A:39:GLU:N	1:A:30:LYS:CG	7	0.11
(2,95)	1:A:39:GLU:N	1:A:30:LYS:CG	20	0.11
(2,89)	1:A:37:VAL:N	1:A:38:VAL:CG1	15	0.11
(2,82)	1:A:36:ILE:N	1:A:94:LEU:CD1	15	0.11
(2,76)	1:A:32:GLU:N	1:A:86:THR:CG2	16	0.11
(2,66)	1:A:29:PHE:N	1:A:27:ILE:CG2	16	0.11
(2,61)	1:A:28:VAL:N	1:A:26:TRP:CB	4	0.11
(2,60)	1:A:28:VAL:H	1:A:49:PHE:HD1	20	0.11
(2,57)	1:A:27:ILE:N	1:A:25:LYS:CD	9	0.11
(2,54)	1:A:27:ILE:N	1:A:14:ARG:CA	18	0.11
(2,48)	1:A:25:LYS:N	1:A:42:GLY:CA	10	0.11
(2,46)	1:A:25:LYS:N	1:A:27:ILE:CA	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,44)	1:A:25:LYS:N	1:A:21:ARG:CA	6	0.11
(2,43)	1:A:25:LYS:N	1:A:18:LEU:CD2	16	0.11
(2,41)	1:A:25:LYS:N	1:A:17:GLU:CA	5	0.11
(2,39)	1:A:21:ARG:N	1:A:43:LYS:CE	9	0.11
(2,277)	1:A:109:HIS:N	1:A:107:GLU:CB	5	0.11
(2,277)	1:A:109:HIS:N	1:A:107:GLU:CB	6	0.11
(2,267)	1:A:106:LEU:N	1:A:70:GLN:CA	7	0.11
(2,267)	1:A:106:LEU:N	1:A:70:GLN:CA	18	0.11
(2,265)	1:A:104:VAL:N	1:A:70:GLN:CA	7	0.11
(2,265)	1:A:104:VAL:N	1:A:70:GLN:CA	18	0.11
(2,26)	1:A:14:ARG:N	1:A:38:VAL:CG1	8	0.11
(2,253)	1:A:98:LEU:N	1:A:62:VAL:CG1	13	0.11
(2,249)	1:A:97:LYS:N	1:A:7:VAL:CG1	14	0.11
(2,24)	1:A:13:ALA:N	1:A:17:GLU:CG	16	0.11
(2,24)	1:A:13:ALA:N	1:A:17:GLU:CG	20	0.11
(2,238)	1:A:93:ALA:N	1:A:97:LYS:CE	14	0.11
(2,234)	1:A:93:ALA:N	1:A:5:MET:CA	8	0.11
(2,233)	1:A:93:ALA:N	1:A:36:ILE:CD1	9	0.11
(2,21)	1:A:11:CYS:N	1:A:14:ARG:CA	10	0.11
(2,187)	1:A:79:ALA:N	1:A:57:ASP:CA	6	0.11
(2,186)	1:A:79:ALA:N	1:A:56:ASN:CA	8	0.11
(2,186)	1:A:79:ALA:N	1:A:56:ASN:CA	20	0.11
(2,183)	1:A:78:ASN:N	1:A:57:ASP:CA	5	0.11
(2,183)	1:A:78:ASN:N	1:A:57:ASP:CA	18	0.11
(2,175)	1:A:73:LEU:N	1:A:105:ALA:CB	13	0.11
(2,167)	1:A:69:ILE:N	1:A:70:GLN:CG	8	0.11
(2,165)	1:A:66:GLY:N	1:A:69:ILE:CG1	4	0.11
(2,165)	1:A:66:GLY:N	1:A:69:ILE:CG1	13	0.11
(2,159)	1:A:65:CYS:N	1:A:67:ASN:CB	14	0.11
(2,155)	1:A:63:TYR:N	1:A:26:TRP:CB	12	0.11
(2,155)	1:A:63:TYR:N	1:A:26:TRP:CB	18	0.11
(2,152)	1:A:62:VAL:N	1:A:29:PHE:CA	4	0.11
(2,152)	1:A:62:VAL:N	1:A:29:PHE:CA	9	0.11
(2,14)	1:A:10:ASN:H	1:A:37:VAL:H	18	0.11
(2,122)	1:A:48:GLU:N	1:A:52:ALA:CB	8	0.11
(2,116)	1:A:46:ALA:N	1:A:50:ARG:CA	10	0.11
(2,110)	1:A:44:GLY:N	1:A:43:LYS:CE	14	0.11
(2,108)	1:A:43:LYS:N	1:A:24:VAL:CA	15	0.11
(2,102)	1:A:41:ASP:N	1:A:25:LYS:CG	18	0.11
(2,1)	1:A:2:ALA:N	1:A:34:THR:CG2	4	0.11
(1,94)	1:A:13:ALA:N	1:A:16:ASN:CA	6	0.11
(1,872)	1:A:117:LEU:N	1:A:115:ALA:CB	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,870)	1:A:115:ALA:N	1:A:117:LEU:CB	16	0.11
(1,827)	1:A:108:ALA:N	1:A:74:TRP:CB	11	0.11
(1,809)	1:A:107:GLU:N	1:A:105:ALA:CB	6	0.11
(1,809)	1:A:107:GLU:N	1:A:105:ALA:CB	14	0.11
(1,774)	1:A:101:ALA:N	1:A:95:LEU:CD2	1	0.11
(1,743)	1:A:97:LYS:N	1:A:96:LYS:CE	19	0.11
(1,737)	1:A:97:LYS:N	1:A:93:ALA:CB	1	0.11
(1,733)	1:A:96:LYS:N	1:A:98:LEU:CG	10	0.11
(1,731)	1:A:96:LYS:N	1:A:97:LYS:CE	5	0.11
(1,714)	1:A:95:LEU:N	1:A:93:ALA:CB	7	0.11
(1,678)	1:A:91:LYS:N	1:A:94:LEU:CG	8	0.11
(1,676)	1:A:91:LYS:N	1:A:93:ALA:CA	1	0.11
(1,62)	1:A:11:CYS:H	1:A:37:VAL:H	2	0.11
(1,62)	1:A:11:CYS:H	1:A:37:VAL:H	18	0.11
(1,596)	1:A:81:VAL:N	1:A:85:MET:CB	7	0.11
(1,596)	1:A:81:VAL:N	1:A:85:MET:CB	13	0.11
(1,596)	1:A:81:VAL:N	1:A:85:MET:CB	20	0.11
(1,573)	1:A:75:CYS:N	1:A:76:PRO:CG	12	0.11
(1,572)	1:A:75:CYS:N	1:A:76:PRO:CB	9	0.11
(1,569)	1:A:75:CYS:N	1:A:73:LEU:CA	13	0.11
(1,545)	1:A:72:VAL:N	1:A:70:GLN:CA	4	0.11
(1,543)	1:A:72:VAL:N	1:A:60:PHE:CB	2	0.11
(1,543)	1:A:72:VAL:N	1:A:60:PHE:CB	7	0.11
(1,515)	1:A:69:ILE:N	1:A:64:ASP:CA	5	0.11
(1,515)	1:A:69:ILE:N	1:A:64:ASP:CA	13	0.11
(1,515)	1:A:69:ILE:N	1:A:64:ASP:CA	18	0.11
(1,515)	1:A:69:ILE:N	1:A:64:ASP:CA	19	0.11
(1,512)	1:A:68:LYS:N	1:A:69:ILE:CD1	6	0.11
(1,493)	1:A:65:CYS:N	1:A:63:TYR:CB	5	0.11
(1,490)	1:A:64:ASP:N	1:A:69:ILE:CG1	17	0.11
(1,486)	1:A:64:ASP:N	1:A:62:VAL:CB	2	0.11
(1,486)	1:A:64:ASP:N	1:A:62:VAL:CB	5	0.11
(1,483)	1:A:63:TYR:N	1:A:64:ASP:CB	4	0.11
(1,472)	1:A:62:VAL:N	1:A:27:ILE:CD1	18	0.11
(1,464)	1:A:61:GLY:N	1:A:29:PHE:CA	4	0.11
(1,464)	1:A:61:GLY:N	1:A:29:PHE:CA	8	0.11
(1,455)	1:A:60:PHE:N	1:A:29:PHE:CA	15	0.11
(1,448)	1:A:58:CYS:N	1:A:59:ARG:CG	17	0.11
(1,445)	1:A:57:ASP:N	1:A:58:CYS:CB	20	0.11
(1,416)	1:A:52:ALA:N	1:A:50:ARG:CB	11	0.11
(1,403)	1:A:51:GLY:N	1:A:47:ASP:CA	8	0.11
(1,37)	1:A:8:ASP:N	1:A:10:ASN:CA	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:A:7:VAL:N	1:A:93:ALA:CB	15	0.11
(1,328)	1:A:43:LYS:N	1:A:41:ASP:CB	6	0.11
(1,316)	1:A:41:ASP:N	1:A:28:VAL:CA	15	0.11
(1,304)	1:A:40:LYS:N	1:A:27:ILE:CA	9	0.11
(1,299)	1:A:39:GLU:N	1:A:40:LYS:CE	2	0.11
(1,299)	1:A:39:GLU:N	1:A:40:LYS:CE	4	0.11
(1,298)	1:A:39:GLU:N	1:A:40:LYS:CD	3	0.11
(1,268)	1:A:37:VAL:H	1:A:11:CYS:H	2	0.11
(1,268)	1:A:37:VAL:H	1:A:11:CYS:H	18	0.11
(1,262)	1:A:36:ILE:N	1:A:31:ILE:CB	18	0.11
(1,241)	1:A:31:ILE:N	1:A:37:VAL:CG2	14	0.11
(1,241)	1:A:31:ILE:N	1:A:37:VAL:CG2	18	0.11
(1,217)	1:A:29:PHE:N	1:A:61:GLY:CA	17	0.11
(1,195)	1:A:28:VAL:N	1:A:27:ILE:CD1	1	0.11
(1,195)	1:A:28:VAL:N	1:A:27:ILE:CD1	6	0.11
(1,186)	1:A:27:ILE:N	1:A:28:VAL:CG2	10	0.11
(1,183)	1:A:27:ILE:N	1:A:25:LYS:CG	14	0.11
(1,175)	1:A:26:TRP:N	1:A:25:LYS:CD	12	0.11
(1,157)	1:A:22:LYS:N	1:A:18:LEU:CB	3	0.11
(1,157)	1:A:22:LYS:N	1:A:18:LEU:CB	11	0.11
(1,136)	1:A:17:GLU:N	1:A:15:PHE:CB	4	0.11
(1,127)	1:A:16:ASN:N	1:A:14:ARG:CB	3	0.11
(1,127)	1:A:16:ASN:N	1:A:14:ARG:CB	5	0.11
(1,125)	1:A:16:ASN:N	1:A:12:VAL:CG1	4	0.11
(1,122)	1:A:15:PHE:N	1:A:27:ILE:CG1	15	0.11
(1,121)	1:A:15:PHE:N	1:A:27:ILE:CD1	11	0.11
(1,120)	1:A:15:PHE:N	1:A:27:ILE:CB	16	0.11
(1,115)	1:A:15:PHE:N	1:A:14:ARG:CD	5	0.11

10 Dihedral-angle violation analysis (i)

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