Full wwPDB NMR Structure Validation Report (i)

Dec 24, 2024 – 03:00 PM EST

PDB ID	:	2LAV
BMRB ID	:	16715
Title	:	NMR solution structure of human Vaccinia-Related Kinase 1
Authors	:	Shin, J.; Yoon, H.S.
Deposited on	:	2011-03-21

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

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

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

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

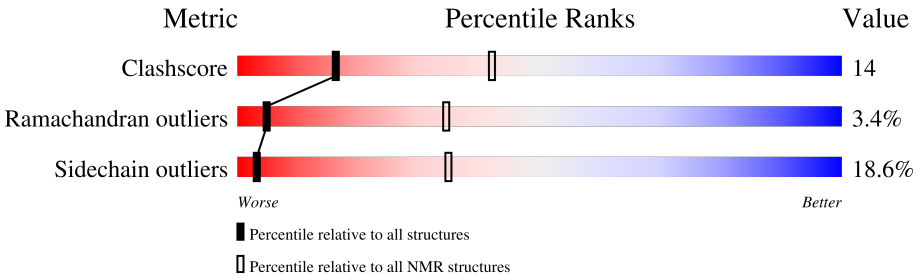
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 73%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	361	51% 33% • 14%

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:23-A:44, A:49-A:61, A:66-A:334, A:351-A:356 (310)	1.01	2

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 5 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5859 atoms, of which 2949 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Vaccinia-related kinase 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	361	5859	1853	2949	509	534	14	0

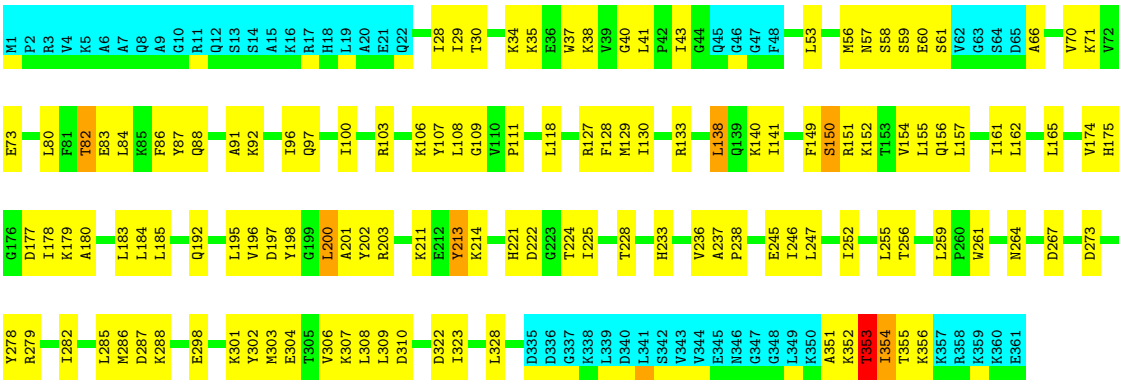
4 Residue-property plots (i)

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: Vaccinia-related kinase 1

Chain A:



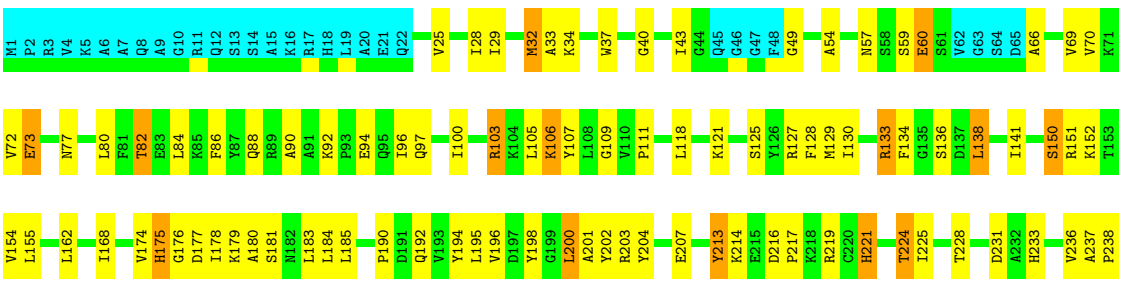
4.2 Scores per residue for each member of the ensemble

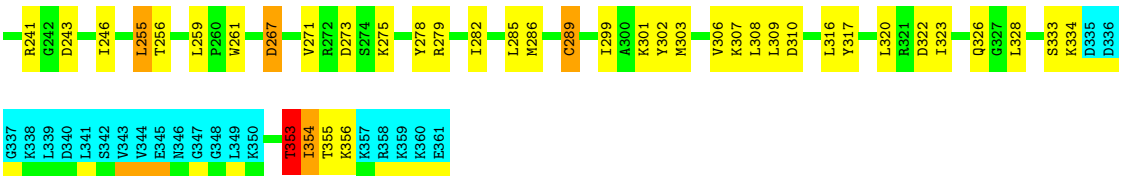
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Vaccinia-related kinase 1

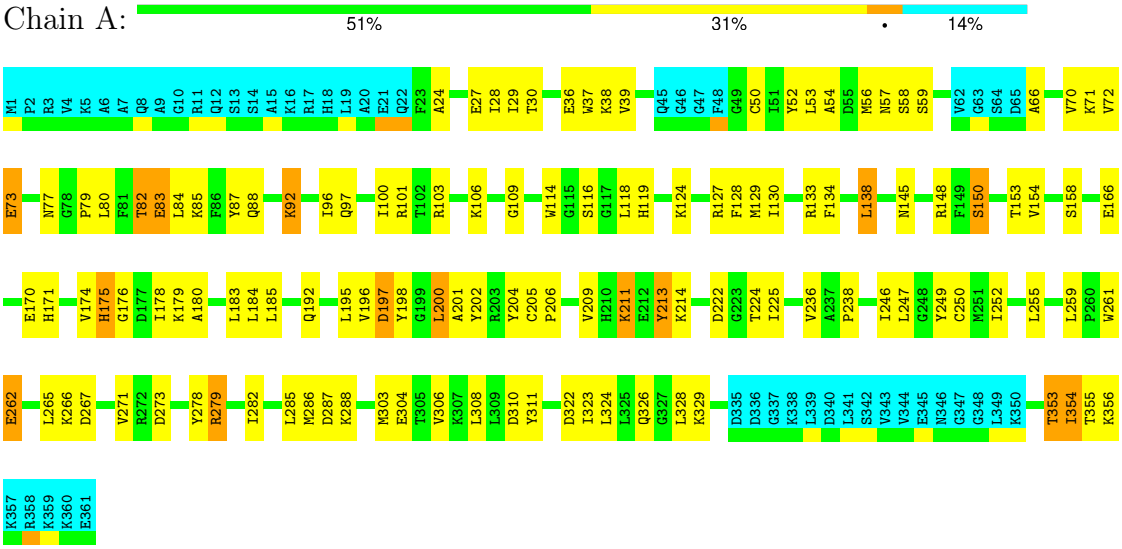
Chain A:





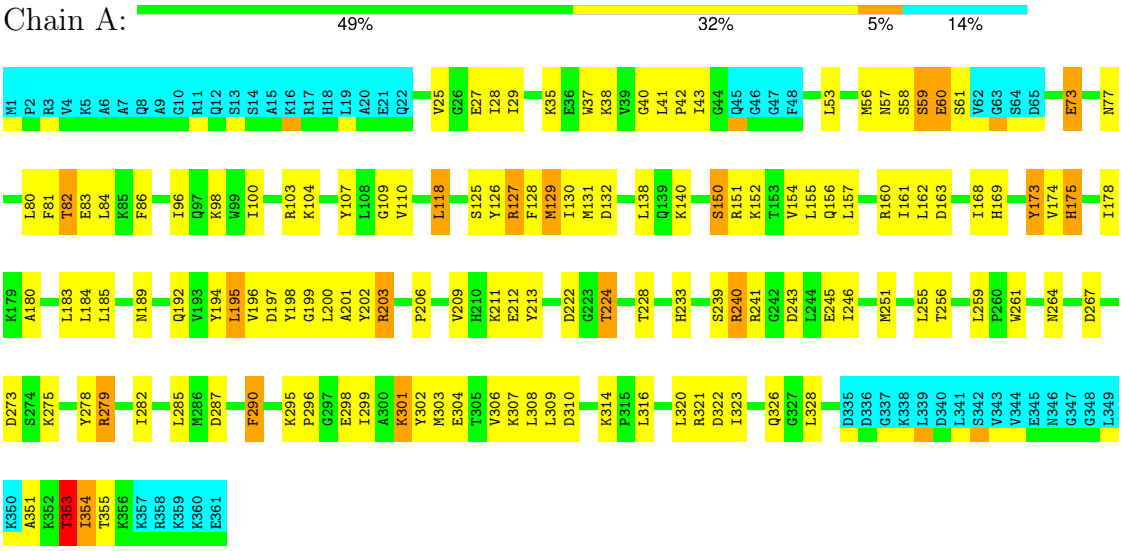
4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Vaccinia-related kinase 1



4.2.3 Score per residue for model 3

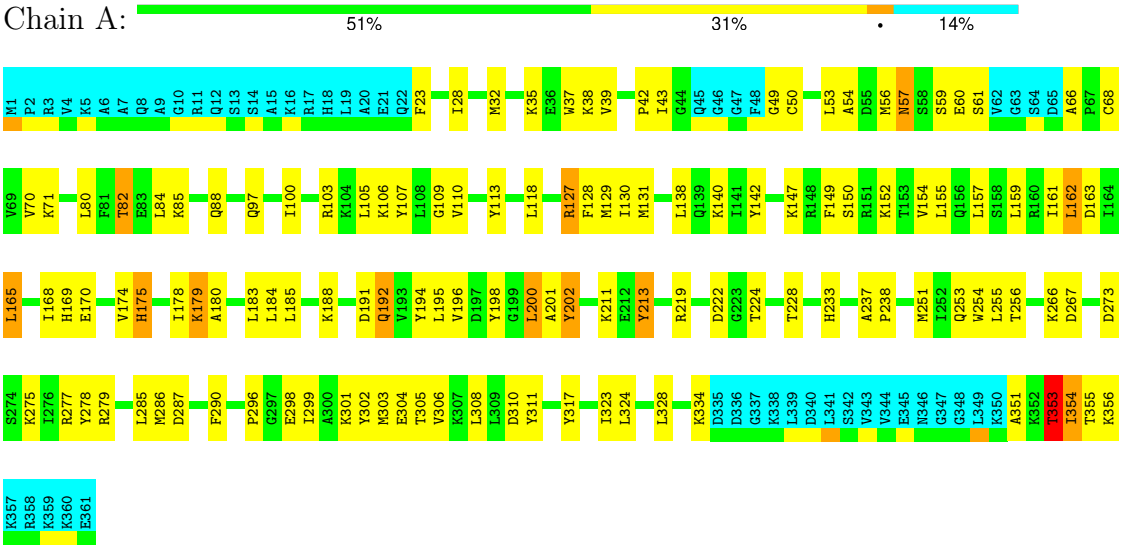
• Molecule 1: Vaccinia-related kinase 1



4.2.4 Score per residue for model 4

• Molecule 1: Vaccinia-related kinase 1

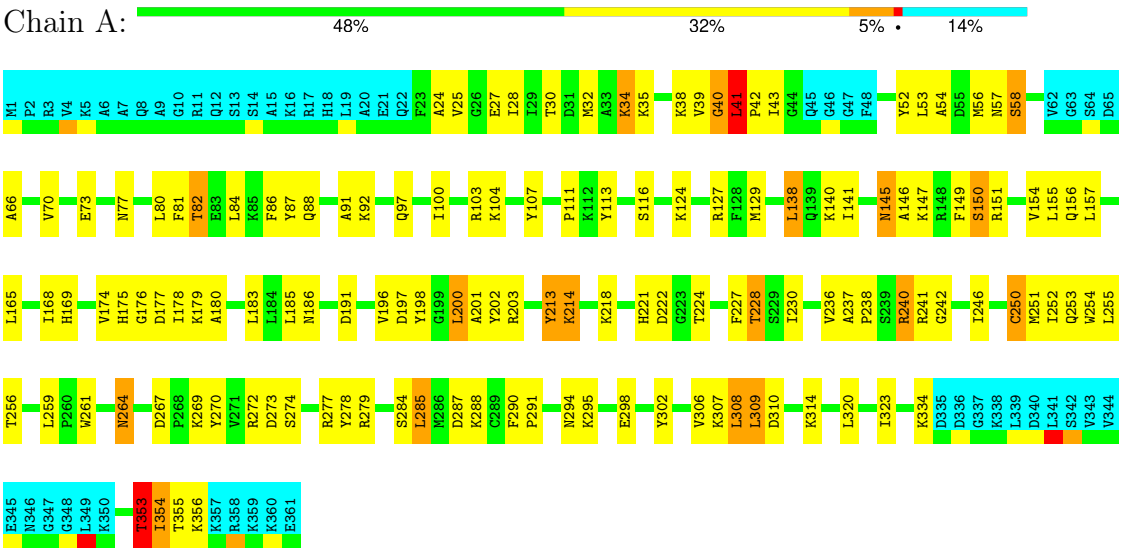
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Vaccinia-related kinase 1

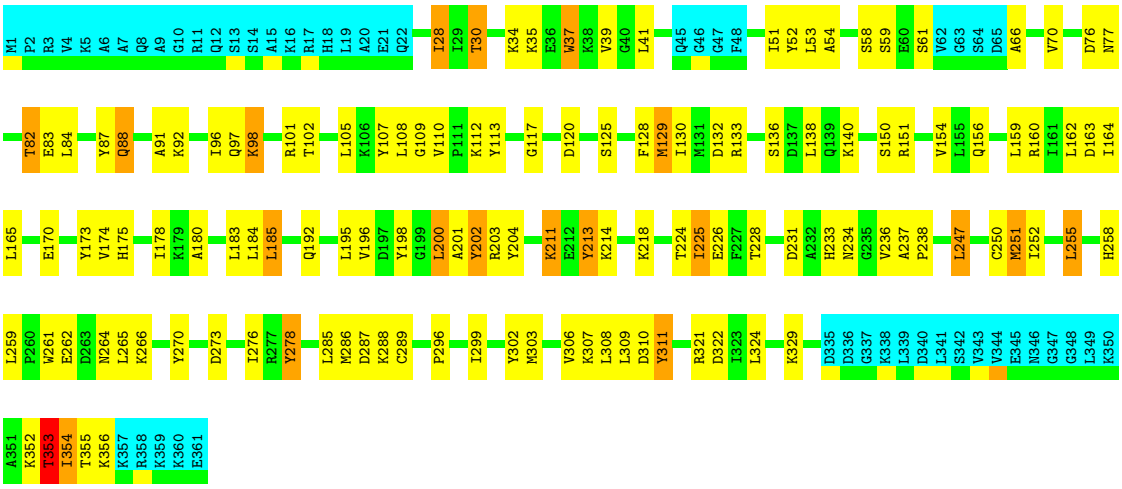
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Vaccinia-related kinase 1

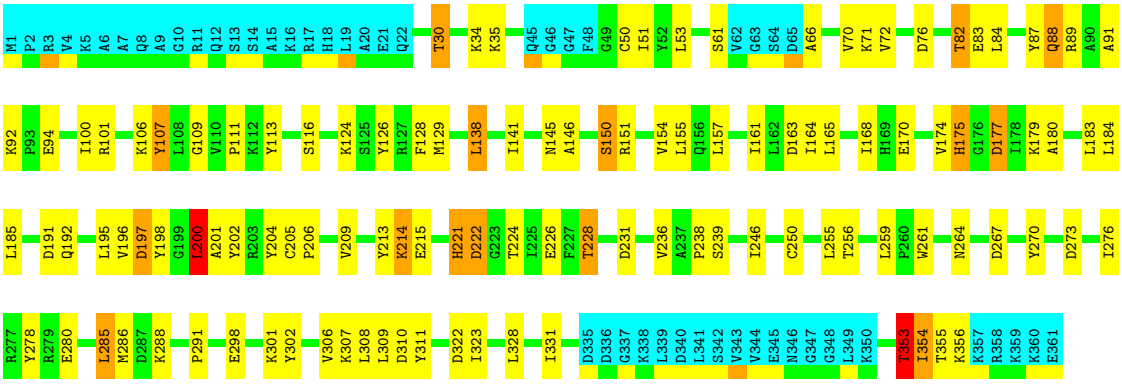
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Vaccinia-related kinase 1

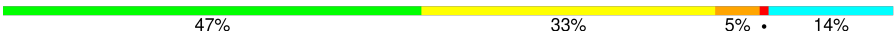
Chain A:

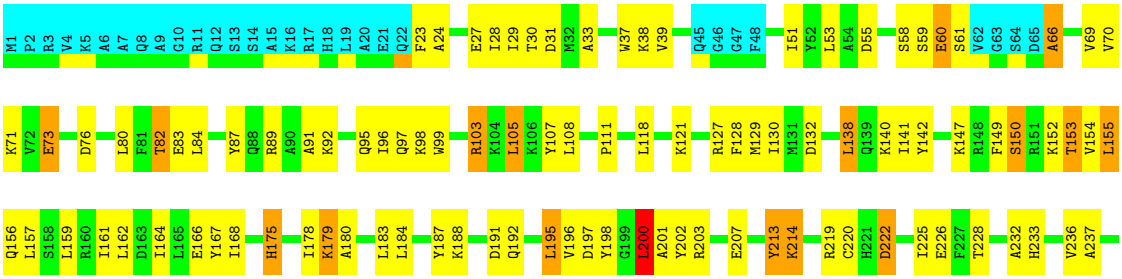


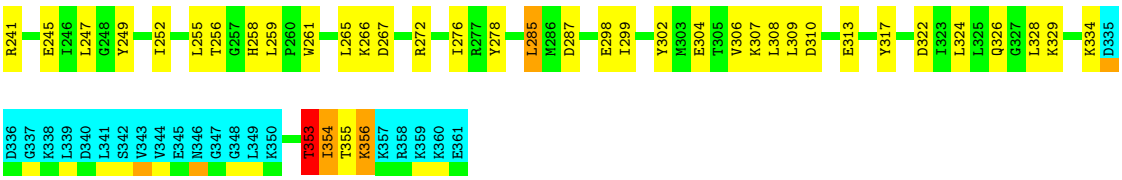
4.2.8 Score per residue for model 8

• Molecule 1: Vaccinia-related kinase 1

Chain A:



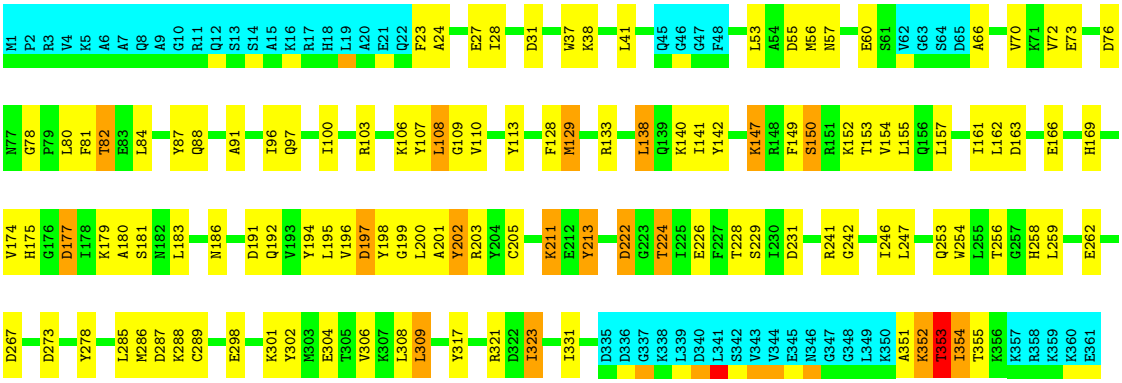




4.2.9 Score per residue for model 9

• Molecule 1: Vaccinia-related kinase 1

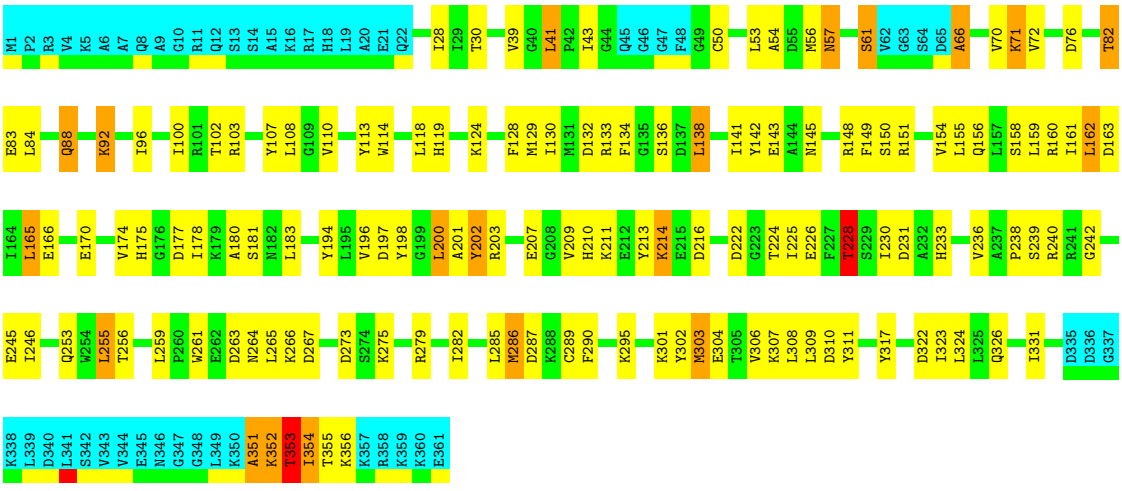
Chain A: 53% 28% 5% 14%



4.2.10 Score per residue for model 10

• Molecule 1: Vaccinia-related kinase 1

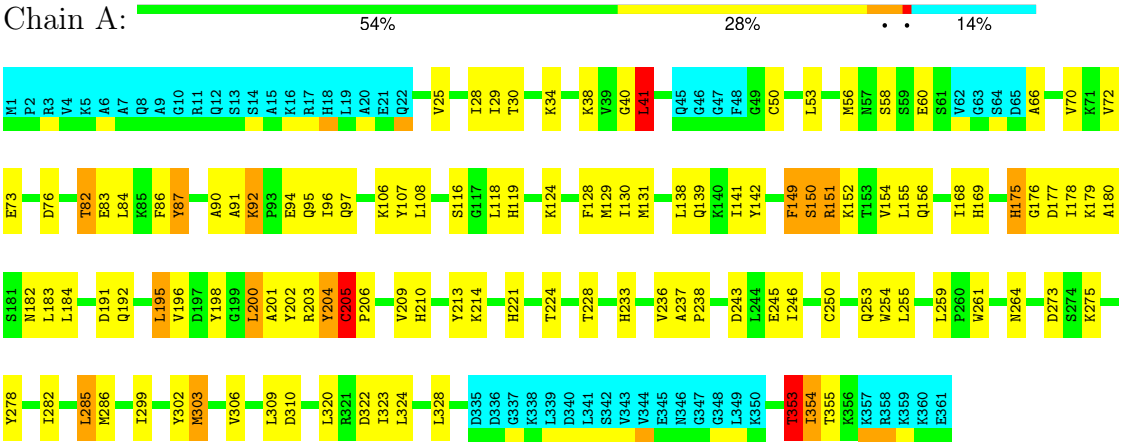
Chain A: 47% 33% 6% • 14%



4.2.11 Score per residue for model 11

• Molecule 1: Vaccinia-related kinase 1

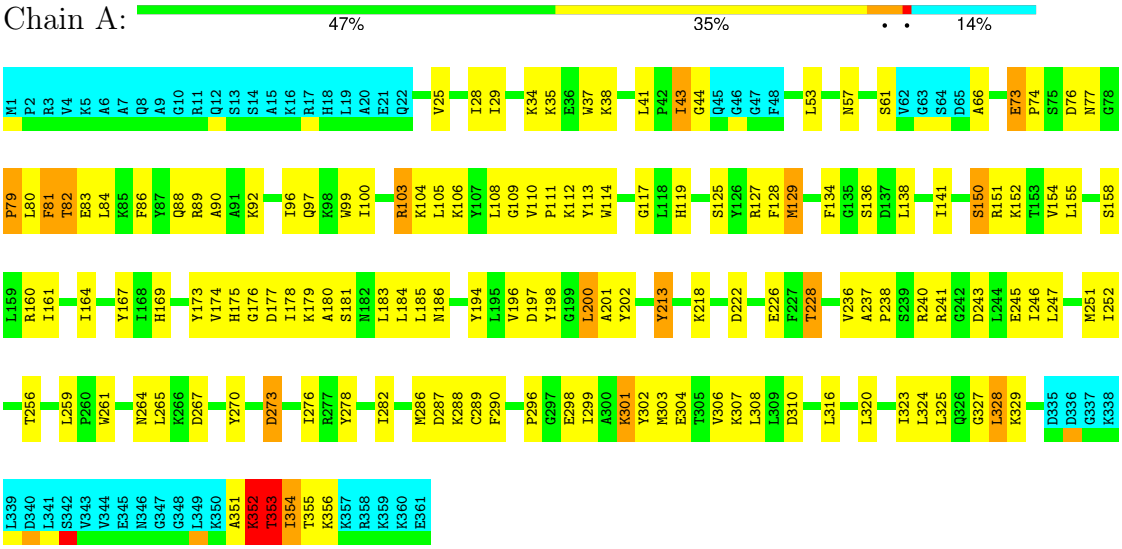
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Vaccinia-related kinase 1

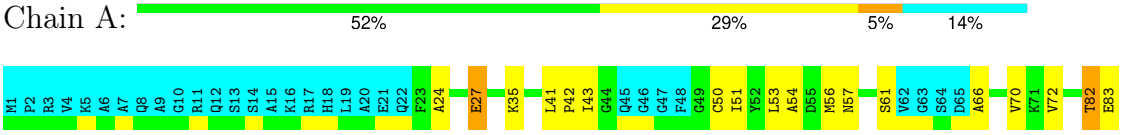
Chain A:

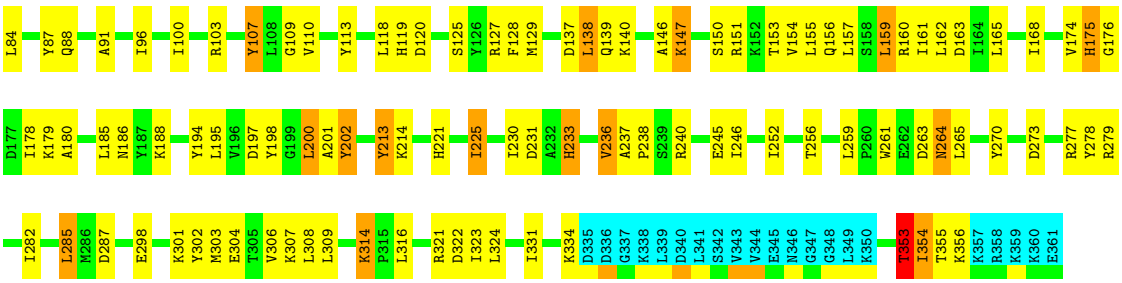


4.2.13 Score per residue for model 13

• Molecule 1: Vaccinia-related kinase 1

Chain A:

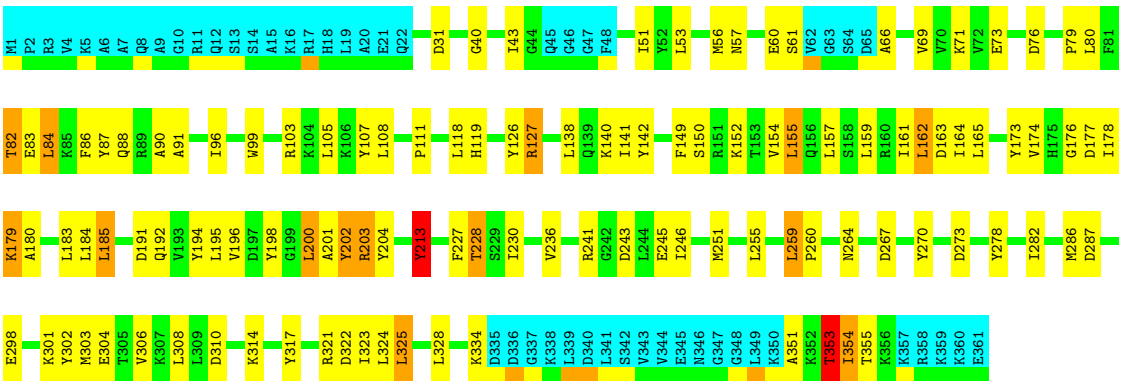




4.2.14 Score per residue for model 14

• Molecule 1: Vaccinia-related kinase 1

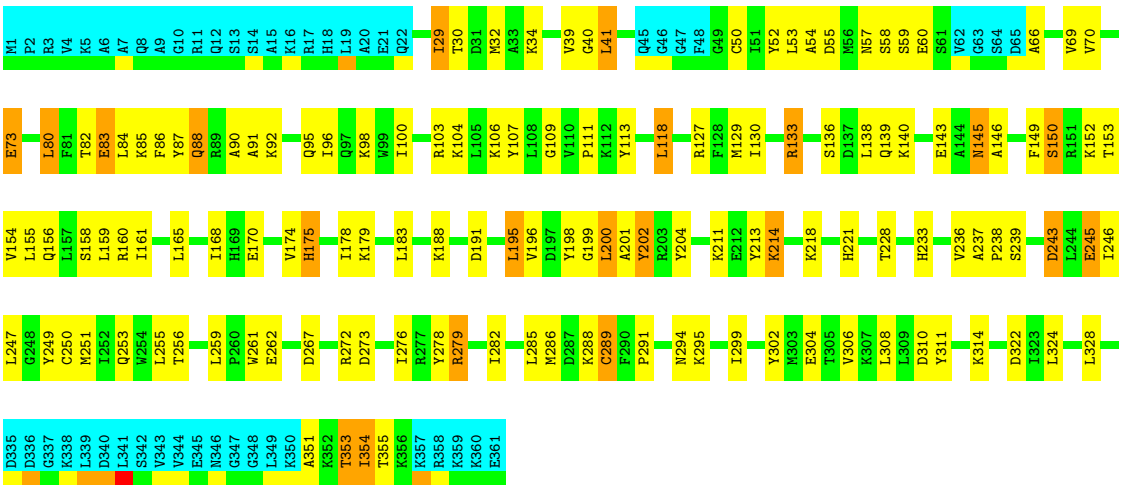
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Vaccinia-related kinase 1

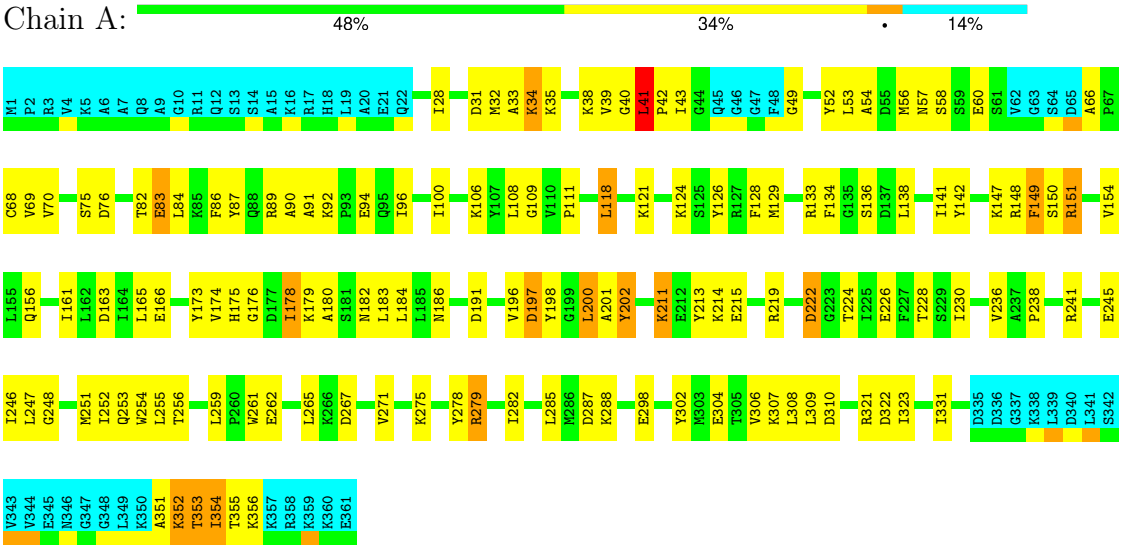
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Vaccinia-related kinase 1

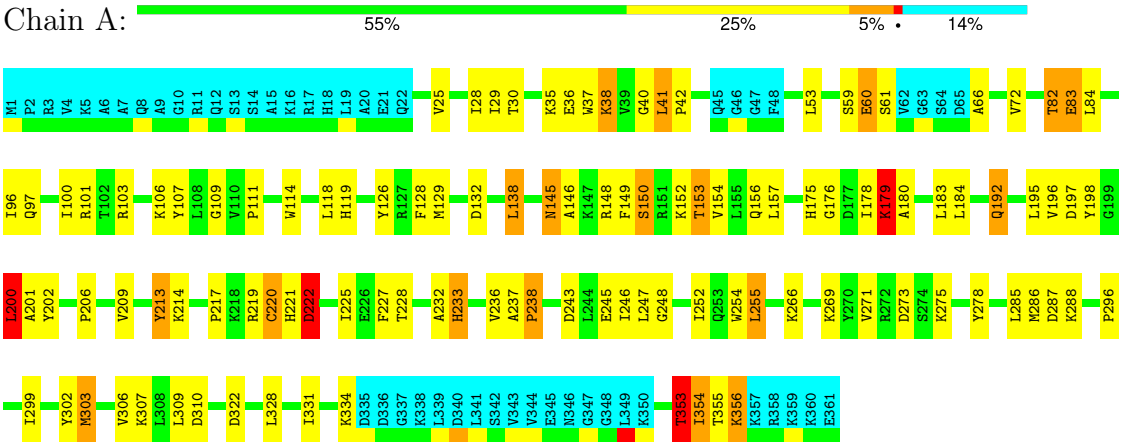
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Vaccinia-related kinase 1

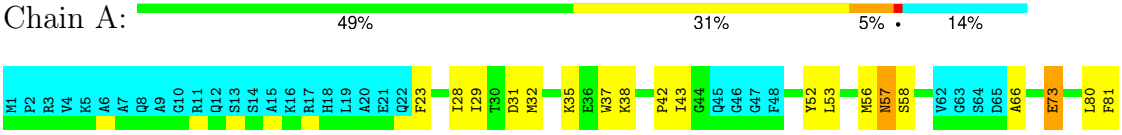
Chain A:

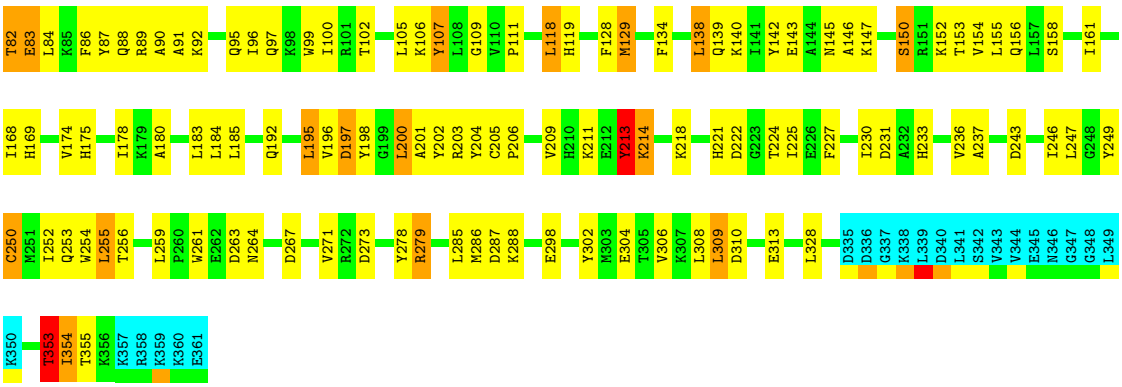


4.2.18 Score per residue for model 18

• Molecule 1: Vaccinia-related kinase 1

Chain A:

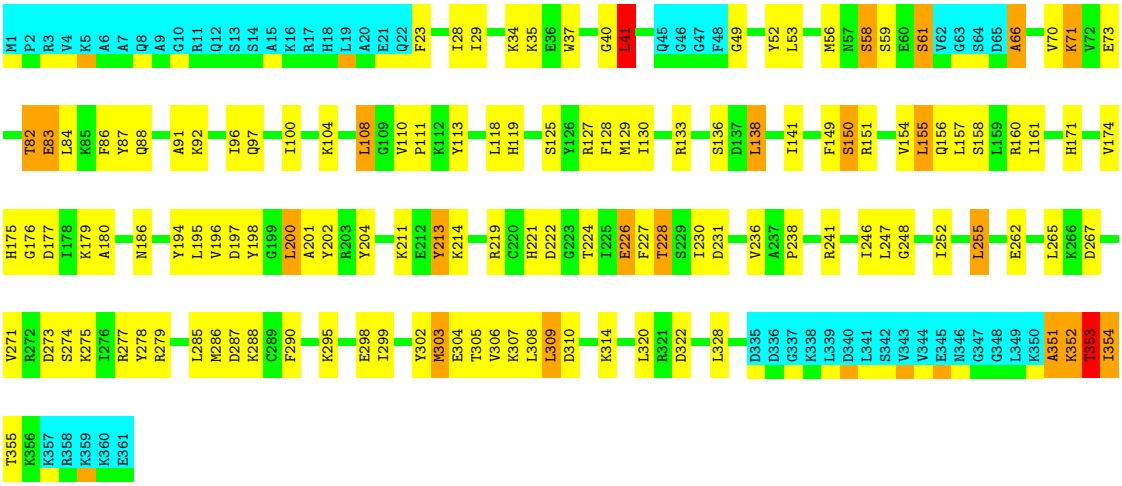




4.2.19 Score per residue for model 19

• Molecule 1: Vaccinia-related kinase 1

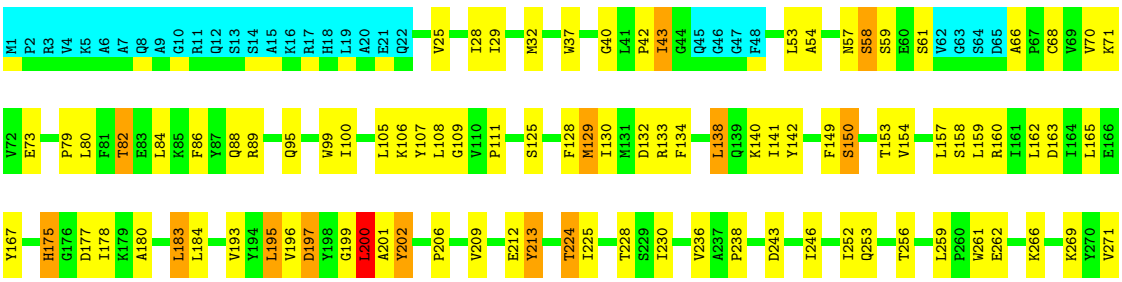
Chain A:

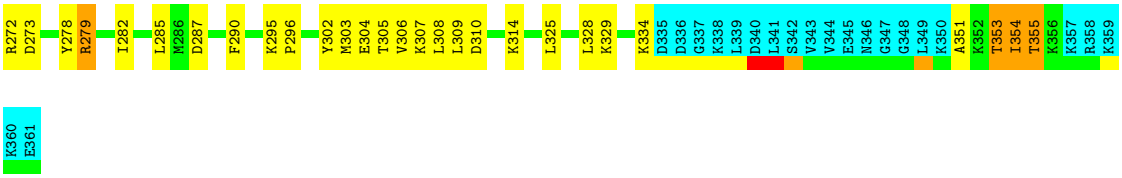


4.2.20 Score per residue for model 20

• Molecule 1: Vaccinia-related kinase 1

Chain A:




R272
D273
Y278
R279
I282
L285
M286
D287
F290
K295
P296
Y302
M303
E304
T305
V306
K307
L308
L309
D310
K314
L325
L328
K329
K334
D335
D336
G337
K338
L339
D340
L341
S342
V343
V344
E345
N346
G347
G348
L349
K350
A351
K352
T353
T354
T355
K356
K357
R358
K359
K360
E361

5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing.*

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

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

Software name	Classification	Version
CNS	refinement	1.2

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	3551
Number of shifts mapped to atoms	3551
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	73%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2527	2553	2545	71±6
All	All	50540	51060	50900	1424

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:LEU:HD21	1:A:195:LEU:HD12	0.98	1.35	8	2
1:A:53:LEU:HD22	1:A:66:ALA:HB3	0.92	1.37	14	10
1:A:29:ILE:HD11	1:A:37:TRP:CZ2	0.89	2.03	2	2
1:A:201:ALA:HB3	1:A:353:THR:HG22	0.87	1.45	4	17
1:A:53:LEU:HD23	1:A:66:ALA:HB3	0.85	1.48	5	4
1:A:37:TRP:CZ2	1:A:130:ILE:HD11	0.84	2.07	8	3
1:A:82:THR:OG1	1:A:354:ILE:HG23	0.83	1.72	9	16
1:A:328:LEU:HD22	1:A:329:LYS:N	0.82	1.89	12	1
1:A:213:TYR:CZ	1:A:236:VAL:HG11	0.80	2.11	12	4
1:A:82:THR:HG21	1:A:354:ILE:HG23	0.79	1.53	12	2
1:A:198:TYR:CD2	1:A:201:ALA:HB2	0.79	2.12	6	14
1:A:222:ASP:OD2	1:A:228:THR:HG23	0.79	1.78	8	1
1:A:70:VAL:HG22	1:A:130:ILE:CD1	0.79	2.08	15	1
1:A:224:THR:O	1:A:228:THR:HG23	0.78	1.79	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:GLY:O	1:A:246:ILE:HD13	0.78	1.79	11	8
1:A:151:ARG:NH2	1:A:331:ILE:HG21	0.77	1.94	16	1
1:A:302:TYR:O	1:A:306:VAL:HG23	0.77	1.80	12	17
1:A:178:ILE:HG23	1:A:195:LEU:HD11	0.76	1.58	14	2
1:A:278:TYR:CG	1:A:285:LEU:HD13	0.76	2.15	3	9
1:A:28:ILE:HD13	1:A:57:ASN:ND2	0.76	1.96	4	1
1:A:252:ILE:O	1:A:256:THR:HG22	0.76	1.81	16	3
1:A:168:ILE:HD13	1:A:175:HIS:CD2	0.76	2.16	3	1
1:A:111:PRO:CG	1:A:196:VAL:HG22	0.76	2.10	12	5
1:A:96:ILE:HG23	1:A:108:LEU:HD22	0.75	1.57	9	1
1:A:201:ALA:HB3	1:A:353:THR:CG2	0.75	2.12	2	16
1:A:150:SER:O	1:A:154:VAL:HG23	0.75	1.82	16	17
1:A:100:ILE:HG22	1:A:108:LEU:HD13	0.75	1.58	10	1
1:A:178:ILE:CD1	1:A:247:LEU:HD12	0.74	2.12	2	1
1:A:150:SER:O	1:A:154:VAL:HG22	0.74	1.82	18	1
1:A:213:TYR:CE1	1:A:236:VAL:HG21	0.74	2.18	13	3
1:A:176:GLY:C	1:A:246:ILE:HD13	0.73	2.03	5	3
1:A:255:LEU:HD13	1:A:299:ILE:HD11	0.73	1.60	19	3
1:A:134:PHE:CZ	1:A:196:VAL:HG11	0.73	2.19	1	4
1:A:174:VAL:HG22	1:A:202:TYR:O	0.73	1.82	9	8
1:A:159:LEU:CD2	1:A:324:LEU:HD13	0.73	2.14	6	3
1:A:111:PRO:HG2	1:A:196:VAL:HG12	0.72	1.61	8	2
1:A:242:GLY:O	1:A:246:ILE:HD12	0.72	1.84	9	3
1:A:259:LEU:HD22	1:A:261:TRP:CH2	0.72	2.20	1	8
1:A:41:LEU:CB	1:A:53:LEU:HD22	0.72	2.15	19	1
1:A:155:LEU:HD21	1:A:298:GLU:OE1	0.71	1.85	14	2
1:A:259:LEU:HD22	1:A:261:TRP:CZ2	0.71	2.19	15	12
1:A:259:LEU:HD13	1:A:260:PRO:HD2	0.71	1.61	14	1
1:A:28:ILE:HG23	1:A:37:TRP:C	0.71	2.06	20	6
1:A:111:PRO:HG3	1:A:196:VAL:HG22	0.71	1.62	12	3
1:A:184:LEU:HD13	1:A:196:VAL:HG22	0.71	1.63	14	1
1:A:251:MET:O	1:A:255:LEU:HD23	0.71	1.86	16	3
1:A:296:PRO:HB2	1:A:299:ILE:HD12	0.70	1.62	4	2
1:A:320:LEU:HA	1:A:323:ILE:HD12	0.70	1.62	12	2
1:A:183:LEU:HD21	1:A:195:LEU:CD1	0.70	2.16	8	1
1:A:247:LEU:HD23	1:A:302:TYR:OH	0.70	1.85	8	7
1:A:165:LEU:HD21	1:A:175:HIS:CE1	0.70	2.21	10	1
1:A:306:VAL:HA	1:A:309:LEU:HD23	0.70	1.64	20	1
1:A:286:MET:CE	1:A:299:ILE:HG21	0.70	2.17	11	3
1:A:177:ASP:HA	1:A:246:ILE:HG21	0.70	1.62	19	4
1:A:103:ARG:HB3	1:A:105:LEU:HD23	0.70	1.64	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ILE:HD13	1:A:57:ASN:OD1	0.70	1.87	18	1
1:A:111:PRO:HG3	1:A:196:VAL:HG12	0.69	1.63	1	5
1:A:174:VAL:HG13	1:A:204:TYR:CE1	0.69	2.22	7	2
1:A:282:ILE:HG21	1:A:303:MET:HB2	0.69	1.64	13	2
1:A:86:PHE:CE2	1:A:201:ALA:HB1	0.69	2.23	19	3
1:A:52:TYR:O	1:A:70:VAL:HG12	0.69	1.86	19	3
1:A:37:TRP:CE2	1:A:130:ILE:HD11	0.69	2.22	8	2
1:A:157:LEU:HD13	1:A:254:TRP:CZ3	0.69	2.22	17	1
1:A:84:LEU:HD12	1:A:129:MET:HB3	0.69	1.64	18	4
1:A:80:LEU:HD12	1:A:351:ALA:CB	0.68	2.19	3	2
1:A:99:TRP:CE3	1:A:108:LEU:HD13	0.68	2.23	20	2
1:A:83:GLU:OE2	1:A:351:ALA:HB1	0.68	1.88	14	1
1:A:304:GLU:O	1:A:308:LEU:HD13	0.68	1.87	18	3
1:A:227:PHE:HB3	1:A:246:ILE:HG23	0.68	1.65	19	4
1:A:154:VAL:HG11	1:A:255:LEU:CD2	0.68	2.18	16	2
1:A:84:LEU:HD11	1:A:116:SER:OG	0.68	1.88	7	3
1:A:253:GLN:OE1	1:A:259:LEU:HD12	0.68	1.88	9	2
1:A:278:TYR:HB3	1:A:285:LEU:HD13	0.68	1.64	20	3
1:A:118:LEU:HD23	1:A:126:TYR:O	0.68	1.89	3	1
1:A:71:LYS:CE	1:A:351:ALA:HB2	0.68	2.18	20	3
1:A:25:VAL:HG11	1:A:41:LEU:HD12	0.67	1.66	12	1
1:A:182:ASN:C	1:A:183:LEU:HD12	0.67	2.08	16	1
1:A:54:ALA:O	1:A:66:ALA:HB1	0.67	1.88	13	4
1:A:28:ILE:HG22	1:A:38:LYS:CA	0.67	2.19	17	6
1:A:43:ILE:HD13	1:A:53:LEU:CD2	0.67	2.20	3	2
1:A:155:LEU:HD21	1:A:298:GLU:OE2	0.67	1.90	9	3
1:A:213:TYR:CZ	1:A:236:VAL:HG21	0.67	2.25	18	1
1:A:53:LEU:HD23	1:A:69:VAL:HG12	0.67	1.67	16	2
1:A:224:THR:C	1:A:228:THR:HG23	0.67	2.10	1	2
1:A:176:GLY:CA	1:A:246:ILE:HD13	0.67	2.19	19	2
1:A:161:ILE:HG21	1:A:178:ILE:HD11	0.67	1.64	16	1
1:A:111:PRO:CG	1:A:196:VAL:HG12	0.67	2.20	7	4
1:A:282:ILE:HD12	1:A:303:MET:SD	0.66	2.31	14	1
1:A:178:ILE:HG22	1:A:246:ILE:HG22	0.66	1.68	16	1
1:A:185:LEU:HD23	1:A:192:GLN:O	0.66	1.90	4	6
1:A:225:ILE:HD11	1:A:271:VAL:HB	0.66	1.65	20	1
1:A:298:GLU:HB2	1:A:324:LEU:HD23	0.66	1.66	8	1
1:A:174:VAL:HG13	1:A:204:TYR:CD1	0.66	2.25	18	7
1:A:255:LEU:HD22	1:A:290:PHE:CZ	0.66	2.26	10	2
1:A:99:TRP:CH2	1:A:105:LEU:HD13	0.65	2.26	8	1
1:A:198:TYR:HB2	1:A:353:THR:HG23	0.65	1.67	19	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:306:VAL:HA	1:A:309:LEU:HD12	0.65	1.69	8	8
1:A:86:PHE:CE1	1:A:201:ALA:HB1	0.65	2.26	20	1
1:A:237:ALA:HB1	1:A:238:PRO:HD2	0.65	1.68	11	9
1:A:82:THR:CG2	1:A:354:ILE:HG23	0.65	2.19	12	2
1:A:273:ASP:HA	1:A:276:ILE:HD12	0.65	1.68	12	1
1:A:243:ASP:HA	1:A:246:ILE:HD12	0.65	1.67	20	5
1:A:28:ILE:HG21	1:A:57:ASN:ND2	0.65	2.06	20	2
1:A:92:LYS:O	1:A:96:ILE:HG22	0.65	1.92	10	6
1:A:157:LEU:O	1:A:161:ILE:HG22	0.65	1.91	4	4
1:A:84:LEU:HD12	1:A:129:MET:HB2	0.64	1.69	9	9
1:A:308:LEU:O	1:A:308:LEU:HD23	0.64	1.92	1	2
1:A:118:LEU:HD23	1:A:119:HIS:N	0.64	2.07	19	2
1:A:41:LEU:O	1:A:53:LEU:HD12	0.64	1.92	3	1
1:A:97:GLN:HA	1:A:100:ILE:HD12	0.64	1.69	1	3
1:A:37:TRP:CZ3	1:A:39:VAL:HG22	0.64	2.28	8	2
1:A:69:VAL:HG13	1:A:133:ARG:HG2	0.64	1.68	15	1
1:A:53:LEU:HD22	1:A:66:ALA:CB	0.64	2.23	8	6
1:A:28:ILE:HD12	1:A:57:ASN:OD1	0.64	1.93	16	2
1:A:41:LEU:CG	1:A:53:LEU:HD22	0.64	2.22	19	1
1:A:138:LEU:HB3	1:A:180:ALA:HB1	0.64	1.70	19	13
1:A:161:ILE:HG21	1:A:178:ILE:HG23	0.64	1.70	3	2
1:A:53:LEU:HD23	1:A:66:ALA:HB2	0.64	1.70	9	2
1:A:84:LEU:HD12	1:A:129:MET:CG	0.64	2.23	20	2
1:A:282:ILE:HD13	1:A:303:MET:HB2	0.64	1.68	20	2
1:A:180:ALA:HA	1:A:183:LEU:HD12	0.63	1.68	10	8
1:A:256:THR:HG21	1:A:289:CYS:SG	0.63	2.32	12	5
1:A:99:TRP:CZ3	1:A:108:LEU:HD13	0.63	2.28	20	2
1:A:155:LEU:HD13	1:A:328:LEU:HD11	0.63	1.68	11	1
1:A:321:ARG:HA	1:A:324:LEU:HD12	0.63	1.70	6	1
1:A:151:ARG:O	1:A:155:LEU:HD13	0.63	1.93	10	2
1:A:39:VAL:HG12	1:A:54:ALA:HB2	0.63	1.70	15	1
1:A:70:VAL:HB	1:A:130:ILE:HD13	0.63	1.69	20	4
1:A:278:TYR:O	1:A:282:ILE:HD13	0.62	1.94	14	2
1:A:304:GLU:O	1:A:308:LEU:HD12	0.62	1.93	20	11
1:A:99:TRP:CZ3	1:A:105:LEU:HD13	0.62	2.29	8	2
1:A:206:PRO:O	1:A:209:VAL:HG12	0.62	1.94	17	1
1:A:255:LEU:CD1	1:A:299:ILE:HD11	0.62	2.24	15	3
1:A:138:LEU:CB	1:A:180:ALA:HB1	0.62	2.24	11	5
1:A:41:LEU:HD13	1:A:42:PRO:HD2	0.62	1.71	17	1
1:A:73:GLU:HB3	1:A:80:LEU:HD22	0.62	1.69	2	4
1:A:301:LYS:HB2	1:A:323:ILE:HG21	0.62	1.72	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:THR:O	1:A:157:LEU:HD12	0.62	1.95	8	1
1:A:43:ILE:HD12	1:A:43:ILE:O	0.61	1.95	4	2
1:A:175:HIS:NE2	1:A:195:LEU:HD13	0.61	2.11	11	2
1:A:298:GLU:HA	1:A:323:ILE:HG22	0.61	1.73	4	3
1:A:175:HIS:CE1	1:A:195:LEU:HD22	0.61	2.30	18	4
1:A:29:ILE:HD13	1:A:128:PHE:CZ	0.61	2.31	18	7
1:A:225:ILE:HD11	1:A:233:HIS:ND1	0.61	2.11	8	1
1:A:301:LYS:CB	1:A:323:ILE:HG21	0.61	2.26	7	3
1:A:155:LEU:HD13	1:A:328:LEU:HB3	0.61	1.73	8	1
1:A:184:LEU:HD13	1:A:196:VAL:CG2	0.60	2.26	2	7
1:A:43:ILE:N	1:A:43:ILE:HD13	0.60	2.11	20	1
1:A:80:LEU:HD12	1:A:351:ALA:HB3	0.60	1.74	15	1
1:A:82:THR:HG22	1:A:353:THR:CG2	0.60	2.26	16	1
1:A:28:ILE:HD12	1:A:36:GLU:CD	0.60	2.16	17	1
1:A:84:LEU:HD13	1:A:127:ARG:CZ	0.60	2.26	3	1
1:A:184:LEU:HD13	1:A:196:VAL:CG1	0.60	2.27	3	2
1:A:252:ILE:HG23	1:A:290:PHE:CZ	0.60	2.31	5	1
1:A:84:LEU:HD22	1:A:127:ARG:NH2	0.60	2.10	14	2
1:A:75:SER:OG	1:A:118:LEU:HD11	0.60	1.95	16	1
1:A:162:LEU:HD22	1:A:317:TYR:CD2	0.60	2.32	8	2
1:A:230:ILE:HD12	1:A:279:ARG:CZ	0.60	2.25	5	1
1:A:155:LEU:HD21	1:A:298:GLU:HG2	0.60	1.73	12	1
1:A:248:GLY:O	1:A:252:ILE:HD12	0.60	1.97	19	3
1:A:24:ALA:HB3	1:A:27:GLU:HG3	0.60	1.72	13	5
1:A:29:ILE:HD11	1:A:37:TRP:HZ2	0.60	1.57	8	1
1:A:279:ARG:NH2	1:A:306:VAL:HG12	0.59	2.11	3	1
1:A:195:LEU:HD23	1:A:198:TYR:CE1	0.59	2.32	4	1
1:A:103:ARG:HB3	1:A:105:LEU:HD12	0.59	1.71	4	2
1:A:154:VAL:HG21	1:A:255:LEU:CD2	0.59	2.28	18	1
1:A:41:LEU:HB3	1:A:53:LEU:HD22	0.59	1.73	19	1
1:A:30:THR:HG22	1:A:34:LYS:HA	0.59	1.73	7	4
1:A:161:ILE:HA	1:A:164:ILE:HD12	0.59	1.74	14	4
1:A:307:LYS:HG3	1:A:308:LEU:HD12	0.59	1.72	7	1
1:A:82:THR:HB	1:A:353:THR:HB	0.59	1.73	20	3
1:A:96:ILE:HG23	1:A:108:LEU:HD23	0.59	1.74	8	1
1:A:138:LEU:HB2	1:A:180:ALA:HB1	0.59	1.73	6	3
1:A:282:ILE:HD13	1:A:303:MET:CB	0.59	2.27	13	1
1:A:202:TYR:CD1	1:A:355:THR:HG22	0.59	2.33	20	1
1:A:155:LEU:HD22	1:A:328:LEU:HD21	0.59	1.75	1	1
1:A:28:ILE:HG21	1:A:57:ASN:HB2	0.58	1.75	12	2
1:A:161:ILE:CG2	1:A:178:ILE:HD11	0.58	2.28	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:LEU:HD22	1:A:183:LEU:HD13	0.58	1.75	17	1
1:A:271:VAL:HG12	1:A:275:LYS:HD2	0.58	1.74	17	1
1:A:118:LEU:HD21	1:A:127:ARG:HD2	0.58	1.74	1	3
1:A:118:LEU:HD12	1:A:127:ARG:CZ	0.58	2.29	15	1
1:A:159:LEU:HG	1:A:324:LEU:HD13	0.58	1.74	4	3
1:A:225:ILE:HG23	1:A:265:LEU:HD22	0.58	1.74	10	1
1:A:54:ALA:HB3	1:A:68:CYS:O	0.58	1.98	20	2
1:A:87:TYR:O	1:A:91:ALA:HB3	0.58	1.99	8	9
1:A:178:ILE:HD12	1:A:178:ILE:N	0.58	2.14	6	2
1:A:230:ILE:HD11	1:A:279:ARG:CZ	0.58	2.29	18	1
1:A:282:ILE:HG21	1:A:303:MET:CB	0.58	2.29	13	2
1:A:161:ILE:HG22	1:A:165:LEU:CD1	0.58	2.28	15	2
1:A:252:ILE:HD11	1:A:303:MET:CE	0.58	2.29	20	2
1:A:80:LEU:HD12	1:A:351:ALA:HB1	0.57	1.76	3	2
1:A:155:LEU:HD13	1:A:328:LEU:CD1	0.57	2.29	11	1
1:A:154:VAL:HG21	1:A:255:LEU:HD22	0.57	1.75	18	1
1:A:305:THR:HB	1:A:320:LEU:HD21	0.57	1.76	19	1
1:A:271:VAL:HG12	1:A:275:LYS:CE	0.57	2.29	19	2
1:A:183:LEU:CD2	1:A:195:LEU:HD12	0.57	2.29	4	2
1:A:255:LEU:CD1	1:A:299:ILE:HG21	0.57	2.30	8	1
1:A:155:LEU:HD21	1:A:298:GLU:CD	0.57	2.20	19	1
1:A:118:LEU:HD12	1:A:118:LEU:N	0.57	2.14	18	3
1:A:74:PRO:O	1:A:80:LEU:HD22	0.57	1.99	12	1
1:A:72:VAL:HG12	1:A:128:PHE:HB3	0.57	1.77	11	6
1:A:184:LEU:HD13	1:A:196:VAL:HB	0.57	1.76	4	3
1:A:237:ALA:HB1	1:A:238:PRO:CD	0.57	2.30	11	2
1:A:301:LYS:HB3	1:A:323:ILE:HD13	0.57	1.77	4	3
1:A:29:ILE:N	1:A:29:ILE:HD13	0.57	2.15	15	1
1:A:175:HIS:CD2	1:A:178:ILE:HD11	0.57	2.35	10	1
1:A:118:LEU:HD13	1:A:126:TYR:O	0.57	2.00	14	1
1:A:161:ILE:HD13	1:A:247:LEU:HD11	0.57	1.76	19	1
1:A:86:PHE:O	1:A:90:ALA:HB3	0.56	2.00	14	7
1:A:278:TYR:HB3	1:A:285:LEU:HD11	0.56	1.77	7	1
1:A:178:ILE:HG21	1:A:247:LEU:HD12	0.56	1.77	18	1
1:A:231:ASP:HA	1:A:236:VAL:HG12	0.56	1.77	1	3
1:A:138:LEU:HD21	1:A:185:LEU:HD11	0.56	1.76	6	1
1:A:151:ARG:HD2	1:A:255:LEU:HD21	0.56	1.77	6	2
1:A:183:LEU:HD23	1:A:193:VAL:CG2	0.56	2.30	20	1
1:A:155:LEU:HD11	1:A:298:GLU:OE1	0.56	2.00	8	1
1:A:351:ALA:O	1:A:352:LYS:CB	0.56	2.51	19	4
1:A:105:LEU:O	1:A:107:TYR:N	0.56	2.38	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:316:LEU:O	1:A:320:LEU:HD13	0.56	2.00	3	2
1:A:183:LEU:C	1:A:184:LEU:HD12	0.56	2.21	6	4
1:A:28:ILE:HD11	1:A:38:LYS:HE3	0.56	1.77	12	1
1:A:28:ILE:HG22	1:A:38:LYS:HA	0.56	1.76	9	6
1:A:24:ALA:HB3	1:A:27:GLU:CG	0.56	2.30	5	1
1:A:230:ILE:HD13	1:A:279:ARG:NH2	0.56	2.15	20	1
1:A:225:ILE:HD11	1:A:233:HIS:NE2	0.56	2.15	13	1
1:A:228:THR:CG2	1:A:232:ALA:HB3	0.56	2.31	8	1
1:A:200:LEU:HD13	1:A:222:ASP:O	0.56	2.01	9	1
1:A:96:ILE:HG13	1:A:108:LEU:HD22	0.56	1.76	19	1
1:A:165:LEU:HD23	1:A:175:HIS:ND1	0.55	2.16	4	1
1:A:159:LEU:HA	1:A:162:LEU:HD12	0.55	1.76	13	1
1:A:70:VAL:HG23	1:A:130:ILE:HD13	0.55	1.79	2	2
1:A:278:TYR:CB	1:A:285:LEU:HD13	0.55	2.31	3	3
1:A:354:ILE:C	1:A:354:ILE:HD12	0.55	2.22	20	16
1:A:328:LEU:H	1:A:328:LEU:HD13	0.55	1.59	12	1
1:A:161:ILE:HD13	1:A:247:LEU:CD1	0.55	2.31	19	1
1:A:175:HIS:CE1	1:A:195:LEU:HD13	0.55	2.36	11	1
1:A:25:VAL:HG13	1:A:40:GLY:C	0.55	2.22	20	2
1:A:25:VAL:HG13	1:A:40:GLY:HA3	0.55	1.77	5	1
1:A:96:ILE:O	1:A:100:ILE:HD12	0.55	2.02	17	8
1:A:30:THR:O	1:A:30:THR:HG23	0.55	2.02	8	1
1:A:41:LEU:HG	1:A:53:LEU:HD22	0.55	1.77	19	1
1:A:41:LEU:O	1:A:53:LEU:HD13	0.55	2.02	9	2
1:A:225:ILE:HD11	1:A:233:HIS:CE1	0.54	2.37	18	3
1:A:198:TYR:HD2	1:A:201:ALA:HB2	0.54	1.61	1	9
1:A:141:ILE:HG22	1:A:145:ASN:ND2	0.54	2.18	7	2
1:A:175:HIS:HE2	1:A:195:LEU:HD13	0.54	1.62	15	1
1:A:174:VAL:HG13	1:A:243:ASP:OD2	0.54	2.03	3	1
1:A:159:LEU:HD23	1:A:324:LEU:HD13	0.54	1.77	6	2
1:A:156:GLN:HA	1:A:159:LEU:HD12	0.54	1.79	8	1
1:A:161:ILE:HG21	1:A:247:LEU:HD11	0.54	1.78	9	1
1:A:213:TYR:CE2	1:A:236:VAL:HG21	0.54	2.38	14	2
1:A:200:LEU:HD21	1:A:222:ASP:O	0.54	2.03	7	3
1:A:53:LEU:CD2	1:A:66:ALA:HB3	0.54	2.30	10	4
1:A:272:ARG:O	1:A:276:ILE:HD12	0.54	2.03	15	2
1:A:205:CYS:HB2	1:A:210:HIS:HA	0.54	1.80	11	1
1:A:162:LEU:HD12	1:A:317:TYR:CD2	0.54	2.38	10	2
1:A:196:VAL:HG12	1:A:197:ASP:OD2	0.54	2.02	9	1
1:A:222:ASP:OD1	1:A:228:THR:HG22	0.54	2.03	3	2
1:A:79:PRO:HG3	1:A:354:ILE:HD11	0.53	1.79	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ILE:HD13	1:A:57:ASN:HD21	0.53	1.63	4	1
1:A:39:VAL:HG13	1:A:53:LEU:O	0.53	2.04	4	2
1:A:118:LEU:HD11	1:A:127:ARG:NE	0.53	2.18	1	1
1:A:37:TRP:CH2	1:A:130:ILE:HD11	0.53	2.38	2	2
1:A:150:SER:HB2	1:A:153:THR:HG23	0.53	1.79	2	1
1:A:25:VAL:HG13	1:A:40:GLY:CA	0.53	2.33	5	1
1:A:276:ILE:HG22	1:A:280:GLU:OE2	0.53	2.04	7	1
1:A:230:ILE:HD12	1:A:241:ARG:NH2	0.53	2.19	19	1
1:A:255:LEU:HD22	1:A:290:PHE:CE2	0.53	2.39	10	1
1:A:184:LEU:HD12	1:A:184:LEU:N	0.53	2.19	14	1
1:A:53:LEU:HD22	1:A:66:ALA:HB1	0.53	1.81	16	1
1:A:214:LYS:O	1:A:236:VAL:HG13	0.53	2.04	16	6
1:A:226:GLU:HG3	1:A:265:LEU:HD21	0.53	1.79	12	2
1:A:73:GLU:CB	1:A:80:LEU:HD13	0.53	2.34	8	4
1:A:151:ARG:O	1:A:155:LEU:HD12	0.53	2.03	7	4
1:A:331:ILE:HG22	1:A:331:ILE:O	0.53	2.03	13	5
1:A:278:TYR:CD1	1:A:285:LEU:HD13	0.53	2.39	15	1
1:A:71:LYS:HE3	1:A:351:ALA:HB2	0.53	1.80	20	1
1:A:70:VAL:O	1:A:70:VAL:HG13	0.53	2.04	8	2
1:A:43:ILE:HD13	1:A:53:LEU:HG	0.53	1.81	18	1
1:A:84:LEU:HD11	1:A:116:SER:CB	0.52	2.33	7	1
1:A:28:ILE:HD12	1:A:28:ILE:O	0.52	2.04	9	1
1:A:178:ILE:HG22	1:A:246:ILE:CG2	0.52	2.33	16	1
1:A:316:LEU:O	1:A:320:LEU:HD12	0.52	2.04	1	1
1:A:70:VAL:HG21	1:A:128:PHE:CD1	0.52	2.39	9	3
1:A:111:PRO:HD3	1:A:196:VAL:HG12	0.52	1.82	16	1
1:A:301:LYS:HB3	1:A:323:ILE:HG21	0.52	1.81	7	3
1:A:321:ARG:O	1:A:325:LEU:HD12	0.52	2.04	14	1
1:A:183:LEU:O	1:A:184:LEU:HD12	0.52	2.05	18	2
1:A:53:LEU:HD23	1:A:66:ALA:CB	0.52	2.34	9	4
1:A:134:PHE:CE2	1:A:196:VAL:HG21	0.52	2.39	12	2
1:A:214:LYS:O	1:A:236:VAL:HG23	0.52	2.05	2	1
1:A:155:LEU:HD13	1:A:328:LEU:CD2	0.52	2.35	3	3
1:A:252:ILE:HG12	1:A:299:ILE:HG21	0.52	1.81	6	2
1:A:138:LEU:HD12	1:A:183:LEU:HB3	0.52	1.81	11	3
1:A:230:ILE:HG22	1:A:245:GLU:OE1	0.51	2.05	10	2
1:A:178:ILE:HD13	1:A:247:LEU:CD1	0.51	2.34	17	1
1:A:261:TRP:CD1	1:A:271:VAL:HG13	0.51	2.40	2	2
1:A:328:LEU:HD12	1:A:329:LYS:N	0.51	2.21	2	2
1:A:251:MET:O	1:A:255:LEU:HD12	0.51	2.04	4	1
1:A:100:ILE:HD11	1:A:106:LYS:C	0.51	2.25	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:HD13	1:A:53:LEU:HD12	0.51	1.81	16	1
1:A:42:PRO:O	1:A:43:ILE:HG23	0.51	2.06	18	7
1:A:111:PRO:HG2	1:A:196:VAL:HG22	0.51	1.80	12	1
1:A:32:MET:CE	1:A:33:ALA:HB2	0.51	2.36	1	1
1:A:185:LEU:HD22	1:A:190:PRO:O	0.51	2.06	1	1
1:A:98:LYS:O	1:A:102:THR:HG22	0.51	2.06	6	1
1:A:41:LEU:HD13	1:A:42:PRO:CD	0.51	2.36	17	1
1:A:142:TYR:CZ	1:A:254:TRP:CZ3	0.51	2.99	11	2
1:A:178:ILE:HD13	1:A:247:LEU:HD13	0.51	1.82	17	1
1:A:176:GLY:HA3	1:A:246:ILE:HD13	0.51	1.83	19	1
1:A:25:VAL:HG13	1:A:40:GLY:HA2	0.51	1.83	17	2
1:A:84:LEU:O	1:A:84:LEU:HD23	0.51	2.06	12	2
1:A:99:TRP:HA	1:A:102:THR:HG22	0.50	1.83	18	1
1:A:108:LEU:HD23	1:A:110:VAL:HB	0.50	1.83	19	2
1:A:271:VAL:HG12	1:A:275:LYS:HE3	0.50	1.82	19	2
1:A:174:VAL:HG12	1:A:240:ARG:NH2	0.50	2.21	5	1
1:A:82:THR:CB	1:A:353:THR:HB	0.50	2.36	15	2
1:A:103:ARG:HG2	1:A:105:LEU:HD12	0.50	1.83	1	1
1:A:178:ILE:O	1:A:178:ILE:HG22	0.50	2.07	8	10
1:A:155:LEU:HD22	1:A:328:LEU:HD23	0.50	1.84	8	1
1:A:165:LEU:HD21	1:A:178:ILE:CD1	0.50	2.37	15	1
1:A:86:PHE:CD1	1:A:198:TYR:CE2	0.50	2.99	18	1
1:A:37:TRP:CH2	1:A:114:TRP:CE3	0.50	3.00	17	2
1:A:43:ILE:C	1:A:43:ILE:HD13	0.50	2.27	12	1
1:A:70:VAL:CG2	1:A:130:ILE:HD13	0.50	2.36	10	2
1:A:154:VAL:HG11	1:A:255:LEU:HG	0.50	1.84	4	1
1:A:41:LEU:HB3	1:A:53:LEU:HD13	0.50	1.82	5	1
1:A:278:TYR:CZ	1:A:285:LEU:HD22	0.50	2.42	6	1
1:A:142:TYR:CD1	1:A:149:PHE:CE2	0.50	3.00	20	4
1:A:199:GLY:CA	1:A:353:THR:HA	0.50	2.37	15	2
1:A:84:LEU:HD13	1:A:127:ARG:NE	0.50	2.22	14	2
1:A:86:PHE:CE1	1:A:198:TYR:CE1	0.50	3.00	5	1
1:A:43:ILE:HD13	1:A:44:GLY:N	0.50	2.21	12	1
1:A:175:HIS:CD2	1:A:198:TYR:CE2	0.50	3.00	7	3
1:A:37:TRP:CE3	1:A:54:ALA:HB1	0.49	2.42	2	1
1:A:255:LEU:HD23	1:A:255:LEU:O	0.49	2.07	2	1
1:A:142:TYR:CE2	1:A:254:TRP:CZ3	0.49	2.99	9	2
1:A:285:LEU:HD23	1:A:286:MET:CE	0.49	2.37	10	1
1:A:155:LEU:HD11	1:A:298:GLU:OE2	0.49	2.08	9	2
1:A:28:ILE:HG21	1:A:57:ASN:CB	0.49	2.37	3	1
1:A:175:HIS:CE1	1:A:178:ILE:HD11	0.49	2.42	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:174:VAL:HG13	1:A:243:ASP:OD1	0.49	2.08	12	1
1:A:29:ILE:HD13	1:A:128:PHE:HZ	0.49	1.65	19	1
1:A:80:LEU:O	1:A:80:LEU:HD13	0.49	2.07	20	1
1:A:231:ASP:CA	1:A:236:VAL:HG12	0.49	2.38	1	2
1:A:37:TRP:CD1	1:A:130:ILE:HD12	0.49	2.43	3	2
1:A:84:LEU:HD12	1:A:129:MET:HG2	0.49	1.84	20	2
1:A:99:TRP:CD1	1:A:167:TYR:CD1	0.49	3.00	20	2
1:A:84:LEU:HD23	1:A:84:LEU:C	0.49	2.28	3	10
1:A:179:LYS:O	1:A:183:LEU:HD13	0.49	2.07	16	2
1:A:201:ALA:CB	1:A:353:THR:HG22	0.49	2.34	10	6
1:A:24:ALA:HB3	1:A:27:GLU:HG2	0.49	1.85	5	1
1:A:236:VAL:HG12	1:A:237:ALA:N	0.49	2.23	15	3
1:A:201:ALA:HB3	1:A:353:THR:HG23	0.49	1.84	15	2
1:A:31:ASP:OD2	1:A:33:ALA:HB3	0.49	2.08	16	2
1:A:28:ILE:HD12	1:A:36:GLU:OE1	0.49	2.08	17	1
1:A:227:PHE:O	1:A:246:ILE:HG23	0.48	2.07	5	1
1:A:28:ILE:HG21	1:A:57:ASN:HD22	0.48	1.68	20	1
1:A:82:THR:HG21	1:A:354:ILE:CG2	0.48	2.32	12	3
1:A:149:PHE:CD2	1:A:254:TRP:CE3	0.48	3.01	4	1
1:A:301:LYS:CB	1:A:323:ILE:HD13	0.48	2.38	1	1
1:A:84:LEU:HD22	1:A:127:ARG:HH21	0.48	1.68	3	1
1:A:43:ILE:HD12	1:A:53:LEU:HG	0.48	1.84	20	1
1:A:175:HIS:CE1	1:A:198:TYR:CE2	0.48	3.02	9	3
1:A:175:HIS:HB3	1:A:178:ILE:HD11	0.48	1.85	13	1
1:A:83:GLU:CD	1:A:351:ALA:HB1	0.48	2.27	14	1
1:A:230:ILE:HG23	1:A:245:GLU:OE1	0.48	2.08	16	1
1:A:39:VAL:HG22	1:A:54:ALA:HB2	0.48	1.83	5	2
1:A:213:TYR:CE1	1:A:236:VAL:HG11	0.48	2.43	12	1
1:A:176:GLY:HA3	1:A:200:LEU:HD12	0.48	1.86	17	1
1:A:199:GLY:O	1:A:200:LEU:HD23	0.48	2.09	20	3
1:A:165:LEU:HD21	1:A:178:ILE:HD11	0.48	1.84	15	2
1:A:178:ILE:HG21	1:A:247:LEU:CD1	0.48	2.39	18	1
1:A:80:LEU:C	1:A:80:LEU:HD13	0.48	2.28	14	1
1:A:158:SER:OG	1:A:324:LEU:HD22	0.48	2.08	12	2
1:A:279:ARG:O	1:A:282:ILE:HD11	0.48	2.08	15	3
1:A:29:ILE:HD13	1:A:29:ILE:H	0.48	1.68	15	1
1:A:168:ILE:HG21	1:A:198:TYR:OH	0.47	2.09	7	2
1:A:278:TYR:CD2	1:A:285:LEU:HD13	0.47	2.44	4	1
1:A:230:ILE:HD12	1:A:279:ARG:NH1	0.47	2.24	5	1
1:A:213:TYR:CD1	1:A:236:VAL:HG21	0.47	2.45	13	1
1:A:142:TYR:CD1	1:A:149:PHE:CD2	0.47	3.02	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:ASN:O	1:A:146:ALA:HB3	0.47	2.09	17	5
1:A:252:ILE:HG23	1:A:290:PHE:HZ	0.47	1.69	5	1
1:A:175:HIS:CD2	1:A:178:ILE:CD1	0.47	2.98	10	2
1:A:255:LEU:HD22	1:A:290:PHE:HZ	0.47	1.69	10	1
1:A:25:VAL:CG1	1:A:41:LEU:HD12	0.47	2.38	12	1
1:A:100:ILE:HG21	1:A:106:LYS:O	0.47	2.10	1	1
1:A:100:ILE:HD11	1:A:107:TYR:N	0.47	2.25	7	1
1:A:103:ARG:HB3	1:A:105:LEU:HD13	0.47	1.84	14	1
1:A:150:SER:O	1:A:154:VAL:HG12	0.47	2.09	19	2
1:A:247:LEU:HD23	1:A:251:MET:HG3	0.47	1.87	6	1
1:A:51:ILE:HG22	1:A:69:VAL:HB	0.47	1.87	8	1
1:A:96:ILE:HG23	1:A:108:LEU:CD2	0.47	2.36	9	2
1:A:222:ASP:OD2	1:A:228:THR:HG22	0.47	2.09	9	1
1:A:114:TRP:CD1	1:A:130:ILE:HG22	0.47	2.45	2	2
1:A:134:PHE:CZ	1:A:196:VAL:HG21	0.47	2.45	10	1
1:A:28:ILE:HD11	1:A:38:LYS:CE	0.47	2.40	18	2
1:A:198:TYR:CB	1:A:353:THR:HG23	0.47	2.40	10	3
1:A:155:LEU:HD13	1:A:328:LEU:HD23	0.47	1.87	7	1
1:A:253:GLN:CD	1:A:259:LEU:HD12	0.47	2.30	15	1
1:A:175:HIS:NE2	1:A:195:LEU:HD22	0.47	2.25	20	1
1:A:118:LEU:HD23	1:A:118:LEU:C	0.46	2.31	10	1
1:A:154:VAL:HA	1:A:157:LEU:HD12	0.46	1.85	20	1
1:A:206:PRO:O	1:A:209:VAL:HG22	0.46	2.10	7	6
1:A:256:THR:HG23	1:A:290:PHE:CZ	0.46	2.44	5	1
1:A:138:LEU:HA	1:A:141:ILE:HD12	0.46	1.86	7	2
1:A:118:LEU:HD21	1:A:127:ARG:CD	0.46	2.40	13	1
1:A:253:GLN:NE2	1:A:254:TRP:CD1	0.46	2.84	4	1
1:A:28:ILE:HA	1:A:37:TRP:O	0.46	2.10	8	1
1:A:23:PHE:CZ	1:A:72:VAL:HG21	0.46	2.45	9	1
1:A:51:ILE:N	1:A:51:ILE:HD12	0.46	2.25	14	2
1:A:214:LYS:C	1:A:236:VAL:HG13	0.46	2.31	10	2
1:A:161:ILE:HG21	1:A:178:ILE:HG21	0.46	1.87	13	1
1:A:184:LEU:HD13	1:A:196:VAL:HG11	0.46	1.85	3	1
1:A:138:LEU:HD12	1:A:183:LEU:CB	0.46	2.41	11	3
1:A:126:TYR:CD1	1:A:126:TYR:N	0.46	2.84	7	2
1:A:28:ILE:HG23	1:A:38:LYS:HD2	0.46	1.87	17	1
1:A:88:GLN:CG	1:A:113:TYR:CE2	0.46	2.99	9	8
1:A:175:HIS:CD2	1:A:178:ILE:CG1	0.46	2.99	5	1
1:A:37:TRP:CE2	1:A:130:ILE:CD1	0.46	2.99	6	2
1:A:103:ARG:CB	1:A:105:LEU:HD23	0.46	2.38	12	1
1:A:183:LEU:HD23	1:A:194:TYR:O	0.46	2.11	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:302:TYR:O	1:A:305:THR:HG22	0.46	2.11	4	1
1:A:252:ILE:HD11	1:A:299:ILE:CG2	0.46	2.41	12	1
1:A:119:HIS:N	1:A:119:HIS:CD2	0.46	2.83	17	1
1:A:183:LEU:HD23	1:A:193:VAL:HG21	0.46	1.86	20	1
1:A:110:VAL:N	1:A:194:TYR:CD2	0.46	2.84	13	5
1:A:256:THR:CG2	1:A:290:PHE:CZ	0.46	2.99	5	1
1:A:29:ILE:HG21	1:A:128:PHE:HZ	0.46	1.70	19	1
1:A:267:ASP:O	1:A:271:VAL:HG23	0.46	2.10	1	1
1:A:249:TYR:HA	1:A:252:ILE:HD12	0.46	1.87	8	3
1:A:52:TYR:HB2	1:A:70:VAL:HG13	0.46	1.88	6	1
1:A:155:LEU:CG	1:A:328:LEU:HD21	0.46	2.40	14	1
1:A:41:LEU:CB	1:A:53:LEU:HD12	0.46	2.41	16	1
1:A:286:MET:HE3	1:A:299:ILE:HG21	0.46	1.88	11	1
1:A:168:ILE:HD11	1:A:175:HIS:ND1	0.46	2.26	13	2
1:A:158:SER:OG	1:A:247:LEU:HD21	0.46	2.11	18	1
1:A:264:ASN:ND2	1:A:270:TYR:CE2	0.45	2.85	7	1
1:A:168:ILE:CD1	1:A:175:HIS:CG	0.45	2.99	8	4
1:A:134:PHE:CE2	1:A:196:VAL:CG2	0.45	2.99	2	1
1:A:134:PHE:CD1	1:A:184:LEU:CB	0.45	3.00	12	1
1:A:217:PRO:CB	1:A:221:HIS:CE1	0.45	2.99	17	1
1:A:29:ILE:HG21	1:A:128:PHE:CZ	0.45	2.47	19	1
1:A:183:LEU:HD23	1:A:195:LEU:HA	0.45	1.87	3	4
1:A:278:TYR:CG	1:A:285:LEU:CD1	0.45	3.00	8	7
1:A:239:SER:CB	1:A:311:TYR:CE2	0.45	2.99	7	2
1:A:28:ILE:HG22	1:A:38:LYS:CB	0.45	2.42	9	3
1:A:182:ASN:ND2	1:A:183:LEU:HD12	0.45	2.27	11	1
1:A:29:ILE:CD1	1:A:128:PHE:CE1	0.45	3.00	17	4
1:A:37:TRP:CD1	1:A:130:ILE:CD1	0.45	3.00	3	1
1:A:175:HIS:NE2	1:A:198:TYR:CE1	0.45	2.84	3	1
1:A:256:THR:CG2	1:A:290:PHE:CE1	0.45	2.99	4	1
1:A:169:HIS:CE1	1:A:240:ARG:CZ	0.45	3.00	5	1
1:A:142:TYR:CZ	1:A:147:LYS:CG	0.45	3.00	8	2
1:A:82:THR:CG2	1:A:354:ILE:HG22	0.45	2.41	20	1
1:A:107:TYR:CZ	1:A:192:GLN:NE2	0.45	2.85	1	2
1:A:107:TYR:CD2	1:A:107:TYR:O	0.45	2.69	5	2
1:A:205:CYS:CB	1:A:209:VAL:O	0.45	2.65	11	1
1:A:251:MET:HE1	1:A:302:TYR:CE2	0.45	2.46	16	1
1:A:282:ILE:HD11	1:A:307:LYS:HD3	0.45	1.87	16	1
1:A:100:ILE:HG23	1:A:108:LEU:HD13	0.45	1.89	9	1
1:A:162:LEU:HD23	1:A:317:TYR:CE2	0.45	2.46	14	1
1:A:179:LYS:CE	1:A:227:PHE:CE2	0.45	3.00	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:TRP:CZ3	1:A:105:LEU:CD1	0.45	3.00	20	1
1:A:37:TRP:CH2	1:A:130:ILE:CD1	0.45	3.00	2	1
1:A:88:GLN:CG	1:A:113:TYR:CE1	0.45	3.00	7	2
1:A:221:HIS:CD2	1:A:356:LYS:N	0.45	2.85	7	1
1:A:165:LEU:CD2	1:A:175:HIS:CE1	0.45	3.00	16	1
1:A:81:PHE:CE2	1:A:127:ARG:NH2	0.45	2.85	5	1
1:A:155:LEU:HD23	1:A:324:LEU:HD23	0.45	1.88	11	1
1:A:99:TRP:CE3	1:A:105:LEU:CD1	0.45	3.00	20	1
1:A:174:VAL:CG2	1:A:204:TYR:CD1	0.45	3.00	1	1
1:A:175:HIS:ND1	1:A:198:TYR:CE2	0.45	2.85	1	1
1:A:37:TRP:CZ2	1:A:130:ILE:CD1	0.45	2.99	2	1
1:A:162:LEU:CD1	1:A:317:TYR:CD2	0.45	3.00	4	2
1:A:224:THR:HG21	1:A:226:GLU:OE2	0.45	2.12	6	1
1:A:278:TYR:CD2	1:A:285:LEU:CD1	0.45	3.00	13	2
1:A:81:PHE:CE2	1:A:127:ARG:CZ	0.45	3.00	12	1
1:A:178:ILE:HG23	1:A:195:LEU:CD1	0.45	2.42	17	2
1:A:134:PHE:CE1	1:A:196:VAL:HG11	0.45	2.46	16	1
1:A:79:PRO:HA	1:A:82:THR:OG1	0.45	2.12	20	1
1:A:103:ARG:CG	1:A:105:LEU:HD12	0.45	2.42	1	1
1:A:184:LEU:HD22	1:A:196:VAL:HG11	0.45	1.89	6	1
1:A:107:TYR:CE1	1:A:192:GLN:NE2	0.45	2.85	14	1
1:A:29:ILE:CD1	1:A:128:PHE:CZ	0.44	3.00	17	2
1:A:70:VAL:CG2	1:A:128:PHE:CD1	0.44	3.01	16	3
1:A:351:ALA:O	1:A:352:LYS:HB3	0.44	2.10	9	1
1:A:142:TYR:CZ	1:A:254:TRP:CE3	0.44	3.05	18	2
1:A:86:PHE:CE2	1:A:201:ALA:CB	0.44	3.00	5	2
1:A:256:THR:HG23	1:A:258:HIS:H	0.44	1.73	8	1
1:A:158:SER:HA	1:A:161:ILE:HD12	0.44	1.87	19	2
1:A:175:HIS:CE1	1:A:178:ILE:CD1	0.44	3.00	12	1
1:A:54:ALA:HB3	1:A:68:CYS:C	0.44	2.32	20	2
1:A:138:LEU:HD21	1:A:157:LEU:HD11	0.44	1.88	19	3
1:A:73:GLU:HB3	1:A:80:LEU:HD13	0.44	1.88	12	1
1:A:202:TYR:CD1	1:A:355:THR:CG2	0.44	2.99	20	1
1:A:233:HIS:CE1	1:A:275:LYS:CD	0.44	3.01	4	1
1:A:199:GLY:HA2	1:A:352:LYS:C	0.44	2.33	9	1
1:A:204:TYR:CD1	1:A:204:TYR:N	0.44	2.85	11	1
1:A:175:HIS:CD2	1:A:198:TYR:CD2	0.44	3.05	19	1
1:A:309:LEU:C	1:A:309:LEU:HD12	0.44	2.31	20	1
1:A:28:ILE:HD12	1:A:36:GLU:HG2	0.44	1.88	2	1
1:A:96:ILE:HG23	1:A:97:GLN:N	0.44	2.28	11	3
1:A:207:GLU:O	1:A:209:VAL:HG23	0.44	2.12	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:TYR:CZ	1:A:203:ARG:CG	0.44	3.00	14	1
1:A:159:LEU:C	1:A:159:LEU:HD23	0.44	2.33	20	1
1:A:225:ILE:HG12	1:A:271:VAL:HG11	0.44	1.88	20	1
1:A:83:GLU:N	1:A:353:THR:OG1	0.44	2.50	19	7
1:A:213:TYR:O	1:A:213:TYR:CD2	0.44	2.71	4	3
1:A:282:ILE:HD11	1:A:303:MET:HG2	0.44	1.89	10	1
1:A:175:HIS:HE1	1:A:195:LEU:HD22	0.44	1.72	11	1
1:A:253:GLN:NE2	1:A:259:LEU:HD12	0.44	2.26	15	2
1:A:205:CYS:N	1:A:206:PRO:CD	0.44	2.81	7	3
1:A:107:TYR:CD2	1:A:192:GLN:NE2	0.44	2.85	9	1
1:A:195:LEU:CD2	1:A:198:TYR:CE1	0.44	3.01	9	1
1:A:51:ILE:CG2	1:A:69:VAL:HG21	0.44	2.43	8	1
1:A:73:GLU:CB	1:A:80:LEU:HD22	0.44	2.43	9	1
1:A:252:ILE:HD11	1:A:303:MET:SD	0.44	2.53	19	1
1:A:84:LEU:HD22	1:A:127:ARG:HH12	0.43	1.71	8	1
1:A:82:THR:HG21	1:A:354:ILE:HG22	0.43	1.89	20	1
1:A:100:ILE:HD11	1:A:107:TYR:CA	0.43	2.43	7	1
1:A:78:GLY:O	1:A:81:PHE:N	0.43	2.50	9	1
1:A:154:VAL:HG13	1:A:155:LEU:N	0.43	2.27	19	2
1:A:168:ILE:HD11	1:A:175:HIS:HB2	0.43	1.90	18	1
1:A:73:GLU:HB2	1:A:80:LEU:HD13	0.43	1.88	2	1
1:A:162:LEU:CD1	1:A:317:TYR:CE2	0.43	3.01	10	2
1:A:100:ILE:HA	1:A:105:LEU:HD12	0.43	1.88	20	1
1:A:69:VAL:HG13	1:A:133:ARG:CD	0.43	2.43	1	1
1:A:225:ILE:CD1	1:A:271:VAL:HG21	0.43	2.42	1	1
1:A:92:LYS:O	1:A:96:ILE:HD12	0.43	2.14	15	4
1:A:303:MET:HA	1:A:306:VAL:HG22	0.43	1.90	2	1
1:A:117:GLY:N	1:A:128:PHE:CE1	0.43	2.86	6	2
1:A:82:THR:CG2	1:A:353:THR:HB	0.43	2.44	16	2
1:A:221:HIS:O	1:A:222:ASP:CB	0.43	2.65	17	1
1:A:225:ILE:HD11	1:A:271:VAL:CG2	0.43	2.44	1	1
1:A:99:TRP:CH2	1:A:105:LEU:CD1	0.43	3.00	8	1
1:A:84:LEU:HD13	1:A:127:ARG:CD	0.43	2.44	14	1
1:A:80:LEU:HD13	1:A:80:LEU:C	0.43	2.34	20	1
1:A:214:LYS:O	1:A:237:ALA:N	0.43	2.51	11	6
1:A:262:GLU:O	1:A:265:LEU:HD23	0.43	2.13	2	1
1:A:142:TYR:CE1	1:A:254:TRP:NE1	0.43	2.86	4	1
1:A:151:ARG:HG3	1:A:255:LEU:HD21	0.43	1.89	19	1
1:A:252:ILE:HG21	1:A:278:TYR:OH	0.43	2.14	6	1
1:A:265:LEU:HD22	1:A:265:LEU:N	0.43	2.29	13	1
1:A:225:ILE:HD11	1:A:271:VAL:HG21	0.43	1.89	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:TYR:CE2	1:A:203:ARG:NH1	0.43	2.87	6	1
1:A:225:ILE:HD12	1:A:228:THR:OG1	0.42	2.13	10	1
1:A:314:LYS:O	1:A:316:LEU:HD22	0.42	2.14	13	1
1:A:226:GLU:CD	1:A:265:LEU:HD21	0.42	2.34	16	1
1:A:28:ILE:HD12	1:A:36:GLU:CG	0.42	2.44	2	1
1:A:87:TYR:O	1:A:91:ALA:N	0.42	2.52	5	4
1:A:184:LEU:HD22	1:A:196:VAL:HG21	0.42	1.90	8	1
1:A:187:TYR:CD1	1:A:188:LYS:N	0.42	2.88	8	1
1:A:204:TYR:O	1:A:205:CYS:CB	0.42	2.67	11	1
1:A:162:LEU:HA	1:A:165:LEU:HD12	0.42	1.90	14	1
1:A:41:LEU:HB3	1:A:53:LEU:HD12	0.42	1.90	16	1
1:A:175:HIS:CE1	1:A:198:TYR:CD2	0.42	3.07	2	1
1:A:73:GLU:CG	1:A:80:LEU:HD13	0.42	2.44	15	1
1:A:352:LYS:CG	1:A:353:THR:N	0.42	2.82	16	1
1:A:236:VAL:HG22	1:A:237:ALA:H	0.42	1.75	18	2
1:A:296:PRO:CG	1:A:299:ILE:HD12	0.42	2.44	3	1
1:A:225:ILE:CD1	1:A:233:HIS:CE1	0.42	3.02	18	1
1:A:82:THR:CG2	1:A:354:ILE:CG2	0.42	2.98	20	1
1:A:29:ILE:N	1:A:29:ILE:CD1	0.42	2.82	15	1
1:A:149:PHE:CE2	1:A:254:TRP:CZ3	0.42	3.07	4	1
1:A:230:ILE:HD12	1:A:245:GLU:OE2	0.42	2.15	13	1
1:A:43:ILE:O	1:A:43:ILE:HG23	0.42	2.14	14	1
1:A:177:ASP:OD1	1:A:246:ILE:HG21	0.42	2.15	14	1
1:A:41:LEU:HD13	1:A:53:LEU:HD22	0.42	1.92	15	1
1:A:157:LEU:CD2	1:A:183:LEU:HD13	0.42	2.44	17	1
1:A:261:TRP:HB2	1:A:271:VAL:HG22	0.42	1.90	18	1
1:A:230:ILE:HG21	1:A:279:ARG:HE	0.42	1.72	16	1
1:A:29:ILE:HD11	1:A:37:TRP:CH2	0.42	2.45	2	1
1:A:37:TRP:CZ3	1:A:39:VAL:CG1	0.42	3.02	6	1
1:A:70:VAL:HG22	1:A:128:PHE:HB2	0.42	1.92	9	2
1:A:99:TRP:CD2	1:A:167:TYR:CD2	0.42	3.08	12	1
1:A:168:ILE:HD11	1:A:175:HIS:CG	0.42	2.50	13	1
1:A:328:LEU:HD22	1:A:328:LEU:C	0.42	2.33	12	1
1:A:111:PRO:CD	1:A:196:VAL:HG12	0.42	2.45	16	1
1:A:71:LYS:HE2	1:A:351:ALA:HB2	0.42	1.89	20	1
1:A:251:MET:CE	1:A:302:TYR:CE2	0.42	3.03	16	1
1:A:175:HIS:HE2	1:A:195:LEU:HD22	0.41	1.75	4	1
1:A:228:THR:O	1:A:228:THR:HG23	0.41	2.14	11	1
1:A:79:PRO:HB3	1:A:352:LYS:CG	0.41	2.45	12	1
1:A:84:LEU:CD1	1:A:127:ARG:NE	0.41	2.83	14	1
1:A:296:PRO:HG2	1:A:299:ILE:HD12	0.41	1.91	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:PHE:O	1:A:81:PHE:CD1	0.41	2.73	18	2
1:A:240:ARG:HH22	1:A:309:LEU:HD22	0.41	1.75	3	1
1:A:307:LYS:CG	1:A:308:LEU:HD12	0.41	2.44	7	1
1:A:23:PHE:CE2	1:A:72:VAL:HG21	0.41	2.50	9	1
1:A:199:GLY:HA2	1:A:353:THR:N	0.41	2.30	20	2
1:A:119:HIS:CE1	1:A:126:TYR:CB	0.41	3.03	17	1
1:A:173:TYR:CZ	1:A:203:ARG:CD	0.41	3.04	3	1
1:A:264:ASN:ND2	1:A:270:TYR:CG	0.41	2.89	5	1
1:A:100:ILE:CG2	1:A:108:LEU:HD13	0.41	2.45	9	1
1:A:155:LEU:HD21	1:A:327:GLY:HA3	0.41	1.92	12	1
1:A:176:GLY:O	1:A:246:ILE:HG21	0.41	2.15	16	1
1:A:43:ILE:HD13	1:A:53:LEU:CG	0.41	2.43	18	1
1:A:134:PHE:CE2	1:A:196:VAL:HG11	0.41	2.50	18	1
1:A:286:MET:HE1	1:A:299:ILE:HG21	0.41	1.91	1	1
1:A:290:PHE:HB3	1:A:294:ASN:O	0.41	2.15	5	1
1:A:32:MET:HE1	1:A:33:ALA:HB2	0.41	1.92	1	1
1:A:160:ARG:O	1:A:164:ILE:HD12	0.41	2.15	6	1
1:A:247:LEU:HD23	1:A:251:MET:CG	0.41	2.45	6	1
1:A:328:LEU:CD1	1:A:328:LEU:N	0.41	2.84	11	1
1:A:72:VAL:HG22	1:A:128:PHE:CB	0.41	2.45	13	1
1:A:119:HIS:CE1	1:A:126:TYR:HB2	0.41	2.51	17	1
1:A:178:ILE:O	1:A:179:LYS:O	0.41	2.38	17	1
1:A:109:GLY:O	1:A:194:TYR:CD2	0.41	2.74	9	2
1:A:255:LEU:HD12	1:A:290:PHE:HZ	0.41	1.75	3	1
1:A:168:ILE:HD12	1:A:169:HIS:N	0.41	2.30	4	2
1:A:211:LYS:O	1:A:311:TYR:CE1	0.41	2.73	6	1
1:A:162:LEU:CD2	1:A:317:TYR:CD2	0.41	3.04	14	1
1:A:39:VAL:HG11	1:A:70:VAL:HG11	0.41	1.91	16	1
1:A:165:LEU:CD2	1:A:175:HIS:ND1	0.41	2.84	16	1
1:A:225:ILE:O	1:A:228:THR:HG22	0.41	2.16	6	1
1:A:71:LYS:HZ3	1:A:83:GLU:CD	0.41	2.19	10	1
1:A:155:LEU:HD12	1:A:328:LEU:HD21	0.41	1.92	14	1
1:A:219:ARG:O	1:A:220:CYS:CB	0.41	2.69	17	1
1:A:175:HIS:CE1	1:A:195:LEU:CD2	0.41	3.02	18	1
1:A:250:CYS:O	1:A:254:TRP:CD1	0.41	2.74	5	2
1:A:290:PHE:N	1:A:290:PHE:CD1	0.41	2.88	5	1
1:A:88:GLN:HG2	1:A:113:TYR:CE1	0.41	2.51	7	1
1:A:28:ILE:HG21	1:A:57:ASN:OD1	0.41	2.15	9	1
1:A:31:ASP:OD2	1:A:37:TRP:CD1	0.41	2.74	9	1
1:A:353:THR:O	1:A:354:ILE:O	0.41	2.38	10	1
1:A:162:LEU:CD2	1:A:317:TYR:CE2	0.41	3.03	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:278:TYR:CG	1:A:285:LEU:HD12	0.41	2.50	19	1
1:A:173:TYR:CZ	1:A:203:ARG:HD2	0.41	2.51	3	1
1:A:189:ASN:OD1	1:A:189:ASN:N	0.41	2.54	3	1
1:A:261:TRP:CD1	1:A:261:TRP:O	0.41	2.74	3	1
1:A:108:LEU:O	1:A:110:VAL:N	0.41	2.54	6	1
1:A:226:GLU:HB3	1:A:265:LEU:HD22	0.41	1.92	6	1
1:A:258:HIS:CG	1:A:262:GLU:OE2	0.41	2.74	6	1
1:A:264:ASN:OD1	1:A:270:TYR:CG	0.41	2.74	7	4
1:A:142:TYR:CZ	1:A:147:LYS:HG2	0.41	2.51	9	1
1:A:282:ILE:HG21	1:A:303:MET:HB3	0.41	1.93	11	1
1:A:161:ILE:HG22	1:A:165:LEU:HD11	0.41	1.90	15	1
1:A:33:ALA:O	1:A:34:LYS:HG3	0.41	2.16	16	1
1:A:83:GLU:HB2	1:A:351:ALA:O	0.41	2.16	16	1
1:A:259:LEU:CD2	1:A:261:TRP:CH2	0.41	3.01	1	1
1:A:169:HIS:CE1	1:A:240:ARG:NH1	0.41	2.89	5	1
1:A:213:TYR:CD1	1:A:213:TYR:O	0.41	2.74	10	1
1:A:128:PHE:CD1	1:A:128:PHE:O	0.41	2.74	13	1
1:A:83:GLU:CA	1:A:353:THR:OG1	0.41	2.69	14	1
1:A:192:GLN:OE1	1:A:194:TYR:CE2	0.41	2.74	14	1
1:A:157:LEU:HD13	1:A:254:TRP:HZ3	0.41	1.72	17	1
1:A:175:HIS:CE1	1:A:178:ILE:HG13	0.41	2.51	17	1
1:A:179:LYS:CD	1:A:227:PHE:CZ	0.41	3.04	17	1
1:A:213:TYR:CD2	1:A:213:TYR:O	0.40	2.75	3	1
1:A:226:GLU:CG	1:A:265:LEU:HD13	0.40	2.46	8	1
1:A:236:VAL:HG13	1:A:237:ALA:O	0.40	2.17	13	1
1:A:83:GLU:HB3	1:A:351:ALA:HB1	0.40	1.91	15	1
1:A:41:LEU:HD13	1:A:53:LEU:CD1	0.40	2.46	16	1
1:A:154:VAL:HG11	1:A:255:LEU:HD23	0.40	1.89	16	1
1:A:182:ASN:O	1:A:183:LEU:HD12	0.40	2.16	16	1
1:A:118:LEU:CD1	1:A:127:ARG:CD	0.40	3.00	3	1
1:A:118:LEU:HD21	1:A:127:ARG:NH1	0.40	2.31	4	1
1:A:162:LEU:HD22	1:A:317:TYR:HD2	0.40	1.69	8	1
1:A:209:VAL:HG12	1:A:210:HIS:N	0.40	2.31	10	1
1:A:146:ALA:O	1:A:147:LYS:CG	0.40	2.69	13	1
1:A:264:ASN:OD1	1:A:270:TYR:CD2	0.40	2.75	13	1
1:A:86:PHE:CD2	1:A:198:TYR:CE2	0.40	3.08	14	1
1:A:245:GLU:OE2	1:A:249:TYR:CE1	0.40	2.75	15	1
1:A:225:ILE:HD11	1:A:233:HIS:HE1	0.40	1.76	17	1
1:A:118:LEU:N	1:A:118:LEU:CD1	0.40	2.84	18	1
1:A:217:PRO:O	1:A:221:HIS:CD2	0.40	2.75	1	1
1:A:174:VAL:CG1	1:A:204:TYR:CE1	0.40	3.04	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:278:TYR:CE1	1:A:285:LEU:HD22	0.40	2.52	6	1
1:A:239:SER:HB3	1:A:311:TYR:CE2	0.40	2.51	7	1
1:A:213:TYR:O	1:A:213:TYR:CG	0.40	2.74	8	1
1:A:258:HIS:CE1	1:A:262:GLU:OE2	0.40	2.75	9	1
1:A:320:LEU:O	1:A:323:ILE:CG1	0.40	2.69	11	1
1:A:186:ASN:OD1	1:A:194:TYR:CE1	0.40	2.74	19	2
1:A:39:VAL:HG12	1:A:53:LEU:O	0.40	2.16	16	1
1:A:253:GLN:OE1	1:A:254:TRP:CH2	0.40	2.75	18	1
1:A:29:ILE:HD13	1:A:128:PHE:CE1	0.40	2.52	20	1
1:A:83:GLU:OE1	1:A:87:TYR:CD1	0.40	2.75	2	1
1:A:118:LEU:HD11	1:A:127:ARG:CD	0.40	2.46	3	1
1:A:166:GLU:OE2	1:A:317:TYR:CD1	0.40	2.75	8	1
1:A:88:GLN:HG2	1:A:113:TYR:CE2	0.40	2.52	13	1
1:A:107:TYR:CD1	1:A:194:TYR:OH	0.40	2.75	13	1
1:A:175:HIS:CD2	1:A:176:GLY:N	0.40	2.90	16	1
1:A:228:THR:OG1	1:A:232:ALA:HB3	0.40	2.16	17	1
1:A:233:HIS:NE2	1:A:275:LYS:CD	0.40	2.85	3	1
1:A:253:GLN:OE1	1:A:254:TRP:CE3	0.40	2.74	5	1
1:A:51:ILE:HD12	1:A:51:ILE:N	0.40	2.32	6	1
1:A:166:GLU:OE1	1:A:317:TYR:CD2	0.40	2.74	9	1
1:A:253:GLN:HG2	1:A:254:TRP:CZ3	0.40	2.52	9	1
1:A:41:LEU:CD1	1:A:43:ILE:HG23	0.40	2.47	10	1
1:A:351:ALA:O	1:A:352:LYS:HB2	0.40	2.16	10	1
1:A:155:LEU:HD22	1:A:328:LEU:N	0.40	2.31	12	1
1:A:83:GLU:OE2	1:A:87:TYR:CE1	0.40	2.75	13	1
1:A:178:ILE:CG2	1:A:246:ILE:HG22	0.40	2.44	16	1
1:A:230:ILE:HD11	1:A:279:ARG:NH2	0.40	2.32	18	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	310/361 (86%)	273±4 (88±1%)	27±4 (9±1%)	10±2 (3±1%)	5	34
All	All	6200/7220 (86%)	5451 (88%)	541 (9%)	208 (3%)	5	34

All 33 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	353	THR	20
1	A	354	ILE	20
1	A	200	LEU	18
1	A	213	TYR	18
1	A	197	ASP	14
1	A	109	GLY	12
1	A	179	LYS	10
1	A	58	SER	9
1	A	57	ASN	8
1	A	60	GLU	7
1	A	238	PRO	7
1	A	228	THR	7
1	A	61	SER	6
1	A	40	GLY	5
1	A	41	LEU	5
1	A	352	LYS	5
1	A	211	LYS	4
1	A	356	LYS	3
1	A	59	SER	3
1	A	23	PHE	3
1	A	266	LYS	3
1	A	291	PRO	3
1	A	177	ASP	3
1	A	66	ALA	3
1	A	296	PRO	2
1	A	220	CYS	2
1	A	351	ALA	2
1	A	205	CYS	1
1	A	79	PRO	1
1	A	294	ASN	1
1	A	222	ASP	1
1	A	106	LYS	1
1	A	49	GLY	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	273/312 (88%)	222±6 (81±2%)	51±6 (19±2%)	3 35
All	All	5460/6240 (88%)	4443 (81%)	1017 (19%)	3 35

All 184 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	202	TYR	20
1	A	355	THR	20
1	A	82	THR	18
1	A	273	ASP	18
1	A	310	ASP	18
1	A	200	LEU	17
1	A	353	THR	16
1	A	287	ASP	16
1	A	267	ASP	15
1	A	150	SER	14
1	A	322	ASP	14
1	A	138	LEU	12
1	A	224	THR	12
1	A	56	MET	12
1	A	73	GLU	11
1	A	103	ARG	11
1	A	152	LYS	11
1	A	279	ARG	11
1	A	307	LYS	11
1	A	83	GLU	11
1	A	222	ASP	11
1	A	286	MET	11
1	A	288	LYS	11
1	A	35	LYS	11
1	A	140	LYS	11
1	A	156	GLN	11
1	A	106	LYS	10
1	A	175	HIS	10
1	A	309	LEU	10
1	A	129	MET	10
1	A	356	LYS	10
1	A	107	TYR	10
1	A	163	ASP	10
1	A	88	GLN	9
1	A	133	ARG	9
1	A	203	ARG	9

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Mol	Chain	Res	Type	Models (Total)
1	A	195	LEU	9
1	A	211	LYS	9
1	A	76	ASP	9
1	A	59	SER	8
1	A	241	ARG	8
1	A	255	LEU	8
1	A	334	LYS	8
1	A	61	SER	8
1	A	32	MET	7
1	A	60	GLU	7
1	A	125	SER	7
1	A	221	HIS	7
1	A	50	CYS	7
1	A	250	CYS	7
1	A	118	LEU	7
1	A	160	ARG	7
1	A	162	LEU	7
1	A	303	MET	7
1	A	314	LYS	7
1	A	41	LEU	7
1	A	214	LYS	7
1	A	228	THR	7
1	A	34	LYS	6
1	A	77	ASN	6
1	A	179	LYS	6
1	A	233	HIS	6
1	A	30	THR	6
1	A	92	LYS	6
1	A	119	HIS	6
1	A	124	LYS	6
1	A	170	GLU	6
1	A	132	ASP	6
1	A	245	GLU	6
1	A	264	ASN	6
1	A	295	LYS	6
1	A	147	LYS	6
1	A	97	GLN	6
1	A	89	ARG	6
1	A	219	ARG	5
1	A	326	GLN	5
1	A	71	LYS	5
1	A	197	ASP	5

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Mol	Chain	Res	Type	Models (Total)
1	A	262	GLU	5
1	A	104	LYS	5
1	A	169	HIS	5
1	A	240	ARG	5
1	A	165	LEU	5
1	A	192	GLN	5
1	A	58	SER	5
1	A	149	PHE	5
1	A	218	LYS	5
1	A	285	LEU	5
1	A	231	ASP	5
1	A	95	GLN	5
1	A	108	LEU	5
1	A	94	GLU	4
1	A	136	SER	4
1	A	151	ARG	4
1	A	177	ASP	4
1	A	181	SER	4
1	A	38	LYS	4
1	A	101	ARG	4
1	A	145	ASN	4
1	A	148	ARG	4
1	A	266	LYS	4
1	A	311	TYR	4
1	A	98	LYS	4
1	A	127	ARG	4
1	A	256	THR	4
1	A	321	ARG	4
1	A	277	ARG	4
1	A	186	ASN	4
1	A	213	TYR	4
1	A	251	MET	4
1	A	226	GLU	4
1	A	153	THR	4
1	A	139	GLN	4
1	A	243	ASP	4
1	A	121	LYS	3
1	A	275	LYS	3
1	A	289	CYS	3
1	A	85	LYS	3
1	A	166	GLU	3
1	A	225	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	323	ILE	3
1	A	173	TYR	3
1	A	290	PHE	3
1	A	188	LYS	3
1	A	269	LYS	3
1	A	155	LEU	3
1	A	143	GLU	3
1	A	253	GLN	3
1	A	263	ASP	3
1	A	52	TYR	3
1	A	207	GLU	2
1	A	216	ASP	2
1	A	171	HIS	2
1	A	27	GLU	2
1	A	212	GLU	2
1	A	239	SER	2
1	A	301	LYS	2
1	A	272	ARG	2
1	A	274	SER	2
1	A	308	LEU	2
1	A	105	LEU	2
1	A	112	LYS	2
1	A	120	ASP	2
1	A	185	LEU	2
1	A	329	LYS	2
1	A	352	LYS	2
1	A	191	ASP	2
1	A	215	GLU	2
1	A	298	GLU	2
1	A	313	GLU	2
1	A	205	CYS	2
1	A	43	ILE	2
1	A	325	LEU	2
1	A	31	ASP	2
1	A	259	LEU	2
1	A	158	SER	2
1	A	333	SER	1
1	A	116	SER	1
1	A	100	ILE	1
1	A	284	SER	1
1	A	28	ILE	1
1	A	37	TRP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	234	ASN	1
1	A	247	LEU	1
1	A	276	ILE	1
1	A	278	TYR	1
1	A	229	SER	1
1	A	102	THR	1
1	A	87	TYR	1
1	A	131	MET	1
1	A	204	TYR	1
1	A	81	PHE	1
1	A	328	LEU	1
1	A	137	ASP	1
1	A	159	LEU	1
1	A	236	VAL	1
1	A	84	LEU	1
1	A	99	TRP	1
1	A	157	LEU	1
1	A	29	ILE	1
1	A	80	LEU	1
1	A	178	ILE	1
1	A	183	LEU	1
1	A	305	THR	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 73% for the well-defined parts and 70% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	3551
Number of shifts mapped to atoms	3551
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	354	0.10 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	317	0.61 ± 0.08	Should be checked
$^{13}C'$	343	0.18 ± 0.06	None needed (< 0.5 ppm)
^{15}N	327	-0.42 ± 0.20	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 73%, i.e. 3187 atoms were assigned a chemical shift out of a possible 4390. 0 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1502/1541 (97%)	599/626 (96%)	614/620 (99%)	289/295 (98%)
Sidechain	1569/2465 (64%)	1144/1594 (72%)	420/770 (55%)	5/101 (5%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	116/384 (30%)	111/182 (61%)	0/181 (0%)	5/21 (24%)
Overall	3187/4390 (73%)	1854/2402 (77%)	1034/1571 (66%)	299/417 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 70%, i.e. 3551 atoms were assigned a chemical shift out of a possible 5064. 0 out of 53 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1702/1801 (95%)	678/734 (92%)	697/722 (97%)	327/345 (95%)
Sidechain	1729/2861 (60%)	1251/1846 (68%)	473/890 (53%)	5/125 (4%)
Aromatic	120/402 (30%)	115/191 (60%)	0/188 (0%)	5/23 (22%)
Overall	3551/5064 (70%)	2044/2771 (74%)	1170/1800 (65%)	337/493 (68%)

7.1.4 Statistically unusual chemical shifts (i)

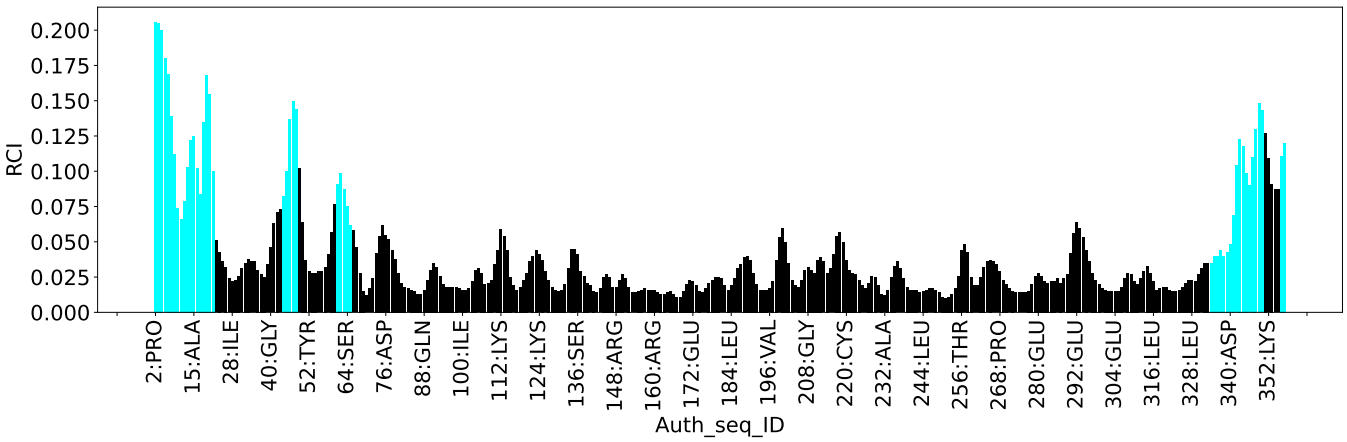
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	29	ILE	HG21	-0.80	-0.56 – 2.11	-5.9
1	A	29	ILE	HG22	-0.80	-0.56 – 2.11	-5.9
1	A	29	ILE	HG23	-0.80	-0.56 – 2.11	-5.9
1	A	29	ILE	HD11	-0.94	-0.72 – 2.09	-5.8
1	A	29	ILE	HD12	-0.94	-0.72 – 2.09	-5.8
1	A	29	ILE	HD13	-0.94	-0.72 – 2.09	-5.8
1	A	130	ILE	HG21	-0.62	-0.56 – 2.11	-5.2
1	A	130	ILE	HG22	-0.62	-0.56 – 2.11	-5.2
1	A	130	ILE	HG23	-0.62	-0.56 – 2.11	-5.2

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
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
2:PRO
15:ALA
28:ILE
40:GLY
52:TYR
64:SER
76:ASP
88:GLN
100:ILE
112:LYS
124:LYS
136:SER
148:ARG
160:ARG
172:GLU
184:LEU
196:VAL
208:GLY
220:CYS
232:ALA
244:LEU
256:THR
268:PRO
280:GLU
292:GLU
304:GLU
316:LEU
328:LEU
340:ASP
352:LYS
Auth_seq_ID

8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	5485
Intra-residue (|i-j|=0)	1070
Sequential (|i-j|=1)	1327
Medium range (|i-j|>1 and |i-j|<5)	986
Long range (|i-j|≥5)	1810
Inter-chain	0
Hydrogen bond restraints	292
Disulfide bond restraints	0
Total dihedral-angle restraints	457
Number of unmapped restraints	0
Number of restraints per residue	16.5
Number of long range restraints per residue[1]	5.3

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.4	0.18
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.0	2.95
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

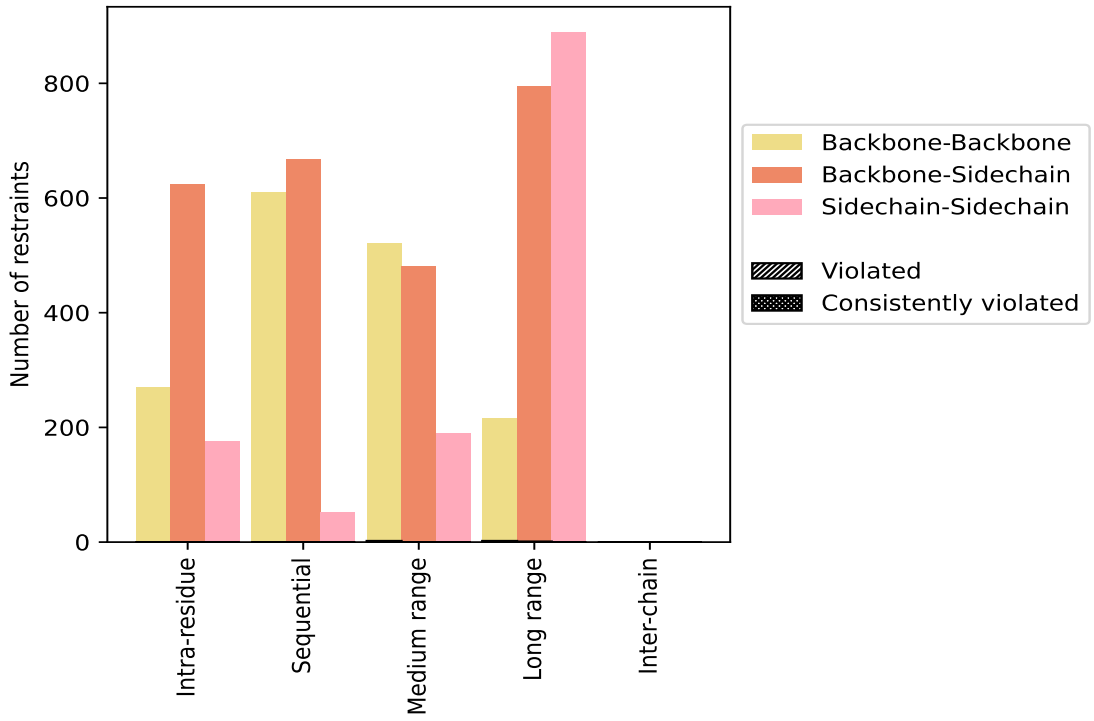
9.1 Summary of distance violations (i)

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)	1070	19.5	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	270	4.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	624	11.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	176	3.2	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	1327	24.2	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	609	11.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	667	12.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	51	0.9	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	986	18.0	2	0.2	0.0	0	0.0	0.0
Backbone-Backbone	520	9.5	2	0.4	0.0	0	0.0	0.0
Backbone-Sidechain	277	5.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	189	3.4	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	1810	33.0	3	0.2	0.1	0	0.0	0.0
Backbone-Backbone	215	3.9	2	0.9	0.0	0	0.0	0.0
Backbone-Sidechain	706	12.9	1	0.1	0.0	0	0.0	0.0
Sidechain-Sidechain	889	16.2	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	292	5.3	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	5485	100.0	5	0.1	0.1	0	0.0	0.0
Backbone-Backbone	1614	29.4	4	0.2	0.1	0	0.0	0.0
Backbone-Sidechain	2566	46.8	1	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	1305	23.8	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



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

9.2 Distance violation statistics for each model

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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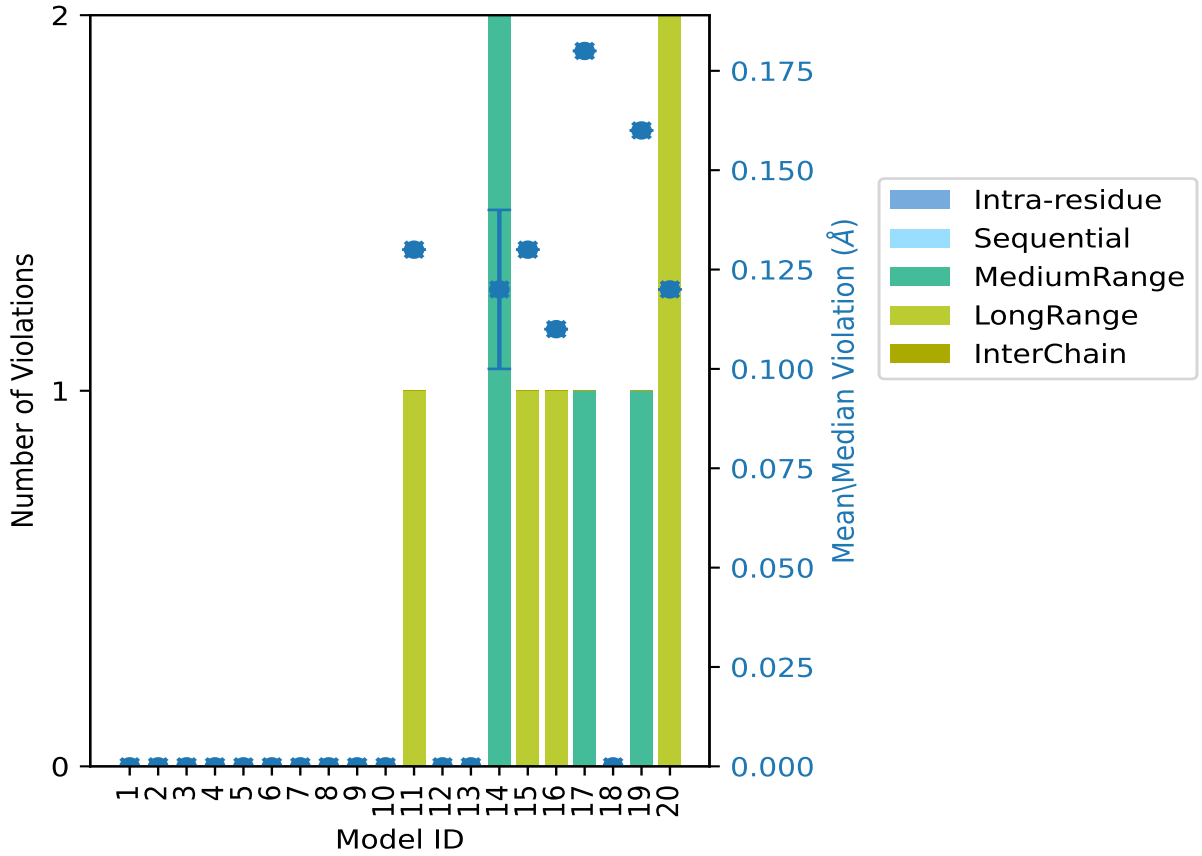
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	0	0	1	0	1	0.13	0.13	0.0	0.13
12	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	2	0	0	2	0.12	0.13	0.02	0.12
15	0	0	0	1	0	1	0.13	0.13	0.0	0.13
16	0	0	0	1	0	1	0.11	0.11	0.0	0.11
17	0	0	1	0	0	1	0.18	0.18	0.0	0.18
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	1	0	0	1	0.16	0.16	0.0	0.16
20	0	0	0	2	0	2	0.12	0.12	0.0	0.12

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

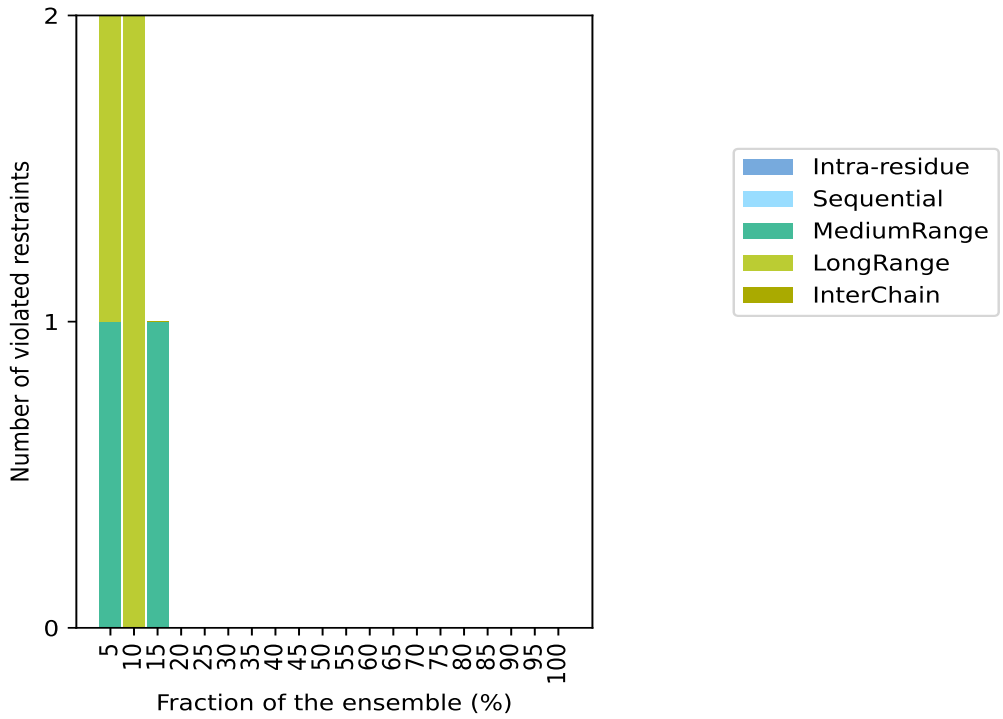
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 5188(IR:1070, SQ:1327, MR:984, LR:1807, 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	0	1	1	0	2	1	5.0
0	0	0	2	0	2	2	10.0
0	0	1	0	0	1	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

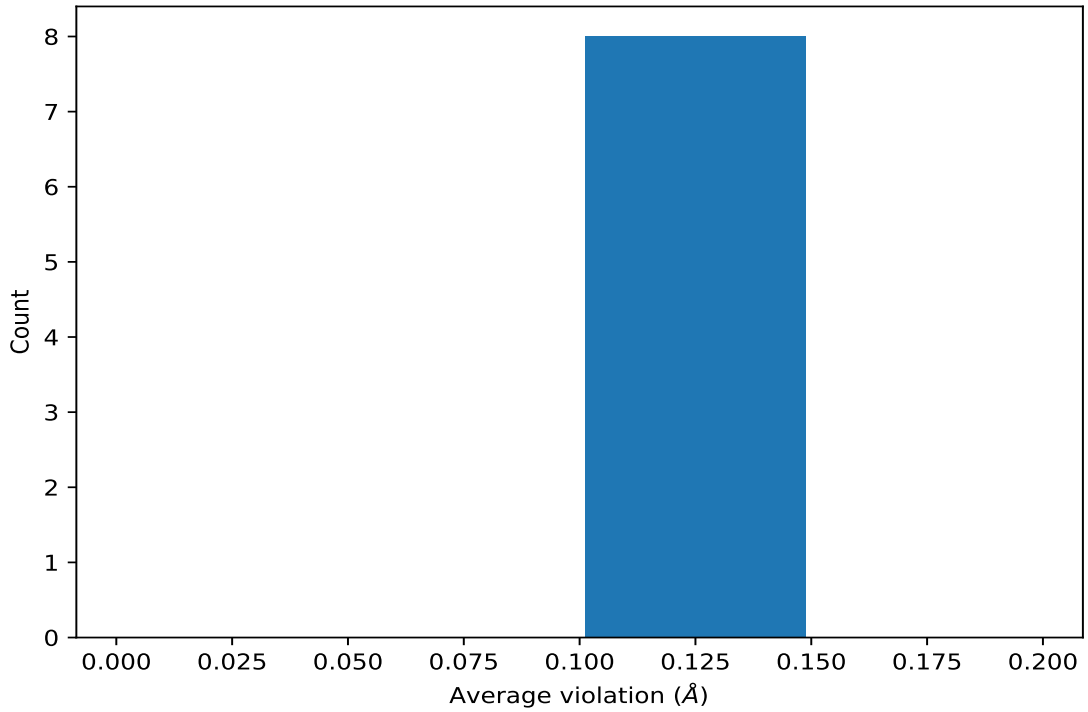
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of theviolation 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.

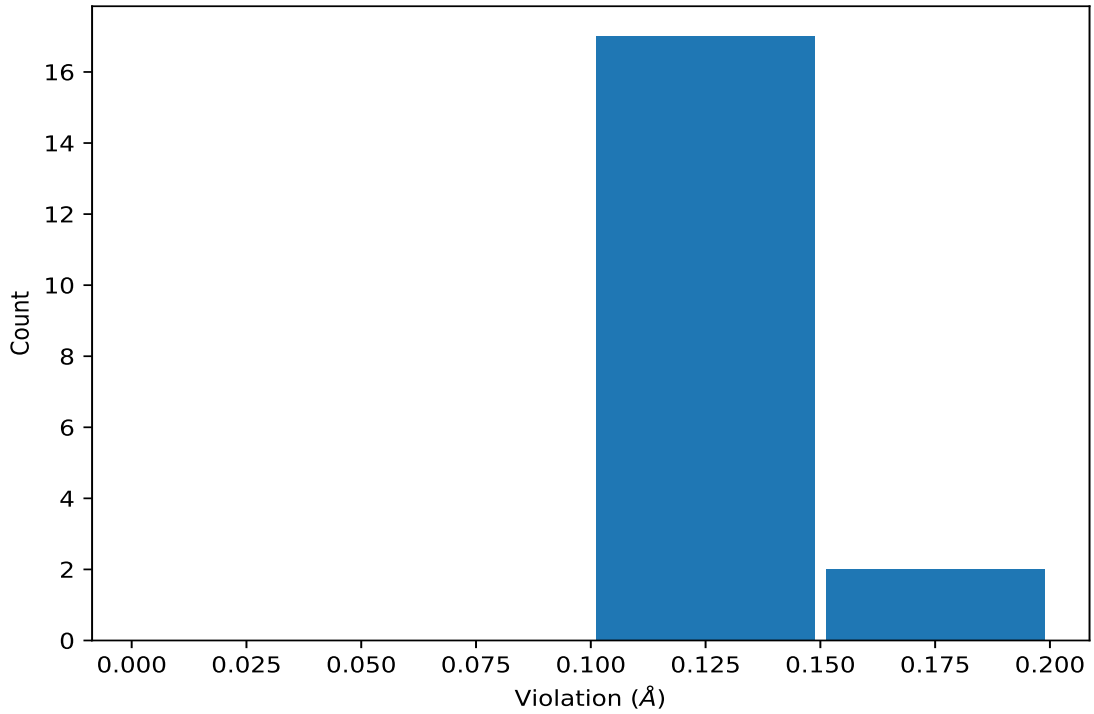
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4963)	1:338:A:LYS:HA	1:340:A:ASP:H	3	0.15	0.03	0.16
(1,1026)	1:82:A:THR:HG21	1:199:A:GLY:HA2	2	0.12	0.01	0.12
(1,1026)	1:82:A:THR:HG21	1:199:A:GLY:HA3	2	0.12	0.01	0.12
(1,1026)	1:82:A:THR:HG22	1:199:A:GLY:HA2	2	0.12	0.01	0.12
(1,1026)	1:82:A:THR:HG22	1:199:A:GLY:HA3	2	0.12	0.01	0.12
(1,1026)	1:82:A:THR:HG23	1:199:A:GLY:HA2	2	0.12	0.01	0.12
(1,1026)	1:82:A:THR:HG23	1:199:A:GLY:HA3	2	0.12	0.01	0.12
(1,5151)	1:82:A:THR:HA	1:354:A:ILE:H	2	0.12	0.0	0.12

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4963)	1:338:A:LYS:HA	1:340:A:ASP:H	17	0.18
(1,4963)	1:338:A:LYS:HA	1:340:A:ASP:H	19	0.16
(1,4949)	1:336:A:ASP:HA	1:338:A:LYS:H	14	0.13
(1,3070)	1:205:A:CYS:HA	1:210:A:HIS:H	11	0.13
(1,1026)	1:82:A:THR:HG21	1:199:A:GLY:HA2	15	0.13
(1,1026)	1:82:A:THR:HG21	1:199:A:GLY:HA3	15	0.13
(1,1026)	1:82:A:THR:HG22	1:199:A:GLY:HA2	15	0.13
(1,1026)	1:82:A:THR:HG22	1:199:A:GLY:HA3	15	0.13
(1,1026)	1:82:A:THR:HG23	1:199:A:GLY:HA2	15	0.13
(1,1026)	1:82:A:THR:HG23	1:199:A:GLY:HA3	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5151)	1:82:A:THR:HA	1:354:A:ILE:H	20	0.12
(1,5151)	1:82:A:THR:HA	1:354:A:ILE:H	16	0.11
(1,1026)	1:82:A:THR:HG21	1:199:A:GLY:HA2	20	0.11
(1,1026)	1:82:A:THR:HG21	1:199:A:GLY:HA3	20	0.11
(1,1026)	1:82:A:THR:HG22	1:199:A:GLY:HA2	20	0.11
(1,1026)	1:82:A:THR:HG22	1:199:A:GLY:HA3	20	0.11
(1,1026)	1:82:A:THR:HG23	1:199:A:GLY:HA2	20	0.11
(1,1026)	1:82:A:THR:HG23	1:199:A:GLY:HA3	20	0.11
(1,4963)	1:338:A:LYS:HA	1:340:A:ASP:H	14	0.1

10 Dihedral-angle violation analysis

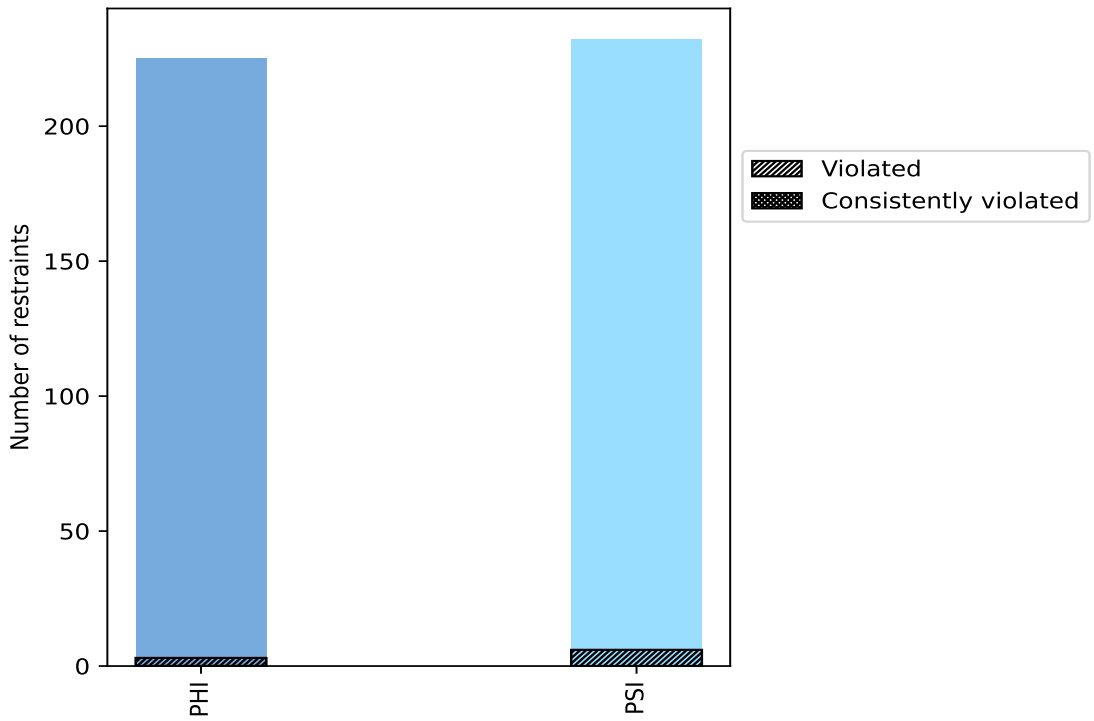
10.1 Summary of dihedral-angle violations

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	225	49.2	3	1.3	0.7	0	0.0	0.0
PSI	232	50.8	6	2.6	1.3	0	0.0	0.0
Total	457	100.0	9	2.0	2.0	0	0.0	0.0

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations



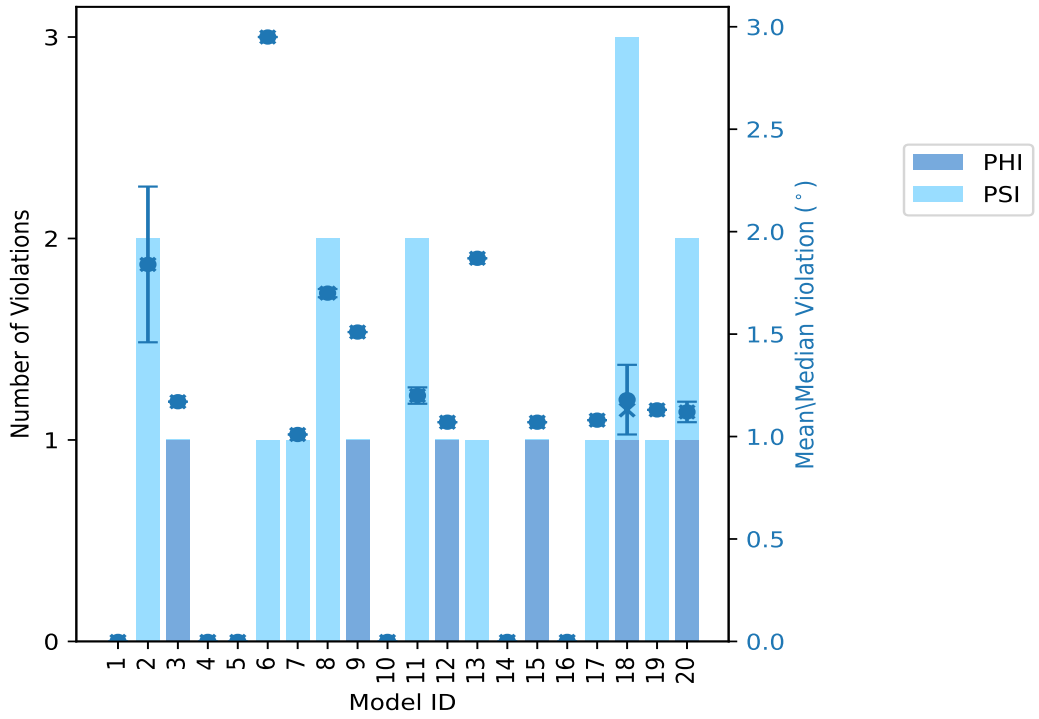
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	0	0	0.0	0.0	0.0	0.0
2	0	2	2	1.84	2.21	0.38	1.84
3	1	0	1	1.17	1.17	0.0	1.17
4	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0.0	0.0	0.0	0.0
6	0	1	1	2.95	2.95	0.0	2.95
7	0	1	1	1.01	1.01	0.0	1.01
8	0	2	2	1.7	1.72	0.02	1.7
9	1	0	1	1.51	1.51	0.0	1.51
10	0	0	0	0.0	0.0	0.0	0.0
11	0	2	2	1.2	1.24	0.04	1.2
12	1	0	1	1.07	1.07	0.0	1.07
13	0	1	1	1.87	1.87	0.0	1.87
14	0	0	0	0.0	0.0	0.0	0.0
15	1	0	1	1.07	1.07	0.0	1.07
16	0	0	0	0.0	0.0	0.0	0.0
17	0	1	1	1.08	1.08	0.0	1.08
18	1	2	3	1.18	1.41	0.17	1.13
19	0	1	1	1.13	1.13	0.0	1.13
20	1	1	2	1.12	1.17	0.05	1.12

10.2.1 Bar graph : Dihedral violation statistics for each model



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

10.3 Dihedral-angle violation statistics for the ensemble

Violation analysis may find that some restraints are violated in very 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 ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
2	4	6	1	5.0
0	1	1	2	10.0
0	0	0	3	15.0
1	0	1	4	20.0
0	0	0	5	25.0
0	0	0	6	30.0
0	0	0	7	35.0
0	1	1	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

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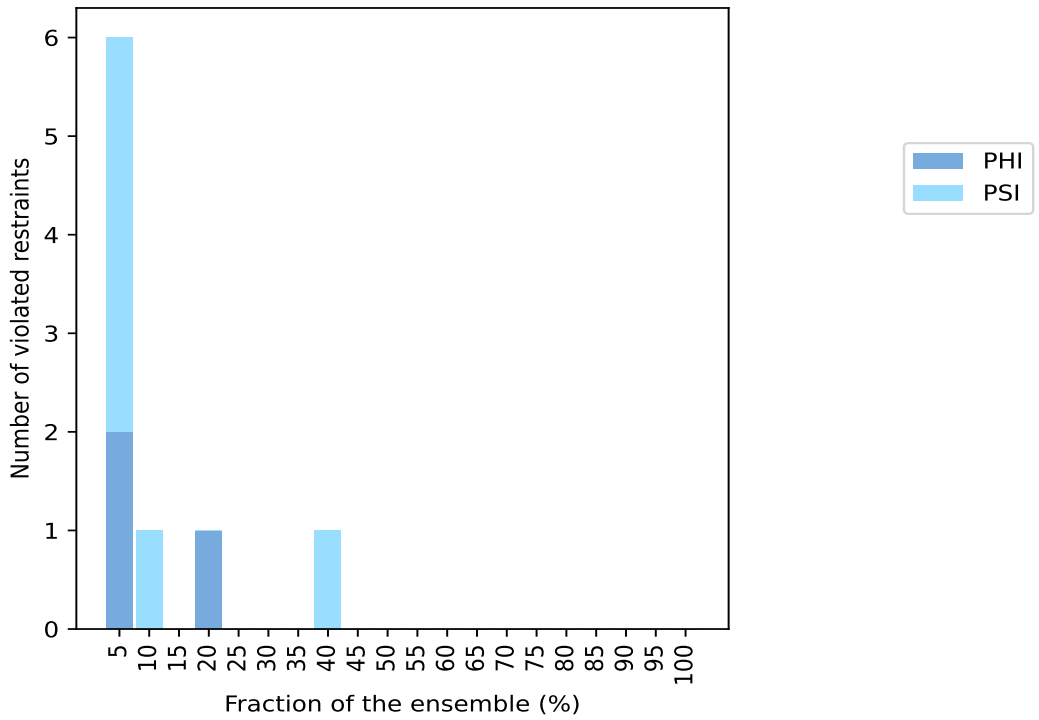
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

[1] Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble

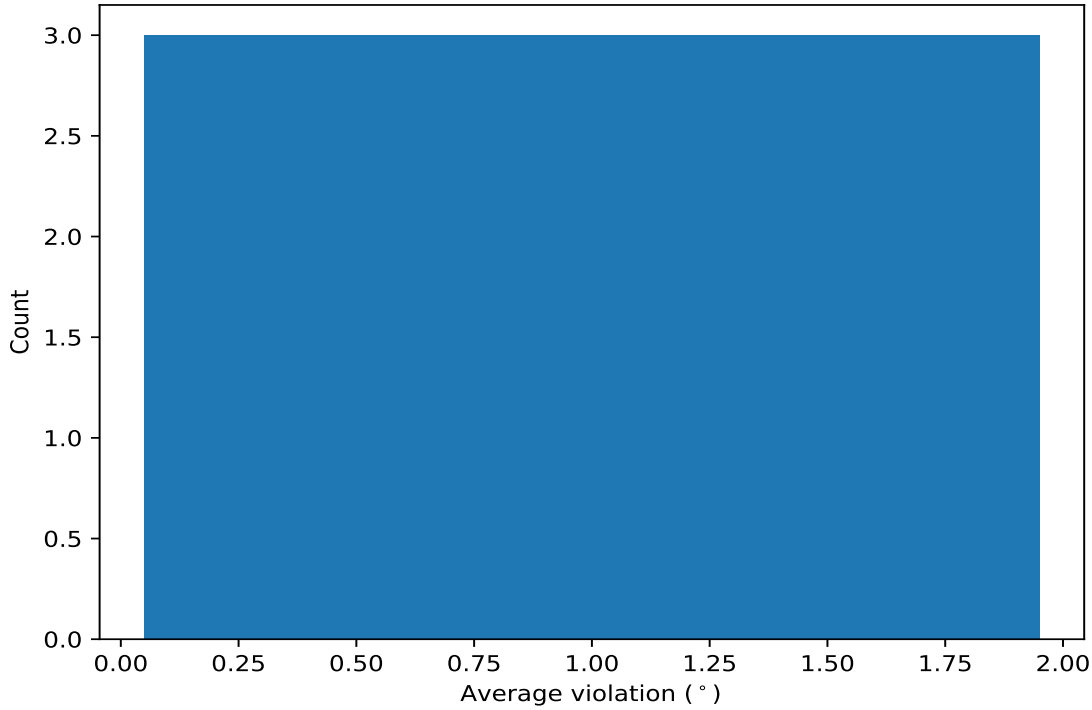


10.4 Most violated dihedral-angle restraints in the ensemble

10.4.1 Histogram : Distribution of mean dihedral-angle violations

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

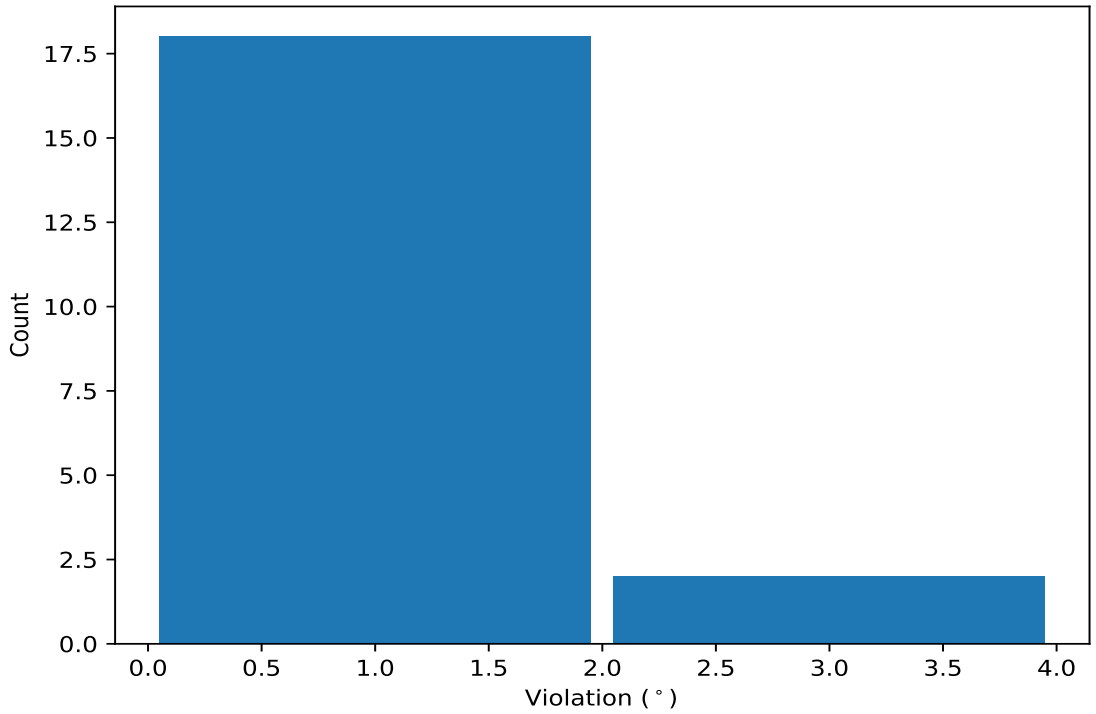
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,8)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:ILE:N	8	1.57	0.64	1.18
(1,248)	1:200:A:LEU:C	1:201:A:ALA:N	1:201:A:ALA:CA	1:201:A:ALA:C	4	1.08	0.06	1.07
(1,10)	1:29:A:ILE:N	1:29:A:ILE:CA	1:29:A:ILE:C	1:30:A:THR:N	2	1.57	0.11	1.57

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



10.5.2 Table: All violated dihedral-angle restraints

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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,8)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:ILE:N	6	2.95
(1,8)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:ILE:N	2	2.21
(1,34)	1:50:A:CYS:N	1:50:A:CYS:CA	1:50:A:CYS:C	1:51:A:ILE:N	13	1.87
(1,8)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:ILE:N	8	1.72
(1,10)	1:29:A:ILE:N	1:29:A:ILE:CA	1:29:A:ILE:C	1:30:A:THR:N	8	1.68
(1,61)	1:80:A:LEU:C	1:81:A:PHE:N	1:81:A:PHE:CA	1:81:A:PHE:C	9	1.51
(1,10)	1:29:A:ILE:N	1:29:A:ILE:CA	1:29:A:ILE:C	1:30:A:THR:N	2	1.46
(1,103)	1:103:A:ARG:N	1:103:A:ARG:CA	1:103:A:ARG:C	1:104:A:LYS:N	18	1.41
(1,8)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:ILE:N	11	1.24
(1,456)	1:354:A:ILE:C	1:355:A:THR:N	1:355:A:THR:CA	1:355:A:THR:C	3	1.17
(1,257)	1:209:A:VAL:N	1:209:A:VAL:CA	1:209:A:VAL:C	1:210:A:HIS:N	11	1.17
(1,248)	1:200:A:LEU:C	1:201:A:ALA:N	1:201:A:ALA:CA	1:201:A:ALA:C	20	1.17
(1,8)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:ILE:N	18	1.13
(1,8)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:ILE:N	19	1.13
(1,8)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:ILE:N	17	1.08
(1,248)	1:200:A:LEU:C	1:201:A:ALA:N	1:201:A:ALA:CA	1:201:A:ALA:C	12	1.07
(1,248)	1:200:A:LEU:C	1:201:A:ALA:N	1:201:A:ALA:CA	1:201:A:ALA:C	15	1.07
(1,8)	1:28:A:ILE:N	1:28:A:ILE:CA	1:28:A:ILE:C	1:29:A:ILE:N	20	1.07
(1,437)	1:325:A:LEU:N	1:325:A:LEU:CA	1:325:A:LEU:C	1:326:A:GLN:N	7	1.01
(1,248)	1:200:A:LEU:C	1:201:A:ALA:N	1:201:A:ALA:CA	1:201:A:ALA:C	18	1.01