Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 01:07 AM BST

PDB ID	:	2LAV
Title	:	NMR solution structure of human Vaccinia-Related Kinase 1
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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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

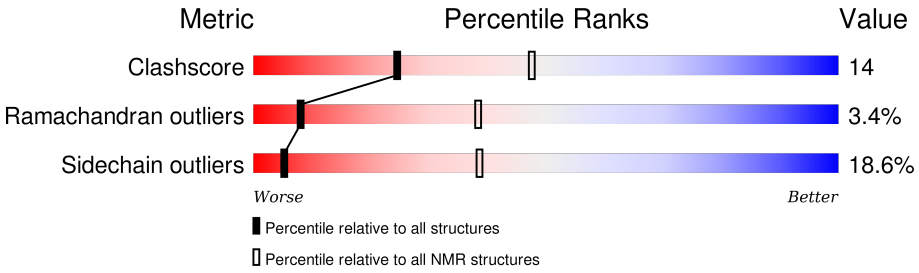
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 72%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	50% 34% • 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)	0.58	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

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

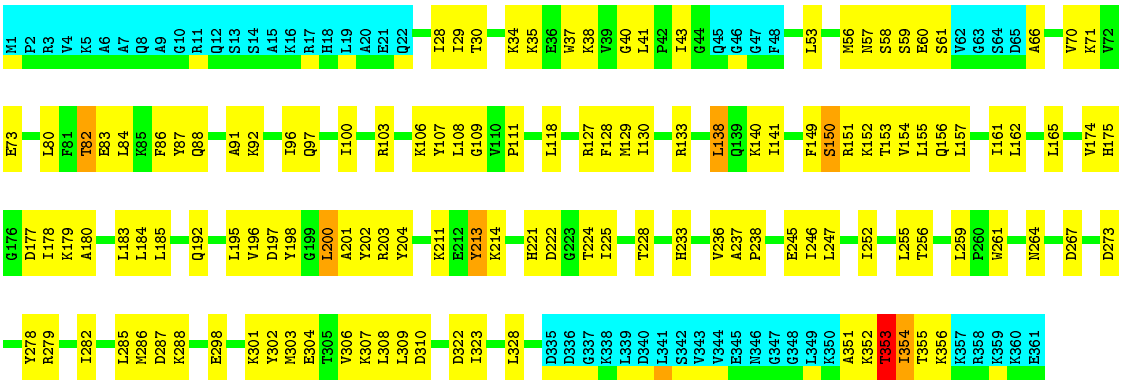
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: 



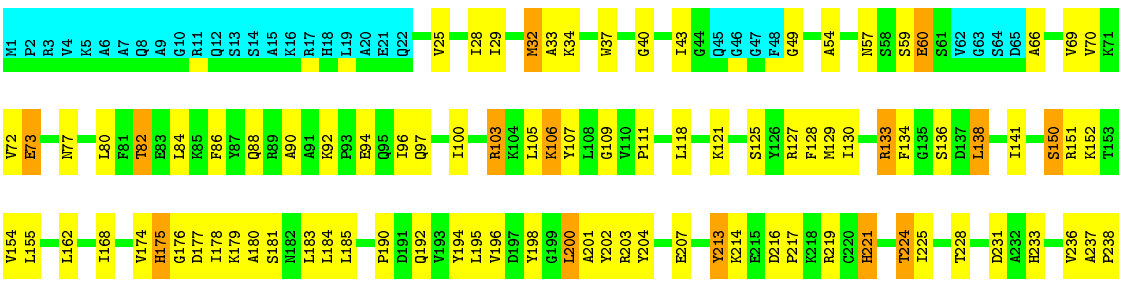
4.2 Scores per residue for each member of the ensemble

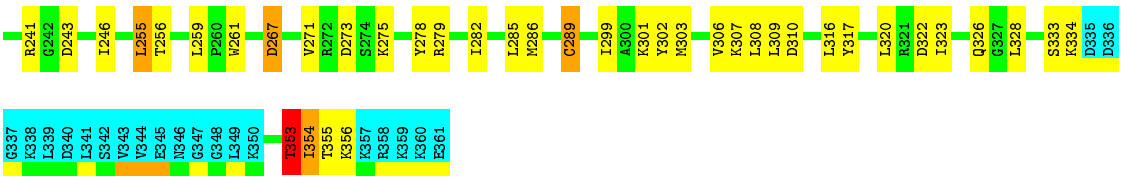
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Vaccinia-related kinase 1

Chain A: 

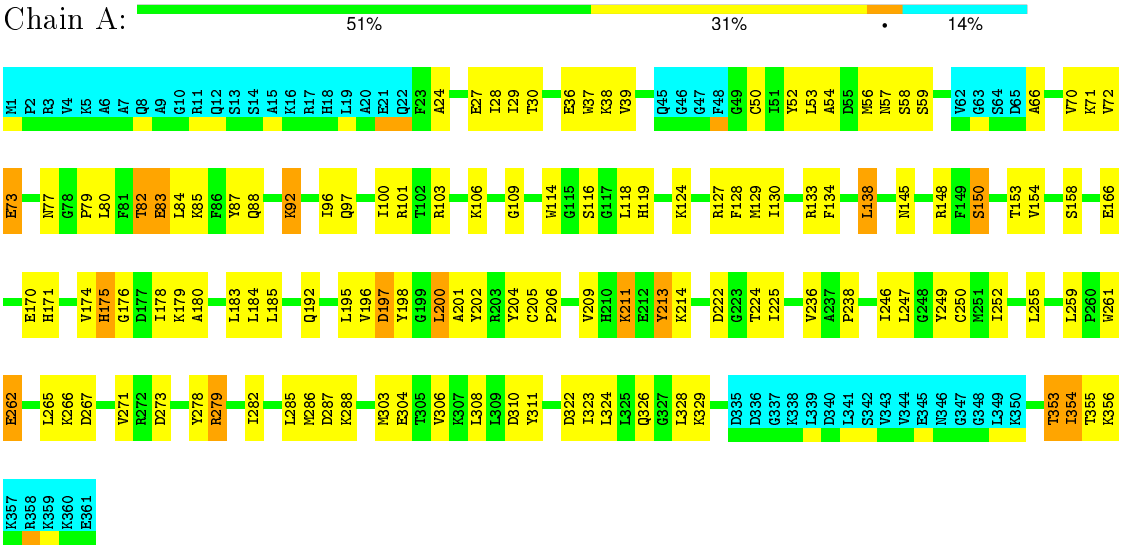




4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Vaccinia-related kinase 1

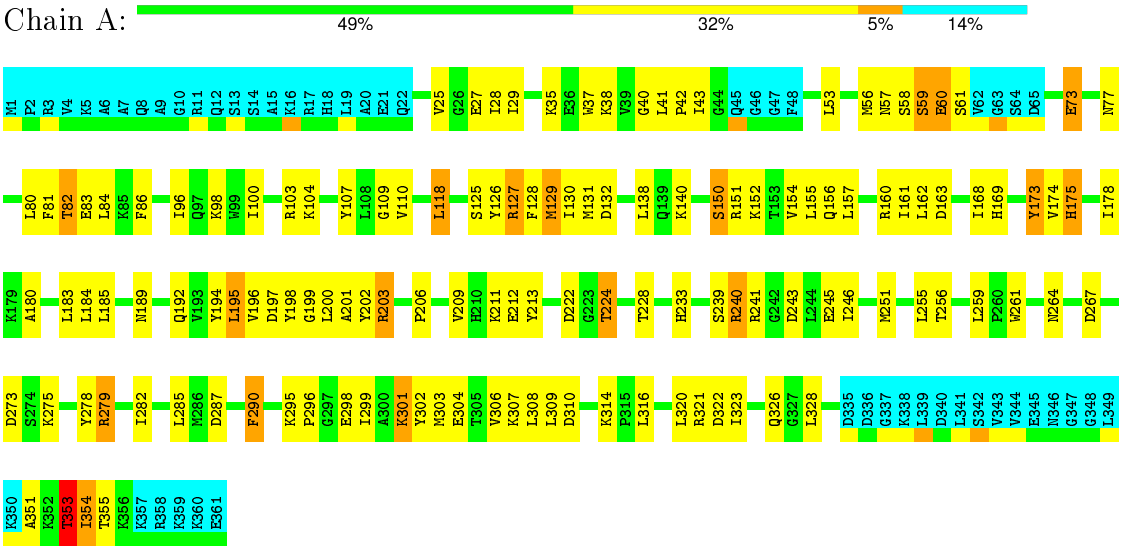
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Vaccinia-related kinase 1

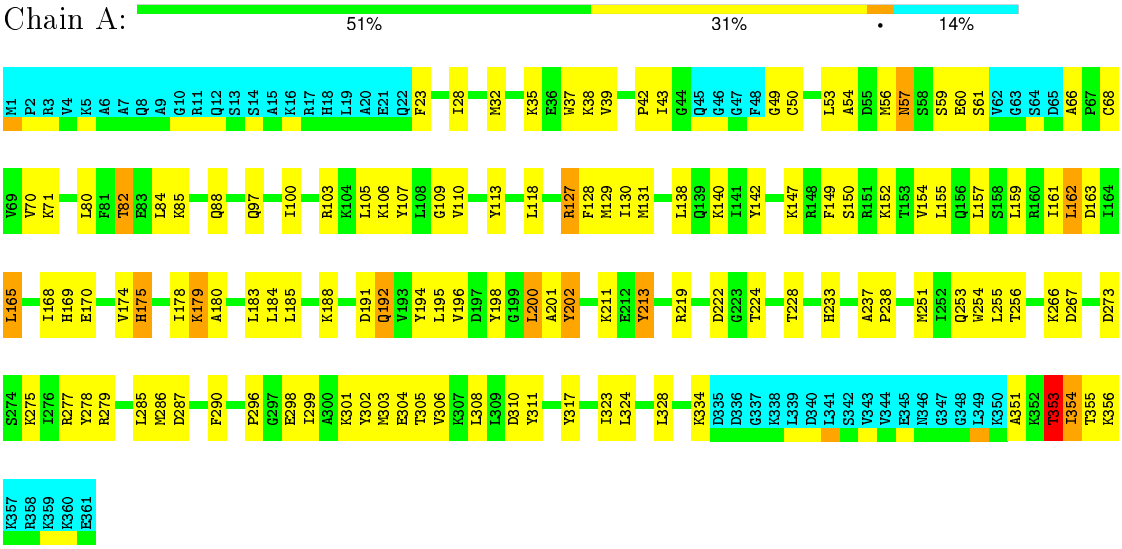
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Vaccinia-related kinase 1

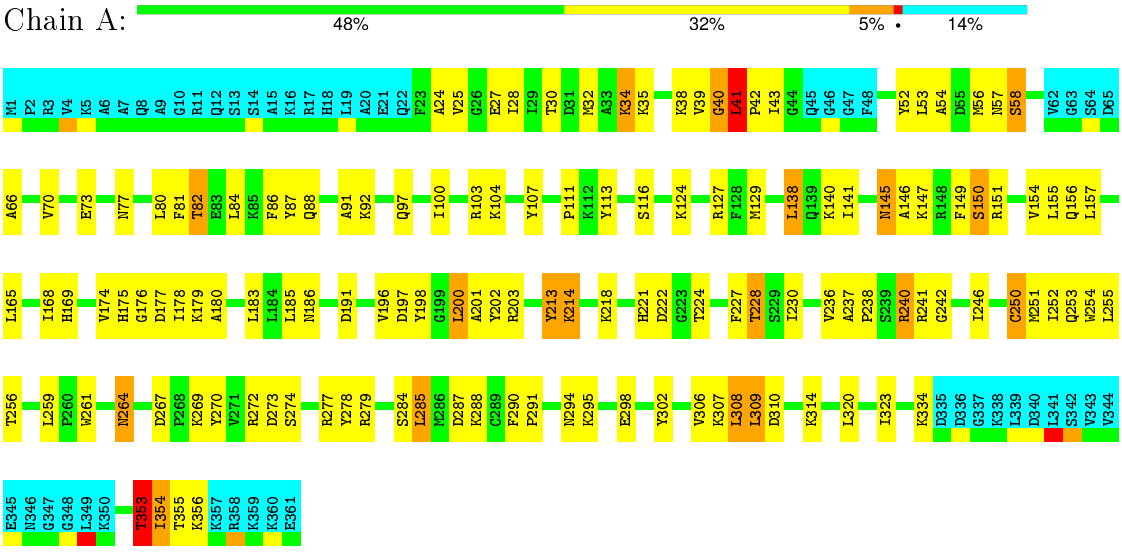
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Vaccinia-related kinase 1

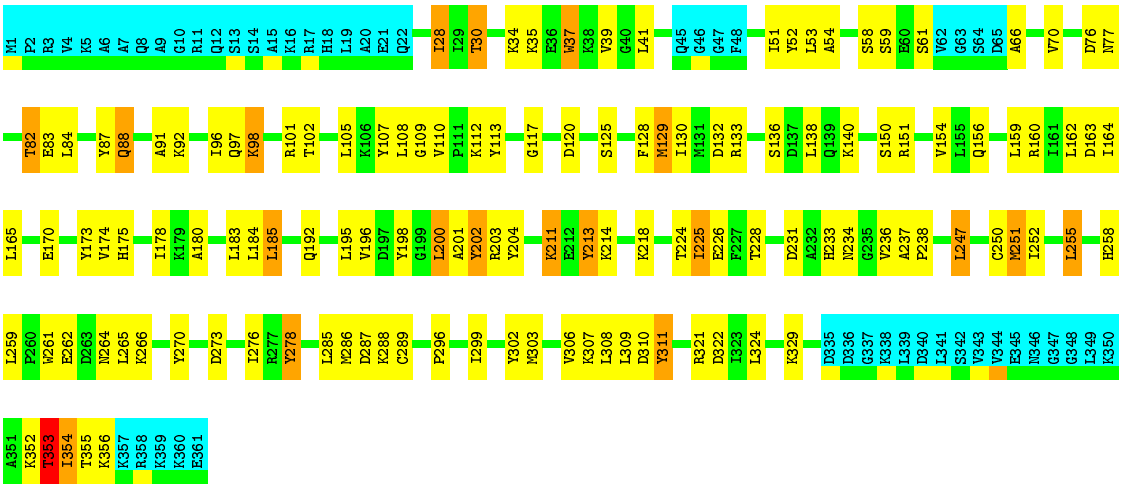
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Vaccinia-related kinase 1

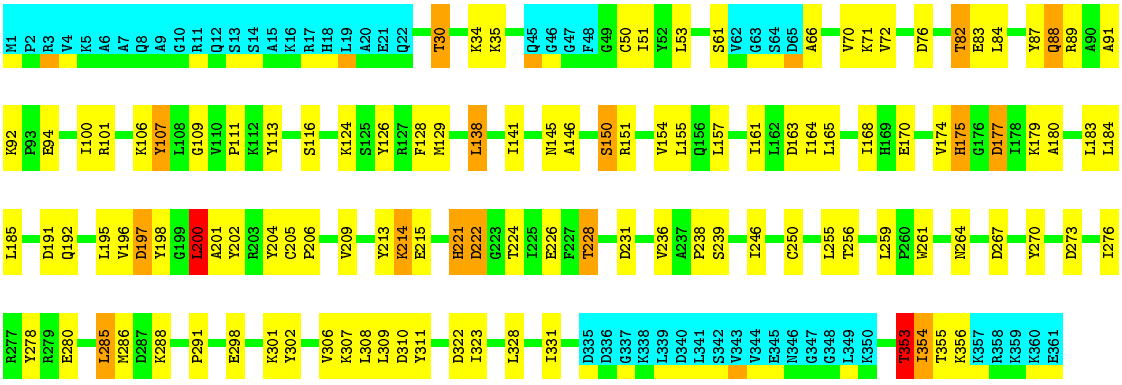
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: Vaccinia-related kinase 1

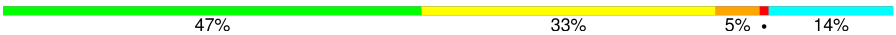
Chain A:

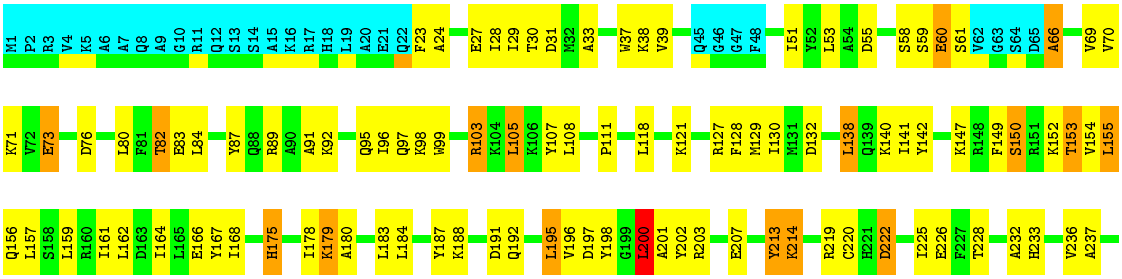


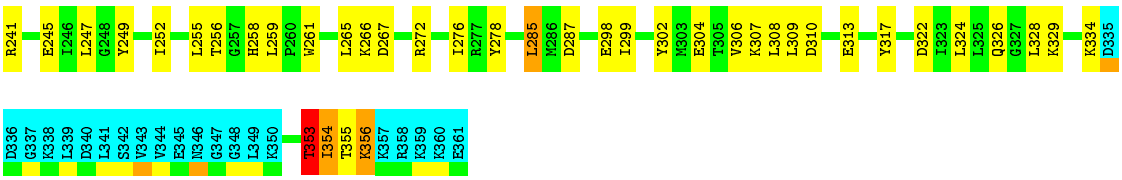
4.2.8 Score per residue for model 8

- Molecule 1: Vaccinia-related kinase 1

Chain A:



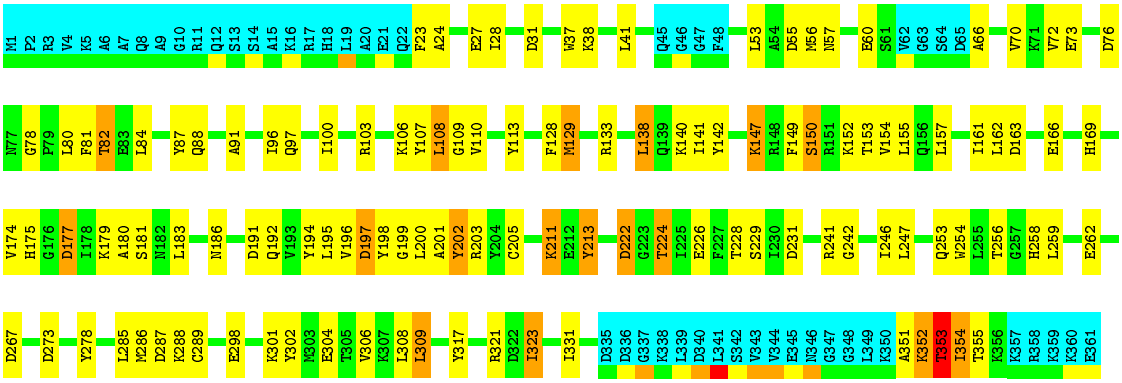




4.2.9 Score per residue for model 9

- Molecule 1: Vaccinia-related kinase 1

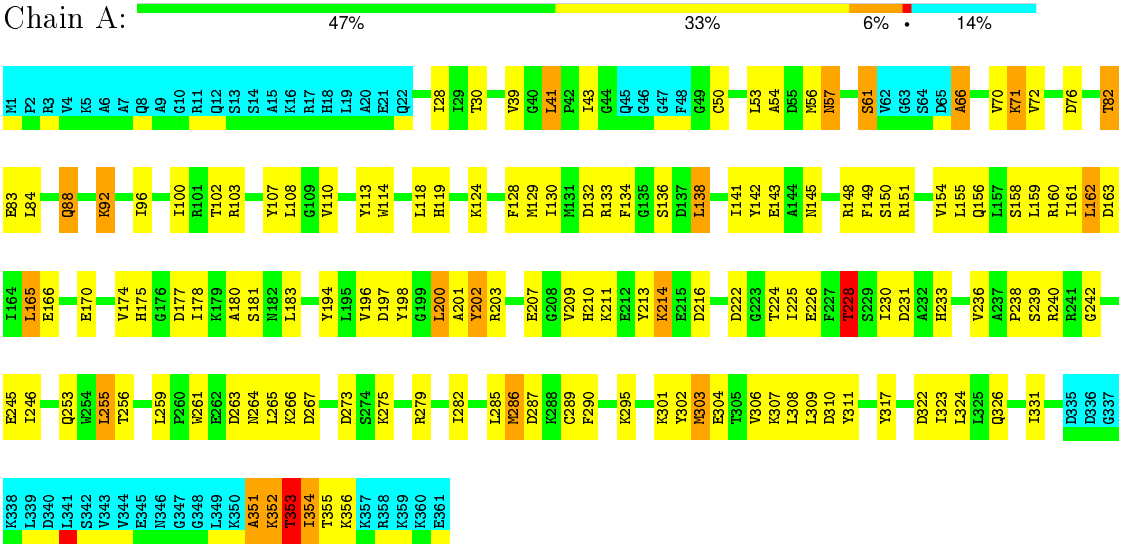
Chain A: 53% 28% 5% 14%



4.2.10 Score per residue for model 10

- Molecule 1: Vaccinia-related kinase 1

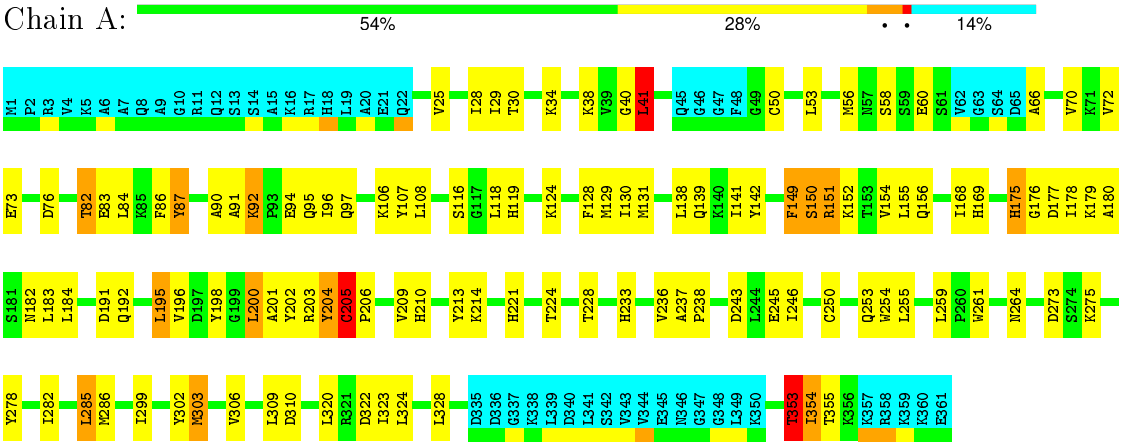
Chain A: 47% 33% 6% 14%



4.2.11 Score per residue for model 11

• Molecule 1: Vaccinia-related kinase 1

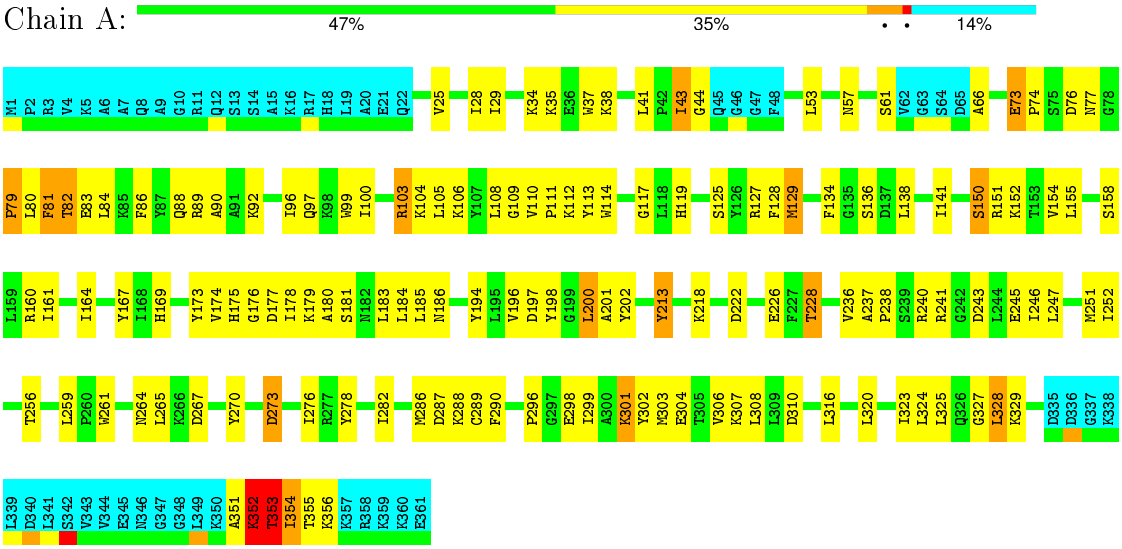
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Vaccinia-related kinase 1

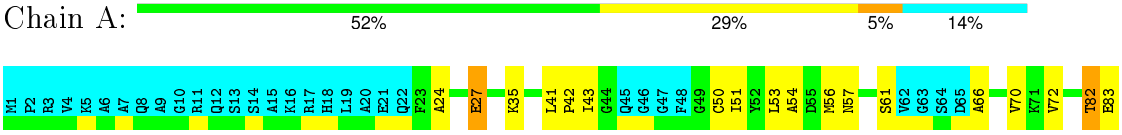
Chain A:

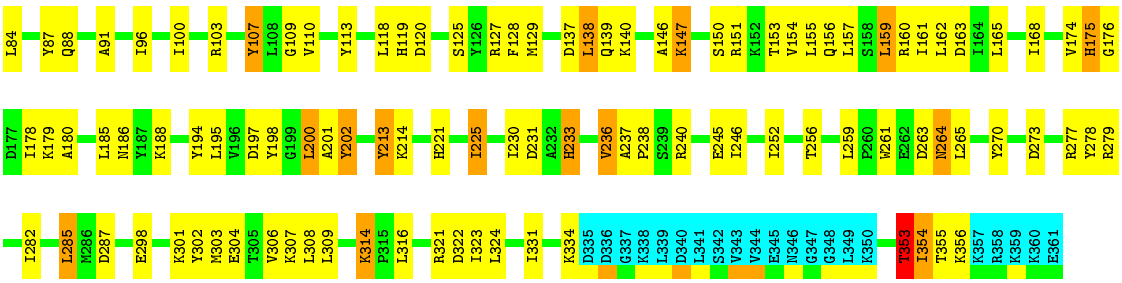


4.2.13 Score per residue for model 13

• Molecule 1: Vaccinia-related kinase 1

Chain A:

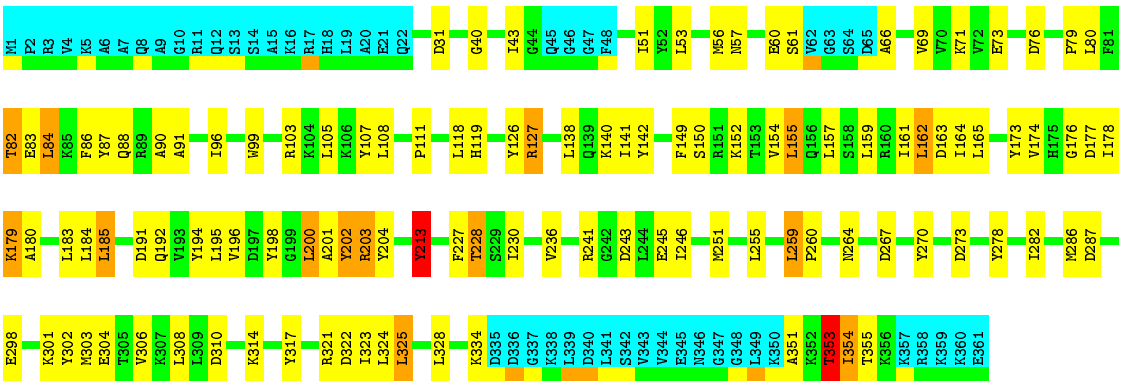




4.2.14 Score per residue for model 14

- Molecule 1: Vaccinia-related kinase 1

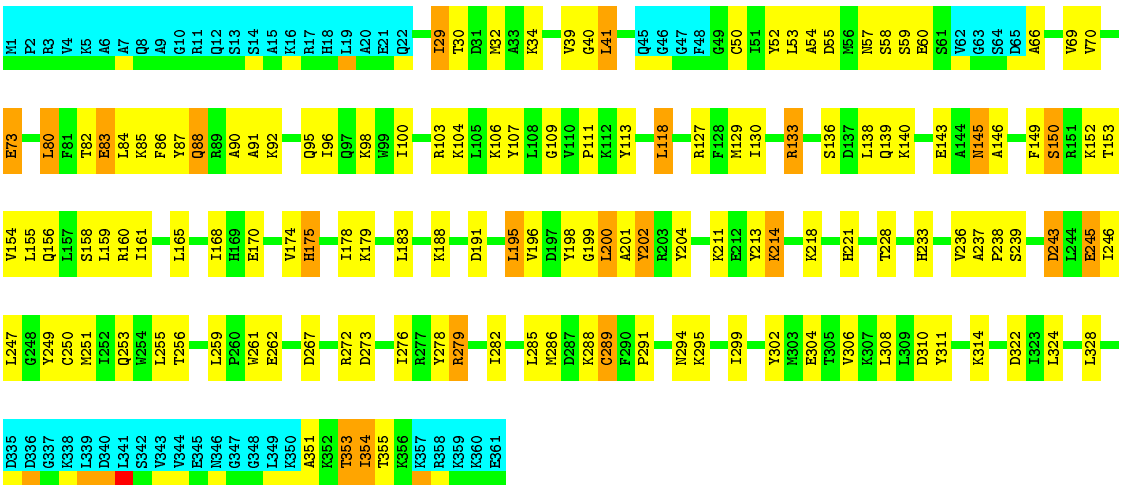
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: Vaccinia-related kinase 1

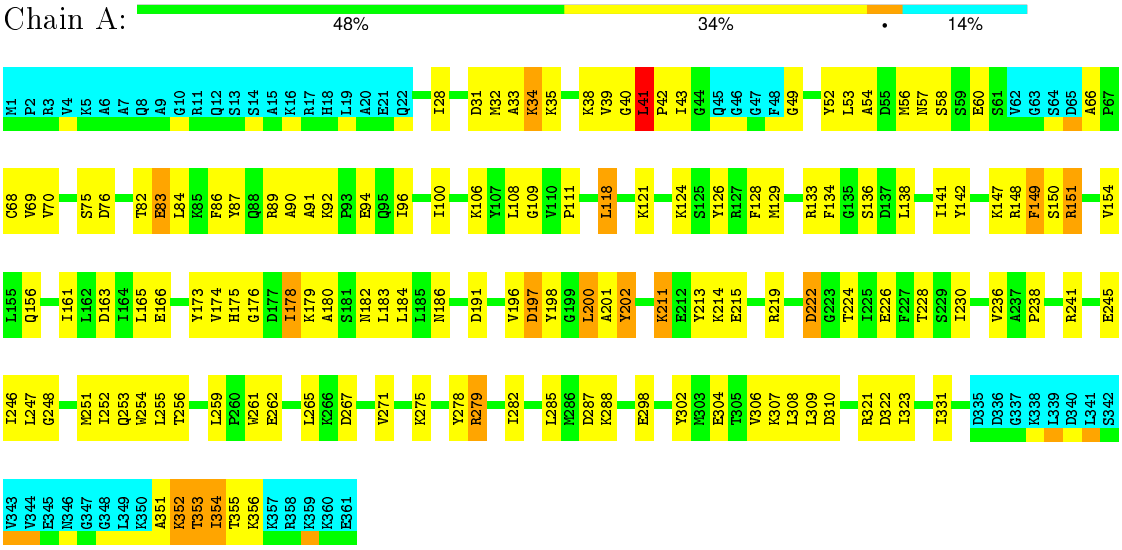
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Vaccinia-related kinase 1

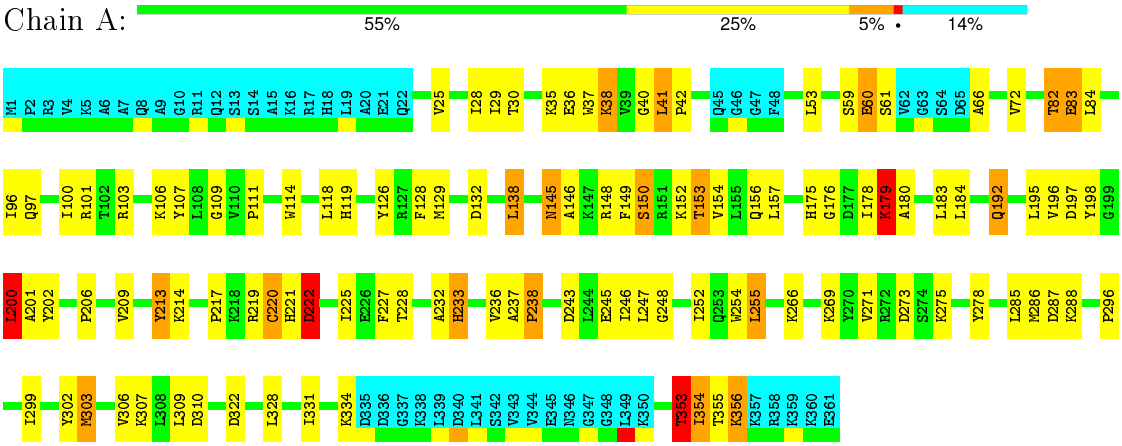
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Vaccinia-related kinase 1

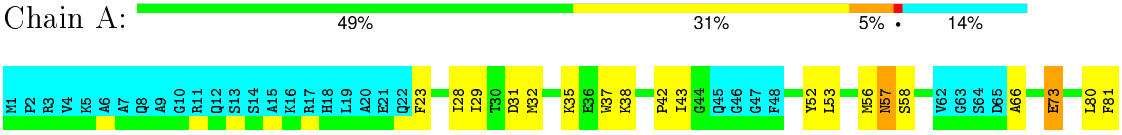
Chain A:

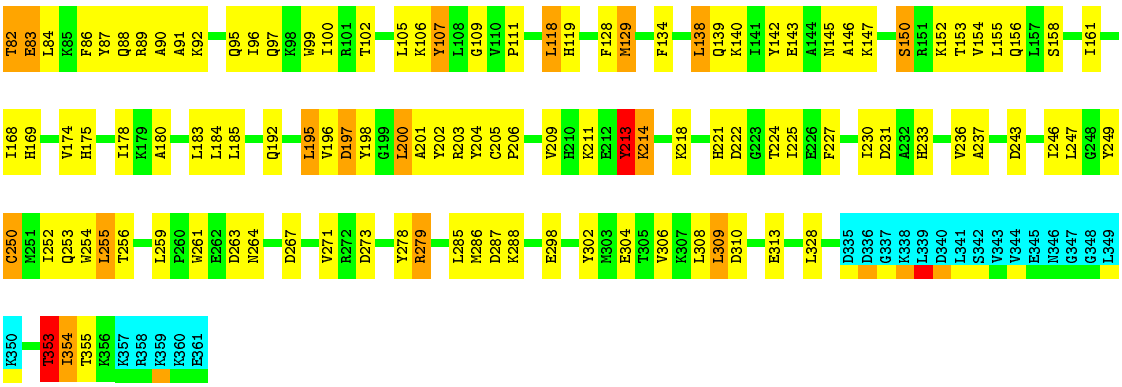


4.2.18 Score per residue for model 18

• Molecule 1: Vaccinia-related kinase 1

Chain A:

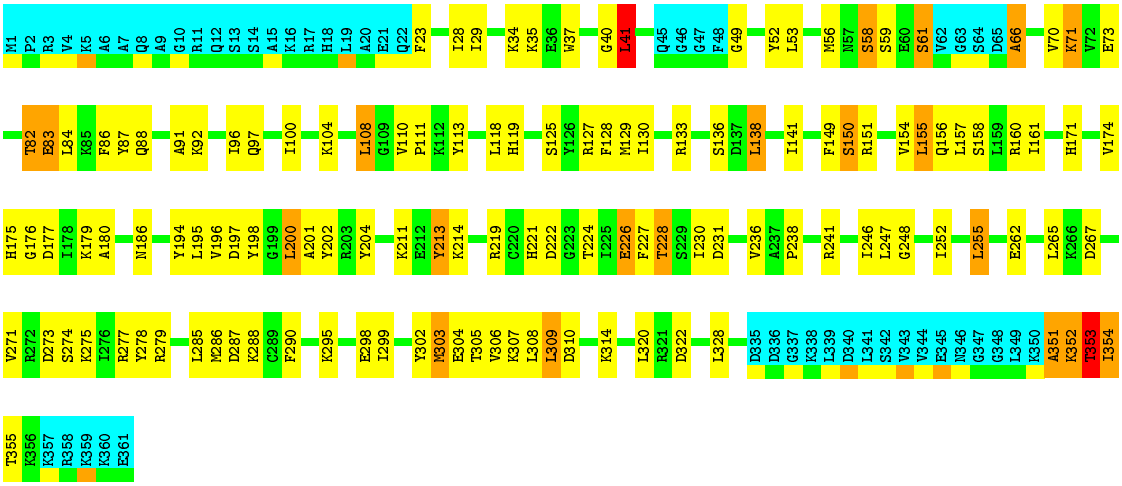




4.2.19 Score per residue for model 19

- Molecule 1: Vaccinia-related kinase 1

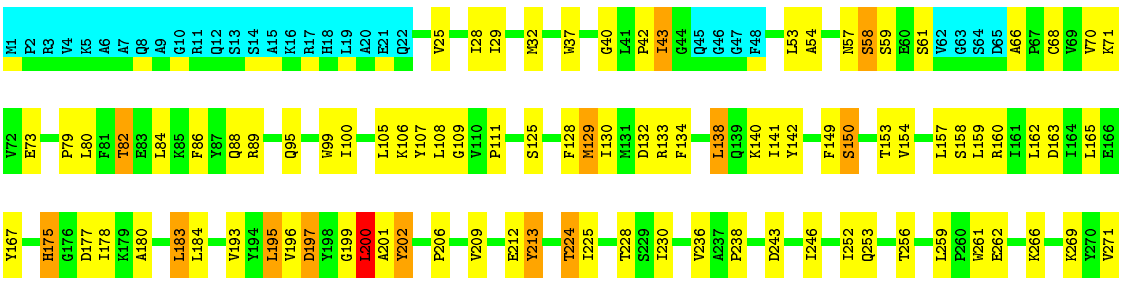
Chain A:

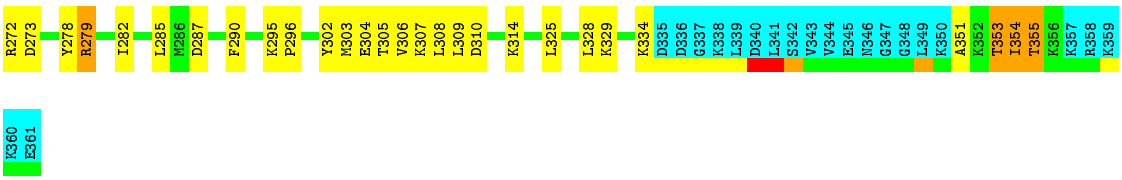


4.2.20 Score per residue for model 20

- 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
I308
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
I354
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)	2lav_cs.str
Number of chemical shift lists	1
Total number of shifts	3545
Number of shifts mapped to atoms	3545
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	72%

No validations of the models with respect to experimental NMR restraints is performed at this time.

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:70:VAL:HG22	1:A:130:ILE:CD1	0.79	2.08	15	1
1:A:222:ASP:OD2	1:A:228:THR:HG23	0.79	1.78	8	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:252:ILE:O	1:A:256:THR:HG22	0.76	1.81	16	3
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: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:28:ILE:HD13	1:A:57:ASN:OD1	0.70	1.87	18	1
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:177:ASP:HA	1:A:246:ILE:HG21	0.70	1.62	19	4
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:253:GLN:OE1	1:A:259:LEU:HD12	0.68	1.88	9	2
1:A:84:LEU:HD11	1:A:116:SER:OG	0.68	1.88	7	3
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:182:ASN:C	1:A:183:LEU:HD12	0.67	2.08	16	1
1:A:25:VAL:HG11	1:A:41:LEU:HD12	0.67	1.66	12	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:213:TYR:CZ	1:A:236:VAL:HG21	0.67	2.25	18	1
1:A:155:LEU:HD21	1:A:298:GLU:OE2	0.67	1.90	9	3
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:225:ILE:HD11	1:A:271:VAL:HB	0.66	1.65	20	1
1:A:185:LEU:HD23	1:A:192:GLN:O	0.66	1.90	4	6
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:86:PHE:CE1	1:A:201:ALA:HB1	0.65	2.26	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:198:TYR:HB2	1:A:353:THR:HG23	0.65	1.67	19	11
1:A:306:VAL:HA	1:A:309:LEU:HD12	0.65	1.69	8	8
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:28:ILE:HG21	1:A:57:ASN:ND2	0.65	2.06	20	2
1:A:243:ASP:HA	1:A:246:ILE:HD12	0.65	1.67	20	5
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:118:LEU:HD23	1:A:119:HIS:N	0.64	2.07	19	2
1:A:308:LEU:O	1:A:308:LEU:HD23	0.64	1.92	1	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:69:VAL:HG13	1:A:133:ARG:HG2	0.64	1.68	15	1
1:A:37:TRP:CZ3	1:A:39:VAL:HG22	0.64	2.28	8	2
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:282:ILE:HD13	1:A:303:MET:HB2	0.64	1.68	20	2
1:A:84:LEU:HD12	1:A:129:MET:CG	0.64	2.23	20	2
1:A:99:TRP:CZ3	1:A:108:LEU:HD13	0.63	2.28	20	2
1:A:256:THR:HG21	1:A:289:CYS:SG	0.63	2.32	12	5
1:A:155:LEU:HD13	1:A:328:LEU:HD11	0.63	1.68	11	1
1:A:180:ALA:HA	1:A:183:LEU:HD12	0.63	1.68	10	8
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:99:TRP:CZ3	1:A:105:LEU:HD13	0.62	2.29	8	2
1:A:304:GLU:O	1:A:308:LEU:HD12	0.62	1.93	20	11
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:43:ILE:HD13	1:A:43:ILE:N	0.60	2.11	20	1
1:A:184:LEU:HD13	1:A:196:VAL:CG2	0.60	2.26	2	7
1:A:82:THR:HG22	1:A:353:THR:CG2	0.60	2.26	16	1
1:A:80:LEU:HD12	1:A:351:ALA:HB3	0.60	1.74	15	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:75:SER:OG	1:A:118:LEU:HD11	0.60	1.95	16	1
1:A:184:LEU:HD13	1:A:196:VAL:CG1	0.60	2.27	3	2
1:A:84:LEU:HD22	1:A:127:ARG:NH2	0.60	2.10	14	2
1:A:252:ILE:HG23	1:A:290:PHE:CZ	0.60	2.31	5	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:154:VAL:HG21	1:A:255:LEU:CD2	0.59	2.28	18	1
1:A:103:ARG:HB3	1:A:105:LEU:HD12	0.59	1.71	4	2
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:82:THR:HB	1:A:353:THR:HB	0.59	1.73	20	3
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: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:202:TYR:CD1	1:A:355:THR:HG22	0.59	2.33	20	1
1:A:282:ILE:HD13	1:A:303:MET:CB	0.59	2.27	13	1
1:A:155:LEU:HD22	1:A:328:LEU:HD21	0.59	1.75	1	1
1:A:161:ILE:CG2	1:A:178:ILE:HD11	0.58	2.28	16	1
1:A:28:ILE:HG21	1:A:57:ASN:HB2	0.58	1.75	12	2

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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:54:ALA:HB3	1:A:68:CYS:O	0.58	1.98	20	2
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:87:TYR:O	1:A:91:ALA:HB3	0.58	1.99	8	9
1:A:178:ILE:N	1:A:178:ILE:HD12	0.58	2.14	6	1
1:A:230:ILE:HD11	1:A:279:ARG:CZ	0.58	2.29	18	1
1:A:252:ILE:HD11	1:A:303:MET:CE	0.58	2.29	20	2
1:A:161:ILE:HG22	1:A:165:LEU:CD1	0.58	2.28	15	2
1:A:282:ILE:HG21	1:A:303:MET:CB	0.58	2.29	13	2
1:A:155:LEU:HD13	1:A:328:LEU:CD1	0.57	2.29	11	1
1:A:80:LEU:HD12	1:A:351:ALA:HB1	0.57	1.76	3	2
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:178:ILE:HD12	1:A:178:ILE:N	0.57	2.14	13	1
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:N	1:A:118:LEU:HD12	0.57	2.14	18	2
1:A:74:PRO:O	1:A:80:LEU:HD22	0.57	1.99	12	1
1:A:237:ALA:HB1	1:A:238:PRO:CD	0.57	2.30	11	2
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:29:ILE:HD13	1:A:29:ILE:N	0.57	2.15	15	1
1:A:301:LYS:HB3	1:A:323:ILE:HD13	0.57	1.77	4	3
1:A:118:LEU:HD13	1:A:126:TYR:O	0.57	2.00	14	1
1:A:175:HIS:CD2	1:A:178:ILE:HD11	0.57	2.35	10	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:178:ILE:HG21	1:A:247:LEU:HD12	0.56	1.77	18	1
1:A:278:TYR:HB3	1:A:285:LEU:HD11	0.56	1.77	7	1
1:A:183:LEU:HD23	1:A:193:VAL:CG2	0.56	2.30	20	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:105:LEU:O	1:A:107:TYR:N	0.56	2.38	18	1
1:A:351:ALA:O	1:A:352:LYS:CB	0.56	2.51	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:LEU:HD11	1:A:298:GLU:OE1	0.56	2.00	8	1
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:96:ILE:HG13	1:A:108:LEU:HD22	0.56	1.76	19	1
1:A:200:LEU:HD13	1:A:222:ASP:O	0.56	2.01	9	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:278:TYR:CB	1:A:285:LEU:HD13	0.55	2.31	3	3
1:A:70:VAL:HG23	1:A:130:ILE:HD13	0.55	1.79	2	2
1:A:354:ILE:C	1:A:354:ILE:HD12	0.55	2.22	20	12
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:175:HIS:HE2	1:A:195:LEU:HD13	0.54	1.62	15	1
1:A:141:ILE:HG22	1:A:145:ASN:ND2	0.54	2.18	7	2
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:272:ARG:O	1:A:276:ILE:HD12	0.54	2.03	15	2
1:A:53:LEU:CD2	1:A:66:ALA:HB3	0.54	2.30	10	4
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:PRO:HG3	1:A:354:ILE:HD11	0.53	1.79	2	2
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: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:118:LEU:HD11	1:A:127:ARG:NE	0.53	2.18	1	1
1:A:276:ILE:HG22	1:A:280:GLU:OE2	0.53	2.04	7	1
1:A:25:VAL:HG13	1:A:40:GLY:CA	0.53	2.33	5	1
1:A:230:ILE:HD12	1:A:241:ARG:NH2	0.53	2.19	19	1
1:A:53:LEU:HD22	1:A:66:ALA:HB1	0.53	1.81	16	1
1:A:184:LEU:HD12	1:A:184:LEU:N	0.53	2.19	14	1
1:A:255:LEU:HD22	1:A:290:PHE:CE2	0.53	2.39	10	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:71:LYS:HE3	1:A:351:ALA:HB2	0.53	1.80	20	1
1:A:73:GLU:CB	1:A:80:LEU:HD13	0.53	2.34	8	4
1:A:278:TYR:CD1	1:A:285:LEU:HD13	0.53	2.39	15	1
1:A:151:ARG:O	1:A:155:LEU:HD12	0.53	2.03	7	4
1:A:331:ILE:O	1:A:331:ILE:HG22	0.53	2.03	13	5
1:A:43:ILE:HD13	1:A:53:LEU:HG	0.53	1.81	18	1
1:A:70:VAL:O	1:A:70:VAL:HG13	0.53	2.04	8	2
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:111:PRO:HD3	1:A:196:VAL:HG12	0.52	1.82	16	1
1:A:70:VAL:HG21	1:A:128:PHE:CD1	0.52	2.39	9	3
1:A:316:LEU:O	1:A:320:LEU:HD12	0.52	2.04	1	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:53:LEU:HD23	1:A:66:ALA:CB	0.52	2.34	9	4
1:A:183:LEU:O	1:A:184:LEU:HD12	0.52	2.05	18	2
1:A:134:PHE:CE2	1:A:196:VAL:HG21	0.52	2.39	12	2
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:214:LYS:O	1:A:236:VAL:HG23	0.52	2.05	2	1
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

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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:100:ILE:HD11	1:A:106:LYS:C	0.51	2.25	7	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: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:185:LEU:HD22	1:A:190:PRO:O	0.51	2.06	1	1
1:A:32:MET:CE	1:A:33:ALA:HB2	0.51	2.36	1	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	1
1:A:99:TRP:HA	1:A:102:THR:HG22	0.50	1.83	18	1
1:A:271:VAL:HG12	1:A:275:LYS:HE3	0.50	1.82	19	2
1:A:84:LEU:HD23	1:A:84:LEU:O	0.50	2.06	11	1
1:A:108:LEU:HD23	1:A:110:VAL:HB	0.50	1.83	19	2
1:A:82:THR:CB	1:A:353:THR:HB	0.50	2.36	15	2
1:A:174:VAL:HG12	1:A:240:ARG:NH2	0.50	2.21	5	1
1:A:178:ILE:O	1:A:178:ILE:HG22	0.50	2.07	8	7
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:155:LEU:HD22	1:A:328:LEU:HD23	0.50	1.84	8	1
1:A:103:ARG:HG2	1:A:105:LEU:HD12	0.50	1.83	1	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:199:GLY:CA	1:A:353:THR:HA	0.50	2.37	15	2
1:A:142:TYR:CD1	1:A:149:PHE:CE2	0.50	3.00	20	4
1:A:70:VAL:CG2	1:A:130:ILE:HD13	0.50	2.36	10	2
1:A:278:TYR:CZ	1:A:285:LEU:HD22	0.50	2.42	6	1
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:84:LEU:HD13	1:A:127:ARG:NE	0.50	2.22	14	2
1:A:43:ILE:HD13	1:A:44:GLY:N	0.50	2.21	12	1
1:A:86:PHE:CE1	1:A:198:TYR:CE1	0.50	3.00	5	1
1:A:175:HIS:CD2	1:A:198:TYR:CE2	0.50	3.00	7	3
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: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:155:LEU:HD11	1:A:298:GLU:OE2	0.49	2.08	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ILE:HG21	1:A:57:ASN:CB	0.49	2.37	3	1
1:A:80:LEU:O	1:A:80:LEU:HD13	0.49	2.07	20	1
1:A:174:VAL:HG13	1:A:243:ASP:OD1	0.49	2.08	12	1
1:A:175:HIS:CE1	1:A:178:ILE:HD11	0.49	2.42	6	1
1:A:29:ILE:HD13	1:A:128:PHE:HZ	0.49	1.65	19	1
1:A:99:TRP:CD1	1:A:167:TYR:CD1	0.49	3.00	20	2
1:A:84:LEU:HD12	1:A:129:MET:HG2	0.49	1.84	20	2
1:A:37:TRP:CD1	1:A:130:ILE:HD12	0.49	2.43	3	2
1:A:231:ASP:CA	1:A:236:VAL:HG12	0.49	2.38	1	2
1:A:84:LEU:HD23	1:A:84:LEU:C	0.49	2.28	3	5
1:A:179:LYS:O	1:A:183:LEU:HD13	0.49	2.07	16	2
1:A:201:ALA:HB3	1:A:353:THR:HG23	0.49	1.84	15	2
1:A:236:VAL:HG12	1:A:237:ALA:N	0.49	2.23	15	3
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: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:28:ILE:HG21	1:A:57:ASN:HD22	0.48	1.68	20	1
1:A:227:PHE:O	1:A:246:ILE:HG23	0.48	2.07	5	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:43:ILE:HD12	1:A:53:LEU:HG	0.48	1.84	20	1
1:A:84:LEU:HD22	1:A:127:ARG:HH21	0.48	1.68	3	1
1:A:301:LYS:CB	1:A:323:ILE:HD13	0.48	2.38	1	1
1:A:230:ILE:HG23	1:A:245:GLU:OE1	0.48	2.08	16	1
1:A:83:GLU:CD	1:A:351:ALA:HB1	0.48	2.27	14	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:213:TYR:CE1	1:A:236:VAL:HG11	0.48	2.43	12	1
1:A:39:VAL:HG22	1:A:54:ALA:HB2	0.48	1.83	5	2
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	2
1:A:29:ILE:HD13	1:A:29:ILE:H	0.48	1.68	15	1
1:A:279:ARG:O	1:A:282:ILE:HD11	0.48	2.08	15	3
1:A:158:SER:OG	1:A:324:LEU:HD22	0.48	2.08	12	2
1:A:84:LEU:C	1:A:84:LEU:HD23	0.47	2.29	19	5
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:213:TYR:CD1	1:A:236:VAL:HG21	0.47	2.45	13	1
1:A:230:ILE:HD12	1:A:279:ARG:NH1	0.47	2.24	5	1
1:A:142:TYR:CD1	1:A:149:PHE:CD2	0.47	3.02	9	2
1:A:145:ASN:O	1:A:146:ALA:HB3	0.47	2.09	17	5
1:A:175:HIS:CD2	1:A:178:ILE:CD1	0.47	2.98	10	2
1:A:25:VAL:CG1	1:A:41:LEU:HD12	0.47	2.38	12	1
1:A:255:LEU:HD22	1:A:290:PHE:HZ	0.47	1.69	10	1
1:A:252:ILE:HG23	1:A:290:PHE:HZ	0.47	1.69	5	1
1:A:150:SER:O	1:A:154:VAL:HG12	0.47	2.09	19	2
1:A:103:ARG:HB3	1:A:105:LEU:HD13	0.47	1.84	14	1
1:A:100:ILE:HD11	1:A:107:TYR:N	0.47	2.25	7	1
1:A:100:ILE:HG21	1:A:106:LYS:O	0.47	2.10	1	1
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:178:ILE:HG22	1:A:178:ILE:O	0.47	2.10	18	3
1:A:175:HIS:NE2	1:A:195:LEU:HD22	0.47	2.25	20	1
1:A:253:GLN:CD	1:A:259:LEU:HD12	0.47	2.30	15	1
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:154:VAL:HA	1:A:157:LEU:HD12	0.46	1.85	20	1
1:A:118:LEU:HD23	1:A:118:LEU:C	0.46	2.31	10	1
1:A:206:PRO:O	1:A:209:VAL:HG22	0.46	2.10	7	6
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:256:THR:HG23	1:A:290:PHE:CZ	0.46	2.44	5	1
1:A:51:ILE:HD12	1:A:51:ILE:N	0.46	2.25	14	2
1:A:28:ILE:HA	1:A:37:TRP:O	0.46	2.10	8	1
1:A:253:GLN:NE2	1:A:254:TRP:CD1	0.46	2.84	4	1
1:A:23:PHE:CZ	1:A:72:VAL:HG21	0.46	2.45	9	1
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:138:LEU:HD12	1:A:183:LEU:CB	0.46	2.41	11	3
1:A:354:ILE:HD12	1:A:354:ILE:C	0.46	2.31	3	4
1:A:184:LEU:HD13	1:A:196:VAL:HG11	0.46	1.85	3	1
1:A:126:TYR:N	1:A:126:TYR:CD1	0.46	2.84	7	1
1:A:28:ILE:HG23	1:A:38:LYS:HD2	0.46	1.87	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:LEU:HD23	1:A:194:TYR:O	0.46	2.11	14	1
1:A:103:ARG:CB	1:A:105:LEU:HD23	0.46	2.38	12	1
1:A:88:GLN:CG	1:A:113:TYR:CE2	0.46	2.99	9	8
1:A:37:TRP:CE2	1:A:130:ILE:CD1	0.46	2.99	6	2
1:A:175:HIS:CD2	1:A:178:ILE:CG1	0.46	2.99	5	1
1:A:183:LEU:HD23	1:A:193:VAL:HG21	0.46	1.86	20	1
1:A:252:ILE:HD11	1:A:299:ILE:CG2	0.46	2.41	12	1
1:A:302:TYR:O	1:A:305:THR:HG22	0.46	2.11	4	1
1:A:119:HIS:N	1:A:119:HIS:CD2	0.46	2.83	17	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:41:LEU:CB	1:A:53:LEU:HD12	0.46	2.41	16	1
1:A:155:LEU:CG	1:A:328:LEU:HD21	0.46	2.40	14	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:267:ASP:O	1:A:271:VAL:HG23	0.46	2.10	1	1
1:A:168:ILE:HD11	1:A:175:HIS:ND1	0.46	2.26	13	2
1:A:286:MET:HE3	1:A:299:ILE:HG21	0.46	1.88	11	1
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:CD1	1:A:184:LEU:CB	0.45	3.00	12	1
1:A:134:PHE:CE2	1:A:196:VAL:CG2	0.45	2.99	2	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:182:ASN:ND2	1:A:183:LEU:HD12	0.45	2.27	11	1
1:A:28:ILE:HG22	1:A:38:LYS:CB	0.45	2.42	9	3
1:A:278:TYR:CG	1:A:285:LEU:CD1	0.45	3.00	8	7
1:A:183:LEU:HD23	1:A:195:LEU:HA	0.45	1.87	3	4
1:A:239:SER:CB	1:A:311:TYR:CE2	0.45	2.99	7	2
1:A:82:THR:CG2	1:A:354:ILE:HG22	0.45	2.41	20	1
1:A:175:HIS:NE2	1:A:198:TYR:CE1	0.45	2.84	3	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:142:TYR:CZ	1:A:147:LYS:CG	0.45	3.00	8	2
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: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:205:CYS:CB	1:A:209:VAL:O	0.45	2.65	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:TYR:CD2	1:A:107:TYR:O	0.45	2.69	5	2
1:A:107:TYR:CZ	1:A:192:GLN:NE2	0.45	2.85	1	2
1:A:99:TRP:CZ3	1:A:105:LEU:CD1	0.45	3.00	20	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
1:A:100:ILE:HG23	1:A:108:LEU:HD13	0.45	1.89	9	1
1:A:165:LEU:CD2	1:A:175:HIS:CE1	0.45	3.00	16	1
1:A:88:GLN:CG	1:A:113:TYR:CE1	0.45	3.00	7	2
1:A:37:TRP:CH2	1:A:130:ILE:CD1	0.45	3.00	2	1
1:A:221:HIS:CD2	1:A:356:LYS:N	0.45	2.85	7	1
1:A:99:TRP:CE3	1:A:105:LEU:CD1	0.45	3.00	20	1
1:A:155:LEU:HD23	1:A:324:LEU:HD23	0.45	1.88	11	1
1:A:81:PHE:CE2	1:A:127:ARG:NH2	0.45	2.85	5	1
1:A:79:PRO:HA	1:A:82:THR:OG1	0.45	2.12	20	1
1:A:134:PHE:CE1	1:A:196:VAL:HG11	0.45	2.46	16	1
1:A:278:TYR:CD2	1:A:285:LEU:CD1	0.45	3.00	13	2
1:A:178:ILE:HG23	1:A:195:LEU:CD1	0.45	2.42	17	2
1:A:81:PHE:CE2	1:A:127:ARG:CZ	0.45	3.00	12	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:37:TRP:CZ2	1:A:130:ILE:CD1	0.45	2.99	2	1
1:A:175:HIS:ND1	1:A:198:TYR:CE2	0.45	2.85	1	1
1:A:174:VAL:CG2	1:A:204:TYR:CD1	0.45	3.00	1	1
1:A:107:TYR:CE1	1:A:192:GLN:NE2	0.45	2.85	14	1
1:A:184:LEU:HD22	1:A:196:VAL:HG11	0.45	1.89	6	1
1:A:103:ARG:CG	1:A:105:LEU:HD12	0.45	2.42	1	1
1:A:70:VAL:CG2	1:A:128:PHE:CD1	0.44	3.01	16	3
1:A:142:TYR:CZ	1:A:254:TRP:CE3	0.44	3.05	18	2
1:A:29:ILE:CD1	1:A:128:PHE:CZ	0.44	3.00	17	2
1:A:351:ALA:O	1:A:352:LYS:HB3	0.44	2.10	9	1
1:A:175:HIS:CE1	1:A:178:ILE:CD1	0.44	3.00	12	1
1:A:158:SER:HA	1:A:161:ILE:HD12	0.44	1.87	19	2
1:A:256:THR:HG23	1:A:258:HIS:H	0.44	1.73	8	1
1:A:86:PHE:CE2	1:A:201:ALA:CB	0.44	3.00	5	2
1:A:54:ALA:HB3	1:A:68:CYS:C	0.44	2.32	20	2
1:A:202:TYR:CD1	1:A:355:THR:CG2	0.44	2.99	20	1
1:A:73:GLU:HB3	1:A:80:LEU:HD13	0.44	1.88	12	1
1:A:138:LEU:HD21	1:A:157:LEU:HD11	0.44	1.88	19	3
1:A:204:TYR:CD1	1:A:204:TYR:N	0.44	2.85	11	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:309:LEU:C	1:A:309:LEU:HD12	0.44	2.31	20	1
1:A:175:HIS:CD2	1:A:198:TYR:CD2	0.44	3.05	19	1
1:A:225:ILE:HG12	1:A:271:VAL:HG11	0.44	1.88	20	1
1:A:159:LEU:HD23	1:A:159:LEU:C	0.44	2.33	20	1
1:A:96:ILE:HG23	1:A:97:GLN:N	0.44	2.28	11	3
1:A:173:TYR:CZ	1:A:203:ARG:CG	0.44	3.00	14	1
1:A:207:GLU:O	1:A:209:VAL:HG23	0.44	2.12	10	1
1:A:28:ILE:HD12	1:A:36:GLU:HG2	0.44	1.88	2	1
1:A:253:GLN:NE2	1:A:259:LEU:HD12	0.44	2.26	15	2
1:A:175:HIS:HE1	1:A:195:LEU:HD22	0.44	1.72	11	1
1:A:83:GLU:N	1:A:353:THR:OG1	0.44	2.50	19	7
1:A:282:ILE:HD11	1:A:303:MET:HG2	0.44	1.89	10	1
1:A:213:TYR:CD2	1:A:213:TYR:O	0.44	2.71	4	2
1:A:205:CYS:N	1:A:206:PRO:CD	0.44	2.81	7	3
1:A:195:LEU:CD2	1:A:198:TYR:CE1	0.44	3.01	9	1
1:A:107:TYR:CD2	1:A:192:GLN:NE2	0.44	2.85	9	1
1:A:126:TYR:CD1	1:A:126:TYR:N	0.44	2.85	16	1
1:A:51:ILE:CG2	1:A:69:VAL:HG21	0.44	2.43	8	1
1:A:252:ILE:HD11	1:A:303:MET:SD	0.44	2.53	19	1
1:A:73:GLU:CB	1:A:80:LEU:HD22	0.44	2.43	9	1
1:A:82:THR:HG21	1:A:354:ILE:HG22	0.43	1.89	20	1
1:A:84:LEU:HD22	1:A:127:ARG:HH12	0.43	1.71	8	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: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:100:ILE:HA	1:A:105:LEU:HD12	0.43	1.88	20	1
1:A:162:LEU:CD1	1:A:317:TYR:CE2	0.43	3.01	10	2
1:A:73:GLU:HB2	1:A:80:LEU:HD13	0.43	1.88	2	1
1:A:225:ILE:CD1	1:A:271:VAL:HG21	0.43	2.42	1	1
1:A:69:VAL:HG13	1:A:133:ARG:CD	0.43	2.43	1	1
1:A:82:THR:CG2	1:A:353:THR:HB	0.43	2.44	16	2
1:A:92:LYS:O	1:A:96:ILE:HD12	0.43	2.14	15	4
1:A:117:GLY:N	1:A:128:PHE:CE1	0.43	2.86	6	2
1:A:303:MET:HA	1:A:306:VAL:HG22	0.43	1.90	2	1
1:A:221:HIS:O	1:A:222:ASP:CB	0.43	2.65	17	1
1:A:99:TRP:CH2	1:A:105:LEU:CD1	0.43	3.00	8	1
1:A:225:ILE:HD11	1:A:271:VAL:CG2	0.43	2.44	1	1
1:A:84:LEU:HD13	1:A:127:ARG:CD	0.43	2.44	14	1
1:A:214:LYS:O	1:A:237:ALA:N	0.43	2.51	11	6
1:A:142:TYR:CE1	1:A:254:TRP:NE1	0.43	2.86	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:262:GLU:O	1:A:265:LEU:HD23	0.43	2.13	2	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:173:TYR:CE2	1:A:203:ARG:NH1	0.43	2.87	6	1
1:A:225:ILE:HD11	1:A:271:VAL:HG21	0.43	1.89	1	1
1:A:226:GLU:CD	1:A:265:LEU:HD21	0.42	2.34	16	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:41:LEU:HB3	1:A:53:LEU:HD12	0.42	1.90	16	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: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:28:ILE:HD12	1:A:36:GLU:CG	0.42	2.44	2	1
1:A:352:LYS:CG	1:A:353:THR:N	0.42	2.82	16	1
1:A:73:GLU:CG	1:A:80:LEU:HD13	0.42	2.44	15	1
1:A:175:HIS:CE1	1:A:198:TYR:CD2	0.42	3.07	2	1
1:A:82:THR:CG2	1:A:354:ILE:CG2	0.42	2.98	20	1
1:A:296:PRO:CG	1:A:299:ILE:HD12	0.42	2.44	3	1
1:A:236:VAL:HG22	1:A:237:ALA:H	0.42	1.75	18	2
1:A:225:ILE:CD1	1:A:233:HIS:CE1	0.42	3.02	18	1
1:A:29:ILE:CD1	1:A:29:ILE:N	0.42	2.82	15	1
1:A:41:LEU:HD13	1:A:53:LEU:HD22	0.42	1.92	15	1
1:A:177:ASP:OD1	1:A:246:ILE:HG21	0.42	2.15	14	1
1:A:43:ILE:O	1:A:43:ILE:HG23	0.42	2.14	14	1
1:A:261:TRP:HB2	1:A:271:VAL:HG22	0.42	1.90	18	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:157:LEU:CD2	1:A:183:LEU:HD13	0.42	2.44	17	1
1:A:230:ILE:HG21	1:A:279:ARG:HE	0.42	1.72	16	1
1:A:99:TRP:CD2	1:A:167:TYR:CD2	0.42	3.08	12	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:29:ILE:HD11	1:A:37:TRP:CH2	0.42	2.45	2	1
1:A:168:ILE:HD11	1:A:175:HIS:CG	0.42	2.50	13	1
1:A:71:LYS:HE2	1:A:351:ALA:HB2	0.42	1.89	20	1
1:A:111:PRO:CD	1:A:196:VAL:HG12	0.42	2.45	16	1
1:A:328:LEU:HD22	1:A:328:LEU:C	0.42	2.33	12	1
1:A:251:MET:CE	1:A:302:TYR:CE2	0.42	3.03	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:228:THR:HG23	1:A:228:THR:O	0.41	2.14	11	1
1:A:84:LEU:CD1	1:A:127:ARG:NE	0.41	2.83	14	1
1:A:79:PRO:HB3	1:A:352:LYS:CG	0.41	2.45	12	1
1:A:175:HIS:HE2	1:A:195:LEU:HD22	0.41	1.75	4	1
1:A:296:PRO:HG2	1:A:299:ILE:HD12	0.41	1.91	17	1
1:A:199:GLY:HA2	1:A:353:THR:N	0.41	2.30	20	2
1:A:240:ARG:HH22	1:A:309:LEU:HD22	0.41	1.75	3	1
1:A:81:PHE:O	1:A:81:PHE:CD1	0.41	2.73	18	2
1:A:213:TYR:O	1:A:213:TYR:CD2	0.41	2.74	17	2
1:A:307:LYS:CG	1:A:308:LEU:HD12	0.41	2.44	7	1
1:A:119:HIS:CE1	1:A:126:TYR:CB	0.41	3.03	17	1
1:A:23:PHE:CE2	1:A:72:VAL:HG21	0.41	2.50	9	1
1:A:176:GLY:O	1:A:246:ILE:HG21	0.41	2.15	16	1
1:A:173:TYR:CZ	1:A:203:ARG:CD	0.41	3.04	3	1
1:A:134:PHE:CE2	1:A:196:VAL:HG11	0.41	2.50	18	1
1:A:43:ILE:HD13	1:A:53:LEU:CG	0.41	2.43	18	1
1:A:155:LEU:HD21	1:A:327:GLY:HA3	0.41	1.92	12	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:290:PHE:HB3	1:A:294:ASN:O	0.41	2.15	5	1
1:A:286:MET:HE1	1:A:299:ILE:HG21	0.41	1.91	1	1
1:A:328:LEU:CD1	1:A:328:LEU:N	0.41	2.84	11	1
1:A:247:LEU:HD23	1:A:251:MET:CG	0.41	2.45	6	1
1:A:160:ARG:O	1:A:164:ILE:HD12	0.41	2.15	6	1
1:A:72:VAL:HG22	1:A:128:PHE:CB	0.41	2.45	13	1
1:A:178:ILE:O	1:A:179:LYS:O	0.41	2.38	17	1
1:A:119:HIS:CE1	1:A:126:TYR:HB2	0.41	2.51	17	1
1:A:32:MET:HE1	1:A:33:ALA:HB2	0.41	1.92	1	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:255:LEU:HD12	1:A:290:PHE:HZ	0.41	1.75	3	1
1:A:162:LEU:CD2	1:A:317:TYR:CD2	0.41	3.04	14	1
1:A:211:LYS:O	1:A:311:TYR:CE1	0.41	2.73	6	1
1:A:168:ILE:HD12	1:A:169:HIS:N	0.41	2.30	4	2
1:A:109:GLY:O	1:A:194:TYR:CD2	0.41	2.74	9	2
1:A:155:LEU:HD12	1:A:328:LEU:HD21	0.41	1.92	14	1
1:A:175:HIS:CE1	1:A:195:LEU:CD2	0.41	3.02	18	1
1:A:71:LYS:HZ3	1:A:83:GLU:CD	0.41	2.19	10	1
1:A:225:ILE:O	1:A:228:THR:HG22	0.41	2.16	6	1
1:A:219:ARG:O	1:A:220:CYS:CB	0.41	2.69	17	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:250:CYS:O	1:A:254:TRP:CD1	0.41	2.74	5	2
1:A:353:THR:O	1:A:354:ILE:O	0.41	2.38	10	1
1:A:88:GLN:HG2	1:A:113:TYR:CE1	0.41	2.51	7	1
1:A:290:PHE:CD1	1:A:290:PHE:N	0.41	2.88	5	1
1:A:278:TYR:CG	1:A:285:LEU:HD12	0.41	2.50	19	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: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:161:ILE:HG22	1:A:165:LEU:HD11	0.41	1.90	15	1
1:A:282:ILE:HG21	1:A:303:MET:HB3	0.41	1.93	11	1
1:A:261:TRP:O	1:A:261:TRP:CD1	0.41	2.74	3	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:264:ASN:OD1	1:A:270:TYR:CG	0.41	2.74	7	4
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:108:LEU:O	1:A:110:VAL:N	0.41	2.54	6	1
1:A:142:TYR:CZ	1:A:147:LYS:HG2	0.41	2.51	9	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: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:169:HIS:CE1	1:A:240:ARG:NH1	0.41	2.89	5	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:259:LEU:CD2	1:A:261:TRP:CH2	0.41	3.01	1	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:41:LEU:HD13	1:A:53:LEU:CD1	0.40	2.46	16	1
1:A:83:GLU:HB3	1:A:351:ALA:HB1	0.40	1.91	15	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:118:LEU:HD12	1:A:118:LEU:N	0.40	2.30	13	1
1:A:245:GLU:OE2	1:A:249:TYR:CE1	0.40	2.75	15	1
1:A:118:LEU:CD1	1:A:127:ARG:CD	0.40	3.00	3	1
1:A:86:PHE:CD2	1:A:198:TYR:CE2	0.40	3.08	14	1
1:A:118:LEU:CD1	1:A:118:LEU:N	0.40	2.84	18	1
1:A:209:VAL:HG12	1:A:210:HIS:N	0.40	2.31	10	1
1:A:162:LEU:HD22	1:A:317:TYR:HD2	0.40	1.69	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:LEU:HD21	1:A:127:ARG:NH1	0.40	2.31	4	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:225:ILE:HD11	1:A:233:HIS:HE1	0.40	1.76	17	1
1:A:29:ILE:HD13	1:A:128:PHE:CE1	0.40	2.52	20	1
1:A:39:VAL:HG12	1:A:53:LEU:O	0.40	2.16	16	1
1:A:320:LEU:O	1:A:323:ILE:CG1	0.40	2.69	11	1
1:A:253:GLN:OE1	1:A:254:TRP:CH2	0.40	2.75	18	1
1:A:186:ASN:OD1	1:A:194:TYR:CE1	0.40	2.74	19	2
1:A:278:TYR:CE1	1:A:285:LEU:HD22	0.40	2.52	6	1
1:A:213:TYR:O	1:A:213:TYR:CG	0.40	2.74	8	1
1:A:174:VAL:CG1	1:A:204:TYR:CE1	0.40	3.04	2	1
1:A:239:SER:HB3	1:A:311:TYR:CE2	0.40	2.51	7	1
1:A:217:PRO:O	1:A:221:HIS:CD2	0.40	2.75	1	1
1:A:258:HIS:CE1	1:A:262:GLU:OE2	0.40	2.75	9	1
1:A:175:HIS:CD2	1:A:176:GLY:N	0.40	2.90	16	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:83:GLU:OE1	1:A:87:TYR:CD1	0.40	2.75	2	1
1:A:107:TYR:CD1	1:A:194:TYR:OH	0.40	2.75	13	1
1:A:88:GLN:HG2	1:A:113:TYR:CE2	0.40	2.52	13	1
1:A:228:THR:OG1	1:A:232:ALA:HB3	0.40	2.16	17	1
1:A:178:ILE:CG2	1:A:246:ILE:HG22	0.40	2.44	16	1
1:A:233:HIS:NE2	1:A:275:LYS:CD	0.40	2.85	3	1
1:A:230:ILE:HD11	1:A:279:ARG:NH2	0.40	2.32	18	1
1:A:155:LEU:HD22	1:A:328:LEU:N	0.40	2.31	12	1
1:A:351:ALA:O	1:A:352:LYS:HB2	0.40	2.16	10	1
1:A:41:LEU:CD1	1:A:43:ILE:HG23	0.40	2.47	10	1
1:A:51:ILE:N	1:A:51:ILE:HD12	0.40	2.32	6	1
1:A:83:GLU:OE2	1:A:87:TYR:CE1	0.40	2.75	13	1
1:A:253:GLN:OE1	1:A:254:TRP:CE3	0.40	2.74	5	1
1:A:253:GLN:HG2	1:A:254:TRP:CZ3	0.40	2.52	9	1
1:A:166:GLU:OE1	1:A:317:TYR:CD2	0.40	2.74	9	1

6.3 Torsion angles

6.3.1 Protein backbone

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

was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	310/361 (86%)	273±4 (88±1%)	27±4 (9±1%)	10±2 (3±1%)	8 38
All	All	6200/7220 (86%)	5451 (88%)	541 (9%)	208 (3%)	8 38

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	354	ILE	20
1	A	353	THR	20
1	A	213	TYR	18
1	A	200	LEU	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	238	PRO	7
1	A	60	GLU	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	266	LYS	3
1	A	356	LYS	3
1	A	177	ASP	3
1	A	23	PHE	3
1	A	59	SER	3
1	A	66	ALA	3
1	A	291	PRO	3
1	A	220	CYS	2
1	A	296	PRO	2
1	A	351	ALA	2
1	A	205	CYS	1
1	A	222	ASP	1
1	A	294	ASN	1
1	A	49	GLY	1
1	A	79	PRO	1
1	A	106	LYS	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%)	5 38
All	All	5460/6240 (88%)	4443 (81%)	1017 (19%)	5 38

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

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Mol	Chain	Res	Type	Models (Total)
1	A	129	MET	10
1	A	356	LYS	10
1	A	106	LYS	10
1	A	309	LEU	10
1	A	76	ASP	9
1	A	88	GLN	9
1	A	211	LYS	9
1	A	195	LEU	9
1	A	203	ARG	9
1	A	133	ARG	9
1	A	241	ARG	8
1	A	61	SER	8
1	A	334	LYS	8
1	A	59	SER	8
1	A	255	LEU	8
1	A	118	LEU	7
1	A	303	MET	7
1	A	314	LYS	7
1	A	60	GLU	7
1	A	214	LYS	7
1	A	32	MET	7
1	A	160	ARG	7
1	A	250	CYS	7
1	A	228	THR	7
1	A	50	CYS	7
1	A	162	LEU	7
1	A	221	HIS	7
1	A	41	LEU	7
1	A	125	SER	7
1	A	233	HIS	6
1	A	97	GLN	6
1	A	132	ASP	6
1	A	147	LYS	6
1	A	77	ASN	6
1	A	295	LYS	6
1	A	245	GLU	6
1	A	92	LYS	6
1	A	264	ASN	6
1	A	179	LYS	6
1	A	124	LYS	6
1	A	34	LYS	6
1	A	170	GLU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	30	THR	6
1	A	119	HIS	6
1	A	89	ARG	6
1	A	71	LYS	5
1	A	262	GLU	5
1	A	149	PHE	5
1	A	192	GLN	5
1	A	58	SER	5
1	A	108	LEU	5
1	A	169	HIS	5
1	A	240	ARG	5
1	A	219	ARG	5
1	A	104	LYS	5
1	A	285	LEU	5
1	A	165	LEU	5
1	A	197	ASP	5
1	A	95	GLN	5
1	A	326	GLN	5
1	A	218	LYS	5
1	A	231	ASP	5
1	A	153	THR	4
1	A	148	ARG	4
1	A	151	ARG	4
1	A	251	MET	4
1	A	256	THR	4
1	A	321	ARG	4
1	A	277	ARG	4
1	A	181	SER	4
1	A	101	ARG	4
1	A	213	TYR	4
1	A	145	ASN	4
1	A	266	LYS	4
1	A	186	ASN	4
1	A	311	TYR	4
1	A	98	LYS	4
1	A	226	GLU	4
1	A	38	LYS	4
1	A	243	ASP	4
1	A	136	SER	4
1	A	177	ASP	4
1	A	139	GLN	4
1	A	94	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	127	ARG	4
1	A	143	GLU	3
1	A	188	LYS	3
1	A	155	LEU	3
1	A	121	LYS	3
1	A	85	LYS	3
1	A	225	ILE	3
1	A	52	TYR	3
1	A	253	GLN	3
1	A	263	ASP	3
1	A	173	TYR	3
1	A	166	GLU	3
1	A	275	LYS	3
1	A	269	LYS	3
1	A	290	PHE	3
1	A	323	ILE	3
1	A	289	CYS	3
1	A	185	LEU	2
1	A	112	LYS	2
1	A	120	ASP	2
1	A	105	LEU	2
1	A	191	ASP	2
1	A	171	HIS	2
1	A	31	ASP	2
1	A	212	GLU	2
1	A	325	LEU	2
1	A	301	LYS	2
1	A	313	GLU	2
1	A	308	LEU	2
1	A	207	GLU	2
1	A	352	LYS	2
1	A	298	GLU	2
1	A	274	SER	2
1	A	216	ASP	2
1	A	27	GLU	2
1	A	239	SER	2
1	A	205	CYS	2
1	A	272	ARG	2
1	A	259	LEU	2
1	A	329	LYS	2
1	A	158	SER	2
1	A	215	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	43	ILE	2
1	A	276	ILE	1
1	A	247	LEU	1
1	A	159	LEU	1
1	A	183	LEU	1
1	A	204	TYR	1
1	A	229	SER	1
1	A	333	SER	1
1	A	29	ILE	1
1	A	84	LEU	1
1	A	102	THR	1
1	A	99	TRP	1
1	A	81	PHE	1
1	A	278	TYR	1
1	A	157	LEU	1
1	A	234	ASN	1
1	A	178	ILE	1
1	A	328	LEU	1
1	A	116	SER	1
1	A	131	MET	1
1	A	236	VAL	1
1	A	137	ASP	1
1	A	80	LEU	1
1	A	305	THR	1
1	A	100	ILE	1
1	A	28	ILE	1
1	A	87	TYR	1
1	A	284	SER	1
1	A	37	TRP	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 carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 72% for the well-defined parts and 69% for the entire structure.

7.1 Chemical shift list 1

File name: 2lav_cs.str

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	3545
Number of shifts mapped to atoms	3545
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 ± 0.05	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	317	0.61 ± 0.07	Should be applied
$^{13}C'$	343	0.18 ± 0.06	None needed (< 0.5 ppm)
^{15}N	327	-0.41 ± 0.16	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 72%, i.e. 2875 atoms were assigned a chemical shift out of a possible 4005. 34 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1481/1520 (97%)	578/605 (96%)	614/620 (99%)	289/295 (98%)
Sidechain	1278/2129 (60%)	860/1258 (68%)	413/770 (54%)	5/101 (5%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	116/356 (33%)	111/182 (61%)	0/153 (0%)	5/21 (24%)
Overall	2875/4005 (72%)	1549/2045 (76%)	1027/1543 (67%)	299/417 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 3200 atoms were assigned a chemical shift out of a possible 4627. 40 out of 53 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	1674/1773 (94%)	650/706 (92%)	697/722 (97%)	327/345 (95%)
Sidechain	1406/2481 (57%)	935/1466 (64%)	466/890 (52%)	5/125 (4%)
Aromatic	120/373 (32%)	115/191 (60%)	0/159 (0%)	5/23 (22%)
Overall	3200/4627 (69%)	1700/2363 (72%)	1163/1771 (66%)	337/493 (68%)

7.1.4 Statistically unusual chemical shifts (i)

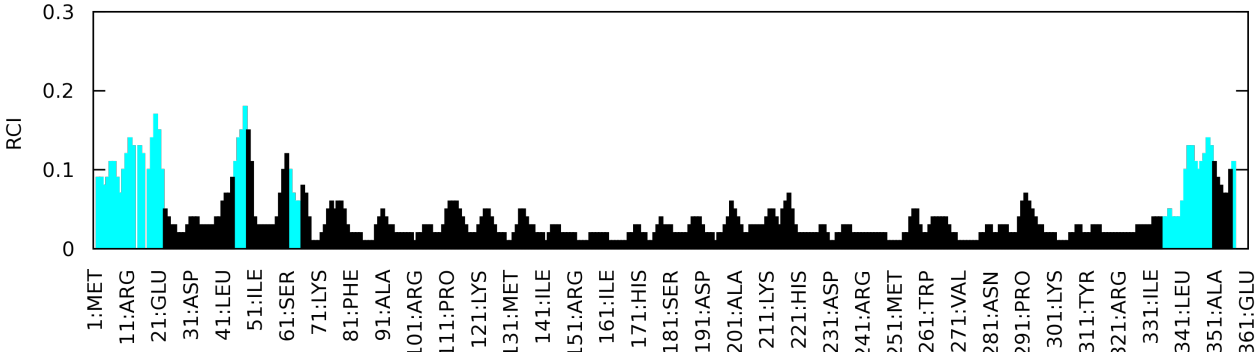
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	29	ILE	HG23	-0.80	2.13 – -0.57	-5.8
1	A	29	ILE	HG22	-0.80	2.13 – -0.57	-5.8
1	A	29	ILE	HG21	-0.80	2.13 – -0.57	-5.8
1	A	29	ILE	HD11	-0.94	2.13 – -0.77	-5.6
1	A	29	ILE	HD12	-0.94	2.13 – -0.77	-5.6
1	A	29	ILE	HD13	-0.94	2.13 – -0.77	-5.6
1	A	130	ILE	HG22	-0.62	2.13 – -0.57	-5.2
1	A	130	ILE	HG23	-0.62	2.13 – -0.57	-5.2
1	A	130	ILE	HG21	-0.62	2.13 – -0.57	-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.

Random coil index (RCI) for chain A:


RCI
0.3
0.2
0.1
0
1:MET
11:ARG
21:GLU
31:ASP
41:LEU
51:ILE
61:SER
71:LYS
81:PHE
91:ALA
101:ARG
111:PRO
121:LYS
131:MET
141:ILE
151:ARG
161:ILE
171:HIS
181:SER
191:ASP
201:ALA
211:LYS
221:HIS
231:ASP
241:ARG
251:MET
261:TRP
271:VAL
281:ASN
291:PRO
301:LYS
311:TYR
321:ARG
331:ILE
341:LEU
351:ALA
361:GLU