



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 05:52 pm GMT

PDB ID : 1CF4  
Title : CDC42/ACK GTPASE-BINDING DOMAIN COMPLEX  
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Deposited on : 1999-03-23

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

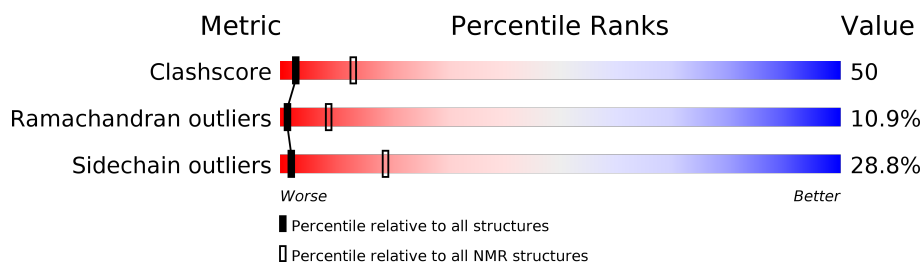
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 63%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	184	<div> <div>28%</div> <div>58%</div> <div>13%</div> <div>.</div> </div>
2	B	44	<div> <div>20%</div> <div>70%</div> <div>9%</div> </div>

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models).

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:1-A:184, B:502-B:545 (228)	0.85	19

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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

### 3 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3602 atoms, of which 1789 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (CDC42 HOMOLOG).

Mol	Chain	Residues	Atoms						Trace
1	A	184	Total	C	H	N	O	S	0
			2899	926	1463	228	275	7	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	LEU	GLN	CONFLICT	UNP P60953
A	?	-	LYS	DELETION	UNP P60953
A	?	-	LYS	DELETION	UNP P60953
A	?	-	SER	DELETION	UNP P60953
A	?	-	ARG	DELETION	UNP P60953
A	?	-	ARG	DELETION	UNP P60953
A	?	-	CYS	DELETION	UNP P60953
A	?	-	VAL	DELETION	UNP P60953

- Molecule 2 is a protein called PROTEIN (ACTIVATED P21CDC42HS KINASE).

Mol	Chain	Residues	Atoms						Trace
2	B	44	Total	C	H	N	O	S	0
			651	210	309	62	69	1	

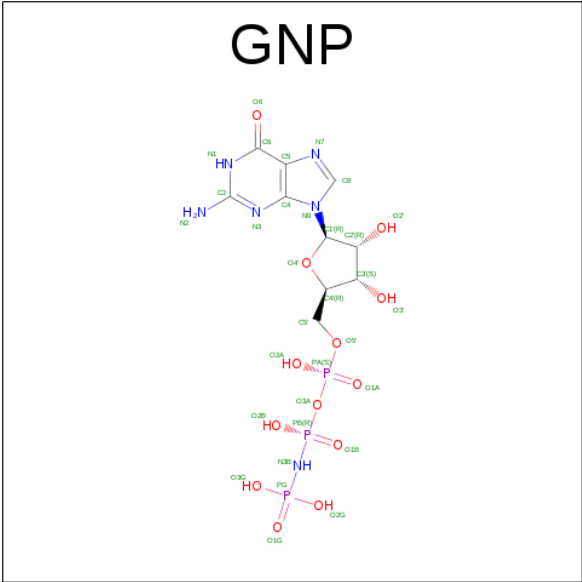
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	502	GLY	VAL	CONFLICT	UNP Q07912
B	503	SER	ALA	CONFLICT	UNP Q07912

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	
3	A	1	Total	Mg
			1	1

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
4	A	1	45	10	13	6	13	3

- Molecule 5 is water.

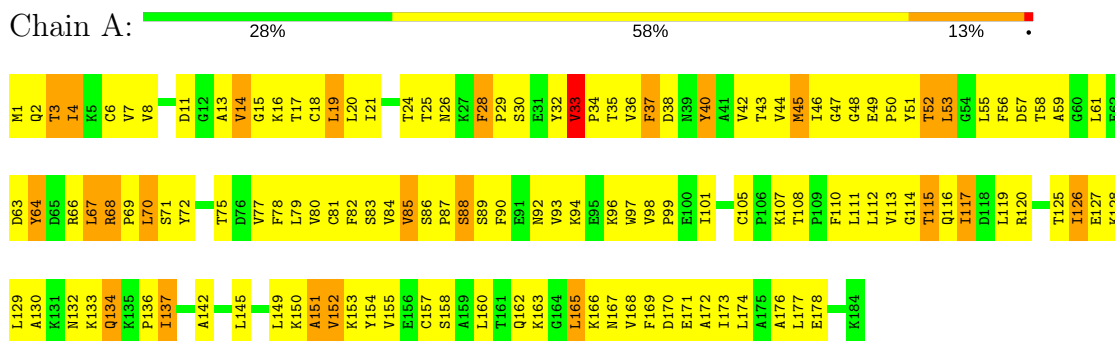
Mol	Chain	Residues	Atoms		
			Total	H	O
5	A	2	6	4	2

## 4 Residue-property plots [i](#)

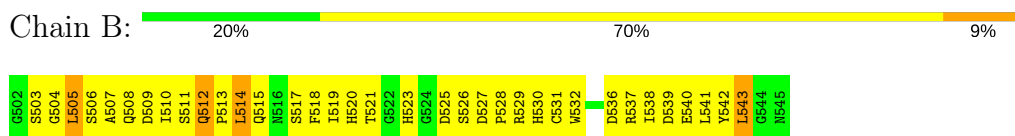
### 4.1 Average score per residue in the NMR ensemble

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: PROTEIN (CDC42 HOMOLOG)



#### • Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

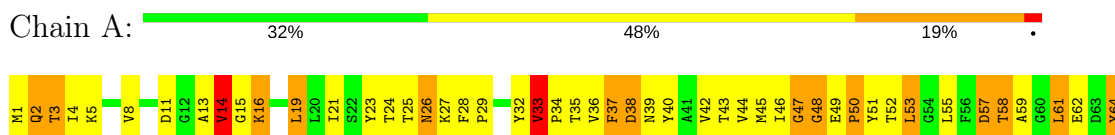


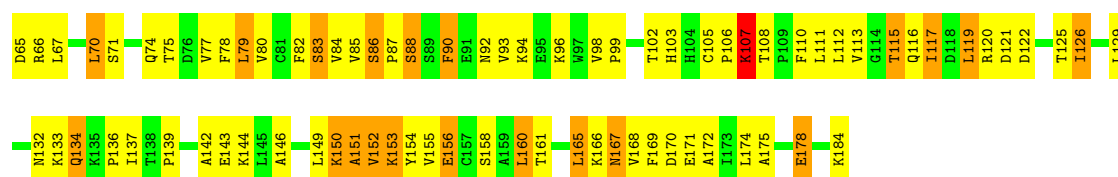
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

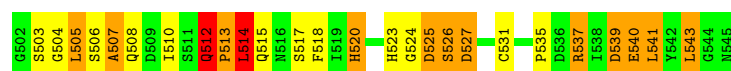
#### 4.2.1 Score per residue for model 1

#### • Molecule 1: PROTEIN (CDC42 HOMOLOG)



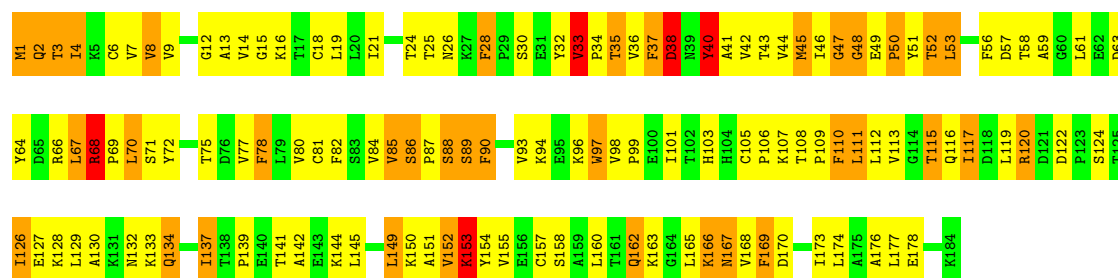


• Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

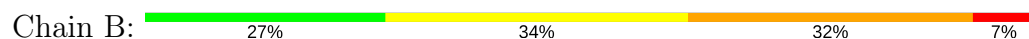


## 4.2.2 Score per residue for model 2

• Molecule 1: PROTEIN (CDC42 HOMOLOG)

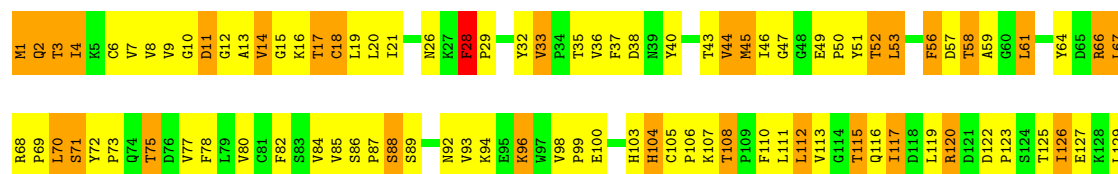


• Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)



## 4.2.3 Score per residue for model 3

• Molecule 1: PROTEIN (CDC42 HOMOLOG)





- Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

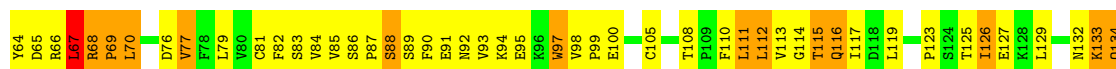
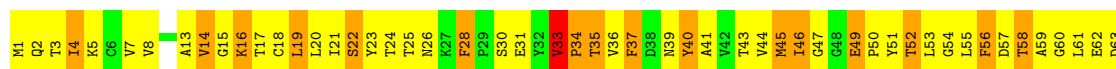
Chain B: 36% 41% 20%



#### 4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (CDC42 HOMOLOG)

Chain A: 32% 48% 19%



- Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

Chain B: 45% 36% 11% 7%



#### 4.2.5 Score per residue for model 5

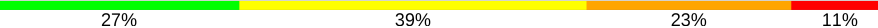
- Molecule 1: PROTEIN (CDC42 HOMOLOG)

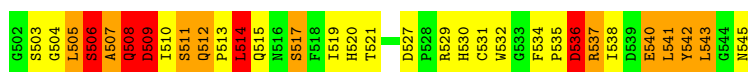
Chain A: 34% 49% 15%



- Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)



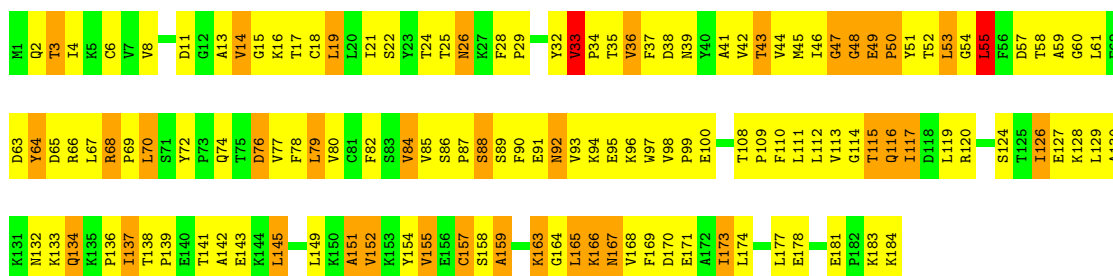
Chain B: 



#### 4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (CDC42 HOMOLOG)

Chain A: 



- Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

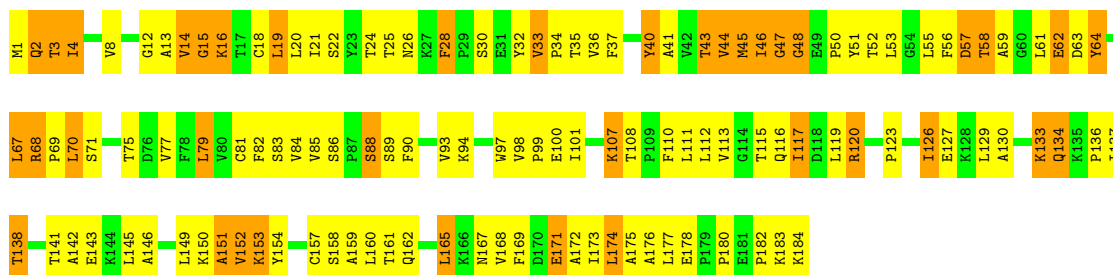
Chain B: 



#### 4.2.7 Score per residue for model 7

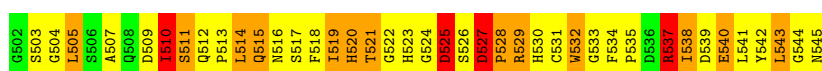
- Molecule 1: PROTEIN (CDC42 HOMOLOG)

Chain A: 



- Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

Chain B: 

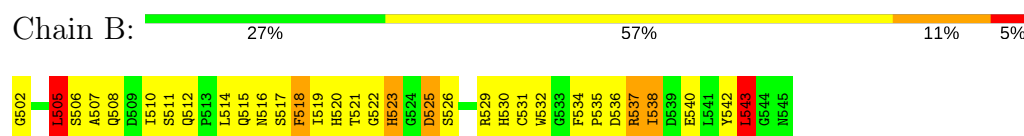


### 4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN (CDC42 HOMOLOG)

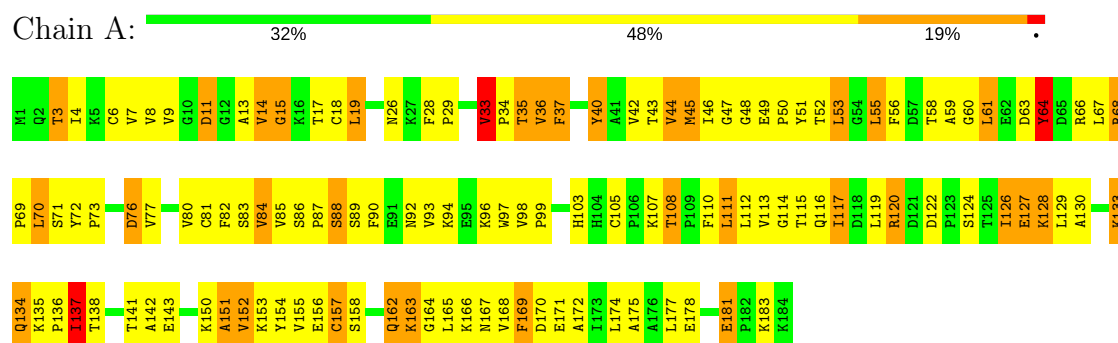


- Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

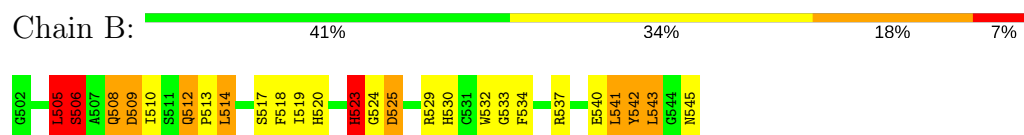


### 4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN (CDC42 HOMOLOG)

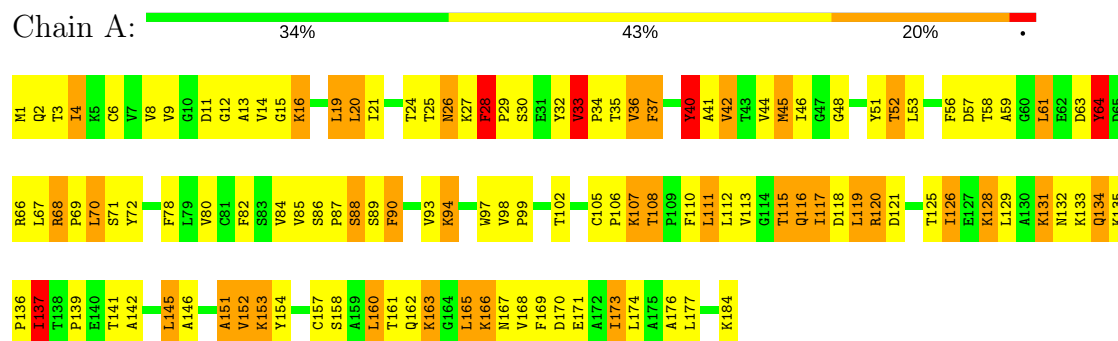


- Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

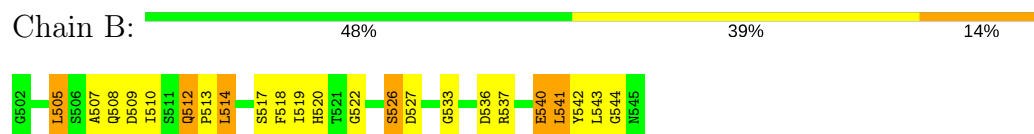


### 4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (CDC42 HOMOLOG)

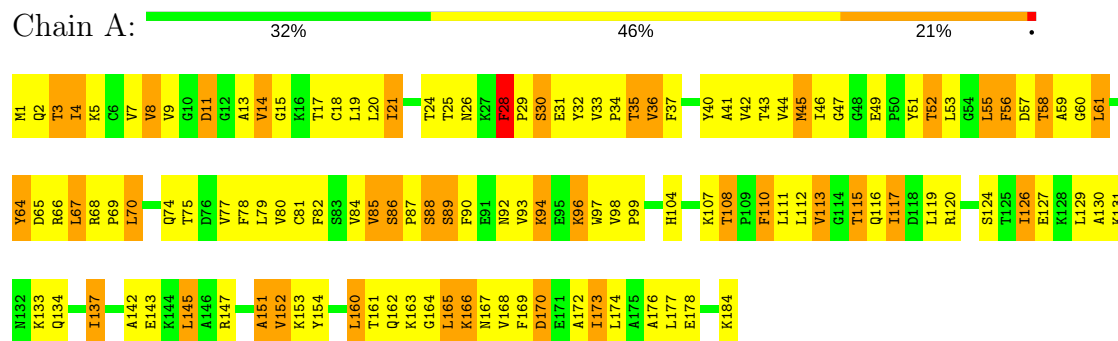


- Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

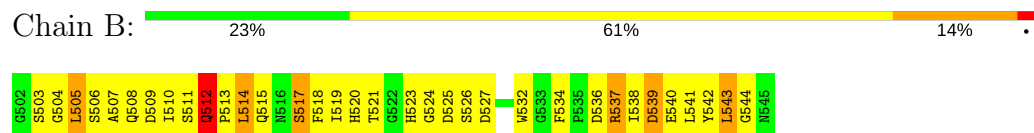


#### 4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (CDC42 HOMOLOG)



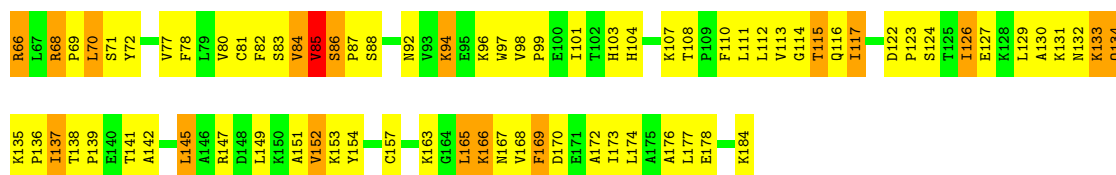
- Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)



#### 4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (CDC42 HOMOLOG)



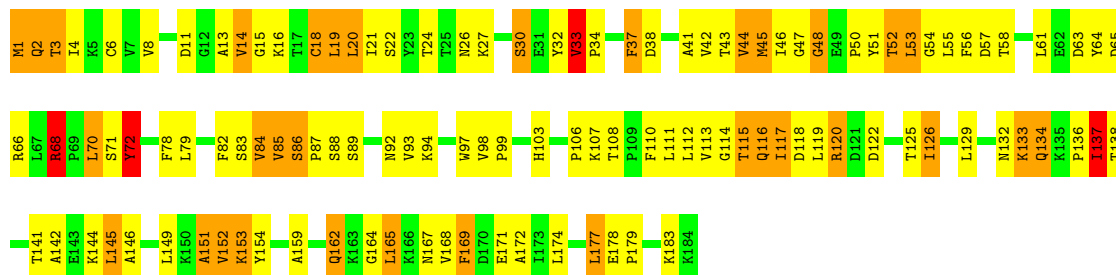


- Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

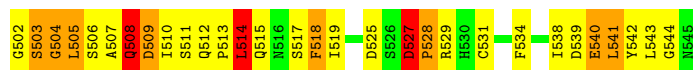
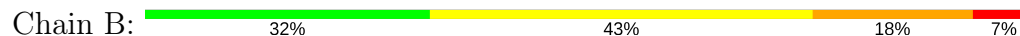


#### 4.2.13 Score per residue for model 13

- Molecule 1: PROTEIN (CDC42 HOMOLOG)

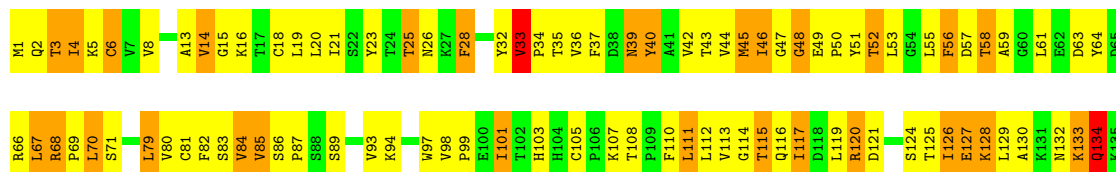


- Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)



#### 4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN (CDC42 HOMOLOG)





• Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

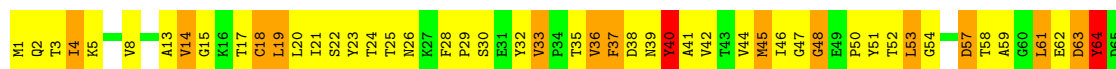
Chain B: 41% 32% 27%



#### 4.2.15 Score per residue for model 15

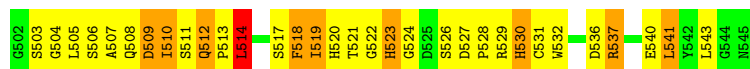
• Molecule 1: PROTEIN (CDC42 HOMOLOG)

Chain A: 33% 46% 18%



• Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

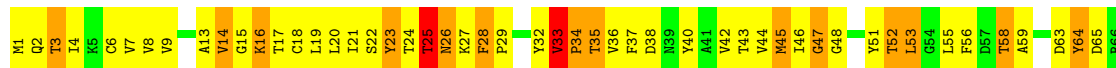
Chain B: 27% 50% 20%



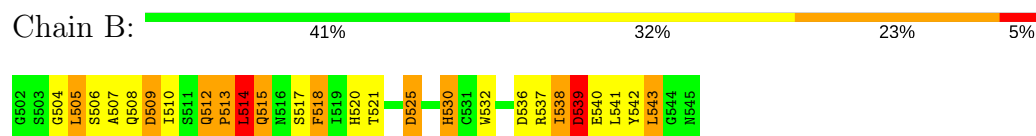
#### 4.2.16 Score per residue for model 16

• Molecule 1: PROTEIN (CDC42 HOMOLOG)

Chain A: 36% 46% 16%

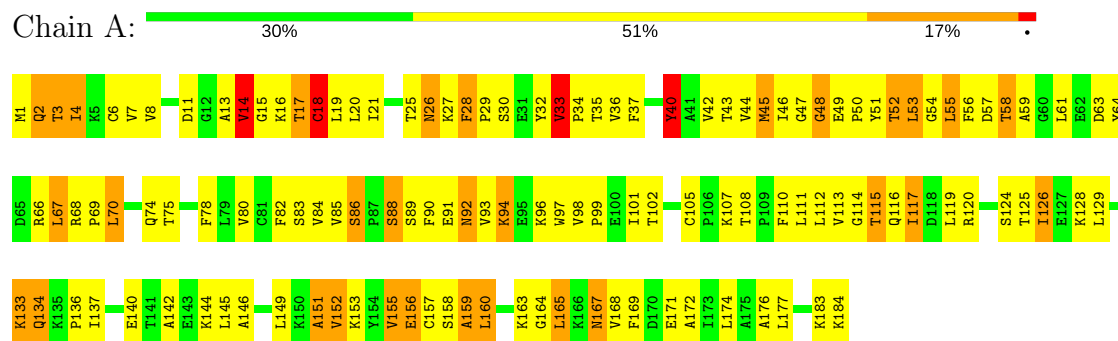


• Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

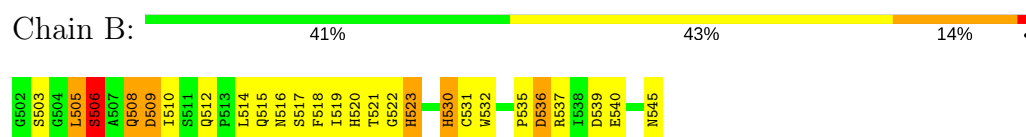


#### 4.2.17 Score per residue for model 17

- Molecule 1: PROTEIN (CDC42 HOMOLOG)

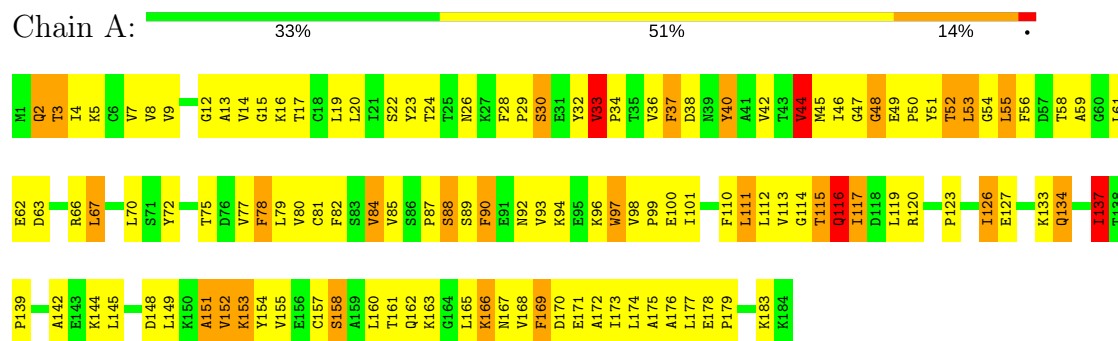


- Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

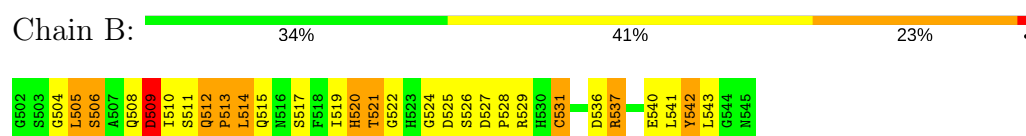


#### 4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN (CDC42 HOMOLOG)

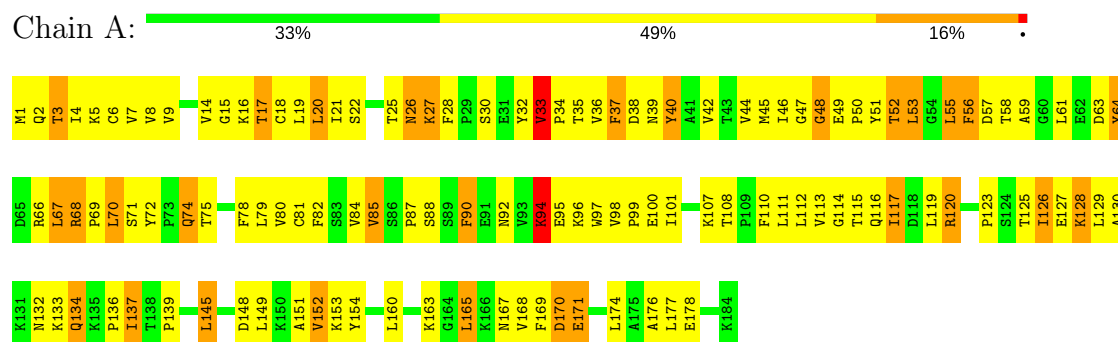


- Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

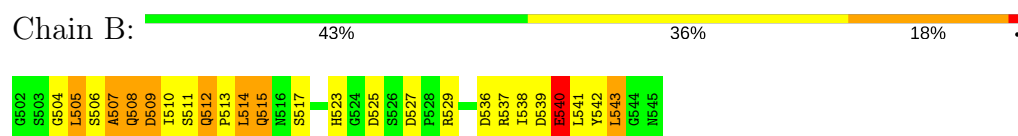


### 4.2.19 Score per residue for model 19 (medoid)

#### • Molecule 1: PROTEIN (CDC42 HOMOLOG)

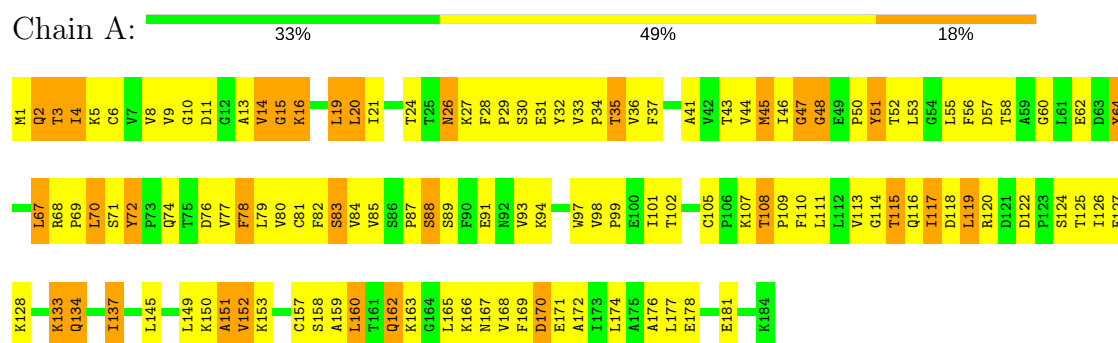


#### • Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)

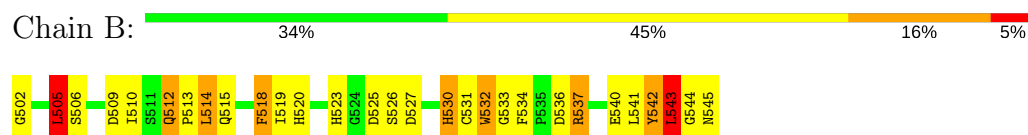


### 4.2.20 Score per residue for model 20

#### • Molecule 1: PROTEIN (CDC42 HOMOLOG)



#### • Molecule 2: PROTEIN (ACTIVATED P21CDC42HS KINASE)



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY, SIMULATED ANNEALING*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851
ANSIG	structure solution	
XPLOR	structure solution	

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)	BMRB entry 4700
Number of chemical shift lists	2
Total number of shifts	2515
Number of shifts mapped to atoms	1988
Number of unparsed shifts	0
Number of shifts with mapping errors	527
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	63%

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



## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, MG

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	1436	1463	1461	166±12
2	B	342	309	303	38±8
4	A	32	13	13	12±3
5	A	2	4	0	0±0
All	All	36260	35780	35540	3580

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 50.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:VAL:HG13	1:A:52:THR:HG21	1.03	1.26	12	1
1:A:113:VAL:HG13	1:A:168:VAL:HG21	1.01	1.33	20	12
1:A:8:VAL:HG11	1:A:14:VAL:HG13	1.01	1.20	3	1
1:A:44:VAL:HG22	1:A:52:THR:HG23	1.00	1.30	19	2
1:A:14:VAL:HG23	1:A:19:LEU:HD21	1.00	1.27	4	1
1:A:112:LEU:HD12	1:A:146:ALA:HB2	0.99	1.28	10	4
1:A:174:LEU:HD13	2:B:505:LEU:HD13	0.98	1.32	19	4
1:A:177:LEU:HD13	2:B:510:ILE:HG21	0.97	1.35	14	3
1:A:36:VAL:HG22	1:A:61:LEU:HD13	0.96	1.33	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:VAL:HG22	1:A:149:LEU:HD13	0.96	1.34	8	2
1:A:58:THR:HG21	1:A:70:LEU:HD22	0.93	1.38	20	2
1:A:46:ILE:HG23	2:B:510:ILE:HG23	0.92	1.36	15	9
1:A:174:LEU:HD23	2:B:505:LEU:HD13	0.91	1.40	10	4
1:A:177:LEU:HD22	2:B:510:ILE:HG21	0.90	1.43	15	2
1:A:82:PHE:CE1	1:A:112:LEU:HD22	0.90	2.02	7	1
1:A:174:LEU:HD21	2:B:505:LEU:HD13	0.90	1.42	6	1
1:A:44:VAL:HG22	1:A:52:THR:CG2	0.90	1.96	19	7
1:A:177:LEU:CD1	2:B:510:ILE:HG21	0.89	1.97	14	3
1:A:17:THR:HG21	1:A:35:THR:HG23	0.89	1.42	9	4
1:A:115:THR:OG1	4:A:185:GNP:H2'	0.88	1.68	19	18
1:A:17:THR:CG2	1:A:35:THR:HG23	0.88	1.99	9	4
1:A:19:LEU:HD23	1:A:169:PHE:CE1	0.88	2.03	10	2
1:A:119:LEU:HD21	1:A:160:LEU:HD22	0.87	1.43	10	1
1:A:177:LEU:CD2	2:B:510:ILE:HG21	0.87	2.00	15	4
1:A:3:THR:HG23	1:A:46:ILE:HG21	0.87	1.43	3	2
1:A:36:VAL:HG23	1:A:59:ALA:HB3	0.87	1.42	8	5
1:A:44:VAL:HG12	1:A:52:THR:CG2	0.87	1.98	18	1
1:A:19:LEU:HD23	1:A:169:PHE:CD2	0.87	2.04	2	3
1:A:116:GLN:NE2	1:A:119:LEU:HD11	0.87	1.85	4	1
1:A:14:VAL:HG11	1:A:113:VAL:HG21	0.86	1.45	14	1
1:A:33:VAL:HG11	2:B:526:SER:O	0.86	1.69	3	2
1:A:19:LEU:HD22	1:A:169:PHE:CD1	0.86	2.04	8	4
1:A:111:LEU:HD12	1:A:152:VAL:HG11	0.86	1.47	16	16
1:A:117:ILE:HD11	1:A:157:CYS:O	0.86	1.71	3	7
1:A:12:GLY:O	1:A:14:VAL:HG13	0.86	1.70	5	1
1:A:35:THR:HG21	2:B:543:LEU:CD2	0.85	2.01	11	2
1:A:113:VAL:CG1	1:A:168:VAL:HG11	0.85	2.02	12	7
1:A:89:SER:O	1:A:93:VAL:HG23	0.85	1.72	5	15
1:A:70:LEU:HD23	2:B:541:LEU:CB	0.85	2.02	3	3
1:A:84:VAL:HG22	1:A:116:GLN:CB	0.84	2.03	12	2
1:A:4:ILE:HG13	1:A:53:LEU:HD13	0.84	1.49	19	3
1:A:19:LEU:HD23	1:A:165:LEU:CD2	0.84	2.02	7	5
1:A:36:VAL:HG12	1:A:59:ALA:CB	0.84	2.00	15	3
1:A:58:THR:HG22	1:A:67:LEU:HD13	0.84	1.50	10	2
1:A:13:ALA:HB2	4:A:185:GNP:O2A	0.84	1.73	14	3
1:A:44:VAL:CG1	2:B:514:LEU:HD13	0.83	2.03	17	2
1:A:80:VAL:HG12	1:A:97:TRP:CH2	0.83	2.09	8	1
1:A:4:ILE:HD11	1:A:53:LEU:HD22	0.83	1.48	3	5
1:A:110:PHE:O	1:A:151:ALA:HB1	0.83	1.73	8	14
1:A:15:GLY:CA	1:A:19:LEU:HD22	0.83	2.04	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:THR:HG23	1:A:38:ASP:OD2	0.83	1.74	2	1
1:A:19:LEU:HD22	1:A:169:PHE:CG	0.83	2.07	12	6
1:A:19:LEU:HD13	1:A:169:PHE:CE1	0.83	2.08	8	6
1:A:14:VAL:HG23	1:A:19:LEU:CD2	0.82	2.04	4	2
1:A:19:LEU:O	1:A:165:LEU:HD13	0.82	1.73	8	4
1:A:173:ILE:HD13	1:A:174:LEU:N	0.82	1.89	10	4
1:A:159:ALA:O	1:A:160:LEU:HD13	0.82	1.74	17	1
1:A:64:TYR:CD2	1:A:67:LEU:HD21	0.82	2.10	11	2
1:A:14:VAL:HG11	1:A:57:ASP:OD2	0.82	1.74	3	1
1:A:58:THR:OG1	1:A:67:LEU:HD21	0.82	1.75	3	2
1:A:61:LEU:HD23	2:B:526:SER:CB	0.82	2.05	6	1
1:A:15:GLY:C	1:A:19:LEU:HD11	0.82	1.93	7	2
1:A:4:ILE:C	1:A:53:LEU:HD23	0.81	1.95	8	3
1:A:14:VAL:CG2	1:A:19:LEU:HD21	0.81	2.04	4	2
1:A:45:MET:O	2:B:514:LEU:HD22	0.81	1.76	11	6
1:A:70:LEU:O	1:A:70:LEU:HD12	0.81	1.75	14	5
1:A:46:ILE:CG1	1:A:52:THR:HG23	0.81	2.06	4	2
1:A:61:LEU:HD23	2:B:526:SER:OG	0.81	1.76	6	1
1:A:9:VAL:HG21	1:A:78:PHE:CE2	0.81	2.10	8	2
1:A:46:ILE:HG12	1:A:52:THR:HG22	0.81	1.53	20	1
1:A:84:VAL:HG11	1:A:120:ARG:HG2	0.80	1.53	18	1
1:A:111:LEU:HD22	1:A:172:ALA:HB2	0.80	1.54	5	2
1:A:9:VAL:HG13	2:B:540:GLU:CD	0.80	1.97	8	1
1:A:136:PRO:C	1:A:137:ILE:HD13	0.80	1.97	17	3
1:A:14:VAL:HG12	4:A:185:GNP:N7	0.80	1.92	6	2
1:A:70:LEU:HD21	2:B:541:LEU:HA	0.79	1.54	2	3
1:A:14:VAL:O	1:A:19:LEU:HD21	0.79	1.77	1	2
1:A:4:ILE:CD1	1:A:53:LEU:HD22	0.79	2.07	9	6
1:A:3:THR:HG23	1:A:53:LEU:HD12	0.79	1.53	10	1
1:A:113:VAL:HG13	1:A:168:VAL:HG11	0.79	1.52	7	13
1:A:125:THR:HG22	1:A:129:LEU:CD1	0.78	2.09	5	3
1:A:58:THR:O	2:B:543:LEU:HD22	0.78	1.79	5	5
2:B:504:GLY:C	2:B:505:LEU:HD13	0.78	1.99	11	2
1:A:86:SER:C	1:A:129:LEU:HD22	0.78	1.99	12	2
1:A:77:VAL:HG11	1:A:176:ALA:HB2	0.78	1.56	12	3
1:A:59:ALA:HB1	1:A:61:LEU:CD1	0.78	2.09	12	4
1:A:58:THR:O	2:B:543:LEU:HD13	0.78	1.78	1	2
1:A:35:THR:HG21	4:A:185:GNP:O2G	0.78	1.79	19	3
1:A:14:VAL:HG21	2:B:543:LEU:HD21	0.78	1.51	3	1
1:A:35:THR:HG21	5:A:187:HOH:O	0.78	1.79	2	1
1:A:19:LEU:CD2	1:A:165:LEU:HD22	0.78	2.09	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:VAL:CG1	1:A:14:VAL:HG13	0.78	2.07	3	1
1:A:19:LEU:HD13	1:A:169:PHE:CE2	0.78	2.14	18	3
4:A:185:GNP:O1G	2:B:543:LEU:HD11	0.77	1.77	14	1
1:A:36:VAL:HG23	1:A:59:ALA:CB	0.77	2.08	1	2
1:A:14:VAL:HG11	1:A:113:VAL:HG11	0.77	1.57	13	1
1:A:13:ALA:HB1	4:A:185:GNP:PA	0.77	2.19	10	1
1:A:98:VAL:CG2	1:A:149:LEU:HD13	0.77	2.08	8	2
1:A:84:VAL:HG22	1:A:116:GLN:HB3	0.77	1.57	7	4
1:A:84:VAL:HG12	1:A:137:ILE:O	0.77	1.79	8	3
1:A:3:THR:HG23	1:A:46:ILE:HD12	0.77	1.54	14	1
1:A:4:ILE:CG1	1:A:53:LEU:HD13	0.77	2.09	19	5
1:A:14:VAL:HG22	1:A:81:CYS:HB3	0.77	1.55	18	2
1:A:8:VAL:HG21	1:A:15:GLY:N	0.76	1.94	8	1
1:A:9:VAL:HG11	1:A:72:TYR:CE1	0.76	2.15	9	1
1:A:70:LEU:HD22	2:B:541:LEU:HA	0.76	1.56	16	2
1:A:14:VAL:HG21	1:A:79:LEU:HD22	0.76	1.57	11	1
1:A:36:VAL:CG2	1:A:61:LEU:HD13	0.76	2.11	14	1
1:A:16:LYS:O	1:A:20:LEU:HD23	0.76	1.80	17	1
1:A:42:VAL:HG13	2:B:517:SER:O	0.76	1.80	19	1
1:A:8:VAL:HG11	1:A:15:GLY:HA2	0.75	1.57	8	1
1:A:17:THR:HG22	1:A:21:ILE:HG13	0.75	1.59	19	1
1:A:19:LEU:HD23	1:A:165:LEU:HD22	0.75	1.58	7	4
1:A:36:VAL:HG12	1:A:59:ALA:HB1	0.75	1.54	15	1
1:A:110:PHE:O	1:A:152:VAL:HG23	0.75	1.80	4	1
1:A:159:ALA:C	1:A:160:LEU:HD13	0.75	2.02	17	1
2:B:504:GLY:O	2:B:505:LEU:HD12	0.75	1.81	18	2
1:A:111:LEU:HD12	1:A:152:VAL:CG1	0.75	2.12	13	18
1:A:19:LEU:HD21	1:A:169:PHE:CE1	0.75	2.17	20	1
1:A:3:THR:HG23	1:A:53:LEU:HD22	0.75	1.57	8	2
1:A:111:LEU:HD12	1:A:152:VAL:HB	0.75	1.59	4	3
1:A:174:LEU:HG	2:B:505:LEU:HD22	0.74	1.57	6	2
1:A:84:VAL:HG11	1:A:120:ARG:CG	0.74	2.12	18	1
1:A:113:VAL:CG1	1:A:168:VAL:HG21	0.74	2.12	5	7
1:A:126:ILE:HD11	1:A:136:PRO:HB3	0.74	1.57	13	9
1:A:113:VAL:HG13	1:A:168:VAL:CG2	0.74	2.11	20	8
1:A:4:ILE:CD1	1:A:53:LEU:HD13	0.74	2.12	15	1
1:A:44:VAL:HB	1:A:52:THR:HG21	0.74	1.60	20	2
1:A:58:THR:CG2	1:A:70:LEU:HD22	0.74	2.12	20	2
1:A:174:LEU:HD13	2:B:505:LEU:HD22	0.74	1.59	9	2
1:A:113:VAL:HG22	1:A:168:VAL:HG11	0.74	1.60	14	1
1:A:8:VAL:HG21	1:A:16:LYS:CG	0.74	2.12	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:VAL:HG22	1:A:116:GLN:OE1	0.74	1.82	11	6
1:A:111:LEU:HD11	1:A:171:GLU:CD	0.74	2.03	5	1
1:A:44:VAL:HG13	2:B:514:LEU:HD13	0.74	1.59	17	2
1:A:77:VAL:HG21	1:A:176:ALA:HB2	0.74	1.59	2	2
2:B:538:ILE:HD11	2:B:542:TYR:CB	0.74	2.13	3	1
1:A:42:VAL:HG23	1:A:52:THR:HG21	0.74	1.57	13	5
1:A:46:ILE:CG1	2:B:510:ILE:HG23	0.74	2.13	11	1
1:A:13:ALA:HB3	4:A:185:GNP:H8	0.73	1.60	10	3
1:A:82:PHE:CE2	1:A:112:LEU:HD22	0.73	2.17	13	1
1:A:36:VAL:HG21	1:A:61:LEU:HB2	0.73	1.60	1	1
1:A:1:MET:CE	1:A:46:ILE:HG23	0.73	2.12	11	2
1:A:19:LEU:O	1:A:165:LEU:HD11	0.73	1.84	5	1
1:A:19:LEU:HA	1:A:165:LEU:HD13	0.73	1.59	7	7
1:A:9:VAL:HG21	1:A:78:PHE:CZ	0.73	2.18	8	1
1:A:19:LEU:HD22	1:A:169:PHE:CD2	0.73	2.19	13	1
1:A:3:THR:O	1:A:4:ILE:HG23	0.73	1.83	4	1
1:A:94:LYS:CG	1:A:145:LEU:HD11	0.73	2.13	12	5
1:A:173:ILE:HD11	1:A:177:LEU:HD22	0.73	1.60	6	1
1:A:163:LYS:HG2	1:A:165:LEU:HD22	0.72	1.57	9	1
1:A:125:THR:HG22	1:A:129:LEU:HD11	0.72	1.61	5	3
1:A:44:VAL:HG12	1:A:52:THR:HG22	0.72	1.61	18	1
1:A:174:LEU:HD13	2:B:505:LEU:CB	0.72	2.14	7	6
1:A:3:THR:HG22	1:A:51:TYR:CE1	0.72	2.20	10	2
1:A:1:MET:HE3	1:A:46:ILE:HG23	0.72	1.61	11	1
1:A:17:THR:HG22	1:A:38:ASP:OD1	0.72	1.84	3	1
1:A:9:VAL:HG21	1:A:78:PHE:CD2	0.72	2.20	2	3
1:A:174:LEU:CD1	2:B:505:LEU:HD13	0.72	2.12	19	3
1:A:19:LEU:CB	1:A:165:LEU:HD12	0.72	2.14	13	1
1:A:177:LEU:HD13	2:B:510:ILE:HB	0.72	1.62	5	9
1:A:174:LEU:HD13	1:A:174:LEU:O	0.72	1.84	13	2
1:A:13:ALA:HB1	4:A:185:GNP:O2A	0.72	1.85	10	2
1:A:93:VAL:HG13	1:A:97:TRP:CE2	0.72	2.20	11	5
1:A:59:ALA:N	1:A:67:LEU:HD21	0.72	1.98	9	3
1:A:84:VAL:HG23	1:A:116:GLN:HB2	0.71	1.61	13	4
1:A:90:PHE:CE2	1:A:137:ILE:HD12	0.71	2.21	1	2
1:A:61:LEU:HD22	2:B:525:ASP:HB3	0.71	1.61	8	1
1:A:58:THR:CB	1:A:67:LEU:HD22	0.71	2.15	4	2
1:A:116:GLN:CD	1:A:119:LEU:HD21	0.71	2.06	4	1
1:A:8:VAL:HG13	2:B:540:GLU:HG2	0.71	1.61	4	1
1:A:3:THR:HG23	1:A:51:TYR:CE1	0.71	2.20	18	10
1:A:46:ILE:HG13	1:A:52:THR:HG23	0.71	1.62	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:ILE:HD11	1:A:53:LEU:CD2	0.71	2.15	9	5
1:A:44:VAL:CG1	1:A:52:THR:HG21	0.71	2.12	12	1
1:A:84:VAL:HG13	1:A:137:ILE:N	0.71	2.00	3	12
1:A:70:LEU:HD22	2:B:541:LEU:N	0.71	2.01	7	1
1:A:4:ILE:HD13	1:A:53:LEU:HD22	0.71	1.63	17	1
1:A:4:ILE:HG22	1:A:176:ALA:HB3	0.71	1.61	10	3
1:A:7:VAL:HG22	1:A:56:PHE:CB	0.71	2.15	3	2
1:A:14:VAL:CG1	1:A:113:VAL:HG21	0.71	2.16	14	2
1:A:67:LEU:O	1:A:67:LEU:HD23	0.71	1.85	14	2
1:A:70:LEU:HD23	2:B:541:LEU:HB2	0.71	1.61	11	3
1:A:8:VAL:HG12	2:B:540:GLU:CG	0.71	2.15	5	1
1:A:8:VAL:CG2	1:A:14:VAL:HG21	0.70	2.16	18	1
1:A:33:VAL:HG13	2:B:545:ASN:ND2	0.70	2.01	5	1
1:A:70:LEU:HD12	1:A:70:LEU:O	0.70	1.85	3	10
1:A:4:ILE:CG2	1:A:176:ALA:HB3	0.70	2.16	10	7
1:A:70:LEU:HD23	2:B:541:LEU:HB3	0.70	1.63	3	1
1:A:17:THR:HG21	1:A:35:THR:OG1	0.70	1.86	11	2
1:A:111:LEU:HD23	1:A:112:LEU:O	0.70	1.85	11	12
1:A:171:GLU:OE2	1:A:174:LEU:HD12	0.70	1.85	6	1
1:A:53:LEU:HD11	2:B:512:GLN:OE1	0.70	1.85	6	1
1:A:8:VAL:HG13	2:B:540:GLU:HG3	0.70	1.63	11	1
1:A:70:LEU:HD11	2:B:541:LEU:CB	0.70	2.16	2	1
1:A:44:VAL:HG23	2:B:514:LEU:HB2	0.70	1.61	12	1
1:A:82:PHE:CE1	1:A:112:LEU:HD12	0.70	2.21	12	1
1:A:4:ILE:O	1:A:53:LEU:HD23	0.70	1.86	11	2
1:A:86:SER:N	1:A:129:LEU:HD22	0.70	2.01	13	10
1:A:78:PHE:CE1	1:A:108:THR:HG21	0.70	2.22	15	3
2:B:502:GLY:N	2:B:511:SER:HG	0.70	1.85	13	1
1:A:7:VAL:HG13	1:A:56:PHE:HB3	0.70	1.61	8	1
1:A:116:GLN:OE1	1:A:119:LEU:HD21	0.70	1.87	4	1
1:A:70:LEU:HD13	2:B:540:GLU:HG2	0.70	1.62	8	1
1:A:21:ILE:HD11	2:B:518:PHE:CE2	0.70	2.22	13	1
1:A:36:VAL:HG11	2:B:525:ASP:CG	0.70	2.07	7	1
1:A:13:ALA:O	1:A:14:VAL:HG13	0.70	1.86	17	1
1:A:85:VAL:HG13	1:A:120:ARG:HD3	0.70	1.63	10	1
1:A:57:ASP:OD2	2:B:543:LEU:HD21	0.70	1.87	1	2
1:A:112:LEU:HD23	1:A:151:ALA:CB	0.69	2.17	4	1
1:A:177:LEU:HD13	2:B:510:ILE:CG2	0.69	2.18	13	3
1:A:58:THR:O	2:B:543:LEU:HD23	0.69	1.86	18	1
1:A:58:THR:OG1	2:B:543:LEU:HD13	0.69	1.86	8	2
1:A:19:LEU:HB3	1:A:165:LEU:HD22	0.69	1.61	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:ILE:HD13	1:A:137:ILE:N	0.69	2.02	19	10
1:A:155:VAL:HG11	1:A:167:ASN:ND2	0.69	2.02	6	5
1:A:84:VAL:HG23	1:A:85:VAL:CG2	0.69	2.18	12	1
1:A:114:GLY:O	1:A:117:ILE:HD11	0.69	1.87	20	2
2:B:505:LEU:HD12	2:B:507:ALA:HB3	0.69	1.60	7	1
1:A:14:VAL:HG21	1:A:79:LEU:CD2	0.69	2.18	11	1
1:A:19:LEU:HD13	1:A:169:PHE:CD2	0.69	2.22	18	1
1:A:70:LEU:HD11	2:B:541:LEU:HB2	0.69	1.64	2	1
1:A:19:LEU:HD13	1:A:169:PHE:CD1	0.69	2.22	11	2
1:A:158:SER:OG	1:A:160:LEU:HD12	0.69	1.87	16	1
1:A:174:LEU:HD13	2:B:505:LEU:CD1	0.69	2.15	19	4
1:A:46:ILE:HD13	2:B:511:SER:O	0.69	1.88	3	3
1:A:33:VAL:HG21	2:B:529:ARG:HD3	0.69	1.63	7	1
1:A:113:VAL:HG22	1:A:168:VAL:CG1	0.69	2.17	14	1
1:A:8:VAL:HG21	1:A:14:VAL:HA	0.69	1.64	3	1
1:A:44:VAL:CG2	1:A:52:THR:HG21	0.69	2.17	14	3
1:A:3:THR:HB	1:A:53:LEU:HD22	0.68	1.64	2	1
1:A:111:LEU:HD12	1:A:152:VAL:CB	0.68	2.17	4	4
1:A:14:VAL:HG21	1:A:113:VAL:HG21	0.68	1.65	14	2
1:A:85:VAL:HG13	1:A:116:GLN:OE1	0.68	1.88	13	1
1:A:54:GLY:C	1:A:55:LEU:HD12	0.68	2.09	6	1
1:A:33:VAL:HG21	2:B:527:ASP:O	0.68	1.89	11	3
1:A:111:LEU:HD21	1:A:171:GLU:OE2	0.68	1.89	5	2
1:A:19:LEU:CA	1:A:165:LEU:HD12	0.68	2.18	13	1
1:A:19:LEU:HD23	1:A:169:PHE:CG	0.68	2.22	9	3
1:A:170:ASP:O	1:A:173:ILE:HD13	0.68	1.88	11	2
1:A:111:LEU:HD11	1:A:171:GLU:HB3	0.68	1.64	7	5
1:A:84:VAL:HG22	1:A:116:GLN:HB2	0.68	1.66	12	1
1:A:19:LEU:HD23	1:A:169:PHE:CD1	0.68	2.23	10	2
1:A:137:ILE:N	1:A:137:ILE:HD13	0.68	2.04	2	8
1:A:8:VAL:HG23	1:A:56:PHE:HB3	0.68	1.64	12	1
1:A:8:VAL:HG11	1:A:16:LYS:HE3	0.68	1.64	19	2
1:A:116:GLN:HG3	1:A:119:LEU:HD13	0.68	1.66	3	1
1:A:90:PHE:CZ	1:A:137:ILE:HG21	0.68	2.24	15	6
1:A:14:VAL:HG11	1:A:113:VAL:CG2	0.68	2.19	14	1
1:A:4:ILE:HD11	1:A:53:LEU:CD1	0.67	2.19	1	4
1:A:19:LEU:HD23	1:A:169:PHE:CE2	0.67	2.25	1	2
2:B:540:GLU:HA	2:B:543:LEU:HD12	0.67	1.65	8	4
1:A:8:VAL:HG22	1:A:15:GLY:HA3	0.67	1.65	14	1
1:A:113:VAL:HG23	4:A:185:GNP:O6	0.67	1.89	11	1
1:A:8:VAL:HG11	2:B:540:GLU:OE2	0.67	1.89	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:505:LEU:CD1	2:B:507:ALA:HB3	0.67	2.18	7	1
1:A:19:LEU:HD13	1:A:169:PHE:CZ	0.67	2.25	8	4
1:A:41:ALA:C	2:B:519:ILE:HD12	0.67	2.10	20	4
1:A:19:LEU:HA	1:A:165:LEU:HD23	0.67	1.66	18	1
1:A:84:VAL:CG2	1:A:117:ILE:HG22	0.67	2.20	1	2
1:A:41:ALA:O	2:B:519:ILE:HD12	0.67	1.90	11	3
1:A:64:TYR:CB	1:A:67:LEU:HD23	0.67	2.19	3	1
1:A:14:VAL:HG12	1:A:81:CYS:SG	0.67	2.30	19	3
2:B:505:LEU:N	2:B:505:LEU:HD13	0.67	2.05	4	1
1:A:46:ILE:HG23	2:B:510:ILE:CG2	0.67	2.20	3	8
2:B:505:LEU:HD22	2:B:505:LEU:N	0.67	2.05	1	1
1:A:174:LEU:HD13	2:B:505:LEU:HG	0.67	1.66	3	1
1:A:70:LEU:CD1	2:B:541:LEU:HD23	0.67	2.20	9	1
1:A:113:VAL:HA	1:A:168:VAL:HG11	0.66	1.66	18	1
1:A:112:LEU:HD12	1:A:146:ALA:CB	0.66	2.14	10	4
1:A:61:LEU:HD22	2:B:544:GLY:HA2	0.66	1.68	3	1
1:A:126:ILE:HD11	1:A:136:PRO:HG3	0.66	1.67	4	2
1:A:67:LEU:HD23	1:A:67:LEU:O	0.66	1.89	18	2
1:A:58:THR:OG1	1:A:67:LEU:HD22	0.66	1.90	4	2
1:A:19:LEU:N	1:A:19:LEU:HD13	0.66	2.05	20	1
1:A:70:LEU:HD11	2:B:541:LEU:HA	0.66	1.66	18	2
1:A:101:ILE:HG21	1:A:110:PHE:CD1	0.66	2.26	7	1
2:B:505:LEU:N	2:B:505:LEU:HD22	0.66	2.04	11	1
1:A:151:ALA:O	1:A:152:VAL:HG23	0.66	1.90	14	17
2:B:505:LEU:HD23	2:B:505:LEU:N	0.66	2.06	13	1
1:A:137:ILE:HG22	1:A:141:THR:HB	0.66	1.68	14	1
1:A:36:VAL:HB	1:A:61:LEU:HD13	0.66	1.67	5	3
1:A:115:THR:O	1:A:117:ILE:HD13	0.65	1.92	10	6
1:A:111:LEU:CD1	1:A:152:VAL:HG11	0.65	2.20	16	6
1:A:97:TRP:O	1:A:101:ILE:HG22	0.65	1.91	8	5
1:A:115:THR:C	1:A:117:ILE:HD13	0.65	2.12	6	8
2:B:538:ILE:HD12	2:B:542:TYR:CB	0.65	2.21	2	2
1:A:53:LEU:N	1:A:53:LEU:HD13	0.65	2.06	16	2
2:B:505:LEU:HD11	2:B:510:ILE:O	0.65	1.91	15	1
1:A:119:LEU:N	1:A:119:LEU:HD13	0.65	2.06	20	1
1:A:43:THR:O	1:A:44:VAL:HG23	0.65	1.91	17	3
1:A:36:VAL:HG11	2:B:524:GLY:HA3	0.65	1.68	4	1
1:A:115:THR:HG22	1:A:157:CYS:CB	0.65	2.20	6	1
1:A:94:LYS:HG3	1:A:145:LEU:HD13	0.65	1.69	7	3
1:A:174:LEU:HD13	2:B:505:LEU:HB3	0.65	1.67	4	5
1:A:7:VAL:HG13	1:A:56:PHE:O	0.65	1.91	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:VAL:HG21	1:A:79:LEU:HD23	0.65	1.69	19	1
1:A:116:GLN:HG2	1:A:119:LEU:HD13	0.65	1.67	2	1
1:A:33:VAL:HG21	2:B:529:ARG:CD	0.65	2.21	7	1
1:A:82:PHE:CE1	1:A:137:ILE:HG21	0.65	2.27	6	5
1:A:44:VAL:HG13	2:B:514:LEU:HB2	0.65	1.67	8	2
1:A:93:VAL:HG22	1:A:97:TRP:CD1	0.65	2.27	8	1
1:A:145:LEU:CD1	1:A:149:LEU:HD23	0.65	2.22	20	1
1:A:58:THR:O	1:A:67:LEU:HD11	0.64	1.92	3	1
1:A:35:THR:HG21	2:B:543:LEU:HD23	0.64	1.66	11	2
1:A:93:VAL:HG22	1:A:97:TRP:CE3	0.64	2.26	4	1
2:B:504:GLY:C	2:B:505:LEU:HD22	0.64	2.12	4	1
1:A:8:VAL:HG23	1:A:81:CYS:SG	0.64	2.31	9	1
1:A:14:VAL:HG21	1:A:113:VAL:CG2	0.64	2.23	14	1
1:A:21:ILE:HG22	1:A:25:THR:OG1	0.64	1.92	5	4
1:A:155:VAL:HG23	1:A:171:GLU:OE2	0.64	1.93	16	2
1:A:44:VAL:HG22	1:A:52:THR:HG22	0.64	1.68	6	3
1:A:55:LEU:HD22	1:A:55:LEU:N	0.64	2.06	11	1
1:A:174:LEU:HD22	2:B:505:LEU:HB3	0.64	1.70	7	3
1:A:64:TYR:HB2	1:A:67:LEU:HD23	0.64	1.67	3	2
4:A:185:GNP:N3	4:A:185:GNP:H2'	0.64	2.06	3	4
1:A:55:LEU:N	1:A:55:LEU:HD22	0.64	2.07	4	1
1:A:160:LEU:N	1:A:160:LEU:HD12	0.64	2.08	3	2
2:B:504:GLY:O	2:B:505:LEU:HD22	0.64	1.92	4	1
1:A:111:LEU:HD13	1:A:172:ALA:N	0.64	2.08	20	8
1:A:159:ALA:HB2	1:A:165:LEU:HD21	0.64	1.69	20	2
1:A:15:GLY:HA2	1:A:19:LEU:HD22	0.64	1.69	5	3
1:A:76:ASP:HA	1:A:108:THR:HG22	0.64	1.68	9	1
1:A:119:LEU:O	1:A:119:LEU:HD12	0.64	1.92	6	1
1:A:35:THR:HG23	2:B:543:LEU:HD23	0.64	1.70	1	3
1:A:126:ILE:HA	1:A:129:LEU:HD12	0.64	1.68	10	2
1:A:111:LEU:C	1:A:112:LEU:HD22	0.64	2.14	9	1
1:A:14:VAL:HA	1:A:19:LEU:HD13	0.63	1.69	9	1
1:A:116:GLN:OE1	4:A:185:GNP:H1'	0.63	1.92	16	2
1:A:119:LEU:HD21	1:A:160:LEU:CD2	0.63	2.23	10	1
1:A:111:LEU:HD21	1:A:171:GLU:CD	0.63	2.14	16	1
1:A:119:LEU:CD2	1:A:160:LEU:HD22	0.63	2.23	10	1
2:B:520:HIS:O	2:B:521:THR:HG23	0.63	1.94	2	1
1:A:17:THR:HG21	1:A:35:THR:HA	0.63	1.71	6	1
1:A:94:LYS:HB2	1:A:145:LEU:HD11	0.63	1.68	18	4
1:A:58:THR:HB	1:A:67:LEU:HD13	0.63	1.69	7	1
1:A:16:LYS:HD3	1:A:55:LEU:HD23	0.63	1.69	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:505:LEU:HD12	2:B:505:LEU:N	0.63	2.08	10	5
1:A:78:PHE:CZ	1:A:108:THR:HG21	0.63	2.29	5	2
1:A:42:VAL:HG23	1:A:52:THR:CG2	0.63	2.24	13	4
1:A:7:VAL:HG22	1:A:56:PHE:HB2	0.63	1.71	3	2
1:A:174:LEU:HD23	2:B:505:LEU:HD23	0.63	1.70	11	1
1:A:4:ILE:O	1:A:53:LEU:HD22	0.63	1.93	7	1
1:A:80:VAL:HG13	1:A:110:PHE:CB	0.62	2.24	20	2
1:A:117:ILE:HD11	1:A:158:SER:N	0.62	2.09	9	1
1:A:111:LEU:HD21	1:A:153:LYS:O	0.62	1.94	2	3
1:A:14:VAL:CG2	1:A:113:VAL:HG11	0.62	2.24	12	1
1:A:3:THR:HG23	1:A:46:ILE:CD1	0.62	2.24	14	1
1:A:8:VAL:HG11	1:A:15:GLY:CA	0.62	2.23	8	1
1:A:54:GLY:O	1:A:55:LEU:HD12	0.62	1.93	6	1
1:A:4:ILE:CG2	1:A:177:LEU:HD23	0.62	2.25	19	3
1:A:126:ILE:HD11	1:A:136:PRO:HD3	0.62	1.70	14	1
1:A:111:LEU:HD11	1:A:171:GLU:CB	0.62	2.25	10	7
1:A:90:PHE:CE2	1:A:137:ILE:HG23	0.62	2.30	1	2
2:B:505:LEU:N	2:B:505:LEU:HD23	0.62	2.10	3	1
1:A:177:LEU:HD13	2:B:505:LEU:HD13	0.62	1.71	15	1
1:A:145:LEU:HD23	1:A:145:LEU:O	0.62	1.94	3	6
1:A:80:VAL:HG13	1:A:110:PHE:HB2	0.62	1.72	1	2
1:A:80:VAL:HG21	1:A:110:PHE:CD1	0.62	2.30	6	3
1:A:19:LEU:CB	1:A:165:LEU:HD22	0.62	2.24	7	4
1:A:70:LEU:HD11	2:B:541:LEU:HD23	0.62	1.69	9	1
1:A:94:LYS:HG2	1:A:145:LEU:HD13	0.62	1.71	17	2
1:A:84:VAL:HG21	1:A:117:ILE:HA	0.62	1.72	11	3
1:A:178:GLU:HB2	2:B:507:ALA:HB1	0.61	1.69	1	1
1:A:9:VAL:HG22	2:B:540:GLU:HG3	0.61	1.70	8	1
1:A:84:VAL:HG21	1:A:120:ARG:HB3	0.61	1.70	7	1
2:B:505:LEU:H	2:B:505:LEU:HD22	0.61	1.55	11	1
1:A:80:VAL:O	1:A:112:LEU:HD13	0.61	1.95	14	1
1:A:46:ILE:O	1:A:46:ILE:HG22	0.61	1.95	18	6
1:A:94:LYS:HG3	1:A:145:LEU:HD11	0.61	1.71	2	6
1:A:21:ILE:HG21	5:A:188:HOH:O	0.61	1.95	1	1
1:A:58:THR:HG23	2:B:540:GLU:O	0.61	1.94	1	2
1:A:36:VAL:HB	1:A:61:LEU:HD12	0.61	1.71	19	2
1:A:8:VAL:HG22	1:A:16:LYS:CB	0.61	2.25	5	1
1:A:114:GLY:O	1:A:117:ILE:HD12	0.61	1.94	15	1
1:A:3:THR:HG22	1:A:53:LEU:HB2	0.61	1.72	11	1
1:A:8:VAL:HG13	2:B:540:GLU:CG	0.61	2.24	4	1
1:A:85:VAL:HG13	1:A:120:ARG:CD	0.61	2.25	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:VAL:HG11	1:A:115:THR:HG21	0.61	1.72	9	1
1:A:44:VAL:CG2	1:A:52:THR:HG23	0.61	2.19	19	2
1:A:23:TYR:HB2	1:A:165:LEU:HD13	0.61	1.71	14	2
2:B:504:GLY:C	2:B:505:LEU:HD23	0.61	2.16	7	2
1:A:46:ILE:HG22	1:A:46:ILE:O	0.61	1.96	19	6
1:A:43:THR:N	2:B:519:ILE:HD11	0.61	2.11	12	2
1:A:36:VAL:CG2	1:A:61:LEU:HD22	0.61	2.26	12	1
1:A:13:ALA:HB3	4:A:185:GNP:C8	0.61	2.24	10	1
1:A:85:VAL:HG11	1:A:125:THR:HG21	0.61	1.71	3	8
1:A:3:THR:HG22	1:A:53:LEU:CD2	0.61	2.25	17	1
1:A:47:GLY:HA3	2:B:510:ILE:HG23	0.60	1.72	6	2
1:A:2:GLN:O	1:A:177:LEU:HD22	0.60	1.96	10	1
1:A:19:LEU:HD23	1:A:165:LEU:HD23	0.60	1.74	18	1
1:A:16:LYS:O	1:A:19:LEU:HD22	0.60	1.95	1	1
1:A:19:LEU:HA	1:A:165:LEU:HD12	0.60	1.72	9	2
1:A:174:LEU:HD11	2:B:505:LEU:HB2	0.60	1.72	6	1
1:A:40:TYR:CE1	2:B:521:THR:HG21	0.60	2.31	7	1
1:A:70:LEU:HG	2:B:541:LEU:HD12	0.60	1.71	4	1
1:A:36:VAL:HG12	1:A:64:TYR:CE2	0.60	2.31	17	1
1:A:14:VAL:HG12	1:A:57:ASP:CG	0.60	2.16	17	1
1:A:170:ASP:OD2	2:B:505:LEU:HD21	0.60	1.96	5	1
5:A:188:HOH:O	2:B:543:LEU:HD21	0.60	1.95	5	1
1:A:14:VAL:HG12	1:A:14:VAL:O	0.60	1.96	8	1
1:A:77:VAL:HG21	1:A:172:ALA:O	0.60	1.97	15	3
1:A:32:TYR:CE2	4:A:185:GNP:PB	0.60	2.94	10	2
2:B:510:ILE:O	2:B:510:ILE:HG22	0.60	1.97	15	1
1:A:177:LEU:HD21	2:B:510:ILE:HG21	0.60	1.72	4	3
1:A:13:ALA:HB1	4:A:185:GNP:O1B	0.60	1.96	13	1
1:A:159:ALA:HB2	1:A:165:LEU:HD11	0.60	1.74	7	2
1:A:36:VAL:CG1	1:A:59:ALA:HB1	0.60	2.27	15	1
1:A:16:LYS:CD	2:B:543:LEU:HD21	0.60	2.26	2	1
1:A:3:THR:HG21	1:A:53:LEU:HD13	0.60	1.72	2	2
1:A:174:LEU:O	1:A:174:LEU:HD12	0.60	1.97	4	3
1:A:174:LEU:HD22	2:B:505:LEU:HD12	0.60	1.73	3	1
1:A:80:VAL:HG12	1:A:97:TRP:CZ2	0.60	2.31	8	1
1:A:82:PHE:CD1	1:A:112:LEU:HD22	0.60	2.32	7	1
1:A:41:ALA:O	2:B:519:ILE:HD13	0.60	1.96	15	1
1:A:15:GLY:O	1:A:19:LEU:HD12	0.60	1.96	18	2
1:A:174:LEU:CD2	2:B:505:LEU:HD13	0.60	2.24	6	3
1:A:14:VAL:HG23	1:A:115:THR:HG21	0.60	1.74	12	1
1:A:14:VAL:HG12	1:A:81:CYS:HB3	0.60	1.72	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:540:GLU:CA	2:B:543:LEU:HD12	0.60	2.26	6	1
1:A:33:VAL:HG12	2:B:526:SER:HA	0.60	1.74	7	1
1:A:111:LEU:HD13	1:A:172:ALA:HA	0.60	1.73	5	3
1:A:78:PHE:CE2	1:A:108:THR:HG21	0.60	2.32	10	1
1:A:46:ILE:HA	2:B:514:LEU:HD11	0.59	1.73	10	1
1:A:59:ALA:HB1	1:A:61:LEU:HD13	0.59	1.74	5	1
1:A:174:LEU:HB2	2:B:505:LEU:HD22	0.59	1.73	12	4
1:A:94:LYS:O	1:A:98:VAL:HG23	0.59	1.97	15	12
1:A:115:THR:O	1:A:117:ILE:HD12	0.59	1.97	8	2
1:A:9:VAL:HG13	1:A:70:LEU:HD13	0.59	1.71	11	1
1:A:44:VAL:HG21	2:B:514:LEU:HB2	0.59	1.75	10	1
1:A:15:GLY:C	1:A:19:LEU:HD12	0.59	2.17	18	1
1:A:8:VAL:HG13	1:A:14:VAL:HG22	0.59	1.75	5	2
1:A:14:VAL:HG11	1:A:81:CYS:HB3	0.59	1.73	4	1
1:A:67:LEU:HD23	1:A:70:LEU:HD23	0.59	1.73	19	1
1:A:77:VAL:HG13	1:A:77:VAL:O	0.59	1.97	12	3
1:A:19:LEU:CG	1:A:165:LEU:HD12	0.59	2.28	13	1
1:A:70:LEU:HD23	2:B:541:LEU:HD23	0.59	1.73	10	1
1:A:77:VAL:O	1:A:77:VAL:HG13	0.59	1.98	16	6
1:A:14:VAL:HG21	1:A:157:CYS:SG	0.59	2.38	6	1
1:A:7:VAL:HG12	2:B:540:GLU:OE2	0.59	1.96	3	1
1:A:125:THR:O	1:A:129:LEU:HD13	0.59	1.98	19	3
1:A:59:ALA:HB1	1:A:61:LEU:HD11	0.59	1.75	12	1
1:A:58:THR:HA	1:A:67:LEU:HD21	0.59	1.74	19	1
1:A:70:LEU:HD21	2:B:541:LEU:O	0.59	1.97	19	1
1:A:8:VAL:HG21	1:A:16:LYS:HG3	0.59	1.74	13	2
1:A:116:GLN:N	4:A:185:GNP:HN22	0.59	1.96	9	4
1:A:8:VAL:HG23	1:A:14:VAL:HG21	0.59	1.73	18	1
1:A:8:VAL:HG12	2:B:540:GLU:HG3	0.59	1.74	5	1
1:A:14:VAL:HG21	1:A:113:VAL:HG11	0.59	1.73	6	1
1:A:8:VAL:HG11	1:A:16:LYS:CE	0.59	2.28	7	2
1:A:8:VAL:HG13	1:A:14:VAL:HB	0.59	1.74	10	2
1:A:70:LEU:HD13	2:B:541:LEU:HD22	0.59	1.74	16	1
1:A:94:LYS:CE	1:A:112:LEU:HD21	0.59	2.27	13	1
1:A:59:ALA:HB1	1:A:61:LEU:HD23	0.59	1.73	17	2
1:A:115:THR:HG22	1:A:157:CYS:SG	0.59	2.37	3	2
1:A:70:LEU:HD21	2:B:541:LEU:CB	0.58	2.28	15	1
1:A:58:THR:HG21	1:A:69:PRO:CG	0.58	2.28	14	2
1:A:113:VAL:HA	1:A:168:VAL:HG21	0.58	1.74	2	6
1:A:45:MET:O	2:B:514:LEU:HD13	0.58	1.98	2	4
1:A:85:VAL:HG12	1:A:129:LEU:HD11	0.58	1.73	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:VAL:HG22	1:A:81:CYS:SG	0.58	2.37	2	1
1:A:117:ILE:N	1:A:117:ILE:HD12	0.58	2.14	20	3
1:A:94:LYS:HE3	1:A:145:LEU:HD22	0.58	1.75	7	1
1:A:13:ALA:HB3	4:A:185:GNP:H5'1	0.58	1.74	9	1
1:A:58:THR:HG23	2:B:540:GLU:CB	0.58	2.28	11	1
1:A:36:VAL:HG22	1:A:61:LEU:HD23	0.58	1.74	17	1
1:A:84:VAL:HG13	1:A:137:ILE:O	0.58	1.98	5	1
1:A:77:VAL:HG21	1:A:175:ALA:HB3	0.58	1.74	9	2
1:A:174:LEU:HD13	2:B:505:LEU:CD2	0.58	2.29	20	3
1:A:80:VAL:HG11	1:A:101:ILE:HD13	0.58	1.75	19	1
1:A:8:VAL:HG21	1:A:16:LYS:HG2	0.58	1.76	16	2
1:A:85:VAL:HG23	1:A:85:VAL:O	0.58	1.98	15	8
1:A:64:TYR:O	1:A:67:LEU:HD23	0.58	1.97	15	3
1:A:53:LEU:O	1:A:53:LEU:HD22	0.58	1.98	12	1
1:A:126:ILE:HD11	1:A:136:PRO:CG	0.58	2.28	4	1
1:A:86:SER:N	1:A:129:LEU:HD21	0.58	2.13	14	2
1:A:61:LEU:HD13	2:B:525:ASP:OD1	0.58	1.98	9	1
1:A:44:VAL:HG11	2:B:517:SER:OG	0.58	1.98	7	1
1:A:4:ILE:HD12	1:A:177:LEU:CD2	0.58	2.28	15	2
1:A:75:THR:HG23	1:A:78:PHE:CE1	0.58	2.33	3	1
1:A:70:LEU:HD12	1:A:70:LEU:C	0.58	2.19	12	5
1:A:80:VAL:O	1:A:80:VAL:HG23	0.58	1.98	10	5
1:A:4:ILE:HG13	1:A:177:LEU:HD12	0.58	1.76	4	1
1:A:4:ILE:N	1:A:4:ILE:HD13	0.57	2.13	14	2
1:A:119:LEU:HD22	1:A:160:LEU:HD22	0.57	1.75	1	1
1:A:45:MET:O	2:B:514:LEU:HD11	0.57	1.99	1	3
1:A:126:ILE:O	1:A:130:ALA:HB2	0.57	1.99	7	1
2:B:541:LEU:HD23	2:B:542:TYR:CD1	0.57	2.33	3	1
1:A:85:VAL:HG11	1:A:125:THR:CG2	0.57	2.30	17	2
1:A:36:VAL:HB	1:A:61:LEU:HD21	0.57	1.75	3	1
1:A:145:LEU:O	1:A:145:LEU:HD23	0.57	1.98	2	5
1:A:58:THR:HG23	2:B:540:GLU:HB3	0.57	1.76	11	1
1:A:3:THR:HG22	1:A:51:TYR:HE1	0.57	1.57	10	1
1:A:3:THR:HG23	1:A:53:LEU:CD1	0.57	2.28	10	1
1:A:174:LEU:O	1:A:174:LEU:HD13	0.57	1.99	5	2
1:A:14:VAL:HG13	1:A:14:VAL:O	0.57	1.98	6	2
1:A:28:PHE:CE1	2:B:532:TRP:CZ2	0.57	2.93	4	1
1:A:58:THR:HG21	1:A:70:LEU:HB3	0.57	1.77	8	2
1:A:70:LEU:HD21	2:B:541:LEU:HB2	0.57	1.76	7	2
1:A:2:GLN:O	2:B:510:ILE:HD13	0.57	2.00	10	1
1:A:58:THR:HB	1:A:67:LEU:HD11	0.57	1.76	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:LEU:HD13	1:A:53:LEU:N	0.57	2.14	18	1
1:A:84:VAL:HG23	1:A:85:VAL:HG22	0.57	1.77	12	1
1:A:85:VAL:HG22	1:A:116:GLN:CD	0.57	2.19	15	2
1:A:59:ALA:HB3	1:A:61:LEU:HD21	0.57	1.77	3	1
1:A:116:GLN:CG	1:A:119:LEU:HD13	0.57	2.30	17	1
1:A:19:LEU:HD23	1:A:165:LEU:CG	0.57	2.29	18	1
1:A:98:VAL:HG13	1:A:149:LEU:HD21	0.57	1.77	1	1
2:B:540:GLU:HA	2:B:543:LEU:HD13	0.57	1.76	3	1
1:A:155:VAL:HB	1:A:168:VAL:HG22	0.56	1.76	14	4
1:A:84:VAL:HG23	4:A:185:GNP:N2	0.56	2.15	6	2
1:A:19:LEU:HG	1:A:165:LEU:HD22	0.56	1.77	2	1
1:A:174:LEU:CG	2:B:505:LEU:HD22	0.56	2.28	6	1
1:A:4:ILE:HD13	1:A:4:ILE:N	0.56	2.14	3	2
1:A:33:VAL:N	1:A:34:PRO:CD	0.56	2.68	20	2
1:A:14:VAL:CG2	1:A:113:VAL:HG21	0.56	2.30	14	1
1:A:33:VAL:HG11	2:B:529:ARG:HG3	0.56	1.76	18	3
1:A:58:THR:O	2:B:543:LEU:HD12	0.56	2.00	2	1
1:A:4:ILE:HG21	1:A:176:ALA:HB3	0.56	1.77	8	3
1:A:114:GLY:O	1:A:117:ILE:HD13	0.56	1.99	9	1
1:A:119:LEU:N	1:A:119:LEU:HD12	0.56	2.15	17	2
1:A:46:ILE:CG1	1:A:52:THR:HG22	0.56	2.27	20	1
2:B:538:ILE:HD12	2:B:542:TYR:HB3	0.56	1.78	2	1
1:A:19:LEU:CG	1:A:165:LEU:HD22	0.56	2.31	3	3
1:A:36:VAL:HG12	1:A:59:ALA:HB2	0.56	1.77	10	2
1:A:84:VAL:HG11	1:A:120:ARG:CB	0.56	2.30	11	2
1:A:127:GLU:O	1:A:130:ALA:HB3	0.56	2.01	5	11
1:A:13:ALA:O	1:A:14:VAL:HG22	0.56	2.01	5	1
1:A:77:VAL:CG2	1:A:176:ALA:HB2	0.56	2.28	2	1
1:A:15:GLY:HA3	1:A:19:LEU:HD22	0.56	1.77	2	1
1:A:82:PHE:CD2	1:A:112:LEU:HD22	0.56	2.36	13	1
1:A:174:LEU:HD11	2:B:506:SER:HB3	0.56	1.78	14	1
1:A:173:ILE:HD12	1:A:177:LEU:CD1	0.56	2.31	15	2
1:A:174:LEU:HD13	2:B:505:LEU:HB2	0.56	1.78	7	4
1:A:85:VAL:HG22	1:A:120:ARG:HA	0.56	1.76	5	1
1:A:174:LEU:C	1:A:174:LEU:HD13	0.56	2.21	8	3
1:A:111:LEU:HD11	1:A:171:GLU:HB2	0.56	1.78	20	1
1:A:33:VAL:HG13	2:B:545:ASN:OXT	0.56	2.01	9	1
1:A:16:LYS:CD	2:B:543:LEU:HD11	0.56	2.30	6	1
1:A:178:GLU:CB	2:B:507:ALA:HB2	0.56	2.30	7	1
1:A:47:GLY:CA	2:B:510:ILE:HG23	0.56	2.30	6	2
1:A:35:THR:O	1:A:35:THR:HG22	0.56	2.01	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ALA:HB1	1:A:18:CYS:HB2	0.56	1.76	9	1
1:A:67:LEU:O	1:A:68:ARG:CB	0.56	2.53	7	2
1:A:177:LEU:HD22	2:B:510:ILE:CG2	0.56	2.28	15	1
1:A:119:LEU:C	1:A:119:LEU:HD12	0.56	2.21	5	2
1:A:128:LYS:HD2	1:A:129:LEU:HD23	0.56	1.77	9	1
1:A:126:ILE:HG13	1:A:129:LEU:HD12	0.56	1.78	13	3
1:A:70:LEU:HD22	2:B:539:ASP:HB2	0.56	1.78	3	1
1:A:4:ILE:HD12	1:A:177:LEU:HD21	0.55	1.78	15	2
1:A:173:ILE:HD12	1:A:177:LEU:HD11	0.55	1.77	15	1
1:A:15:GLY:CA	1:A:19:LEU:HD13	0.55	2.31	16	1
1:A:21:ILE:HD11	2:B:518:PHE:CZ	0.55	2.36	13	2
1:A:111:LEU:HD13	1:A:172:ALA:CA	0.55	2.32	5	6
2:B:538:ILE:C	2:B:538:ILE:HD13	0.55	2.21	16	1
1:A:70:LEU:HD13	2:B:541:LEU:HA	0.55	1.79	9	1
1:A:174:LEU:HD13	1:A:174:LEU:C	0.55	2.21	16	3
1:A:17:THR:HG21	1:A:35:THR:CG2	0.55	2.24	9	1
1:A:82:PHE:CZ	1:A:137:ILE:HG21	0.55	2.37	10	2
1:A:19:LEU:HD11	1:A:169:PHE:CE1	0.55	2.37	3	1
1:A:58:THR:C	1:A:67:LEU:HD11	0.55	2.22	3	1
1:A:14:VAL:C	1:A:19:LEU:HD11	0.55	2.22	11	1
1:A:35:THR:HG21	2:B:543:LEU:HD22	0.55	1.78	11	1
1:A:118:ASP:CG	1:A:161:THR:HG21	0.55	2.20	10	1
1:A:85:VAL:O	1:A:85:VAL:HG23	0.55	2.01	11	6
1:A:61:LEU:HD23	1:A:61:LEU:N	0.55	2.17	3	1
1:A:64:TYR:CG	1:A:67:LEU:HD21	0.55	2.36	11	1
1:A:3:THR:HG22	1:A:53:LEU:HD22	0.55	1.79	17	1
1:A:46:ILE:CG2	2:B:510:ILE:HG23	0.55	2.32	14	1
1:A:70:LEU:C	1:A:70:LEU:HD12	0.55	2.22	15	5
1:A:102:THR:HG22	1:A:107:LYS:HA	0.55	1.79	1	2
1:A:177:LEU:HD21	2:B:510:ILE:CG2	0.55	2.31	4	1
2:B:505:LEU:HD21	2:B:510:ILE:O	0.55	2.01	4	1
1:A:19:LEU:HD12	1:A:165:LEU:HD22	0.55	1.79	20	1
1:A:13:ALA:C	1:A:14:VAL:HG23	0.55	2.23	18	1
1:A:19:LEU:HG	1:A:165:LEU:HD13	0.55	1.79	5	1
1:A:68:ARG:N	1:A:69:PRO:CD	0.55	2.70	11	9
1:A:8:VAL:HG13	2:B:540:GLU:OE1	0.55	2.01	20	1
1:A:116:GLN:N	4:A:185:GNP:N2	0.55	2.55	9	4
2:B:538:ILE:HG23	2:B:543:LEU:HD12	0.55	1.76	19	3
1:A:94:LYS:CB	1:A:145:LEU:HD11	0.55	2.32	5	2
1:A:44:VAL:HG22	1:A:52:THR:HG21	0.55	1.79	2	4
1:A:45:MET:HE2	1:A:45:MET:C	0.55	2.22	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:146:ALA:HB1	1:A:151:ALA:HB3	0.55	1.78	4	1
1:A:15:GLY:HA2	1:A:19:LEU:HD13	0.54	1.78	5	4
1:A:5:LYS:N	1:A:53:LEU:HD23	0.54	2.17	4	2
1:A:14:VAL:HG23	4:A:185:GNP:C8	0.54	2.31	13	1
1:A:14:VAL:HG22	1:A:14:VAL:O	0.54	2.02	11	1
1:A:119:LEU:HD22	1:A:119:LEU:N	0.54	2.17	18	2
1:A:113:VAL:HG13	1:A:168:VAL:CB	0.54	2.32	5	1
1:A:116:GLN:CD	1:A:119:LEU:HD11	0.54	2.23	13	1
1:A:35:THR:CG2	2:B:543:LEU:HD23	0.54	2.32	3	3
1:A:8:VAL:HG23	1:A:14:VAL:CG1	0.54	2.33	11	1
1:A:177:LEU:HD13	2:B:510:ILE:CB	0.54	2.33	13	3
1:A:61:LEU:HD13	2:B:526:SER:HB2	0.54	1.79	15	1
1:A:14:VAL:HB	2:B:543:LEU:HD21	0.54	1.78	15	1
1:A:6:CYS:SG	1:A:77:VAL:HG23	0.54	2.42	3	1
1:A:4:ILE:N	1:A:53:LEU:HD12	0.54	2.17	14	1
1:A:111:LEU:HD11	1:A:171:GLU:OE1	0.54	2.02	5	1
1:A:19:LEU:CD1	1:A:169:PHE:CE1	0.54	2.91	3	5
1:A:21:ILE:HD11	1:A:37:PHE:CZ	0.54	2.38	6	1
1:A:16:LYS:CB	1:A:56:PHE:CE1	0.54	2.91	19	1
1:A:42:VAL:HG23	1:A:52:THR:HB	0.54	1.78	10	1
1:A:44:VAL:HG21	2:B:514:LEU:CB	0.54	2.33	10	1
1:A:14:VAL:HG21	1:A:113:VAL:CB	0.54	2.32	14	2
1:A:19:LEU:HA	1:A:165:LEU:HD22	0.54	1.77	12	2
1:A:58:THR:HG21	2:B:540:GLU:O	0.54	2.02	9	1
1:A:12:GLY:O	1:A:14:VAL:HG23	0.54	2.02	7	1
1:A:59:ALA:H	1:A:67:LEU:HD21	0.54	1.58	9	1
1:A:6:CYS:CB	1:A:55:LEU:HD13	0.54	2.32	13	1
1:A:45:MET:HE1	1:A:47:GLY:O	0.54	2.03	12	1
1:A:112:LEU:N	1:A:112:LEU:HD22	0.54	2.18	3	3
1:A:90:PHE:CE1	1:A:145:LEU:HD12	0.54	2.37	10	1
1:A:4:ILE:HG21	1:A:173:ILE:O	0.54	2.03	2	1
1:A:80:VAL:HG12	1:A:97:TRP:CZ3	0.54	2.38	6	2
1:A:19:LEU:CA	1:A:165:LEU:HD13	0.54	2.33	19	1
1:A:5:LYS:O	1:A:75:THR:HG21	0.54	2.01	19	1
1:A:47:GLY:N	2:B:510:ILE:HG23	0.54	2.18	6	2
1:A:13:ALA:C	1:A:14:VAL:HG22	0.54	2.23	17	1
1:A:158:SER:OG	1:A:161:THR:HG22	0.53	2.03	5	2
1:A:174:LEU:HD12	1:A:174:LEU:O	0.53	2.03	9	1
1:A:21:ILE:HG22	1:A:26:ASN:HB2	0.53	1.80	16	1
1:A:93:VAL:CG1	1:A:97:TRP:CZ3	0.53	2.92	20	1
1:A:155:VAL:HG11	1:A:167:ASN:HD22	0.53	1.62	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:LEU:HD21	2:B:512:GLN:NE2	0.53	2.18	9	1
1:A:14:VAL:O	1:A:14:VAL:HG23	0.53	2.03	19	1
1:A:3:THR:CG2	1:A:51:TYR:CE1	0.53	2.91	4	5
1:A:82:PHE:CE2	1:A:112:LEU:HD12	0.53	2.38	9	5
1:A:1:MET:CE	1:A:51:TYR:CD1	0.53	2.92	12	2
1:A:142:ALA:HB1	1:A:154:TYR:CD2	0.53	2.38	13	4
1:A:13:ALA:HB3	4:A:185:GNP:PA	0.53	2.43	13	1
1:A:14:VAL:HG12	1:A:81:CYS:CB	0.53	2.34	16	2
1:A:8:VAL:O	1:A:9:VAL:HG13	0.53	2.03	10	2
1:A:9:VAL:CG2	1:A:78:PHE:CE1	0.53	2.92	18	1
1:A:43:THR:HG22	2:B:519:ILE:HD13	0.53	1.80	9	1
1:A:119:LEU:HD12	1:A:119:LEU:C	0.53	2.23	19	4
1:A:4:ILE:HD13	1:A:4:ILE:H	0.53	1.61	3	2
1:A:19:LEU:HD23	1:A:165:LEU:HD21	0.53	1.79	11	1
1:A:36:VAL:CG1	1:A:59:ALA:HB2	0.53	2.34	10	1
1:A:4:ILE:H	1:A:4:ILE:HD13	0.53	1.61	14	1
1:A:33:VAL:HG11	2:B:529:ARG:CD	0.53	2.34	18	2
1:A:42:VAL:HG13	2:B:517:SER:C	0.53	2.24	9	3
1:A:61:LEU:HD22	2:B:526:SER:HB2	0.53	1.79	15	1
1:A:32:TYR:CD2	4:A:185:GNP:N3B	0.53	2.77	14	5
1:A:58:THR:HA	1:A:67:LEU:HD11	0.53	1.80	14	2
1:A:84:VAL:C	1:A:85:VAL:HG23	0.53	2.24	5	2
2:B:504:GLY:C	2:B:505:LEU:HD12	0.53	2.24	5	1
1:A:119:LEU:HD12	1:A:119:LEU:N	0.53	2.17	15	3
2:B:511:SER:O	2:B:514:LEU:HD11	0.53	2.03	8	3
1:A:51:TYR:O	1:A:51:TYR:CD1	0.53	2.62	11	2
1:A:142:ALA:CB	1:A:154:TYR:CD2	0.53	2.92	13	6
1:A:32:TYR:CE1	4:A:185:GNP:N3B	0.53	2.77	8	1
1:A:19:LEU:CD1	1:A:169:PHE:CD1	0.53	2.92	14	2
1:A:133:LYS:O	1:A:134:GLN:CB	0.53	2.57	15	19
1:A:78:PHE:CZ	1:A:108:THR:CG2	0.53	2.92	12	2
1:A:82:PHE:CZ	1:A:90:PHE:CE1	0.53	2.97	19	2
1:A:90:PHE:CD2	1:A:137:ILE:HD12	0.53	2.38	1	1
1:A:58:THR:OG1	2:B:543:LEU:HD22	0.53	2.03	13	2
1:A:19:LEU:CA	1:A:165:LEU:HD21	0.53	2.34	16	2
1:A:115:THR:C	4:A:185:GNP:N2	0.53	2.61	18	1
1:A:85:VAL:HG12	1:A:129:LEU:CD2	0.53	2.33	5	1
1:A:32:TYR:CD1	4:A:185:GNP:N3B	0.53	2.77	2	1
1:A:137:ILE:CD1	1:A:137:ILE:N	0.53	2.71	6	6
1:A:15:GLY:CA	1:A:19:LEU:HD11	0.53	2.35	13	2
1:A:4:ILE:O	1:A:53:LEU:HD13	0.53	2.03	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:534:PHE:CZ	2:B:538:ILE:HG22	0.53	2.39	7	1
2:B:538:ILE:HD11	2:B:542:TYR:HB3	0.53	1.79	3	1
1:A:19:LEU:HD13	1:A:169:PHE:CG	0.52	2.39	11	2
1:A:64:TYR:CD2	1:A:67:LEU:CD1	0.52	2.92	2	1
1:A:8:VAL:HG21	1:A:15:GLY:C	0.52	2.25	6	1
1:A:116:GLN:NE2	1:A:119:LEU:HD21	0.52	2.18	13	1
1:A:70:LEU:CD2	2:B:541:LEU:CA	0.52	2.86	7	1
1:A:8:VAL:HG22	2:B:540:GLU:CG	0.52	2.35	19	1
1:A:44:VAL:HG13	1:A:52:THR:CG2	0.52	2.18	12	1
1:A:6:CYS:CB	1:A:56:PHE:CE2	0.52	2.92	12	1
1:A:58:THR:CB	1:A:67:LEU:HD21	0.52	2.34	14	4
1:A:84:VAL:HG11	1:A:120:ARG:HB3	0.52	1.81	5	3
1:A:32:TYR:CD2	4:A:185:GNP:PG	0.52	3.02	3	1
1:A:33:VAL:O	1:A:36:VAL:HG12	0.52	2.05	3	1
1:A:36:VAL:HG12	1:A:64:TYR:HE2	0.52	1.63	17	1
1:A:1:MET:HE1	1:A:51:TYR:CD1	0.52	2.39	12	2
1:A:113:VAL:HG13	1:A:168:VAL:CG1	0.52	2.31	12	7
1:A:115:THR:HG22	1:A:163:LYS:HE3	0.52	1.80	9	1
1:A:58:THR:CB	1:A:67:LEU:HD13	0.52	2.33	7	1
1:A:174:LEU:HD13	2:B:505:LEU:CG	0.52	2.34	3	1
1:A:14:VAL:CG2	1:A:15:GLY:N	0.52	2.73	16	1
2:B:532:TRP:CZ2	2:B:537:ARG:NH2	0.52	2.78	20	1
1:A:36:VAL:HA	1:A:59:ALA:HB3	0.52	1.79	14	2
1:A:130:ALA:HB2	1:A:134:GLN:CD	0.52	2.25	5	2
1:A:59:ALA:CB	1:A:61:LEU:HD13	0.52	2.35	5	1
2:B:527:ASP:CB	2:B:528:PRO:CD	0.52	2.87	7	3
1:A:21:ILE:HD12	2:B:518:PHE:CZ	0.52	2.38	12	2
1:A:70:LEU:HD21	2:B:539:ASP:HB3	0.52	1.80	11	1
1:A:117:ILE:HD13	1:A:117:ILE:H	0.52	1.65	3	2
2:B:508:GLN:O	2:B:509:ASP:CB	0.52	2.58	13	11
1:A:46:ILE:HG22	1:A:51:TYR:O	0.52	2.05	2	1
1:A:77:VAL:HG21	1:A:175:ALA:CB	0.52	2.35	1	1
1:A:119:LEU:HD12	1:A:119:LEU:O	0.52	2.05	11	1
2:B:532:TRP:CE2	2:B:537:ARG:NH2	0.52	2.78	20	1
1:A:14:VAL:CG1	1:A:79:LEU:HD11	0.52	2.35	14	1
1:A:14:VAL:HG22	1:A:81:CYS:CB	0.52	2.33	18	1
1:A:17:THR:HG22	1:A:38:ASP:CG	0.52	2.25	3	2
1:A:64:TYR:CD1	1:A:64:TYR:N	0.52	2.77	15	5
1:A:80:VAL:HG11	1:A:101:ILE:HD11	0.52	1.81	17	1
1:A:16:LYS:C	1:A:20:LEU:HD23	0.52	2.24	17	1
1:A:14:VAL:HG21	1:A:113:VAL:CG1	0.52	2.34	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:VAL:CA	1:A:19:LEU:HD13	0.52	2.35	9	1
1:A:80:VAL:CG2	1:A:110:PHE:CD1	0.52	2.92	6	2
1:A:32:TYR:CD2	4:A:185:GNP:O1G	0.52	2.63	1	2
1:A:42:VAL:HG12	2:B:518:PHE:HA	0.52	1.82	8	1
1:A:36:VAL:HG11	1:A:63:ASP:HB2	0.52	1.81	15	1
1:A:3:THR:HG23	1:A:4:ILE:N	0.52	2.20	10	1
1:A:85:VAL:HG12	1:A:129:LEU:HD21	0.52	1.81	5	1
1:A:32:TYR:CD2	4:A:185:GNP:O1A	0.52	2.63	1	2
1:A:70:LEU:CD2	2:B:541:LEU:N	0.52	2.73	7	3
1:A:43:THR:O	1:A:43:THR:HG23	0.52	2.05	17	2
1:A:116:GLN:CD	4:A:185:GNP:HO2'	0.52	2.07	6	1
1:A:40:TYR:CE1	2:B:521:THR:CG2	0.52	2.92	7	1
1:A:13:ALA:HB1	4:A:185:GNP:O3A	0.52	2.04	3	1
1:A:101:ILE:CD1	1:A:110:PHE:CE2	0.51	2.94	14	1
1:A:42:VAL:HG12	2:B:517:SER:C	0.51	2.25	10	3
1:A:82:PHE:CE1	1:A:90:PHE:CE1	0.51	2.98	4	4
2:B:510:ILE:N	2:B:510:ILE:HD12	0.51	2.20	15	2
1:A:70:LEU:HD22	2:B:541:LEU:CA	0.51	2.31	16	1
1:A:19:LEU:HD23	1:A:165:LEU:HG	0.51	1.81	18	1
1:A:14:VAL:HG21	1:A:113:VAL:HB	0.51	1.81	12	1
1:A:82:PHE:HE2	1:A:112:LEU:HD22	0.51	1.63	13	1
1:A:32:TYR:CE2	4:A:185:GNP:N3B	0.51	2.78	15	1
1:A:58:THR:HB	1:A:67:LEU:HD22	0.51	1.80	4	1
1:A:4:ILE:CD1	1:A:4:ILE:N	0.51	2.74	14	1
1:A:32:TYR:CG	2:B:537:ARG:NH2	0.51	2.79	18	1
1:A:4:ILE:CG2	1:A:176:ALA:CB	0.51	2.88	17	3
1:A:78:PHE:CE1	1:A:108:THR:CG2	0.51	2.93	15	2
1:A:13:ALA:HB2	2:B:537:ARG:CD	0.51	2.35	3	1
1:A:9:VAL:HG13	1:A:70:LEU:CD1	0.51	2.35	11	1
2:B:538:ILE:HD12	2:B:542:TYR:HB2	0.51	1.81	11	2
1:A:36:VAL:CB	1:A:61:LEU:HD12	0.51	2.34	19	1
1:A:58:THR:HB	1:A:67:LEU:HD21	0.51	1.82	14	2
1:A:68:ARG:HG2	2:B:541:LEU:HD11	0.51	1.80	14	1
1:A:53:LEU:HD13	1:A:53:LEU:H	0.51	1.63	12	2
1:A:145:LEU:HD21	1:A:149:LEU:HD11	0.51	1.83	16	2
1:A:174:LEU:HD13	2:B:505:LEU:HD23	0.51	1.82	1	1
1:A:111:LEU:HD23	1:A:112:LEU:N	0.51	2.21	15	3
1:A:115:THR:O	4:A:185:GNP:N2	0.51	2.44	18	1
1:A:51:TYR:CD1	1:A:52:THR:N	0.51	2.78	15	7
1:A:43:THR:OG1	2:B:519:ILE:HD11	0.51	2.06	2	1
1:A:159:ALA:HB2	1:A:165:LEU:CD1	0.51	2.36	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:N	1:A:20:LEU:HD23	0.51	2.19	3	2
1:A:155:VAL:HG23	1:A:171:GLU:CD	0.51	2.26	16	1
2:B:511:SER:HB2	2:B:514:LEU:HD21	0.51	1.82	19	2
1:A:44:VAL:CG2	1:A:52:THR:CG2	0.51	2.89	7	9
1:A:113:VAL:HG22	1:A:168:VAL:CG2	0.51	2.36	10	2
1:A:116:GLN:CD	1:A:119:LEU:HD13	0.51	2.26	9	1
1:A:32:TYR:CD2	4:A:185:GNP:O1B	0.51	2.64	7	1
1:A:155:VAL:CB	1:A:168:VAL:HG22	0.51	2.35	15	1
1:A:24:THR:HG23	1:A:25:THR:HG23	0.51	1.82	11	1
1:A:13:ALA:HB3	4:A:185:GNP:C5'	0.51	2.36	9	1
1:A:4:ILE:HD11	1:A:53:LEU:HD13	0.51	1.82	15	1
1:A:113:VAL:HG12	1:A:115:THR:HG23	0.51	1.83	18	1
1:A:4:ILE:HD11	1:A:53:LEU:HD12	0.51	1.81	1	2
1:A:4:ILE:CG1	1:A:53:LEU:HD22	0.51	2.35	9	3
1:A:59:ALA:CB	1:A:61:LEU:HD21	0.51	2.36	3	1
1:A:46:ILE:CA	2:B:514:LEU:HD11	0.51	2.36	10	1
1:A:45:MET:HE1	1:A:48:GLY:C	0.50	2.27	14	1
1:A:8:VAL:HG22	1:A:16:LYS:HB2	0.50	1.83	5	1
1:A:19:LEU:CD2	1:A:169:PHE:CG	0.50	2.93	9	1
2:B:532:TRP:CD1	2:B:537:ARG:NH2	0.50	2.79	9	2
1:A:130:ALA:HB1	1:A:134:GLN:HG2	0.50	1.82	7	1
1:A:36:VAL:HG22	1:A:36:VAL:O	0.50	2.06	4	1
2:B:530:HIS:O	2:B:530:HIS:CG	0.50	2.64	2	1
1:A:64:TYR:CG	1:A:67:LEU:HD23	0.50	2.40	1	1
1:A:45:MET:HE3	1:A:46:ILE:N	0.50	2.22	8	3
1:A:43:THR:HG23	2:B:516:ASN:HB3	0.50	1.82	8	1
1:A:33:VAL:HG13	2:B:545:ASN:C	0.50	2.26	9	1
1:A:116:GLN:CG	1:A:119:LEU:HD21	0.50	2.36	6	2
1:A:110:PHE:CE1	1:A:151:ALA:HB2	0.50	2.42	1	2
2:B:530:HIS:CG	2:B:530:HIS:O	0.50	2.64	15	2
1:A:32:TYR:CD2	4:A:185:GNP:O2B	0.50	2.65	11	3
1:A:4:ILE:HG12	1:A:53:LEU:HD13	0.50	1.82	15	2
1:A:32:TYR:CE1	4:A:185:GNP:O1B	0.50	2.65	3	1
1:A:14:VAL:HG23	1:A:79:LEU:HD23	0.50	1.83	16	1
1:A:98:VAL:N	1:A:99:PRO:CD	0.50	2.75	14	15
1:A:70:LEU:HD21	2:B:541:LEU:CA	0.50	2.33	2	1
1:A:64:TYR:CD1	1:A:67:LEU:HD23	0.50	2.42	1	2
1:A:174:LEU:HD23	2:B:505:LEU:HD22	0.50	1.84	8	1
1:A:1:MET:HE3	1:A:51:TYR:CD1	0.50	2.41	3	1
1:A:64:TYR:HB2	1:A:67:LEU:HD12	0.50	1.84	4	1
1:A:94:LYS:HD2	1:A:145:LEU:HD13	0.50	1.82	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LYS:HD3	2:B:543:LEU:HD21	0.50	1.84	2	1
1:A:90:PHE:CZ	1:A:137:ILE:HG23	0.50	2.40	1	1
1:A:3:THR:O	1:A:4:ILE:CG2	0.50	2.59	4	3
1:A:115:THR:HG22	1:A:157:CYS:O	0.50	2.06	12	1
1:A:32:TYR:CE2	4:A:185:GNP:O3A	0.50	2.65	20	2
1:A:36:VAL:HG13	1:A:59:ALA:HB3	0.50	1.82	17	3
1:A:3:THR:HG23	1:A:51:TYR:CZ	0.50	2.41	18	1
2:B:517:SER:O	2:B:518:PHE:CD1	0.50	2.65	11	6
1:A:43:THR:O	1:A:44:VAL:HG13	0.50	2.07	7	3
2:B:505:LEU:HD12	2:B:506:SER:N	0.50	2.22	9	1
4:A:185:GNP:C4'	2:B:537:ARG:NH2	0.50	2.75	6	1
1:A:110:PHE:N	1:A:110:PHE:CD1	0.50	2.79	11	2
1:A:46:ILE:HD11	2:B:510:ILE:CG2	0.50	2.37	11	1
1:A:101:ILE:CD1	1:A:110:PHE:CD2	0.50	2.94	5	2
1:A:32:TYR:CE2	4:A:185:GNP:O1A	0.50	2.65	18	4
1:A:51:TYR:CG	1:A:52:THR:N	0.50	2.80	19	3
1:A:9:VAL:HG12	1:A:70:LEU:HB2	0.50	1.84	3	1
1:A:4:ILE:HD12	1:A:4:ILE:O	0.50	2.06	4	1
1:A:32:TYR:CZ	4:A:185:GNP:O3A	0.50	2.65	17	1
1:A:116:GLN:CB	4:A:185:GNP:HN22	0.50	2.19	14	6
1:A:68:ARG:N	1:A:69:PRO:HD3	0.50	2.22	11	5
1:A:168:VAL:HG13	1:A:169:PHE:N	0.50	2.22	1	13
1:A:117:ILE:HD12	1:A:117:ILE:N	0.50	2.22	8	1
1:A:43:THR:HG23	1:A:43:THR:O	0.50	2.07	8	1
1:A:14:VAL:HG13	1:A:18:CYS:H	0.50	1.66	15	1
1:A:4:ILE:HG23	1:A:177:LEU:HD23	0.50	1.84	16	2
1:A:82:PHE:CZ	1:A:142:ALA:HB2	0.50	2.42	1	2
1:A:42:VAL:HG11	2:B:517:SER:O	0.50	2.06	1	2
1:A:28:PHE:CD1	4:A:185:GNP:O2A	0.50	2.65	8	2
1:A:80:VAL:CG1	1:A:101:ILE:HD12	0.50	2.37	12	1
1:A:28:PHE:CD1	4:A:185:GNP:O1A	0.50	2.65	9	2
1:A:36:VAL:HG13	1:A:61:LEU:HD23	0.49	1.84	18	1
1:A:28:PHE:N	1:A:29:PRO:CD	0.49	2.75	6	8
1:A:19:LEU:HD23	1:A:169:PHE:HB2	0.49	1.83	5	2
1:A:19:LEU:CD2	1:A:169:PHE:CE1	0.49	2.95	20	1
2:B:512:GLN:CB	2:B:513:PRO:CD	0.49	2.90	18	14
2:B:538:ILE:CD1	2:B:542:TYR:CB	0.49	2.91	2	2
1:A:160:LEU:HD22	1:A:160:LEU:N	0.49	2.21	17	1
1:A:37:PHE:O	1:A:40:TYR:CG	0.49	2.65	10	2
1:A:46:ILE:O	1:A:46:ILE:HG23	0.49	2.06	2	1
1:A:79:LEU:CD2	1:A:172:ALA:HB1	0.49	2.37	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:VAL:CG2	1:A:78:PHE:CE2	0.49	2.92	8	1
1:A:82:PHE:HE2	1:A:112:LEU:HD12	0.49	1.66	9	1
1:A:67:LEU:O	1:A:67:LEU:HD12	0.49	2.06	10	1
1:A:61:LEU:N	1:A:61:LEU:HD22	0.49	2.22	18	2
1:A:61:LEU:HD12	2:B:525:ASP:HB2	0.49	1.83	18	1
1:A:28:PHE:CE1	4:A:185:GNP:O2A	0.49	2.65	8	2
1:A:9:VAL:HG13	2:B:540:GLU:OE1	0.49	2.06	8	1
1:A:142:ALA:CB	1:A:154:TYR:CE2	0.49	2.96	12	3
1:A:128:LYS:CD	1:A:129:LEU:HD23	0.49	2.37	9	1
1:A:19:LEU:HD12	1:A:165:LEU:CD1	0.49	2.37	9	1
1:A:72:TYR:N	1:A:72:TYR:CD1	0.49	2.78	20	2
1:A:61:LEU:HD12	2:B:526:SER:CB	0.49	2.38	3	1
1:A:21:ILE:CG2	1:A:22:SER:N	0.49	2.75	4	1
1:A:33:VAL:HG23	1:A:34:PRO:CD	0.49	2.36	17	3
1:A:14:VAL:HG11	1:A:113:VAL:CG1	0.49	2.33	13	1
1:A:33:VAL:HG11	2:B:525:ASP:O	0.49	2.08	11	1
1:A:3:THR:HG21	1:A:53:LEU:H	0.49	1.66	10	1
1:A:84:VAL:CG1	1:A:137:ILE:N	0.49	2.75	14	2
1:A:19:LEU:CD1	1:A:169:PHE:CE2	0.49	2.91	18	1
1:A:90:PHE:CE1	1:A:137:ILE:HG21	0.49	2.43	15	2
1:A:18:CYS:SG	4:A:185:GNP:PA	0.49	3.11	5	3
1:A:110:PHE:CD1	1:A:110:PHE:N	0.49	2.80	8	4
1:A:25:THR:O	1:A:26:ASN:CB	0.49	2.59	1	1
1:A:21:ILE:HD11	1:A:37:PHE:HZ	0.49	1.65	6	1
1:A:145:LEU:CD2	1:A:149:LEU:HD12	0.49	2.37	7	1
1:A:46:ILE:CG2	1:A:52:THR:HG23	0.49	2.38	11	1
1:A:80:VAL:CG2	1:A:112:LEU:HD22	0.49	2.37	11	1
1:A:173:ILE:C	1:A:173:ILE:HD13	0.49	2.27	4	1
1:A:3:THR:HG21	1:A:51:TYR:OH	0.49	2.07	15	4
1:A:3:THR:HG1	1:A:51:TYR:HE1	0.49	1.51	2	1
1:A:36:VAL:CG2	1:A:59:ALA:HB3	0.49	2.29	8	2
1:A:43:THR:HG22	2:B:519:ILE:HD11	0.49	1.85	17	1
1:A:158:SER:O	1:A:159:ALA:HB2	0.49	2.08	6	2
2:B:534:PHE:CE1	2:B:538:ILE:HG22	0.49	2.42	7	1
1:A:120:ARG:O	1:A:126:ILE:HD13	0.49	2.08	14	4
1:A:33:VAL:HG11	2:B:529:ARG:CG	0.49	2.37	18	2
2:B:505:LEU:CD2	2:B:505:LEU:N	0.49	2.75	1	3
1:A:169:PHE:CD2	2:B:512:GLN:OE1	0.49	2.66	12	1
1:A:42:VAL:HG23	1:A:52:THR:CB	0.49	2.38	13	2
1:A:94:LYS:HE2	1:A:112:LEU:HD21	0.49	1.85	13	1
1:A:90:PHE:CE2	1:A:137:ILE:CG2	0.49	2.95	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LEU:CG	2:B:541:LEU:HD12	0.49	2.38	4	1
2:B:505:LEU:N	2:B:505:LEU:CD1	0.49	2.75	4	2
2:B:508:GLN:CB	2:B:510:ILE:CD1	0.49	2.91	19	1
1:A:46:ILE:O	1:A:46:ILE:CG2	0.49	2.60	2	5
1:A:61:LEU:HD11	2:B:544:GLY:HA3	0.49	1.84	2	1
1:A:9:VAL:HG13	2:B:540:GLU:OE2	0.49	2.08	8	1
1:A:115:THR:N	4:A:185:GNP:N2	0.49	2.61	9	1
1:A:110:PHE:CE1	1:A:151:ALA:CB	0.49	2.96	9	1
1:A:80:VAL:HG12	1:A:97:TRP:HZ3	0.49	1.68	6	1
1:A:116:GLN:HG3	1:A:119:LEU:HD21	0.49	1.84	11	2
1:A:13:ALA:HB3	4:A:185:GNP:O1A	0.49	2.08	13	1
1:A:58:THR:HA	1:A:67:LEU:HD22	0.48	1.84	7	2
1:A:20:LEU:HD23	1:A:20:LEU:N	0.48	2.22	15	2
1:A:4:ILE:CB	1:A:176:ALA:HB3	0.48	2.38	2	1
1:A:55:LEU:HD22	1:A:55:LEU:H	0.48	1.68	17	2
1:A:137:ILE:N	1:A:137:ILE:CD1	0.48	2.73	4	7
1:A:87:PRO:N	1:A:129:LEU:HD22	0.48	2.22	12	1
1:A:3:THR:HG23	1:A:51:TYR:HE1	0.48	1.68	12	2
1:A:15:GLY:O	1:A:169:PHE:CZ	0.48	2.66	3	5
1:A:40:TYR:CE2	2:B:518:PHE:CZ	0.48	3.00	15	1
2:B:507:ALA:O	2:B:510:ILE:HD13	0.48	2.08	3	1
1:A:119:LEU:H	1:A:119:LEU:HD13	0.48	1.67	20	1
1:A:108:THR:O	1:A:110:PHE:CD2	0.48	2.66	5	1
1:A:1:MET:CE	1:A:46:ILE:CG2	0.48	2.91	11	2
1:A:115:THR:OG1	4:A:185:GNP:N3	0.48	2.45	18	2
1:A:45:MET:HE1	1:A:49:GLU:N	0.48	2.23	11	4
1:A:45:MET:CE	1:A:46:ILE:N	0.48	2.76	10	5
1:A:133:LYS:CG	1:A:134:GLN:N	0.48	2.75	19	6
2:B:519:ILE:HG22	2:B:520:HIS:N	0.48	2.23	7	1
1:A:4:ILE:HB	1:A:176:ALA:HB1	0.48	1.83	15	2
1:A:28:PHE:CE2	4:A:185:GNP:O3'	0.48	2.66	16	2
1:A:33:VAL:N	1:A:34:PRO:HD3	0.48	2.22	20	1
1:A:80:VAL:HG13	1:A:110:PHE:HB3	0.48	1.85	20	1
1:A:133:LYS:O	1:A:134:GLN:CG	0.48	2.62	14	16
1:A:86:SER:N	1:A:129:LEU:CD2	0.48	2.76	14	1
1:A:79:LEU:HD12	1:A:111:LEU:O	0.48	2.08	18	2
1:A:82:PHE:CD1	1:A:82:PHE:O	0.48	2.66	2	2
1:A:34:PRO:O	1:A:37:PHE:CD1	0.48	2.66	1	4
1:A:32:TYR:CE2	4:A:185:GNP:O2A	0.48	2.66	12	1
2:B:523:HIS:CD2	2:B:524:GLY:N	0.48	2.81	12	3
1:A:19:LEU:HD12	1:A:165:LEU:HD12	0.48	1.84	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:SER:N	1:A:133:LYS:CB	0.48	2.77	9	2
1:A:177:LEU:HD11	2:B:510:ILE:HG21	0.48	1.81	17	1
1:A:58:THR:CA	1:A:67:LEU:HD21	0.48	2.38	19	1
1:A:94:LYS:HG2	1:A:145:LEU:HD11	0.48	1.85	12	1
1:A:8:VAL:CG2	1:A:14:VAL:CG1	0.48	2.91	11	1
1:A:81:CYS:O	1:A:97:TRP:CZ3	0.48	2.67	20	1
1:A:82:PHE:O	1:A:82:PHE:CD1	0.48	2.67	18	3
1:A:4:ILE:CD1	1:A:53:LEU:HD12	0.48	2.38	1	2
1:A:113:VAL:HG11	1:A:168:VAL:HG11	0.48	1.80	12	1
1:A:37:PHE:O	1:A:40:TYR:CD2	0.48	2.67	12	1
1:A:37:PHE:CG	1:A:37:PHE:O	0.48	2.67	13	2
1:A:112:LEU:HD23	1:A:151:ALA:HB1	0.48	1.82	4	1
1:A:80:VAL:CG2	1:A:110:PHE:CD2	0.48	2.97	19	1
1:A:43:THR:H	2:B:519:ILE:HD11	0.48	1.69	14	3
1:A:4:ILE:CG2	1:A:177:LEU:CD2	0.48	2.92	5	6
1:A:36:VAL:HG13	1:A:59:ALA:O	0.48	2.09	2	1
1:A:44:VAL:HG22	2:B:515:GLN:O	0.48	2.09	8	1
1:A:85:VAL:HG22	1:A:116:GLN:NE2	0.48	2.24	15	1
1:A:61:LEU:HD12	2:B:526:SER:HB2	0.48	1.85	3	1
2:B:532:TRP:CZ2	2:B:534:PHE:O	0.48	2.67	3	2
1:A:20:LEU:HD22	1:A:20:LEU:H	0.48	1.69	19	1
1:A:68:ARG:CG	2:B:541:LEU:HD21	0.48	2.38	2	1
1:A:16:LYS:NZ	1:A:55:LEU:HD12	0.48	2.24	8	1
1:A:36:VAL:CG2	1:A:59:ALA:CB	0.48	2.92	8	1
1:A:19:LEU:CD2	1:A:169:PHE:CD1	0.48	2.95	17	2
1:A:21:ILE:CD1	2:B:518:PHE:CZ	0.48	2.97	12	1
1:A:78:PHE:CD2	1:A:108:THR:OG1	0.48	2.67	12	1
1:A:84:VAL:HG23	1:A:85:VAL:HG23	0.48	1.83	12	1
1:A:116:GLN:OE1	1:A:119:LEU:HD11	0.48	2.09	13	1
1:A:15:GLY:H	1:A:19:LEU:HD11	0.48	1.69	13	1
1:A:4:ILE:N	1:A:4:ILE:CD1	0.48	2.76	15	2
1:A:28:PHE:CB	1:A:29:PRO:CD	0.48	2.92	10	4
1:A:6:CYS:CB	1:A:55:LEU:HD23	0.48	2.38	20	1
1:A:28:PHE:CZ	4:A:185:GNP:O3'	0.48	2.67	5	4
1:A:112:LEU:CD2	1:A:151:ALA:CB	0.48	2.92	2	1
1:A:61:LEU:HD12	1:A:61:LEU:N	0.48	2.23	12	1
1:A:70:LEU:O	1:A:72:TYR:CD2	0.48	2.67	9	1
1:A:80:VAL:HG11	1:A:101:ILE:CD1	0.48	2.37	19	1
1:A:13:ALA:O	1:A:15:GLY:N	0.48	2.46	1	8
1:A:84:VAL:HG21	1:A:117:ILE:N	0.48	2.24	5	1
1:A:8:VAL:HG11	1:A:16:LYS:CG	0.48	2.39	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:TYR:CE1	1:A:52:THR:O	0.48	2.67	15	3
1:A:66:ARG:N	1:A:66:ARG:CD	0.48	2.77	12	1
1:A:36:VAL:CG1	1:A:59:ALA:CB	0.48	2.92	10	2
1:A:70:LEU:HD21	2:B:539:ASP:OD2	0.48	2.07	3	1
1:A:36:VAL:CG1	2:B:524:GLY:CA	0.48	2.92	11	1
1:A:21:ILE:O	1:A:25:THR:HG22	0.48	2.09	4	1
1:A:3:THR:HG22	1:A:4:ILE:H	0.47	1.68	14	1
1:A:46:ILE:O	1:A:48:GLY:N	0.47	2.47	7	12
1:A:111:LEU:CD1	1:A:152:VAL:CG1	0.47	2.91	2	4
1:A:112:LEU:CD2	1:A:151:ALA:HB1	0.47	2.39	2	1
1:A:68:ARG:CB	1:A:69:PRO:CD	0.47	2.92	8	3
1:A:84:VAL:HG11	1:A:120:ARG:HB2	0.47	1.85	11	1
1:A:156:GLU:O	1:A:168:VAL:HG13	0.47	2.09	17	1
2:B:515:GLN:O	2:B:516:ASN:HB3	0.47	2.09	17	1
1:A:70:LEU:HD11	2:B:541:LEU:HD22	0.47	1.85	18	1
1:A:37:PHE:CE2	1:A:39:ASN:O	0.47	2.67	8	1
1:A:174:LEU:CB	2:B:505:LEU:HD22	0.47	2.37	12	2
1:A:70:LEU:CD1	2:B:541:LEU:CD2	0.47	2.92	9	1
1:A:33:VAL:CG1	2:B:526:SER:CB	0.47	2.91	3	2
1:A:54:GLY:C	1:A:55:LEU:HD22	0.47	2.30	4	1
1:A:70:LEU:CD2	2:B:541:LEU:HD12	0.47	2.39	4	1
1:A:36:VAL:HG22	1:A:61:LEU:CD2	0.47	2.39	17	1
1:A:40:TYR:CZ	1:A:42:VAL:CG1	0.47	2.97	18	1
1:A:32:TYR:CE2	4:A:185:GNP:PA	0.47	3.08	12	2
1:A:28:PHE:CD1	1:A:32:TYR:OH	0.47	2.67	1	1
1:A:51:TYR:CZ	1:A:52:THR:O	0.47	2.67	19	2
1:A:43:THR:HG22	2:B:519:ILE:CD1	0.47	2.40	17	2
1:A:112:LEU:CD1	1:A:146:ALA:HB2	0.47	2.31	13	1
1:A:15:GLY:N	1:A:19:LEU:HD11	0.47	2.24	13	1
1:A:93:VAL:O	1:A:97:TRP:CG	0.47	2.67	13	1
1:A:36:VAL:O	1:A:38:ASP:N	0.47	2.48	15	1
1:A:42:VAL:HA	2:B:519:ILE:HD12	0.47	1.87	15	1
1:A:59:ALA:HB1	1:A:61:LEU:CD2	0.47	2.39	4	2
1:A:37:PHE:CZ	2:B:522:GLY:O	0.47	2.68	10	1
1:A:119:LEU:N	1:A:119:LEU:CD2	0.47	2.77	18	2
2:B:506:SER:O	2:B:507:ALA:HB2	0.47	2.08	5	3
1:A:32:TYR:CE1	4:A:185:GNP:PA	0.47	3.07	2	1
1:A:178:GLU:CB	2:B:507:ALA:HB1	0.47	2.39	1	1
2:B:505:LEU:HD12	2:B:507:ALA:CB	0.47	2.35	7	1
1:A:59:ALA:N	1:A:67:LEU:CD2	0.47	2.77	15	1
1:A:32:TYR:CD1	4:A:185:GNP:O1B	0.47	2.66	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:LEU:HD12	1:A:149:LEU:HD23	0.47	1.84	20	1
2:B:533:GLY:O	2:B:534:PHE:CG	0.47	2.67	20	1
1:A:68:ARG:CB	2:B:541:LEU:HD21	0.47	2.39	2	1
1:A:99:PRO:O	1:A:103:HIS:CG	0.47	2.68	2	2
1:A:40:TYR:OH	2:B:520:HIS:CE1	0.47	2.67	1	1
1:A:61:LEU:HD23	2:B:525:ASP:OD1	0.47	2.09	12	1
1:A:174:LEU:C	1:A:174:LEU:HD12	0.47	2.28	7	2
4:A:185:GNP:N3	4:A:185:GNP:C2'	0.47	2.77	13	2
1:A:27:LYS:O	1:A:32:TYR:CE1	0.47	2.67	20	1
1:A:132:ASN:O	1:A:133:LYS:CG	0.47	2.63	14	1
1:A:20:LEU:N	1:A:20:LEU:CD2	0.47	2.78	14	2
1:A:53:LEU:H	1:A:53:LEU:HD13	0.47	1.70	6	4
1:A:8:VAL:CG2	1:A:16:LYS:CB	0.47	2.92	5	1
1:A:130:ALA:HB2	1:A:134:GLN:NE2	0.47	2.25	5	1
1:A:64:TYR:CB	1:A:67:LEU:CD2	0.47	2.93	3	2
1:A:32:TYR:CD2	4:A:185:GNP:PB	0.47	3.07	7	2
1:A:16:LYS:CD	2:B:543:LEU:CD2	0.47	2.93	2	1
1:A:64:TYR:CD1	1:A:67:LEU:CD2	0.47	2.97	1	1
1:A:61:LEU:HD23	2:B:526:SER:HB2	0.47	1.81	6	1
1:A:14:VAL:HG23	4:A:185:GNP:N7	0.47	2.24	13	1
1:A:86:SER:H	1:A:129:LEU:HD22	0.47	1.69	7	2
1:A:28:PHE:CG	1:A:32:TYR:OH	0.47	2.68	15	1
1:A:4:ILE:CD1	1:A:53:LEU:CD1	0.47	2.92	15	1
1:A:4:ILE:HG21	1:A:176:ALA:CB	0.47	2.39	3	1
1:A:150:LYS:N	1:A:150:LYS:CD	0.47	2.77	16	1
2:B:539:ASP:OD2	2:B:542:TYR:CD2	0.47	2.67	16	1
1:A:36:VAL:CG2	1:A:63:ASP:CB	0.47	2.92	16	1
1:A:151:ALA:O	1:A:153:LYS:N	0.47	2.48	4	1
1:A:6:CYS:SG	1:A:55:LEU:HD23	0.47	2.50	20	1
1:A:16:LYS:HB2	1:A:56:PHE:CE1	0.47	2.45	19	1
1:A:111:LEU:HD23	1:A:112:LEU:H	0.47	1.69	10	1
1:A:8:VAL:HG23	1:A:14:VAL:HG11	0.47	1.87	18	1
1:A:32:TYR:CZ	4:A:185:GNP:O1A	0.47	2.68	2	2
1:A:115:THR:HG22	1:A:157:CYS:HB3	0.47	1.84	6	1
1:A:80:VAL:CG2	1:A:110:PHE:CG	0.47	2.98	6	1
1:A:20:LEU:H	1:A:20:LEU:HD22	0.47	1.70	10	2
1:A:15:GLY:O	1:A:169:PHE:CE1	0.47	2.67	7	1
1:A:174:LEU:HD22	1:A:174:LEU:O	0.47	2.09	16	1
1:A:3:THR:HG21	1:A:53:LEU:N	0.47	2.23	10	1
1:A:82:PHE:O	4:A:185:GNP:N1	0.47	2.48	14	11
1:A:142:ALA:HB3	1:A:154:TYR:CE2	0.47	2.45	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:174:LEU:HD21	2:B:505:LEU:O	0.47	2.10	8	2
1:A:28:PHE:CE1	4:A:185:GNP:O3'	0.47	2.67	12	5
1:A:160:LEU:H	1:A:160:LEU:HD12	0.47	1.70	8	2
1:A:139:PRO:O	1:A:154:TYR:CE1	0.47	2.68	12	2
1:A:14:VAL:CG1	4:A:185:GNP:N7	0.47	2.78	12	1
1:A:40:TYR:CD1	1:A:40:TYR:N	0.47	2.82	19	2
1:A:117:ILE:HG21	1:A:154:TYR:OH	0.47	2.10	6	1
1:A:173:ILE:HD13	1:A:173:ILE:C	0.47	2.30	6	1
1:A:53:LEU:CD1	1:A:53:LEU:N	0.47	2.77	16	1
1:A:37:PHE:O	1:A:40:TYR:CD1	0.47	2.68	4	1
1:A:114:GLY:CA	1:A:154:TYR:CE2	0.47	2.98	12	3
1:A:33:VAL:HG23	1:A:34:PRO:HD3	0.47	1.87	19	3
1:A:63:ASP:OD2	1:A:64:TYR:CE1	0.47	2.67	9	1
1:A:16:LYS:HD3	2:B:543:LEU:HD11	0.47	1.87	6	1
2:B:530:HIS:CD2	2:B:531:CYS:O	0.47	2.68	6	1
1:A:178:GLU:HB2	2:B:507:ALA:HB2	0.47	1.86	7	1
1:A:34:PRO:O	1:A:37:PHE:CZ	0.46	2.69	14	1
1:A:3:THR:OG1	1:A:51:TYR:CD1	0.46	2.68	14	1
1:A:8:VAL:HG22	1:A:15:GLY:CA	0.46	2.38	14	1
1:A:43:THR:O	1:A:44:VAL:CG1	0.46	2.63	7	9
1:A:56:PHE:O	1:A:56:PHE:CG	0.46	2.67	18	1
1:A:90:PHE:CZ	1:A:137:ILE:CG2	0.46	2.99	18	3
1:A:45:MET:O	2:B:514:LEU:HD21	0.46	2.08	1	2
1:A:63:ASP:OD2	1:A:64:TYR:CZ	0.46	2.68	8	1
1:A:78:PHE:CD1	1:A:108:THR:CG2	0.46	2.98	6	1
1:A:28:PHE:CD1	4:A:185:GNP:PA	0.46	3.09	3	1
1:A:19:LEU:HD21	1:A:165:LEU:HD22	0.46	1.84	19	1
1:A:174:LEU:HD22	2:B:505:LEU:HD22	0.46	1.87	19	1
1:A:46:ILE:CG2	1:A:51:TYR:O	0.46	2.63	11	3
2:B:505:LEU:O	2:B:506:SER:CB	0.46	2.64	15	3
1:A:82:PHE:CE1	1:A:113:VAL:O	0.46	2.68	20	3
1:A:6:CYS:HB2	1:A:56:PHE:CZ	0.46	2.45	12	1
1:A:40:TYR:CD1	2:B:521:THR:CB	0.46	2.98	7	1
1:A:98:VAL:HG11	1:A:149:LEU:HD22	0.46	1.87	7	1
1:A:4:ILE:CD1	1:A:177:LEU:HD21	0.46	2.41	15	1
1:A:142:ALA:O	1:A:146:ALA:HB2	0.46	2.10	4	2
1:A:2:GLN:O	1:A:177:LEU:HD11	0.46	2.10	4	1
1:A:79:LEU:HD13	1:A:172:ALA:HB1	0.46	1.86	5	1
1:A:13:ALA:HB2	4:A:185:GNP:H8	0.46	1.87	8	1
1:A:173:ILE:HD12	1:A:177:LEU:HD12	0.46	1.85	7	1
1:A:174:LEU:CD1	2:B:505:LEU:CB	0.46	2.91	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LYS:O	1:A:20:LEU:HD22	0.46	2.10	20	1
1:A:116:GLN:HE21	1:A:119:LEU:HD22	0.46	1.70	17	1
1:A:174:LEU:HA	1:A:177:LEU:HD12	0.46	1.85	14	1
1:A:93:VAL:CG1	1:A:97:TRP:CE2	0.46	2.98	13	2
2:B:512:GLN:CB	2:B:513:PRO:HD3	0.46	2.39	13	14
1:A:84:VAL:HG22	1:A:137:ILE:O	0.46	2.10	18	4
1:A:8:VAL:CG2	1:A:14:VAL:CG2	0.46	2.91	18	1
1:A:15:GLY:O	1:A:19:LEU:HD11	0.46	2.09	7	1
1:A:36:VAL:HA	1:A:59:ALA:HB2	0.46	1.85	16	1
1:A:115:THR:HG1	4:A:185:GNP:H2'	0.46	1.65	4	1
1:A:79:LEU:HD21	1:A:172:ALA:CB	0.46	2.41	14	1
1:A:88:SER:CB	1:A:133:LYS:CG	0.46	2.94	20	4
1:A:98:VAL:N	1:A:99:PRO:HD2	0.46	2.26	13	14
1:A:32:TYR:CE1	4:A:185:GNP:O1A	0.46	2.69	2	1
1:A:8:VAL:HG11	1:A:16:LYS:HG3	0.46	1.88	2	1
1:A:34:PRO:O	1:A:36:VAL:N	0.46	2.49	4	4
1:A:98:VAL:HG21	1:A:149:LEU:HD13	0.46	1.87	7	2
1:A:75:THR:HG22	1:A:77:VAL:H	0.46	1.70	7	1
1:A:174:LEU:HD22	2:B:504:GLY:O	0.46	2.10	15	1
1:A:1:MET:SD	1:A:51:TYR:CE1	0.46	3.09	11	1
1:A:151:ALA:O	1:A:152:VAL:CG2	0.46	2.62	14	18
4:A:185:GNP:O4'	2:B:537:ARG:CZ	0.46	2.64	1	2
1:A:56:PHE:O	1:A:56:PHE:CD2	0.46	2.68	18	1
1:A:112:LEU:CD2	1:A:112:LEU:N	0.46	2.79	9	1
1:A:21:ILE:CD1	2:B:518:PHE:CE2	0.46	2.98	13	1
1:A:94:LYS:CE	1:A:145:LEU:HD22	0.46	2.39	7	1
1:A:23:TYR:CG	1:A:165:LEU:HD13	0.46	2.45	16	1
1:A:19:LEU:CD1	1:A:19:LEU:N	0.46	2.76	20	1
1:A:23:TYR:CE2	1:A:166:LYS:HD3	0.46	2.45	18	1
1:A:13:ALA:HB2	2:B:537:ARG:HG3	0.46	1.88	2	1
1:A:126:ILE:HG13	1:A:129:LEU:HD11	0.46	1.86	7	1
1:A:44:VAL:HG12	2:B:515:GLN:O	0.46	2.10	7	1
1:A:36:VAL:O	1:A:64:TYR:CE2	0.46	2.69	11	1
1:A:44:VAL:HG11	2:B:512:GLN:O	0.46	2.10	20	1
1:A:15:GLY:CA	1:A:169:PHE:CZ	0.46	2.99	17	1
1:A:21:ILE:CG2	1:A:27:LYS:CG	0.46	2.93	19	1
1:A:174:LEU:HD13	2:B:504:GLY:O	0.46	2.11	14	1
1:A:114:GLY:O	1:A:157:CYS:N	0.46	2.49	17	3
1:A:114:GLY:C	1:A:117:ILE:HD12	0.46	2.31	5	2
1:A:37:PHE:CE2	1:A:63:ASP:OD1	0.46	2.68	2	1
1:A:43:THR:HG23	2:B:516:ASN:CB	0.46	2.40	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:PHE:CD1	1:A:137:ILE:HG13	0.46	2.46	9	1
1:A:7:VAL:HG22	1:A:56:PHE:HB3	0.46	1.85	3	1
1:A:14:VAL:CG2	2:B:543:LEU:HD21	0.46	2.35	3	1
1:A:3:THR:HG21	1:A:53:LEU:HG	0.46	1.88	20	1
1:A:125:THR:C	1:A:129:LEU:HD13	0.46	2.31	5	2
2:B:542:TYR:N	2:B:542:TYR:CD1	0.46	2.82	8	2
2:B:508:GLN:HE21	2:B:510:ILE:HD11	0.46	1.71	8	1
1:A:93:VAL:O	1:A:97:TRP:CD1	0.46	2.69	13	1
1:A:17:THR:O	1:A:21:ILE:N	0.46	2.49	4	3
1:A:125:THR:O	1:A:128:LYS:N	0.46	2.49	14	3
1:A:58:THR:HG21	1:A:69:PRO:HG2	0.46	1.88	14	2
1:A:45:MET:O	2:B:514:LEU:CD1	0.46	2.64	6	14
1:A:158:SER:HB3	1:A:161:THR:HG22	0.46	1.87	18	2
1:A:20:LEU:HD21	1:A:169:PHE:CE2	0.46	2.45	5	2
1:A:112:LEU:HD23	1:A:146:ALA:CB	0.46	2.40	1	1
1:A:93:VAL:HG13	1:A:94:LYS:N	0.46	2.25	8	2
1:A:119:LEU:HD11	1:A:160:LEU:CD2	0.46	2.41	3	1
1:A:15:GLY:O	1:A:56:PHE:CD2	0.46	2.69	16	1
1:A:134:GLN:O	1:A:134:GLN:CG	0.45	2.64	14	1
1:A:101:ILE:HD11	1:A:110:PHE:HB3	0.45	1.87	2	1
1:A:36:VAL:HG22	1:A:61:LEU:HD22	0.45	1.86	12	1
1:A:45:MET:CE	1:A:47:GLY:O	0.45	2.64	7	4
1:A:177:LEU:HD21	2:B:510:ILE:CB	0.45	2.41	4	1
1:A:40:TYR:CZ	2:B:521:THR:O	0.45	2.69	17	1
1:A:70:LEU:HD23	2:B:541:LEU:CD2	0.45	2.40	10	1
1:A:114:GLY:HA2	1:A:154:TYR:CE2	0.45	2.46	18	1
1:A:23:TYR:CE2	1:A:166:LYS:CD	0.45	2.99	18	1
1:A:98:VAL:O	1:A:102:THR:HG23	0.45	2.11	5	3
1:A:46:ILE:CG2	1:A:46:ILE:O	0.45	2.64	1	6
1:A:18:CYS:CB	4:A:185:GNP:O3A	0.45	2.64	8	1
1:A:37:PHE:O	1:A:37:PHE:CD1	0.45	2.70	9	1
1:A:35:THR:CG2	2:B:543:LEU:CD2	0.45	2.93	6	2
2:B:539:ASP:O	2:B:543:LEU:CD1	0.45	2.63	13	2
1:A:142:ALA:HB3	1:A:154:TYR:CZ	0.45	2.47	14	2
1:A:36:VAL:HG21	2:B:524:GLY:HA3	0.45	1.87	18	1
1:A:114:GLY:CA	1:A:154:TYR:CE1	0.45	3.00	9	1
2:B:505:LEU:HD13	2:B:505:LEU:N	0.45	2.26	11	1
2:B:508:GLN:O	2:B:509:ASP:HB2	0.45	2.11	17	1
1:A:32:TYR:CE2	4:A:185:GNP:O1B	0.45	2.69	10	1
2:B:512:GLN:O	2:B:514:LEU:N	0.45	2.50	18	2
1:A:115:THR:OG1	4:A:185:GNP:C2'	0.45	2.63	1	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:505:LEU:HD22	2:B:505:LEU:H	0.45	1.71	1	1
1:A:37:PHE:CB	2:B:522:GLY:CA	0.45	2.94	8	2
1:A:3:THR:CG2	1:A:53:LEU:HD12	0.45	2.42	12	1
1:A:79:LEU:HD13	1:A:80:VAL:N	0.45	2.26	6	1
1:A:119:LEU:HD11	1:A:160:LEU:HD21	0.45	1.88	3	1
1:A:94:LYS:CD	1:A:145:LEU:HD13	0.45	2.42	20	1
1:A:19:LEU:C	1:A:165:LEU:HD11	0.45	2.30	5	1
1:A:84:VAL:O	1:A:85:VAL:HG23	0.45	2.10	5	1
1:A:82:PHE:CZ	1:A:90:PHE:CZ	0.45	3.05	6	2
1:A:84:VAL:HG23	1:A:116:GLN:CB	0.45	2.37	13	1
1:A:16:LYS:NZ	2:B:543:LEU:CD2	0.45	2.80	13	1
1:A:129:LEU:HD12	1:A:130:ALA:N	0.45	2.27	7	1
1:A:4:ILE:HG22	1:A:176:ALA:CB	0.45	2.41	20	2
1:A:32:TYR:CE2	4:A:185:GNP:O2B	0.45	2.69	19	1
1:A:21:ILE:O	1:A:25:THR:N	0.45	2.49	10	12
1:A:82:PHE:O	4:A:185:GNP:C2	0.45	2.65	8	6
1:A:60:GLY:C	1:A:61:LEU:HD22	0.45	2.31	4	1
1:A:67:LEU:C	1:A:67:LEU:HD23	0.45	2.31	20	1
1:A:93:VAL:CG1	1:A:97:TRP:CE3	0.45	3.00	20	1
2:B:505:LEU:N	2:B:505:LEU:HD12	0.45	2.27	19	1
1:A:80:VAL:HG23	1:A:112:LEU:HD13	0.45	1.89	18	1
1:A:8:VAL:CG1	1:A:12:GLY:O	0.45	2.65	5	1
1:A:45:MET:HG3	1:A:45:MET:O	0.45	2.12	7	1
1:A:15:GLY:HA2	1:A:19:LEU:HD11	0.45	1.88	15	1
1:A:59:ALA:CA	1:A:67:LEU:HD21	0.45	2.41	15	1
2:B:505:LEU:N	2:B:505:LEU:CD2	0.45	2.74	11	1
1:A:3:THR:OG1	1:A:51:TYR:CE1	0.45	2.68	14	4
1:A:45:MET:O	2:B:514:LEU:CD2	0.45	2.65	5	13
1:A:82:PHE:HZ	1:A:142:ALA:HB1	0.45	1.72	18	1
1:A:18:CYS:O	1:A:22:SER:CB	0.45	2.65	19	7
1:A:18:CYS:CA	4:A:185:GNP:O2B	0.45	2.65	9	1
1:A:90:PHE:CE2	1:A:137:ILE:HG21	0.45	2.46	7	1
1:A:9:VAL:HG21	1:A:78:PHE:HD2	0.45	1.72	3	1
1:A:45:MET:HE2	1:A:46:ILE:N	0.45	2.27	10	2
2:B:507:ALA:O	2:B:508:GLN:CB	0.45	2.65	19	3
1:A:18:CYS:CB	4:A:185:GNP:O2A	0.45	2.65	2	2
1:A:116:GLN:CG	4:A:185:GNP:HN22	0.45	2.25	9	3
2:B:538:ILE:O	2:B:543:LEU:HD11	0.45	2.12	13	1
1:A:114:GLY:HA3	1:A:154:TYR:CE2	0.45	2.47	4	1
1:A:40:TYR:N	1:A:40:TYR:CD1	0.45	2.84	10	1
1:A:33:VAL:CB	1:A:34:PRO:CD	0.45	2.95	9	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:THR:OG1	1:A:116:GLN:N	0.45	2.50	1	3
1:A:84:VAL:HG21	1:A:117:ILE:CA	0.45	2.42	5	1
1:A:19:LEU:HD23	1:A:169:PHE:CZ	0.45	2.46	1	2
1:A:44:VAL:HG11	2:B:515:GLN:O	0.45	2.12	1	1
1:A:168:VAL:CG1	1:A:169:PHE:N	0.45	2.80	7	6
1:A:32:TYR:OH	2:B:532:TRP:CD1	0.45	2.68	8	1
1:A:51:TYR:C	1:A:51:TYR:CD1	0.45	2.89	3	5
2:B:532:TRP:CE3	2:B:533:GLY:O	0.45	2.70	12	1
1:A:64:TYR:N	1:A:64:TYR:CD1	0.44	2.81	9	1
1:A:130:ALA:HB2	1:A:134:GLN:HG3	0.44	1.89	11	2
1:A:72:TYR:CZ	1:A:104:HIS:O	0.44	2.70	3	1
1:A:82:PHE:HZ	1:A:142:ALA:HB2	0.44	1.72	16	1
1:A:21:ILE:HG21	1:A:27:LYS:CG	0.44	2.42	19	1
1:A:4:ILE:HD11	1:A:53:LEU:CG	0.44	2.42	1	1
1:A:6:CYS:CB	1:A:56:PHE:CZ	0.44	3.00	12	1
1:A:9:VAL:HG12	2:B:541:LEU:CD2	0.44	2.41	16	1
1:A:32:TYR:CB	4:A:185:GNP:O3G	0.44	2.65	17	2
4:A:185:GNP:O1G	2:B:537:ARG:CG	0.44	2.65	20	1
1:A:114:GLY:O	1:A:117:ILE:CD1	0.44	2.66	14	5
1:A:28:PHE:CD1	1:A:28:PHE:C	0.44	2.90	5	3
2:B:517:SER:O	2:B:518:PHE:CG	0.44	2.70	11	4
1:A:117:ILE:HD12	1:A:157:CYS:N	0.44	2.28	9	1
1:A:13:ALA:CB	4:A:185:GNP:O1B	0.44	2.65	13	2
1:A:18:CYS:CB	4:A:185:GNP:O1A	0.44	2.66	7	1
1:A:20:LEU:HD13	1:A:20:LEU:N	0.44	2.27	20	1
1:A:16:LYS:HA	1:A:19:LEU:HD22	0.44	1.88	10	1
1:A:53:LEU:H	1:A:53:LEU:HD22	0.44	1.72	18	1
2:B:511:SER:O	2:B:514:LEU:HD12	0.44	2.13	5	2
1:A:4:ILE:HD11	1:A:53:LEU:HG	0.44	1.89	1	1
1:A:82:PHE:CD2	1:A:83:SER:N	0.44	2.85	20	2
1:A:33:VAL:O	1:A:35:THR:N	0.44	2.50	6	4
1:A:15:GLY:N	1:A:19:LEU:HD22	0.44	2.27	9	1
4:A:185:GNP:O2A	2:B:537:ARG:NE	0.44	2.50	9	1
1:A:13:ALA:CB	4:A:185:GNP:O5'	0.44	2.65	6	1
1:A:15:GLY:CA	1:A:19:LEU:HD12	0.44	2.43	6	1
1:A:116:GLN:O	1:A:119:LEU:N	0.44	2.50	16	2
1:A:51:TYR:CD1	1:A:51:TYR:O	0.44	2.70	10	2
1:A:116:GLN:NE2	1:A:119:LEU:HD22	0.44	2.27	14	1
1:A:28:PHE:CE1	4:A:185:GNP:O5'	0.44	2.70	15	2
1:A:123:PRO:O	1:A:127:GLU:CG	0.44	2.66	5	8
1:A:8:VAL:O	1:A:8:VAL:HG13	0.44	2.12	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:ARG:O	1:A:126:ILE:CD1	0.44	2.66	6	6
1:A:4:ILE:CG1	1:A:4:ILE:O	0.44	2.65	12	1
1:A:78:PHE:CG	1:A:108:THR:OG1	0.44	2.70	12	1
1:A:26:ASN:ND2	1:A:26:ASN:N	0.44	2.65	19	2
1:A:32:TYR:CE2	2:B:537:ARG:NH2	0.44	2.85	15	1
1:A:40:TYR:CE2	2:B:518:PHE:CE2	0.44	3.05	15	1
1:A:15:GLY:HA3	1:A:169:PHE:CZ	0.44	2.47	17	2
1:A:170:ASP:OD1	2:B:505:LEU:HD21	0.44	2.13	19	1
1:A:46:ILE:CB	2:B:514:LEU:HD11	0.44	2.42	10	1
1:A:137:ILE:HG23	1:A:141:THR:HG21	0.44	1.88	14	2
1:A:82:PHE:C	1:A:82:PHE:CD1	0.44	2.91	14	2
1:A:82:PHE:O	4:A:185:GNP:C6	0.44	2.66	20	6
1:A:178:GLU:CB	2:B:507:ALA:CB	0.44	2.95	1	1
4:A:185:GNP:O4'	2:B:537:ARG:NE	0.44	2.51	1	1
1:A:37:PHE:CD1	1:A:37:PHE:C	0.44	2.90	19	4
2:B:523:HIS:CD2	2:B:523:HIS:C	0.44	2.91	17	2
1:A:28:PHE:C	1:A:28:PHE:CD1	0.44	2.90	17	2
1:A:13:ALA:CB	4:A:185:GNP:O3A	0.44	2.64	12	1
1:A:22:SER:O	1:A:26:ASN:ND2	0.44	2.50	6	2
1:A:26:ASN:N	1:A:26:ASN:ND2	0.44	2.64	20	3
1:A:4:ILE:HG21	1:A:177:LEU:CD2	0.44	2.42	19	1
1:A:174:LEU:HD22	2:B:504:GLY:HA2	0.44	1.89	14	1
1:A:79:LEU:HD13	1:A:111:LEU:HB3	0.44	1.89	18	1
1:A:9:VAL:HG23	1:A:78:PHE:CE1	0.44	2.47	18	1
1:A:77:VAL:HG11	1:A:175:ALA:HB3	0.44	1.89	5	1
1:A:85:VAL:HG21	1:A:119:LEU:CD1	0.44	2.42	5	1
1:A:35:THR:CG2	4:A:185:GNP:O2G	0.44	2.65	1	1
1:A:85:VAL:HG13	1:A:120:ARG:CG	0.44	2.43	1	1
1:A:46:ILE:CG1	1:A:51:TYR:O	0.44	2.66	16	6
2:B:527:ASP:N	2:B:528:PRO:CD	0.44	2.80	6	2
1:A:4:ILE:O	1:A:53:LEU:CB	0.44	2.66	17	4
1:A:32:TYR:CB	4:A:185:GNP:O2G	0.44	2.65	3	1
1:A:63:ASP:OD1	1:A:64:TYR:CE2	0.44	2.70	16	1
2:B:507:ALA:HB3	2:B:510:ILE:HG12	0.44	1.89	14	1
1:A:93:VAL:O	1:A:97:TRP:N	0.44	2.51	8	3
1:A:13:ALA:O	1:A:14:VAL:CB	0.44	2.65	15	3
1:A:3:THR:CG2	1:A:51:TYR:OH	0.44	2.66	15	4
1:A:41:ALA:O	2:B:519:ILE:CG1	0.44	2.66	8	5
1:A:37:PHE:O	1:A:39:ASN:N	0.44	2.50	15	2
1:A:25:THR:HG22	1:A:26:ASN:N	0.44	2.27	12	1
1:A:3:THR:HG21	1:A:51:TYR:CE1	0.44	2.48	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:VAL:O	1:A:171:GLU:CG	0.44	2.66	16	1
4:A:185:GNP:O3G	2:B:537:ARG:CZ	0.44	2.66	16	1
1:A:93:VAL:HG12	1:A:97:TRP:CE3	0.44	2.48	20	1
1:A:20:LEU:HD22	1:A:20:LEU:N	0.44	2.28	19	1
1:A:166:LYS:O	1:A:170:ASP:CB	0.44	2.66	9	5
1:A:120:ARG:CZ	1:A:139:PRO:CD	0.44	2.96	18	1
1:A:113:VAL:CG1	1:A:168:VAL:CG2	0.44	2.93	5	1
1:A:164:GLY:O	1:A:166:LYS:N	0.44	2.51	5	5
1:A:51:TYR:CD1	1:A:51:TYR:C	0.44	2.91	2	5
1:A:14:VAL:O	1:A:19:LEU:CD2	0.44	2.65	12	1
1:A:36:VAL:HG13	1:A:61:LEU:HD13	0.44	1.89	12	1
1:A:115:THR:HG22	1:A:157:CYS:HB2	0.44	1.89	6	1
2:B:540:GLU:HA	2:B:543:LEU:CD1	0.44	2.43	19	2
1:A:126:ILE:O	1:A:130:ALA:N	0.44	2.50	7	1
1:A:9:VAL:HG12	2:B:541:LEU:HD21	0.44	1.90	16	1
1:A:1:MET:HE3	1:A:46:ILE:CG2	0.44	2.43	20	1
1:A:15:GLY:O	1:A:19:LEU:CG	0.43	2.66	19	2
1:A:42:VAL:CG1	2:B:517:SER:O	0.43	2.66	15	5
1:A:139:PRO:HA	1:A:154:TYR:CE1	0.43	2.48	1	4
1:A:70:LEU:HD11	2:B:541:LEU:CG	0.43	2.43	2	1
1:A:117:ILE:O	1:A:120:ARG:CG	0.43	2.66	3	6
1:A:139:PRO:O	1:A:154:TYR:CD1	0.43	2.70	1	1
1:A:18:CYS:CB	4:A:185:GNP:O5'	0.43	2.66	8	1
1:A:11:ASP:O	2:B:537:ARG:N	0.43	2.51	9	2
1:A:14:VAL:CG2	1:A:19:LEU:CD2	0.43	2.96	6	1
1:A:19:LEU:HG	1:A:165:LEU:HD12	0.43	1.89	13	1
1:A:15:GLY:CA	1:A:19:LEU:HD21	0.43	2.43	7	1
1:A:174:LEU:HD13	2:B:505:LEU:HA	0.43	1.88	15	1
1:A:42:VAL:HG23	1:A:42:VAL:O	0.43	2.13	11	1
1:A:4:ILE:O	1:A:4:ILE:CD1	0.43	2.66	4	1
1:A:149:LEU:N	1:A:149:LEU:HD22	0.43	2.28	19	1
2:B:523:HIS:C	2:B:523:HIS:CD2	0.43	2.92	2	1
1:A:12:GLY:CA	2:B:536:ASP:O	0.43	2.66	2	1
1:A:12:GLY:O	2:B:537:ARG:NH1	0.43	2.52	8	1
1:A:82:PHE:HE1	1:A:112:LEU:HD12	0.43	1.68	12	2
1:A:17:THR:HG21	1:A:38:ASP:CG	0.43	2.33	12	1
1:A:115:THR:CA	1:A:117:ILE:HD13	0.43	2.43	6	2
2:B:530:HIS:O	2:B:532:TRP:N	0.43	2.51	15	1
1:A:3:THR:O	1:A:177:LEU:HD23	0.43	2.13	10	1
1:A:6:CYS:SG	1:A:169:PHE:CZ	0.43	3.09	14	1
1:A:87:PRO:O	1:A:88:SER:CB	0.43	2.66	5	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:VAL:HG12	1:A:137:ILE:HB	0.43	1.90	12	1
1:A:68:ARG:O	1:A:71:SER:CB	0.43	2.67	12	2
1:A:36:VAL:HG13	1:A:59:ALA:HB1	0.43	1.90	6	1
1:A:46:ILE:HD11	2:B:512:GLN:OE1	0.43	2.14	6	1
2:B:512:GLN:HB3	2:B:513:PRO:HD3	0.43	1.91	6	2
1:A:62:GLU:CB	2:B:524:GLY:O	0.43	2.67	7	1
1:A:116:GLN:HB2	4:A:185:GNP:HN22	0.43	1.73	20	2
1:A:116:GLN:CG	1:A:119:LEU:HD22	0.43	2.42	17	1
1:A:32:TYR:HA	4:A:185:GNP:PG	0.43	2.53	17	1
4:A:185:GNP:O3A	2:B:537:ARG:NE	0.43	2.50	19	1
1:A:2:GLN:O	1:A:177:LEU:CD2	0.43	2.67	14	2
1:A:15:GLY:O	1:A:19:LEU:CD1	0.43	2.67	4	3
1:A:45:MET:C	1:A:45:MET:CE	0.43	2.87	9	2
2:B:508:GLN:NE2	2:B:510:ILE:HD11	0.43	2.29	8	1
1:A:20:LEU:CD2	1:A:20:LEU:N	0.43	2.82	11	1
2:B:503:SER:HB3	2:B:505:LEU:HD11	0.43	1.90	11	1
1:A:46:ILE:HG12	2:B:510:ILE:HG23	0.43	1.88	11	1
1:A:16:LYS:CE	1:A:58:THR:OG1	0.43	2.67	16	1
1:A:21:ILE:O	1:A:25:THR:CG2	0.43	2.66	4	1
1:A:37:PHE:N	1:A:37:PHE:CD1	0.43	2.83	4	1
1:A:3:THR:HB	1:A:51:TYR:CE1	0.43	2.48	4	1
1:A:160:LEU:HD22	4:A:185:GNP:O3'	0.43	2.13	20	1
1:A:44:VAL:CG1	2:B:512:GLN:O	0.43	2.67	20	1
1:A:45:MET:C	1:A:45:MET:HE2	0.43	2.34	10	1
2:B:540:GLU:OE1	2:B:543:LEU:HD13	0.43	2.13	18	1
1:A:82:PHE:O	4:A:185:GNP:C5	0.43	2.66	15	4
1:A:45:MET:CE	1:A:49:GLU:C	0.43	2.87	1	3
1:A:32:TYR:N	1:A:32:TYR:CD1	0.43	2.84	8	1
1:A:75:THR:HG21	1:A:78:PHE:HD1	0.43	1.73	8	1
1:A:1:MET:CE	1:A:2:GLN:O	0.43	2.66	20	2
1:A:33:VAL:CG1	2:B:526:SER:O	0.43	2.66	15	1
1:A:15:GLY:HA3	1:A:169:PHE:CE1	0.43	2.49	3	1
1:A:59:ALA:CB	1:A:61:LEU:CD2	0.43	2.97	3	1
1:A:174:LEU:HD23	2:B:505:LEU:CD2	0.43	2.42	11	1
1:A:119:LEU:CD1	1:A:119:LEU:N	0.43	2.77	20	1
1:A:15:GLY:O	1:A:19:LEU:CD2	0.43	2.67	20	1
2:B:508:GLN:HB2	2:B:510:ILE:CD1	0.43	2.44	19	1
1:A:84:VAL:HG22	1:A:117:ILE:HG22	0.43	1.88	10	1
1:A:46:ILE:HG21	2:B:510:ILE:HG23	0.43	1.90	14	1
1:A:3:THR:CG2	1:A:51:TYR:CZ	0.43	3.02	18	1
1:A:113:VAL:HG12	1:A:115:THR:CG2	0.43	2.44	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:VAL:O	2:B:540:GLU:CG	0.43	2.67	5	2
1:A:158:SER:OG	1:A:163:LYS:N	0.43	2.51	10	2
1:A:13:ALA:O	1:A:16:LYS:N	0.43	2.52	1	1
1:A:43:THR:O	2:B:516:ASN:CB	0.43	2.67	8	1
1:A:14:VAL:CG2	1:A:113:VAL:CG1	0.43	2.94	12	1
1:A:6:CYS:HB3	1:A:56:PHE:CE2	0.43	2.47	12	1
1:A:88:SER:N	1:A:133:LYS:HB3	0.43	2.28	7	3
1:A:45:MET:CE	1:A:45:MET:C	0.43	2.87	16	3
1:A:1:MET:HE1	1:A:46:ILE:HB	0.43	1.90	4	1
1:A:44:VAL:CG2	1:A:52:THR:OG1	0.43	2.67	4	1
1:A:55:LEU:N	1:A:55:LEU:CD2	0.43	2.77	4	1
1:A:79:LEU:HD21	1:A:113:VAL:CG2	0.43	2.43	4	1
1:A:64:TYR:CD1	1:A:67:LEU:HD12	0.43	2.49	20	1
1:A:119:LEU:HD21	1:A:160:LEU:HD13	0.43	1.90	10	1
1:A:18:CYS:SG	4:A:185:GNP:C5'	0.43	3.06	14	2
1:A:30:SER:O	2:B:531:CYS:CB	0.43	2.67	18	2
1:A:155:VAL:HG12	1:A:156:GLU:H	0.43	1.73	1	1
1:A:86:SER:CA	1:A:129:LEU:HD22	0.43	2.44	12	1
1:A:59:ALA:N	2:B:542:TYR:O	0.43	2.52	9	1
1:A:97:TRP:O	1:A:100:GLU:CG	0.43	2.67	4	2
1:A:33:VAL:CG1	2:B:525:ASP:O	0.43	2.67	11	1
1:A:170:ASP:OD1	2:B:503:SER:CB	0.43	2.67	11	1
1:A:166:LYS:O	1:A:170:ASP:N	0.43	2.52	9	11
1:A:15:GLY:O	1:A:19:LEU:CB	0.43	2.67	18	2
1:A:46:ILE:CD1	1:A:53:LEU:HD11	0.43	2.44	18	1
1:A:69:PRO:O	1:A:73:PRO:N	0.43	2.52	5	1
1:A:84:VAL:HG12	1:A:85:VAL:H	0.43	1.74	5	1
1:A:16:LYS:HD2	2:B:543:LEU:HD21	0.43	1.88	2	1
1:A:85:VAL:HB	1:A:129:LEU:HD21	0.43	1.89	17	3
1:A:85:VAL:CG2	1:A:116:GLN:OE1	0.43	2.67	7	1
1:A:24:THR:HG23	1:A:25:THR:N	0.43	2.29	15	2
1:A:58:THR:CA	1:A:67:LEU:HD22	0.43	2.43	11	1
1:A:36:VAL:HG13	2:B:524:GLY:CA	0.43	2.43	11	1
1:A:92:ASN:O	1:A:96:LYS:CB	0.43	2.67	11	7
4:A:185:GNP:O1A	2:B:537:ARG:NE	0.43	2.50	2	1
1:A:36:VAL:CG1	1:A:59:ALA:O	0.43	2.67	2	1
1:A:19:LEU:HA	1:A:165:LEU:HD21	0.43	1.91	1	2
1:A:38:ASP:CB	1:A:64:TYR:OH	0.43	2.67	8	1
1:A:16:LYS:N	1:A:19:LEU:HD11	0.43	2.28	13	1
1:A:11:ASP:CB	2:B:537:ARG:O	0.43	2.67	3	2
1:A:46:ILE:CD1	2:B:510:ILE:HG23	0.43	2.44	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:THR:HG23	2:B:540:GLU:C	0.43	2.34	4	1
1:A:118:ASP:CG	1:A:160:LEU:HD11	0.43	2.34	20	1
1:A:44:VAL:HG13	2:B:514:LEU:CD1	0.43	2.44	20	1
1:A:19:LEU:O	1:A:165:LEU:CD1	0.43	2.67	17	1
1:A:58:THR:OG1	2:B:540:GLU:CB	0.43	2.67	17	2
1:A:5:LYS:O	1:A:75:THR:CB	0.43	2.66	19	1
1:A:88:SER:OG	1:A:133:LYS:CG	0.43	2.67	6	7
1:A:87:PRO:O	1:A:132:ASN:CB	0.43	2.67	5	9
1:A:13:ALA:O	1:A:14:VAL:CG2	0.43	2.67	5	1
2:B:534:PHE:O	2:B:536:ASP:N	0.43	2.52	5	2
1:A:21:ILE:CG2	1:A:25:THR:OG1	0.43	2.66	6	4
4:A:185:GNP:O4'	2:B:537:ARG:NH2	0.43	2.52	6	1
1:A:20:LEU:HD21	1:A:169:PHE:CD2	0.43	2.49	7	1
1:A:14:VAL:O	1:A:18:CYS:CB	0.43	2.67	15	2
1:A:13:ALA:C	1:A:14:VAL:HG13	0.43	2.35	16	1
1:A:19:LEU:HG	1:A:169:PHE:CD1	0.43	2.49	20	1
1:A:14:VAL:HG12	1:A:81:CYS:HB2	0.43	1.91	19	1
1:A:13:ALA:HB1	1:A:18:CYS:HB3	0.42	1.91	14	1
1:A:125:THR:O	1:A:129:LEU:CD1	0.42	2.67	19	3
1:A:70:LEU:HD23	1:A:70:LEU:H	0.42	1.73	18	1
2:B:511:SER:O	2:B:514:LEU:CD1	0.42	2.67	13	6
1:A:36:VAL:HG11	1:A:61:LEU:HB2	0.42	1.91	2	1
2:B:502:GLY:CA	2:B:509:ASP:O	0.42	2.67	2	2
1:A:95:GLU:O	1:A:99:PRO:CD	0.42	2.67	8	2
1:A:19:LEU:O	1:A:23:TYR:CB	0.42	2.67	12	1
1:A:60:GLY:N	2:B:543:LEU:O	0.42	2.52	9	2
1:A:181:GLU:CG	1:A:181:GLU:O	0.42	2.67	6	2
2:B:538:ILE:HG12	2:B:539:ASP:N	0.42	2.29	7	1
2:B:530:HIS:O	2:B:530:HIS:CD2	0.42	2.72	15	1
1:A:12:GLY:O	2:B:537:ARG:CB	0.42	2.67	3	1
2:B:541:LEU:CD2	2:B:542:TYR:CD1	0.42	3.01	3	1
1:A:174:LEU:HD23	2:B:505:LEU:CD1	0.42	2.27	10	1
1:A:33:VAL:CG1	2:B:526:SER:HB2	0.42	2.44	10	1
1:A:54:GLY:O	1:A:56:PHE:N	0.42	2.52	18	1
1:A:14:VAL:O	1:A:79:LEU:CD2	0.42	2.67	5	1
1:A:51:TYR:OH	1:A:53:LEU:CD1	0.42	2.68	2	1
2:B:524:GLY:O	2:B:525:ASP:CB	0.42	2.67	1	1
1:A:14:VAL:CG2	2:B:538:ILE:O	0.42	2.67	8	1
2:B:505:LEU:O	2:B:507:ALA:N	0.42	2.53	12	1
1:A:117:ILE:CG2	1:A:154:TYR:OH	0.42	2.66	6	1
1:A:36:VAL:CG1	1:A:63:ASP:CB	0.42	2.97	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:LEU:CD2	1:A:112:LEU:O	0.42	2.67	3	4
2:B:537:ARG:CZ	2:B:537:ARG:N	0.42	2.82	7	1
1:A:58:THR:CB	2:B:540:GLU:O	0.42	2.68	20	2
1:A:58:THR:HG21	1:A:69:PRO:HD2	0.42	1.90	17	1
1:A:61:LEU:HD22	2:B:526:SER:OG	0.42	2.14	10	1
1:A:40:TYR:OH	2:B:518:PHE:CZ	0.42	2.67	14	1
4:A:185:GNP:O4'	2:B:537:ARG:CD	0.42	2.67	5	1
1:A:137:ILE:HG23	1:A:141:THR:CG2	0.42	2.45	2	1
1:A:111:LEU:CD2	1:A:153:LYS:O	0.42	2.67	2	2
1:A:12:GLY:N	2:B:538:ILE:O	0.42	2.52	2	1
1:A:99:PRO:O	1:A:103:HIS:CB	0.42	2.67	8	1
2:B:502:GLY:CA	2:B:511:SER:OG	0.42	2.68	8	1
1:A:117:ILE:HG22	1:A:120:ARG:HD3	0.42	1.91	13	1
1:A:68:ARG:O	1:A:71:SER:N	0.42	2.52	13	1
1:A:14:VAL:HG12	1:A:79:LEU:HD12	0.42	1.92	7	1
1:A:20:LEU:O	1:A:23:TYR:N	0.42	2.52	4	2
1:A:95:GLU:O	1:A:99:PRO:CG	0.42	2.67	4	2
1:A:1:MET:O	2:B:510:ILE:CD1	0.42	2.67	20	1
1:A:14:VAL:HG12	1:A:57:ASP:OD1	0.42	2.13	17	1
1:A:159:ALA:HB3	1:A:160:LEU:HD22	0.42	1.91	17	1
1:A:57:ASP:CB	2:B:540:GLU:OE1	0.42	2.67	17	1
1:A:39:ASN:CB	1:A:55:LEU:O	0.42	2.68	14	1
1:A:6:CYS:O	1:A:56:PHE:CB	0.42	2.67	14	1
1:A:32:TYR:CD1	2:B:532:TRP:CE3	0.42	3.07	14	1
2:B:512:GLN:HB2	2:B:513:PRO:CD	0.42	2.45	18	1
1:A:82:PHE:O	4:A:185:GNP:C4	0.42	2.67	15	4
1:A:49:GLU:CB	1:A:50:PRO:CD	0.42	2.97	2	1
1:A:58:THR:O	2:B:543:LEU:CD1	0.42	2.66	2	1
1:A:6:CYS:O	1:A:56:PHE:N	0.42	2.52	2	1
1:A:46:ILE:HG12	2:B:510:ILE:CG2	0.42	2.44	10	2
4:A:185:GNP:O2A	4:A:185:GNP:H4'	0.42	2.14	8	1
1:A:13:ALA:HB3	4:A:185:GNP:O3A	0.42	2.14	12	1
1:A:71:SER:OG	1:A:72:TYR:N	0.42	2.53	12	1
1:A:33:VAL:HB	1:A:34:PRO:CD	0.42	2.44	4	3
1:A:157:CYS:O	1:A:163:LYS:CB	0.42	2.67	6	1
1:A:35:THR:HG21	2:B:543:LEU:HD21	0.42	1.89	6	2
2:B:507:ALA:O	2:B:508:GLN:CG	0.42	2.67	13	1
1:A:22:SER:OG	1:A:26:ASN:ND2	0.42	2.52	15	2
1:A:84:VAL:N	1:A:116:GLN:OE1	0.42	2.52	3	1
2:B:527:ASP:O	2:B:529:ARG:CG	0.42	2.67	3	1
1:A:43:THR:O	1:A:44:VAL:CG2	0.42	2.67	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:THR:O	1:A:141:THR:N	0.42	2.50	14	6
1:A:21:ILE:O	1:A:25:THR:CB	0.42	2.68	14	1
1:A:92:ASN:O	1:A:96:LYS:N	0.42	2.53	9	5
1:A:80:VAL:HG21	1:A:110:PHE:CG	0.42	2.50	6	1
1:A:82:PHE:N	4:A:185:GNP:O6	0.42	2.52	13	1
2:B:504:GLY:C	2:B:505:LEU:CD2	0.42	2.88	13	1
1:A:68:ARG:N	1:A:69:PRO:HD2	0.42	2.30	7	1
1:A:59:ALA:O	1:A:61:LEU:N	0.42	2.52	11	2
1:A:174:LEU:HD22	2:B:505:LEU:HA	0.42	1.90	15	1
1:A:17:THR:O	1:A:21:ILE:HG22	0.42	2.14	15	1
1:A:8:VAL:HG12	1:A:57:ASP:OD1	0.42	2.15	15	1
1:A:142:ALA:CB	1:A:154:TYR:CD1	0.42	3.03	3	1
1:A:4:ILE:HG21	1:A:177:LEU:N	0.42	2.29	3	1
1:A:1:MET:SD	1:A:2:GLN:N	0.42	2.92	17	2
2:B:510:ILE:HD12	2:B:510:ILE:N	0.42	2.30	11	1
1:A:8:VAL:O	1:A:9:VAL:CG1	0.42	2.67	16	1
1:A:37:PHE:CG	2:B:521:THR:OG1	0.42	2.73	16	1
1:A:70:LEU:CD2	2:B:541:LEU:O	0.42	2.67	16	2
2:B:505:LEU:CD2	2:B:510:ILE:O	0.42	2.67	4	1
1:A:35:THR:CG2	1:A:57:ASP:OD2	0.42	2.67	20	1
1:A:83:SER:CB	1:A:116:GLN:OE1	0.42	2.67	17	1
1:A:116:GLN:HA	1:A:119:LEU:HD13	0.42	1.91	14	2
1:A:46:ILE:HD11	1:A:53:LEU:HD11	0.42	1.92	18	1
1:A:94:LYS:O	1:A:98:VAL:CG2	0.42	2.68	18	3
2:B:504:GLY:O	2:B:506:SER:N	0.42	2.51	18	1
1:A:88:SER:CB	1:A:133:LYS:HG3	0.42	2.45	15	3
1:A:33:VAL:CG1	2:B:526:SER:OG	0.42	2.68	2	1
1:A:149:LEU:O	1:A:150:LYS:CD	0.42	2.67	1	1
1:A:40:TYR:OH	2:B:520:HIS:ND1	0.42	2.52	1	1
1:A:113:VAL:O	4:A:185:GNP:N1	0.42	2.53	7	2
1:A:119:LEU:O	1:A:122:ASP:N	0.42	2.53	16	4
1:A:173:ILE:O	1:A:176:ALA:HB3	0.42	2.15	12	1
1:A:61:LEU:CD2	2:B:525:ASP:OD1	0.42	2.68	12	1
1:A:28:PHE:N	1:A:29:PRO:HD2	0.42	2.29	15	2
1:A:28:PHE:HA	1:A:32:TYR:CE1	0.42	2.50	7	1
2:B:523:HIS:N	2:B:523:HIS:ND1	0.42	2.68	15	1
1:A:17:THR:O	1:A:21:ILE:HB	0.42	2.15	4	2
1:A:78:PHE:O	1:A:110:PHE:CB	0.42	2.68	3	1
1:A:40:TYR:OH	2:B:518:PHE:CE1	0.42	2.67	11	1
1:A:157:CYS:SG	1:A:168:VAL:HG12	0.42	2.54	4	1
1:A:170:ASP:O	1:A:174:LEU:CB	0.42	2.68	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:544:GLY:O	2:B:545:ASN:ND2	0.42	2.53	20	1
1:A:8:VAL:HG11	1:A:14:VAL:CA	0.42	2.45	17	1
1:A:44:VAL:HG12	2:B:515:GLN:CB	0.42	2.45	19	1
1:A:44:VAL:HB	1:A:52:THR:CG2	0.42	2.45	5	1
1:A:44:VAL:CG2	1:A:52:THR:HG22	0.42	2.44	1	2
1:A:75:THR:HG21	1:A:78:PHE:CD1	0.42	2.50	8	1
1:A:88:SER:CB	1:A:133:LYS:HG2	0.42	2.44	10	3
1:A:53:LEU:HD21	2:B:512:GLN:OE1	0.42	2.15	9	1
1:A:9:VAL:HG11	1:A:72:TYR:HE1	0.42	1.69	9	1
1:A:8:VAL:HG23	1:A:57:ASP:OD1	0.42	2.15	6	1
1:A:58:THR:OG1	2:B:543:LEU:CD1	0.42	2.67	6	1
1:A:80:VAL:CG1	1:A:97:TRP:CE3	0.42	3.03	6	1
1:A:126:ILE:O	1:A:130:ALA:CB	0.42	2.67	7	1
1:A:173:ILE:CD1	1:A:177:LEU:HD11	0.42	2.43	15	2
1:A:8:VAL:O	1:A:9:VAL:CG2	0.42	2.68	11	1
2:B:538:ILE:CD1	2:B:542:TYR:HB2	0.42	2.44	11	1
1:A:19:LEU:C	1:A:165:LEU:HD21	0.42	2.35	16	1
1:A:40:TYR:CD1	1:A:40:TYR:O	0.42	2.72	4	1
1:A:79:LEU:CD1	1:A:111:LEU:O	0.42	2.68	20	1
1:A:5:LYS:O	1:A:77:VAL:HG13	0.42	2.15	20	1
1:A:92:ASN:O	1:A:96:LYS:CD	0.42	2.68	17	1
1:A:148:ASP:HB3	1:A:149:LEU:HD22	0.42	1.92	19	1
1:A:90:PHE:HE1	1:A:145:LEU:HD12	0.42	1.75	10	1
1:A:59:ALA:CA	2:B:542:TYR:O	0.42	2.67	18	2
2:B:508:GLN:HB2	2:B:510:ILE:HD12	0.42	1.91	12	1
1:A:19:LEU:HB3	1:A:169:PHE:CD2	0.42	2.49	9	1
1:A:39:ASN:ND2	1:A:64:TYR:OH	0.42	2.53	6	1
1:A:76:ASP:O	1:A:109:PRO:CG	0.42	2.67	20	2
1:A:33:VAL:CB	1:A:34:PRO:HD3	0.42	2.45	13	2
2:B:527:ASP:O	2:B:529:ARG:N	0.42	2.53	13	1
1:A:133:LYS:HG2	1:A:134:GLN:N	0.42	2.30	4	2
1:A:158:SER:O	1:A:165:LEU:HD12	0.42	2.15	7	1
1:A:157:CYS:SG	1:A:168:VAL:CG1	0.42	3.08	20	2
1:A:17:THR:O	1:A:21:ILE:CB	0.42	2.68	15	1
1:A:17:THR:OG1	1:A:18:CYS:N	0.42	2.52	11	1
1:A:8:VAL:CG2	1:A:9:VAL:N	0.42	2.83	11	1
1:A:83:SER:HG	4:A:185:GNP:HI'	0.42	1.75	16	1
1:A:21:ILE:CD1	2:B:518:PHE:CE1	0.42	3.02	16	1
2:B:504:GLY:O	2:B:505:LEU:CD2	0.42	2.65	4	1
1:A:60:GLY:N	2:B:542:TYR:O	0.42	2.53	4	1
2:B:530:HIS:O	2:B:531:CYS:CB	0.42	2.68	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:504:GLY:CA	2:B:509:ASP:OD2	0.42	2.68	19	1
1:A:158:SER:O	1:A:162:GLN:CA	0.42	2.67	18	2
1:A:133:LYS:O	1:A:134:GLN:HB3	0.42	2.15	2	10
2:B:542:TYR:O	2:B:544:GLY:N	0.42	2.52	2	2
1:A:14:VAL:CG1	1:A:14:VAL:O	0.42	2.67	6	1
1:A:10:GLY:O	2:B:539:ASP:N	0.42	2.53	3	1
1:A:1:MET:SD	1:A:51:TYR:CZ	0.42	3.13	11	1
1:A:58:THR:HG1	1:A:67:LEU:HD22	0.42	1.73	4	1
1:A:124:SER:OG	1:A:125:THR:N	0.42	2.52	20	1
4:A:185:GNP:C2'	4:A:185:GNP:N3	0.42	2.82	20	1
1:A:19:LEU:HD13	1:A:19:LEU:H	0.42	1.72	20	1
1:A:13:ALA:CB	1:A:18:CYS:SG	0.42	3.08	17	1
1:A:64:TYR:O	1:A:67:LEU:CD1	0.42	2.68	19	1
1:A:37:PHE:CE1	2:B:522:GLY:O	0.42	2.73	10	1
1:A:170:ASP:OD1	1:A:173:ILE:HD11	0.42	2.15	18	1
1:A:9:VAL:HG21	1:A:78:PHE:CE1	0.42	2.50	18	1
1:A:111:LEU:HD11	1:A:171:GLU:CG	0.42	2.45	5	2
1:A:28:PHE:CB	1:A:29:PRO:HD3	0.42	2.45	11	4
1:A:139:PRO:HA	1:A:154:TYR:CE2	0.42	2.50	8	1
1:A:3:THR:C	1:A:4:ILE:CG2	0.42	2.88	8	3
2:B:530:HIS:CD2	2:B:530:HIS:O	0.42	2.73	8	1
1:A:114:GLY:HA3	1:A:154:TYR:CZ	0.42	2.50	12	2
1:A:26:ASN:ND2	1:A:31:GLU:O	0.42	2.53	12	1
2:B:534:PHE:O	2:B:537:ARG:NH1	0.42	2.53	9	1
1:A:116:GLN:NE2	4:A:185:GNP:O2'	0.42	2.53	3	1
1:A:142:ALA:O	1:A:146:ALA:CB	0.42	2.68	4	1
1:A:117:ILE:CD1	1:A:158:SER:OG	0.42	2.67	20	1
1:A:131:LYS:HD2	1:A:132:ASN:N	0.42	2.30	10	1
1:A:88:SER:OG	1:A:133:LYS:CE	0.42	2.68	10	1
1:A:2:GLN:NE2	1:A:177:LEU:O	0.42	2.53	10	1
1:A:71:SER:OG	1:A:72:TYR:CE2	0.42	2.69	10	1
1:A:4:ILE:HB	1:A:176:ALA:HB3	0.41	1.93	18	1
1:A:160:LEU:N	1:A:160:LEU:CD1	0.41	2.81	5	2
1:A:4:ILE:CG2	1:A:173:ILE:O	0.41	2.68	2	1
1:A:1:MET:HE1	1:A:51:TYR:HD1	0.41	1.74	2	1
1:A:64:TYR:CG	1:A:67:LEU:HD12	0.41	2.50	2	1
1:A:158:SER:OG	1:A:162:GLN:N	0.41	2.53	10	2
1:A:1:MET:HE2	1:A:2:GLN:O	0.41	2.15	1	1
1:A:3:THR:C	1:A:4:ILE:HG23	0.41	2.36	1	3
2:B:512:GLN:HB2	2:B:513:PRO:HD2	0.41	1.92	1	1
1:A:61:LEU:CD2	2:B:526:SER:OG	0.41	2.67	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:N	1:A:20:LEU:HD22	0.41	2.30	8	1
1:A:119:LEU:CD1	1:A:119:LEU:O	0.41	2.67	6	1
1:A:69:PRO:O	1:A:74:GLN:NE2	0.41	2.53	6	2
1:A:84:VAL:HG13	1:A:137:ILE:CB	0.41	2.45	13	1
1:A:16:LYS:O	1:A:20:LEU:CD2	0.41	2.67	20	2
1:A:175:ALA:HB1	1:A:180:PRO:HG3	0.41	1.91	7	1
1:A:28:PHE:CE1	4:A:185:GNP:H4'	0.41	2.50	15	1
1:A:67:LEU:O	2:B:541:LEU:CD1	0.41	2.68	11	1
1:A:93:VAL:HG22	1:A:97:TRP:CD2	0.41	2.50	4	1
2:B:512:GLN:HB3	2:B:513:PRO:CD	0.41	2.45	20	2
1:A:100:GLU:N	1:A:100:GLU:OE1	0.41	2.53	19	1
1:A:8:VAL:HG23	1:A:14:VAL:HG13	0.41	1.92	19	1
1:A:84:VAL:C	1:A:85:VAL:CG2	0.41	2.88	5	1
2:B:519:ILE:O	2:B:519:ILE:HG22	0.41	2.15	5	1
1:A:105:CYS:O	1:A:107:LYS:N	0.41	2.53	2	2
1:A:33:VAL:CG2	1:A:34:PRO:HD3	0.41	2.45	2	1
1:A:40:TYR:CE1	2:B:521:THR:O	0.41	2.74	2	1
2:B:507:ALA:O	2:B:508:GLN:HB3	0.41	2.15	1	1
1:A:158:SER:N	1:A:163:LYS:HB2	0.41	2.30	9	1
1:A:70:LEU:O	1:A:72:TYR:CE2	0.41	2.72	9	1
1:A:23:TYR:CE2	1:A:165:LEU:HB3	0.41	2.49	16	1
1:A:44:VAL:HG12	2:B:515:GLN:HB2	0.41	1.92	16	1
1:A:44:VAL:CG1	1:A:45:MET:N	0.41	2.83	17	1
1:A:19:LEU:HD11	1:A:169:PHE:CD1	0.41	2.49	19	1
1:A:13:ALA:CB	4:A:185:GNP:O2A	0.41	2.64	10	1
1:A:4:ILE:O	1:A:53:LEU:CD2	0.41	2.66	2	1
1:A:33:VAL:HG12	1:A:61:LEU:HD21	0.41	1.92	1	1
1:A:38:ASP:CB	1:A:57:ASP:HB2	0.41	2.45	1	1
1:A:115:THR:C	1:A:117:ILE:HD12	0.41	2.36	8	1
2:B:523:HIS:O	2:B:525:ASP:N	0.41	2.54	7	2
2:B:516:ASN:ND2	2:B:518:PHE:O	0.41	2.53	6	1
2:B:541:LEU:HD23	2:B:542:TYR:CE1	0.41	2.50	7	1
1:A:145:LEU:O	1:A:145:LEU:CD2	0.41	2.68	3	3
1:A:28:PHE:O	1:A:32:TYR:CE1	0.41	2.73	3	1
1:A:117:ILE:HD13	1:A:117:ILE:N	0.41	2.30	11	1
1:A:126:ILE:CG2	1:A:127:GLU:N	0.41	2.83	11	1
1:A:142:ALA:HB3	1:A:154:TYR:CD2	0.41	2.50	11	1
1:A:78:PHE:CE1	1:A:108:THR:CB	0.41	3.04	16	1
1:A:158:SER:O	1:A:162:GLN:N	0.41	2.53	20	1
1:A:27:LYS:O	1:A:32:TYR:CZ	0.41	2.73	20	1
1:A:94:LYS:HD2	1:A:145:LEU:HD22	0.41	1.92	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:LEU:CD2	1:A:165:LEU:O	0.41	2.68	19	1
1:A:18:CYS:HB2	4:A:185:GNP:PB	0.41	2.55	14	1
1:A:64:TYR:HB2	1:A:67:LEU:CD2	0.41	2.46	5	1
1:A:15:GLY:HA2	1:A:19:LEU:CD2	0.41	2.45	2	2
1:A:14:VAL:O	1:A:14:VAL:CG1	0.41	2.67	8	1
1:A:37:PHE:HB3	2:B:522:GLY:CA	0.41	2.46	12	1
1:A:33:VAL:HG21	2:B:529:ARG:HG3	0.41	1.92	9	1
1:A:32:TYR:O	2:B:545:ASN:ND2	0.41	2.54	6	2
2:B:539:ASP:HB3	2:B:541:LEU:HD12	0.41	1.92	13	1
1:A:13:ALA:CB	2:B:537:ARG:HD3	0.41	2.45	3	1
1:A:24:THR:CG2	1:A:25:THR:N	0.41	2.83	11	1
2:B:531:CYS:O	2:B:533:GLY:N	0.41	2.53	4	1
2:B:542:TYR:O	2:B:543:LEU:CB	0.41	2.68	20	1
1:A:113:VAL:HG22	1:A:168:VAL:HG21	0.41	1.92	10	1
1:A:3:THR:CG2	1:A:53:LEU:HG	0.41	2.45	10	1
1:A:28:PHE:CE1	1:A:32:TYR:OH	0.41	2.69	14	1
1:A:78:PHE:N	1:A:109:PRO:O	0.41	2.52	2	2
2:B:532:TRP:CD2	2:B:532:TRP:O	0.41	2.74	2	1
1:A:32:TYR:C	1:A:33:VAL:HG22	0.41	2.36	17	4
1:A:18:CYS:HB3	4:A:185:GNP:PB	0.41	2.56	8	1
2:B:523:HIS:CD2	2:B:523:HIS:N	0.41	2.88	9	1
2:B:538:ILE:CG1	2:B:542:TYR:HB2	0.41	2.46	7	2
2:B:538:ILE:HG13	2:B:539:ASP:N	0.41	2.31	11	1
1:A:26:ASN:ND2	1:A:159:ALA:O	0.41	2.53	4	1
1:A:82:PHE:CD1	1:A:90:PHE:CE1	0.41	3.08	4	1
1:A:80:VAL:HG22	1:A:110:PHE:HB2	0.41	1.92	20	1
1:A:58:THR:HB	1:A:67:LEU:CD2	0.41	2.45	19	1
1:A:1:MET:HE2	1:A:46:ILE:HG23	0.41	1.92	10	1
1:A:8:VAL:HG13	1:A:14:VAL:CB	0.41	2.44	10	1
1:A:14:VAL:HG12	1:A:79:LEU:HD11	0.41	1.92	14	1
1:A:115:THR:HA	1:A:117:ILE:HD13	0.41	1.91	18	1
1:A:13:ALA:O	1:A:14:VAL:HG23	0.41	2.15	18	1
1:A:23:TYR:CZ	1:A:166:LYS:HD3	0.41	2.50	18	1
1:A:37:PHE:CB	2:B:522:GLY:HA3	0.41	2.45	12	1
1:A:94:LYS:HG3	1:A:145:LEU:CD1	0.41	2.46	12	1
1:A:6:CYS:SG	1:A:77:VAL:HG13	0.41	2.55	9	1
1:A:63:ASP:HB3	1:A:64:TYR:CE1	0.41	2.50	7	1
1:A:36:VAL:HG13	1:A:61:LEU:HD21	0.41	1.93	15	1
1:A:157:CYS:SG	1:A:165:LEU:HD23	0.41	2.56	3	1
1:A:75:THR:O	1:A:108:THR:HG22	0.41	2.16	11	1
1:A:178:GLU:OE1	2:B:506:SER:CB	0.41	2.69	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:CD2	1:A:169:PHE:CE2	0.41	3.04	18	1
2:B:532:TRP:O	2:B:532:TRP:CE3	0.41	2.73	2	1
1:A:170:ASP:O	1:A:173:ILE:CD1	0.41	2.64	8	1
1:A:56:PHE:CE2	1:A:74:GLN:NE2	0.41	2.88	8	1
1:A:42:VAL:HG12	1:A:43:THR:N	0.41	2.30	9	1
2:B:532:TRP:O	2:B:534:PHE:N	0.41	2.53	9	1
2:B:534:PHE:CZ	2:B:537:ARG:O	0.41	2.73	7	1
1:A:13:ALA:O	1:A:14:VAL:HB	0.41	2.15	15	1
1:A:40:TYR:OH	2:B:518:PHE:CD2	0.41	2.70	15	1
1:A:16:LYS:CB	1:A:38:ASP:OD2	0.41	2.69	3	1
1:A:55:LEU:CD2	1:A:55:LEU:N	0.41	2.78	11	1
1:A:36:VAL:N	1:A:57:ASP:OD2	0.41	2.53	11	1
1:A:173:ILE:HG21	2:B:512:GLN:OE1	0.41	2.16	4	1
1:A:10:GLY:O	2:B:540:GLU:N	0.41	2.53	20	1
1:A:44:VAL:CB	1:A:52:THR:HG21	0.41	2.40	20	1
1:A:18:CYS:O	1:A:21:ILE:N	0.41	2.53	17	1
1:A:37:PHE:HB3	2:B:522:GLY:N	0.41	2.30	17	1
1:A:28:PHE:HB3	1:A:29:PRO:HD3	0.41	1.92	10	1
1:A:126:ILE:HD11	1:A:136:PRO:CD	0.41	2.42	14	1
1:A:49:GLU:HB3	1:A:50:PRO:CD	0.41	2.46	2	1
1:A:4:ILE:CG2	1:A:177:LEU:CD1	0.41	2.99	6	1
1:A:19:LEU:O	1:A:165:LEU:CD2	0.41	2.68	6	1
1:A:54:GLY:O	1:A:56:PHE:CE2	0.41	2.74	13	1
2:B:508:GLN:HB3	2:B:510:ILE:CD1	0.41	2.45	3	1
1:A:13:ALA:O	1:A:14:VAL:CG1	0.41	2.65	17	1
1:A:163:LYS:O	1:A:163:LYS:CG	0.41	2.69	19	1
1:A:44:VAL:HG22	1:A:45:MET:H	0.41	1.75	18	1
1:A:7:VAL:CG2	1:A:56:PHE:CZ	0.41	3.03	18	1
2:B:540:GLU:CD	2:B:543:LEU:HD13	0.41	2.36	18	1
1:A:78:PHE:CZ	1:A:108:THR:CB	0.41	3.04	5	1
1:A:31:GLU:CG	2:B:530:HIS:HA	0.41	2.45	5	1
2:B:532:TRP:NE1	2:B:536:ASP:O	0.41	2.53	5	1
1:A:84:VAL:HG12	1:A:85:VAL:N	0.41	2.31	5	1
1:A:32:TYR:CZ	4:A:185:GNP:PA	0.41	3.14	2	1
2:B:538:ILE:CD1	2:B:542:TYR:HB3	0.41	2.45	3	2
4:A:185:GNP:PA	2:B:537:ARG:HG2	0.41	2.55	1	1
1:A:58:THR:CG2	2:B:540:GLU:O	0.41	2.67	1	1
1:A:37:PHE:HB2	2:B:522:GLY:CA	0.41	2.46	8	1
1:A:68:ARG:CB	1:A:69:PRO:HD3	0.41	2.46	8	2
1:A:25:THR:CG2	1:A:26:ASN:N	0.41	2.84	12	1
1:A:174:LEU:CD1	2:B:505:LEU:HB2	0.41	2.45	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:ILE:HG21	1:A:177:LEU:HD13	0.41	1.93	6	1
4:A:185:GNP:H4'	2:B:537:ARG:NH2	0.41	2.31	6	1
1:A:38:ASP:OD2	1:A:57:ASP:N	0.41	2.52	13	1
1:A:145:LEU:HD21	1:A:149:LEU:HD12	0.41	1.92	7	1
1:A:45:MET:CG	1:A:45:MET:O	0.41	2.69	7	1
1:A:58:THR:O	2:B:540:GLU:O	0.41	2.39	7	1
1:A:72:TYR:CE1	1:A:104:HIS:O	0.41	2.74	15	1
2:B:510:ILE:N	2:B:510:ILE:CD1	0.41	2.84	15	1
1:A:174:LEU:HD13	2:B:505:LEU:CA	0.41	2.46	15	1
1:A:85:VAL:CG2	1:A:85:VAL:O	0.41	2.69	20	2
1:A:13:ALA:O	4:A:185:GNP:O2B	0.41	2.39	3	1
1:A:53:LEU:H	1:A:53:LEU:HD23	0.41	1.76	3	1
1:A:1:MET:HE1	1:A:2:GLN:O	0.41	2.16	3	1
1:A:73:PRO:HG2	1:A:78:PHE:CE2	0.41	2.51	3	1
1:A:30:SER:O	2:B:532:TRP:N	0.41	2.53	11	1
1:A:49:GLU:HB2	1:A:51:TYR:CE2	0.41	2.51	11	1
2:B:510:ILE:CD1	2:B:510:ILE:N	0.41	2.84	11	1
1:A:8:VAL:HG13	1:A:14:VAL:CG2	0.41	2.46	16	1
1:A:82:PHE:CD1	1:A:82:PHE:C	0.41	2.93	4	1
1:A:105:CYS:CB	1:A:108:THR:OG1	0.41	2.68	20	1
1:A:4:ILE:HD12	1:A:177:LEU:HG	0.41	1.93	17	1
1:A:88:SER:OG	1:A:133:LYS:CB	0.41	2.69	17	1
1:A:164:GLY:O	1:A:165:LEU:CB	0.41	2.69	17	1
1:A:139:PRO:O	1:A:154:TYR:CE2	0.41	2.74	19	1
1:A:128:LYS:O	1:A:131:LYS:HG3	0.41	2.14	10	1
1:A:58:THR:CA	1:A:67:LEU:HD11	0.41	2.45	14	1
1:A:115:THR:HG1	4:A:185:GNP:C2	0.41	2.29	18	1
1:A:1:MET:O	1:A:2:GLN:O	0.41	2.39	3	3
1:A:21:ILE:CG2	1:A:26:ASN:CB	0.41	2.99	1	1
1:A:80:VAL:CG1	1:A:97:TRP:CZ3	0.41	3.03	6	1
1:A:162:GLN:NE2	1:A:162:GLN:O	0.41	2.53	13	1
2:B:504:GLY:N	2:B:509:ASP:OD1	0.41	2.53	7	1
1:A:61:LEU:CB	2:B:525:ASP:HB2	0.41	2.46	7	1
2:B:505:LEU:HD13	2:B:510:ILE:HB	0.41	1.93	15	1
1:A:116:GLN:HG2	1:A:119:LEU:HD11	0.41	1.93	11	1
1:A:45:MET:HE2	1:A:47:GLY:N	0.41	2.31	11	1
1:A:14:VAL:HG23	1:A:79:LEU:CD2	0.41	2.45	16	1
1:A:73:PRO:HG2	1:A:78:PHE:CZ	0.41	2.51	16	1
1:A:37:PHE:CB	2:B:522:GLY:N	0.41	2.84	17	1
1:A:94:LYS:NZ	1:A:112:LEU:HD11	0.41	2.31	19	1
1:A:25:THR:OG1	1:A:26:ASN:N	0.41	2.53	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:CYS:O	1:A:16:LYS:CE	0.41	2.70	10	1
1:A:59:ALA:CB	1:A:61:LEU:CD1	0.40	2.93	5	1
2:B:538:ILE:O	2:B:538:ILE:HG23	0.40	2.15	5	1
1:A:16:LYS:HE2	1:A:169:PHE:CZ	0.40	2.51	8	1
1:A:96:LYS:CG	1:A:96:LYS:O	0.40	2.69	8	1
1:A:162:GLN:O	1:A:163:LYS:O	0.40	2.40	9	1
1:A:77:VAL:O	1:A:77:VAL:CG1	0.40	2.68	6	1
1:A:11:ASP:OD1	2:B:539:ASP:N	0.40	2.54	13	1
1:A:37:PHE:O	1:A:40:TYR:N	0.40	2.53	7	1
1:A:85:VAL:O	1:A:85:VAL:CG2	0.40	2.69	16	1
1:A:79:LEU:HD23	1:A:111:LEU:O	0.40	2.16	4	1
1:A:85:VAL:CG1	1:A:125:THR:HG21	0.40	2.46	19	1
1:A:63:ASP:C	1:A:64:TYR:CG	0.40	2.92	10	1
2:B:519:ILE:HD13	2:B:519:ILE:N	0.40	2.31	18	1
1:A:77:VAL:CG1	1:A:77:VAL:O	0.40	2.68	1	1
1:A:90:PHE:O	1:A:93:VAL:CG2	0.40	2.70	1	1
1:A:45:MET:SD	1:A:50:PRO:N	0.40	2.94	6	2
1:A:53:LEU:HD23	1:A:55:LEU:HG	0.40	1.93	6	1
1:A:44:VAL:HG23	1:A:52:THR:CG2	0.40	2.45	7	1
1:A:14:VAL:CG1	1:A:81:CYS:SG	0.40	3.09	11	1
1:A:8:VAL:CG2	1:A:14:VAL:HG13	0.40	2.46	11	1
1:A:113:VAL:CG2	4:A:185:GNP:O6	0.40	2.67	11	1
1:A:22:SER:HA	1:A:26:ASN:CB	0.40	2.46	16	1
1:A:4:ILE:HG21	1:A:176:ALA:C	0.40	2.36	4	1
1:A:89:SER:O	1:A:93:VAL:HG12	0.40	2.17	4	1
1:A:21:ILE:O	1:A:24:THR:N	0.40	2.53	20	1
1:A:174:LEU:CD1	2:B:505:LEU:HD22	0.40	2.39	20	1
1:A:119:LEU:N	1:A:119:LEU:CD1	0.40	2.84	17	1
1:A:14:VAL:CG2	5:A:188:HOH:O	0.40	2.68	17	1
1:A:168:VAL:HG23	1:A:169:PHE:N	0.40	2.31	17	1
1:A:38:ASP:N	1:A:57:ASP:OD1	0.40	2.54	19	1
1:A:64:TYR:O	1:A:67:LEU:CD2	0.40	2.69	10	1
1:A:115:THR:CB	1:A:157:CYS:O	0.40	2.69	18	1
1:A:77:VAL:CG1	1:A:175:ALA:HB3	0.40	2.46	18	1
1:A:53:LEU:HD21	2:B:513:PRO:HG3	0.40	1.93	18	1
1:A:133:LYS:HG3	1:A:134:GLN:N	0.40	2.31	9	1
1:A:4:ILE:CG2	1:A:177:LEU:HG	0.40	2.46	13	1
1:A:159:ALA:HA	1:A:165:LEU:HD12	0.40	1.93	7	1
2:B:510:ILE:HG22	2:B:510:ILE:O	0.40	2.16	7	1
1:A:66:ARG:O	1:A:67:LEU:CB	0.40	2.70	3	1
1:A:130:ALA:HB2	1:A:134:GLN:CG	0.40	2.47	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ILE:HG21	1:A:52:THR:HG23	0.40	1.92	11	1
1:A:16:LYS:HG3	1:A:17:THR:HG23	0.40	1.93	4	1
1:A:33:VAL:HG12	1:A:61:LEU:HD12	0.40	1.93	4	1
1:A:64:TYR:HB2	1:A:67:LEU:CD1	0.40	2.46	4	1
1:A:118:ASP:HB3	1:A:119:LEU:HD13	0.40	1.93	20	1
1:A:119:LEU:O	1:A:122:ASP:OD1	0.40	2.40	20	1
1:A:6:CYS:SG	1:A:55:LEU:CD2	0.40	3.10	20	1
1:A:45:MET:O	1:A:45:MET:CG	0.40	2.70	14	1
1:A:177:LEU:HB3	2:B:510:ILE:HD12	0.40	1.93	2	1
1:A:58:THR:OG1	1:A:67:LEU:CD1	0.40	2.69	1	1
1:A:77:VAL:HG13	1:A:109:PRO:HB2	0.40	1.93	8	1
1:A:160:LEU:HD12	1:A:160:LEU:N	0.40	2.32	8	1
1:A:69:PRO:O	1:A:72:TYR:O	0.40	2.40	8	1
1:A:82:PHE:HE1	1:A:137:ILE:HG21	0.40	1.71	6	1
1:A:58:THR:CG2	1:A:67:LEU:HD13	0.40	2.44	6	1
1:A:142:ALA:HB1	1:A:154:TYR:CD1	0.40	2.52	3	1
1:A:64:TYR:HB2	1:A:67:LEU:CG	0.40	2.46	11	1
1:A:157:CYS:SG	1:A:167:ASN:CB	0.40	3.10	16	1
1:A:155:VAL:CG2	1:A:171:GLU:OE2	0.40	2.68	16	1
1:A:22:SER:HA	1:A:26:ASN:HA	0.40	1.92	18	1
1:A:2:GLN:CG	2:B:510:ILE:CD1	0.40	3.00	18	1
1:A:45:MET:CE	1:A:46:ILE:C	0.40	2.90	18	1
1:A:32:TYR:OH	4:A:185:GNP:O2A	0.40	2.40	8	1
1:A:37:PHE:CB	2:B:522:GLY:HA2	0.40	2.46	8	1
1:A:56:PHE:CE1	1:A:169:PHE:CE1	0.40	3.09	12	1
4:A:185:GNP:O5'	2:B:537:ARG:NE	0.40	2.54	12	1
1:A:71:SER:C	1:A:72:TYR:CD2	0.40	2.95	12	1
1:A:88:SER:N	1:A:133:LYS:HB2	0.40	2.32	9	1
1:A:28:PHE:CE1	4:A:185:GNP:O1A	0.40	2.74	9	1
1:A:72:TYR:O	1:A:72:TYR:CG	0.40	2.72	15	1
1:A:71:SER:O	1:A:104:HIS:CD2	0.40	2.74	3	1
1:A:58:THR:O	1:A:67:LEU:CD1	0.40	2.67	3	1
1:A:7:VAL:CG1	2:B:540:GLU:OE2	0.40	2.67	3	1
1:A:28:PHE:CE2	1:A:160:LEU:HB3	0.40	2.51	11	1
1:A:33:VAL:N	1:A:34:PRO:HD2	0.40	2.30	11	1
2:B:512:GLN:N	2:B:513:PRO:CD	0.40	2.85	16	1
1:A:14:VAL:CG2	1:A:81:CYS:SG	0.40	3.10	20	1
2:B:532:TRP:NE1	2:B:537:ARG:CZ	0.40	2.85	20	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	182/184 (99%)	127±4 (70±2%)	40±5 (22±3%)	16±3 (9±2%)	2	13
2	B	42/44 (95%)	19±2 (45±5%)	15±2 (35±6%)	9±2 (21±5%)	0	2
All	All	4480/4560 (98%)	2907 (65%)	1086 (24%)	487 (11%)	1	9

All 96 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	152	VAL	20
1	A	134	GLN	18
1	A	47	GLY	18
1	A	50	PRO	17
1	A	33	VAL	17
2	B	514	LEU	16
1	A	48	GLY	15
1	A	151	ALA	14
1	A	14	VAL	13
2	B	512	GLN	11
2	B	536	ASP	11
1	A	2	GLN	10
2	B	509	ASP	10
2	B	507	ALA	9
1	A	137	ILE	9
1	A	85	VAL	9
2	B	531	CYS	9
1	A	107	LYS	9
1	A	67	LEU	8
1	A	68	ARG	8
1	A	28	PHE	8
1	A	40	TYR	8
2	B	523	HIS	7
2	B	543	LEU	7
1	A	84	VAL	7
2	B	508	GLN	7

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Mol	Chain	Res	Type	Models (Total)
1	A	35	THR	6
1	A	75	THR	6
2	B	520	HIS	6
2	B	522	GLY	6
2	B	505	LEU	6
2	B	535	PRO	6
2	B	527	ASP	6
2	B	525	ASP	6
2	B	506	SER	6
1	A	106	PRO	6
1	A	44	VAL	5
1	A	30	SER	5
2	B	528	PRO	5
1	A	153	LYS	5
1	A	15	GLY	4
2	B	533	GLY	4
1	A	55	LEU	4
2	B	544	GLY	4
1	A	18	CYS	4
1	A	38	ASP	4
1	A	72	TYR	3
2	B	532	TRP	3
2	B	539	ASP	3
2	B	513	PRO	3
2	B	524	GLY	3
1	A	64	TYR	3
1	A	34	PRO	3
1	A	12	GLY	3
2	B	503	SER	3
1	A	179	PRO	3
2	B	521	THR	3
2	B	515	GLN	2
2	B	510	ILE	2
1	A	159	ALA	2
1	A	162	GLN	2
1	A	26	ASN	2
1	A	36	VAL	2
1	A	77	VAL	2
2	B	540	GLU	2
1	A	27	LYS	2
1	A	19	LEU	2
2	B	530	HIS	2

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Mol	Chain	Res	Type	Models (Total)
2	B	504	GLY	2
1	A	54	GLY	2
2	B	538	ILE	2
1	A	60	GLY	2
1	A	21	ILE	2
1	A	167	ASN	1
1	A	163	LYS	1
1	A	164	GLY	1
1	A	165	LEU	1
2	B	537	ARG	1
1	A	37	PHE	1
1	A	25	THR	1
1	A	39	ASN	1
1	A	180	PRO	1
2	B	511	SER	1
2	B	526	SER	1
1	A	90	PHE	1
1	A	87	PRO	1
1	A	182	PRO	1
1	A	116	GLN	1
1	A	94	LYS	1
1	A	62	GLU	1
1	A	69	PRO	1
1	A	133	LYS	1
1	A	150	LYS	1
1	A	46	ILE	1
2	B	519	ILE	1
1	A	73	PRO	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	164/164 (100%)	118±5 (72±3%)	46±5 (28±3%)	2	20
2	B	37/37 (100%)	25±3 (68±9%)	12±3 (32±9%)	1	13
All	All	4020/4020 (100%)	2861 (71%)	1159 (29%)	2	19

All 168 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	126	ILE	20
1	A	117	ILE	20
1	A	70	LEU	19
1	A	167	ASN	17
1	A	88	SER	17
1	A	66	ARG	17
2	B	505	LEU	17
1	A	115	THR	17
1	A	3	THR	16
1	A	108	THR	16
1	A	160	LEU	15
1	A	64	TYR	15
1	A	33	VAL	15
1	A	45	MET	15
1	A	26	ASN	14
1	A	52	THR	14
1	A	153	LYS	14
1	A	165	LEU	13
1	A	37	PHE	13
1	A	178	GLU	13
1	A	53	LEU	13
2	B	506	SER	12
2	B	520	HIS	12
2	B	537	ARG	12
1	A	120	ARG	12
1	A	56	PHE	11
2	B	512	GLN	11
1	A	4	ILE	11
2	B	543	LEU	11
2	B	521	THR	11
1	A	40	TYR	11
1	A	128	LYS	10
1	A	86	SER	10
1	A	137	ILE	10
1	A	166	LYS	10
1	A	68	ARG	10
2	B	518	PHE	10
1	A	55	LEU	10
1	A	183	LYS	10
1	A	19	LEU	9
1	A	83	SER	9

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Mol	Chain	Res	Type	Models (Total)
2	B	515	GLN	9
2	B	541	LEU	9
1	A	97	TRP	9
1	A	169	PHE	9
1	A	78	PHE	9
2	B	514	LEU	9
2	B	530	HIS	9
1	A	163	LYS	9
1	A	24	THR	9
2	B	527	ASP	9
1	A	184	LYS	9
1	A	124	SER	9
1	A	58	THR	9
1	A	145	LEU	9
1	A	107	LYS	9
2	B	517	SER	9
1	A	30	SER	8
1	A	16	LYS	8
1	A	61	LEU	8
2	B	540	GLU	8
1	A	63	ASP	8
1	A	149	LEU	8
1	A	105	CYS	8
1	A	94	LYS	8
1	A	150	LYS	8
1	A	28	PHE	8
1	A	57	ASP	8
1	A	103	HIS	7
1	A	11	ASP	7
1	A	49	GLU	7
2	B	526	SER	7
1	A	1	MET	7
1	A	133	LYS	7
2	B	503	SER	7
1	A	65	ASP	7
2	B	542	TYR	7
2	B	529	ARG	7
1	A	71	SER	7
1	A	72	TYR	6
1	A	6	CYS	6
1	A	162	GLN	6
1	A	96	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	67	LEU	6
2	B	523	HIS	6
2	B	536	ASP	6
1	A	27	LYS	6
1	A	62	GLU	6
1	A	74	GLN	6
1	A	116	GLN	6
1	A	111	LEU	6
1	A	144	LYS	6
2	B	525	ASP	6
1	A	122	ASP	5
1	A	79	LEU	5
1	A	5	LYS	5
1	A	92	ASN	5
1	A	143	GLU	5
1	A	20	LEU	5
1	A	90	PHE	5
1	A	158	SER	5
1	A	7	VAL	5
1	A	121	ASP	5
2	B	508	GLN	5
1	A	2	GLN	5
1	A	173	ILE	5
2	B	532	TRP	4
1	A	36	VAL	4
1	A	95	GLU	4
1	A	39	ASN	4
1	A	31	GLU	4
1	A	91	GLU	4
1	A	155	VAL	4
1	A	161	THR	4
2	B	539	ASP	4
1	A	170	ASP	4
1	A	135	LYS	4
1	A	43	THR	4
1	A	76	ASP	4
1	A	156	GLU	4
1	A	100	GLU	4
1	A	131	LYS	4
1	A	134	GLN	3
1	A	14	VAL	3
1	A	147	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	110	PHE	3
1	A	119	LEU	3
1	A	8	VAL	3
2	B	509	ASP	3
1	A	17	THR	3
2	B	531	CYS	3
1	A	89	SER	3
1	A	127	GLU	3
1	A	171	GLU	3
2	B	538	ILE	3
1	A	104	HIS	3
1	A	177	LEU	3
2	B	519	ILE	3
1	A	148	ASP	3
1	A	138	THR	2
1	A	51	TYR	2
1	A	42	VAL	2
2	B	545	ASN	2
1	A	85	VAL	2
1	A	118	ASP	2
1	A	112	LEU	2
2	B	511	SER	2
1	A	140	GLU	2
1	A	25	THR	2
2	B	534	PHE	2
1	A	46	ILE	2
1	A	181	GLU	2
1	A	38	ASP	2
1	A	157	CYS	2
1	A	44	VAL	1
1	A	75	THR	1
1	A	22	SER	1
1	A	113	VAL	1
2	B	510	ILE	1
1	A	141	THR	1
1	A	101	ILE	1
1	A	132	ASN	1
1	A	174	LEU	1
1	A	18	CYS	1
1	A	81	CYS	1
2	B	516	ASN	1
1	A	23	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	80	VAL	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	GNP	A	185	3	29,34,34	1.64±0.01	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	GNP	A	185	3	27,54,54	1.62±0.02	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GNP	A	185	3	-	0±0,13,38,38	0±0,3,3,3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	185	GNP	O1G-PG-N3B-PB	3
4	A	185	GNP	O1B-PB-N3B-PG	2

There are no ring outliers.

## 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 63% for the well-defined parts and 63% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 4700

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	1988
Number of shifts mapped to atoms	1988
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	184	$-0.23 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	150	$0.53 \pm 0.13$	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	165	$2.23 \pm 0.49$	Should be applied

#### 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 63%, i.e. 1729 atoms were assigned a chemical shift out of a possible 2752. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	689/1104 (62%)	340/438 (78%)	184/456 (40%)	165/210 (79%)
Sidechain	927/1430 (65%)	585/839 (70%)	333/541 (62%)	9/50 (18%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	113/218 (52%)	66/114 (58%)	46/92 (50%)	1/12 (8%)
Overall	1729/2752 (63%)	991/1391 (71%)	563/1089 (52%)	175/272 (64%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 63%, i.e. 1729 atoms were assigned a chemical shift out of a possible 2752. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	689/1104 (62%)	340/438 (78%)	184/456 (40%)	165/210 (79%)
Sidechain	927/1430 (65%)	585/839 (70%)	333/541 (62%)	9/50 (18%)
Aromatic	113/218 (52%)	66/114 (58%)	46/92 (50%)	1/12 (8%)
Overall	1729/2752 (63%)	991/1391 (71%)	563/1089 (52%)	175/272 (64%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

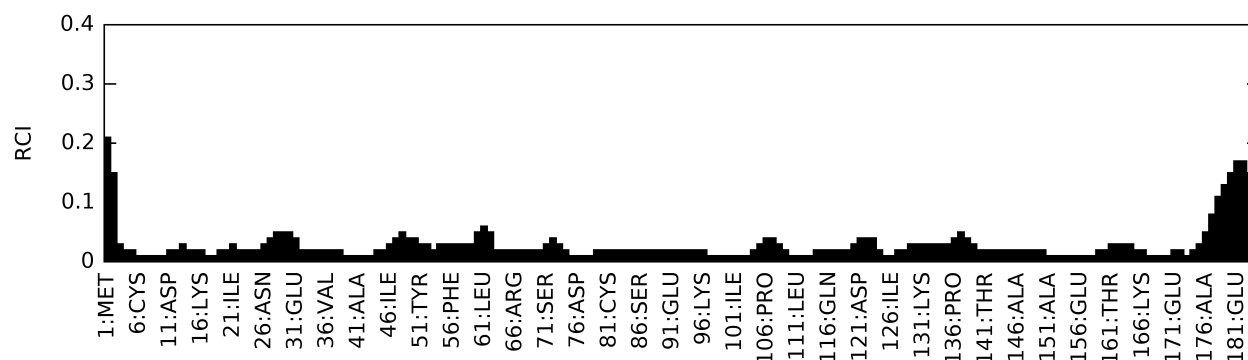
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	92	ASN	HD22	10.33	9.59 – 4.69	6.5
1	A	10	GLY	HA3	1.71	5.80 – 2.00	-5.8
1	A	63	ASP	HB3	1.16	4.07 – 1.27	-5.4

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



## 7.2 Chemical shift list 2

File name: BMRB entry 4700

Chemical shift list name: *assigned\_chem\_shift\_list\_2*

### 7.2.1 Bookkeeping [i](#)

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

Total number of shifts	527
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	527
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Chain not found in structure. All 527 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	30	GLN	HE21	6.991	0.005	2
UNMAPPED	39	ASN	HA	4.798	0.012	1
UNMAPPED	42	LYS	HE2	3.048	0.018	1
UNMAPPED	27	MET	HG2	2.593	0.017	2
UNMAPPED	42	LYS	HD3	1.729	0.018	1
UNMAPPED	21	THR	CA	61.64	0.03	1
UNMAPPED	8	ASP	CA	54.93	0.09	1
UNMAPPED	41	THR	H	8.274	0.012	1
UNMAPPED	9	PHE	CE1	131.24	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	16	GLY	HA2	4.641	0.005	2
UNMAPPED	14	HIS	HE1	8.415	0.0	1
UNMAPPED	21	THR	HG23	1.177	0.011	1
UNMAPPED	27	MET	CA	53.39	0.08	1
UNMAPPED	14	HIS	HA	5.474	0.005	1
UNMAPPED	27	MET	CG	31.87	0.06	1
UNMAPPED	7	SER	HA	4.787	0.007	1
UNMAPPED	38	SER	H	8.226	0.014	1
UNMAPPED	35	LEU	HD13	0.744	0.01	2
UNMAPPED	13	ILE	HB	1.605	0.01	1
UNMAPPED	29	GLU	HG3	2.32	0.013	2
UNMAPPED	45	GLN	HB3	2.033	0.015	2
UNMAPPED	37	THR	CG2	21.41	0.05	1
UNMAPPED	32	ALA	HB3	1.503	0.02	1
UNMAPPED	32	ALA	N	121.03	0.04	1
UNMAPPED	32	ALA	CB	17.73	0.05	1
UNMAPPED	27	MET	HB2	2.038	0.019	2
UNMAPPED	30	GLN	HA	4.122	0.014	1
UNMAPPED	42	LYS	HG2	1.49	0.019	2
UNMAPPED	5	LEU	H	8.234	0.011	1
UNMAPPED	45	GLN	CB	29.28	0.06	1
UNMAPPED	20	VAL	H	8.265	0.015	1
UNMAPPED	7	SER	N	115.25	0.02	1
UNMAPPED	25	THR	CA	59.73	0.04	1
UNMAPPED	12	THR	HB	3.955	0.013	1
UNMAPPED	13	ILE	H	7.37	0.021	1
UNMAPPED	42	LYS	HA	4.407	0.017	1
UNMAPPED	17	PHE	HB2	2.848	0.003	2
UNMAPPED	15	VAL	HG11	1.018	0.016	2
UNMAPPED	4	SER	CB	65.76	0.03	1
UNMAPPED	36	GLN	CA	56.73	0.04	1
UNMAPPED	4	SER	N	125.93	0.04	1
UNMAPPED	18	ASP	N	128.17	0.05	1
UNMAPPED	30	GLN	HG3	2.494	0.012	2
UNMAPPED	5	LEU	HD21	1.133	0.002	2
UNMAPPED	20	VAL	HG22	1.034	0.01	2
UNMAPPED	39	ASN	HD21	6.968	0.012	2
UNMAPPED	23	GLU	CB	32.1	0.03	1
UNMAPPED	5	LEU	HD13	1.06	0.003	2
UNMAPPED	23	GLU	HB3	1.705	0.015	2
UNMAPPED	21	THR	CG2	21.51	0.07	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	46	LYS	CB	33.5	0.06	1
UNMAPPED	6	PRO	HB2	1.827	0.018	2
UNMAPPED	31	TRP	HA	4.568	0.014	1
UNMAPPED	44	GLU	HA	4.359	0.012	1
UNMAPPED	27	MET	HE3	1.656	0.015	1
UNMAPPED	36	GLN	H	7.759	0.012	1
UNMAPPED	3	ILE	CB	39.19	0.08	1
UNMAPPED	33	ARG	HA	4.188	0.011	1
UNMAPPED	8	ASP	HB2	2.879	0.017	1
UNMAPPED	41	THR	HB	4.241	0.008	1
UNMAPPED	19	ALA	HA	3.867	0.011	1
UNMAPPED	37	THR	CA	62.39	0.1	1
UNMAPPED	41	THR	CB	69.71	0.15	1
UNMAPPED	33	ARG	HG2	1.815	0.01	2
UNMAPPED	36	GLN	HA	4.382	0.008	1
UNMAPPED	7	SER	HB3	3.746	0.009	2
UNMAPPED	15	VAL	HG23	1.145	0.016	2
UNMAPPED	33	ARG	HD3	3.27	0.015	1
UNMAPPED	33	ARG	CA	58.42	0.08	1
UNMAPPED	15	VAL	CB	32.15	0.02	1
UNMAPPED	33	ARG	CG	27.19	0.06	1
UNMAPPED	41	THR	HG23	1.255	0.01	1
UNMAPPED	3	ILE	HD13	0.84	0.013	1
UNMAPPED	24	PHE	CA	57.8	0.03	1
UNMAPPED	40	ILE	H	8.127	0.013	1
UNMAPPED	19	ALA	HB2	1.523	0.012	1
UNMAPPED	11	HIS	HB3	2.891	0.016	2
UNMAPPED	44	GLU	HB3	1.976	0.007	2
UNMAPPED	20	VAL	CG2	22.07	0.05	2
UNMAPPED	35	LEU	HD21	0.767	0.014	2
UNMAPPED	4	SER	HB2	4.002	0.01	1
UNMAPPED	26	GLY	HA2	4.451	0.013	2
UNMAPPED	33	ARG	HE	7.457	0.017	1
UNMAPPED	5	LEU	HG	1.802	0.008	1
UNMAPPED	27	MET	HG3	2.469	0.012	2
UNMAPPED	3	ILE	HG21	1.036	0.019	1
UNMAPPED	35	LEU	H	7.996	0.014	1
UNMAPPED	36	GLN	NE2	111.39	0.04	1
UNMAPPED	5	LEU	HA	4.496	0.013	1
UNMAPPED	46	LYS	HE3	3.031	0.013	1
UNMAPPED	16	GLY	HA3	3.557	0.013	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	21	THR	HG22	1.177	0.011	1
UNMAPPED	7	SER	H	9.163	0.015	1
UNMAPPED	6	PRO	CA	62.56	0.04	1
UNMAPPED	33	ARG	H	7.893	0.012	1
UNMAPPED	44	GLU	CA	56.26	0.04	1
UNMAPPED	42	LYS	CD	28.84	0.02	1
UNMAPPED	13	ILE	HA	4.37	0.018	1
UNMAPPED	13	ILE	CB	41.76	0.07	1
UNMAPPED	13	ILE	HD12	0.755	0.015	1
UNMAPPED	44	GLU	CG	35.99	0.1	1
UNMAPPED	5	LEU	CD2	22.7	0.09	2
UNMAPPED	5	LEU	CD1	25.04	0.08	2
UNMAPPED	14	HIS	CA	55.0	0.05	1
UNMAPPED	12	THR	HG23	1.09	0.018	1
UNMAPPED	13	ILE	HG13	1.093	0.021	2
UNMAPPED	42	LYS	CA	56.21	0.03	1
UNMAPPED	32	ALA	HB2	1.503	0.02	1
UNMAPPED	34	LEU	HB2	1.912	0.018	2
UNMAPPED	16	GLY	CA	43.0	0.05	1
UNMAPPED	14	HIS	CB	31.01	0.01	1
UNMAPPED	30	GLN	CA	58.55	0.02	1
UNMAPPED	13	ILE	HG12	1.522	0.018	2
UNMAPPED	3	ILE	CG1	28.21	0.11	1
UNMAPPED	23	GLU	H	7.126	0.011	1
UNMAPPED	16	GLY	N	114.32	0.03	1
UNMAPPED	46	LYS	H	8.092	0.021	1
UNMAPPED	15	VAL	HA	4.91	0.014	1
UNMAPPED	44	GLU	H	8.523	0.014	1
UNMAPPED	2	SER	HB3	3.894	0.017	1
UNMAPPED	34	LEU	HD21	0.91	0.0	2
UNMAPPED	9	PHE	HE2	7.015	0.009	1
UNMAPPED	8	ASP	CB	38.73	0.06	1
UNMAPPED	9	PHE	CA	59.44	0.03	1
UNMAPPED	10	GLU	HG3	2.044	0.015	2
UNMAPPED	4	SER	CA	59.02	0.05	1
UNMAPPED	11	HIS	CE1	136.12	0.0	1
UNMAPPED	18	ASP	CA	52.08	0.04	1
UNMAPPED	24	PHE	HZ	7.32	0.014	1
UNMAPPED	31	TRP	HE3	7.268	0.017	1
UNMAPPED	30	GLN	HG2	2.568	0.012	2
UNMAPPED	24	PHE	CD1	131.99	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	20	VAL	HG21	1.034	0.01	2
UNMAPPED	21	THR	HA	4.291	0.023	1
UNMAPPED	37	THR	HG21	1.306	0.018	1
UNMAPPED	34	LEU	CD2	25.41	0.04	2
UNMAPPED	31	TRP	CZ3	119.7	0.08	1
UNMAPPED	20	VAL	N	117.67	0.05	1
UNMAPPED	13	ILE	HG22	0.866	0.014	1
UNMAPPED	23	GLU	HB2	2.055	0.015	2
UNMAPPED	34	LEU	H	7.616	0.012	1
UNMAPPED	39	ASN	CA	53.26	0.07	1
UNMAPPED	6	PRO	HB3	1.595	0.014	2
UNMAPPED	36	GLN	HB3	2.252	0.016	1
UNMAPPED	15	VAL	H	8.383	0.012	1
UNMAPPED	28	PRO	CD	50.29	0.07	1
UNMAPPED	17	PHE	N	119.22	0.01	1
UNMAPPED	29	GLU	HA	4.022	0.009	1
UNMAPPED	35	LEU	HG	1.737	0.007	1
UNMAPPED	28	PRO	CB	31.84	0.02	1
UNMAPPED	29	GLU	CG	35.68	0.05	1
UNMAPPED	24	PHE	CE2	131.13	0.1	1
UNMAPPED	45	GLN	CG	33.66	0.08	1
UNMAPPED	24	PHE	HE1	7.302	0.011	1
UNMAPPED	38	SER	N	116.96	0.05	1
UNMAPPED	20	VAL	HG11	0.926	0.014	2
UNMAPPED	37	THR	N	112.8	0.04	1
UNMAPPED	38	SER	CB	63.55	0.04	1
UNMAPPED	25	THR	HG23	1.135	0.013	1
UNMAPPED	15	VAL	HG22	1.145	0.016	2
UNMAPPED	18	ASP	HA	4.588	0.007	1
UNMAPPED	33	ARG	CB	29.9	0.06	1
UNMAPPED	40	ILE	CB	38.46	0.03	1
UNMAPPED	35	LEU	CA	55.95	0.04	1
UNMAPPED	24	PHE	HD2	7.502	0.012	1
UNMAPPED	41	THR	HG22	1.255	0.01	1
UNMAPPED	40	ILE	N	120.33	0.01	1
UNMAPPED	25	THR	HB	4.241	0.009	1
UNMAPPED	19	ALA	HB3	1.523	0.012	1
UNMAPPED	18	ASP	HB3	2.237	0.011	2
UNMAPPED	45	GLN	CA	55.68	0.06	1
UNMAPPED	9	PHE	HD1	6.91	0.011	1
UNMAPPED	17	PHE	HD2	6.49	0.007	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	20	VAL	CG1	20.66	0.07	2
UNMAPPED	11	HIS	CD2	116.65	0.05	1
UNMAPPED	3	ILE	HG22	1.036	0.019	1
UNMAPPED	46	LYS	HE2	3.031	0.013	1
UNMAPPED	45	GLN	N	121.82	0.02	1
UNMAPPED	2	SER	CA	58.11	0.03	1
UNMAPPED	34	LEU	CA	56.89	0.06	1
UNMAPPED	9	PHE	HA	4.883	0.009	1
UNMAPPED	6	PRO	HA	5.067	0.005	1
UNMAPPED	31	TRP	HB2	3.26	0.024	2
UNMAPPED	7	SER	CA	57.03	0.06	1
UNMAPPED	8	ASP	H	8.796	0.013	1
UNMAPPED	42	LYS	N	123.86	0.06	1
UNMAPPED	13	ILE	HD13	0.755	0.015	1
UNMAPPED	7	SER	CB	66.27	0.08	1
UNMAPPED	41	THR	CG2	21.46	0.03	1
UNMAPPED	9	PHE	CZ	128.47	0.08	1
UNMAPPED	42	LYS	CB	32.84	0.05	1
UNMAPPED	17	PHE	CE2	130.43	0.02	1
UNMAPPED	32	ALA	HB1	1.503	0.02	1
UNMAPPED	9	PHE	HB3	2.73	0.014	2
UNMAPPED	12	THR	H	8.066	0.021	1
UNMAPPED	44	GLU	CB	30.17	0.04	1
UNMAPPED	15	VAL	CG2	22.45	0.06	2
UNMAPPED	3	ILE	CG2	17.96	0.05	1
UNMAPPED	35	LEU	CD2	25.28	0.04	2
UNMAPPED	10	GLU	N	126.68	0.08	1
UNMAPPED	34	LEU	CB	41.98	0.06	1
UNMAPPED	15	VAL	HB	2.099	0.017	1
UNMAPPED	2	SER	HB2	3.894	0.017	1
UNMAPPED	34	LEU	HD11	0.904	0.011	2
UNMAPPED	34	LEU	HD22	0.91	0.0	2
UNMAPPED	34	LEU	HD13	0.904	0.011	2
UNMAPPED	34	LEU	HD12	0.904	0.011	2
UNMAPPED	31	TRP	NE1	127.27	0.01	1
UNMAPPED	43	SER	HB3	3.901	0.012	1
UNMAPPED	9	PHE	CD1	131.27	0.02	1
UNMAPPED	42	LYS	HB2	1.909	0.014	2
UNMAPPED	29	GLU	HB3	2.032	0.01	2
UNMAPPED	38	SER	HA	4.548	0.012	1
UNMAPPED	5	LEU	CG	27.59	0.08	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	12	THR	CG2	22.36	0.06	1
UNMAPPED	5	LEU	HB2	1.746	0.018	2
UNMAPPED	20	VAL	CA	65.4	0.07	1
UNMAPPED	5	LEU	CA	62.56	0.0	1
UNMAPPED	13	ILE	CG1	26.71	0.07	1
UNMAPPED	31	TRP	CZ2	113.31	0.06	1
UNMAPPED	23	GLU	N	117.37	0.02	1
UNMAPPED	13	ILE	HG23	0.866	0.014	1
UNMAPPED	46	LYS	N	128.51	0.02	1
UNMAPPED	39	ASN	CB	38.6	0.07	1
UNMAPPED	36	GLN	N	117.83	0.03	1
UNMAPPED	26	GLY	CA	45.71	0.06	1
UNMAPPED	22	GLY	N	111.68	0.05	1
UNMAPPED	28	PRO	CG	26.85	0.05	1
UNMAPPED	31	TRP	HD1	6.907	0.005	1
UNMAPPED	27	MET	HE1	1.656	0.015	1
UNMAPPED	40	ILE	HD12	0.902	0.014	1
UNMAPPED	23	GLU	HG2	2.228	0.018	2
UNMAPPED	19	ALA	CA	53.74	0.03	1
UNMAPPED	13	ILE	CD1	12.15	0.05	1
UNMAPPED	25	THR	HG22	1.135	0.013	1
UNMAPPED	41	THR	N	118.12	0.03	1
UNMAPPED	36	GLN	CB	28.6	0.04	1
UNMAPPED	15	VAL	HG21	1.145	0.016	2
UNMAPPED	30	GLN	NE2	111.6	0.03	1
UNMAPPED	11	HIS	CB	29.4	0.07	1
UNMAPPED	17	PHE	HA	4.93	0.009	1
UNMAPPED	38	SER	HB3	3.945	0.016	2
UNMAPPED	35	LEU	N	118.5	0.01	1
UNMAPPED	15	VAL	N	127.78	0.07	1
UNMAPPED	35	LEU	CB	42.08	0.05	1
UNMAPPED	41	THR	HG21	1.255	0.01	1
UNMAPPED	3	ILE	HD11	0.84	0.013	1
UNMAPPED	6	PRO	HD2	3.487	0.021	2
UNMAPPED	17	PHE	H	8.605	0.013	1
UNMAPPED	42	LYS	H	8.404	0.013	1
UNMAPPED	18	ASP	HB2	2.899	0.015	2
UNMAPPED	6	PRO	HG3	0.745	0.022	2
UNMAPPED	12	THR	N	119.09	0.12	1
UNMAPPED	30	GLN	HE22	7.595	0.003	2
UNMAPPED	17	PHE	HD1	6.49	0.007	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	35	LEU	HD23	0.767	0.014	2
UNMAPPED	12	THR	CB	68.44	0.07	1
UNMAPPED	31	TRP	CA	58.09	0.03	1
UNMAPPED	37	THR	H	8.074	0.014	1
UNMAPPED	3	ILE	HG23	1.036	0.019	1
UNMAPPED	5	LEU	HD23	1.133	0.002	2
UNMAPPED	9	PHE	CE2	131.24	0.05	1
UNMAPPED	27	MET	CB	33.08	0.04	1
UNMAPPED	30	GLN	HB2	2.138	0.017	1
UNMAPPED	6	PRO	CG	26.7	0.09	1
UNMAPPED	31	TRP	HB3	3.113	0.017	2
UNMAPPED	42	LYS	CE	41.93	0.05	1
UNMAPPED	12	THR	HG22	1.09	0.018	1
UNMAPPED	17	PHE	CE1	130.43	0.02	1
UNMAPPED	9	PHE	HB2	2.903	0.029	2
UNMAPPED	24	PHE	HB3	3.012	0.011	2
UNMAPPED	32	ALA	CA	55.25	0.05	1
UNMAPPED	36	GLN	HB2	2.252	0.016	1
UNMAPPED	30	GLN	CG	33.54	0.03	1
UNMAPPED	17	PHE	HE1	6.935	0.002	1
UNMAPPED	15	VAL	CG1	22.93	0.03	2
UNMAPPED	31	TRP	HZ2	6.901	0.008	1
UNMAPPED	25	THR	N	114.56	0.06	1
UNMAPPED	35	LEU	CD1	22.67	0.06	2
UNMAPPED	40	ILE	CG1	27.05	0.03	1
UNMAPPED	39	ASN	H	8.449	0.014	1
UNMAPPED	35	LEU	HB2	1.781	0.012	2
UNMAPPED	34	LEU	HD23	0.91	0.0	2
UNMAPPED	15	VAL	HG12	1.018	0.016	2
UNMAPPED	8	ASP	N	115.82	0.04	1
UNMAPPED	14	HIS	H	8.876	0.013	1
UNMAPPED	27	MET	HA	4.307	0.018	1
UNMAPPED	31	TRP	HE1	9.778	0.003	1
UNMAPPED	30	GLN	H	9.128	0.019	1
UNMAPPED	43	SER	HB2	3.901	0.012	1
UNMAPPED	37	THR	HB	4.4	0.006	1
UNMAPPED	42	LYS	HB3	1.82	0.01	2
UNMAPPED	29	GLU	HB2	2.132	0.014	2
UNMAPPED	17	PHE	CD1	131.47	0.02	1
UNMAPPED	5	LEU	N	117.35	0.02	1
UNMAPPED	39	ASN	HD22	7.647	0.015	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	33	ARG	HB2	1.95	0.015	1
UNMAPPED	5	LEU	HB3	1.693	0.013	2
UNMAPPED	35	LEU	HB3	1.659	0.011	2
UNMAPPED	23	GLU	CA	54.49	0.04	1
UNMAPPED	13	ILE	CG2	17.4	0.02	1
UNMAPPED	23	GLU	CG	35.52	0.04	1
UNMAPPED	10	GLU	H	8.676	0.015	1
UNMAPPED	26	GLY	N	109.88	0.05	1
UNMAPPED	13	ILE	HG21	0.866	0.014	1
UNMAPPED	46	LYS	CE	41.94	0.01	1
UNMAPPED	22	GLY	HA3	3.545	0.012	2
UNMAPPED	40	ILE	HG13	1.236	0.015	2
UNMAPPED	35	LEU	HA	4.232	0.013	1
UNMAPPED	5	LEU	HD11	1.06	0.003	2
UNMAPPED	17	PHE	CB	42.26	0.05	1
UNMAPPED	46	LYS	HA	4.213	0.018	1
UNMAPPED	31	TRP	CD1	123.17	0.02	1
UNMAPPED	20	VAL	HB	2.323	0.011	1
UNMAPPED	3	ILE	CA	60.75	0.05	1
UNMAPPED	44	GLU	HG3	2.31	0.012	1
UNMAPPED	46	LYS	HD2	1.706	0.008	1
UNMAPPED	23	GLU	HG3	2.138	0.015	2
UNMAPPED	37	THR	CB	69.5	0.14	1
UNMAPPED	19	ALA	CB	18.45	0.07	1
UNMAPPED	41	THR	CA	61.85	0.03	1
UNMAPPED	40	ILE	HG21	0.956	0.012	1
UNMAPPED	17	PHE	HZ	7.143	0.011	1
UNMAPPED	39	ASN	HB3	2.831	0.007	2
UNMAPPED	46	LYS	CG	24.52	0.02	1
UNMAPPED	17	PHE	CZ	128.98	0.01	1
UNMAPPED	24	PHE	CZ	129.3	0.04	1
UNMAPPED	31	TRP	CH2	123.41	0.04	1
UNMAPPED	27	MET	H	8.133	0.011	1
UNMAPPED	15	VAL	CA	60.14	0.06	1
UNMAPPED	40	ILE	HB	1.942	0.014	1
UNMAPPED	33	ARG	N	115.1	0.02	1
UNMAPPED	40	ILE	HA	4.269	0.008	1
UNMAPPED	24	PHE	N	118.85	0.04	1
UNMAPPED	33	ARG	NE	84.04	0.02	1
UNMAPPED	9	PHE	CB	39.45	0.01	1
UNMAPPED	45	GLN	HE21	6.912	0.001	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	24	PHE	CB	40.92	0.05	1
UNMAPPED	6	PRO	HD3	3.333	0.019	2
UNMAPPED	34	LEU	HA	4.225	0.018	1
UNMAPPED	19	ALA	HB1	1.523	0.012	1
UNMAPPED	6	PRO	HG2	1.412	0.002	2
UNMAPPED	43	SER	CB	63.71	0.02	1
UNMAPPED	31	TRP	N	117.85	0.04	1
UNMAPPED	34	LEU	HG	1.884	0.004	1
UNMAPPED	35	LEU	HD22	0.767	0.014	2
UNMAPPED	10	GLU	HB3	1.749	0.011	2
UNMAPPED	43	SER	N	117.03	0.01	1
UNMAPPED	31	TRP	CB	29.41	0.01	1
UNMAPPED	32	ALA	HA	4.044	0.015	1
UNMAPPED	23	GLU	HA	4.498	0.015	1
UNMAPPED	21	THR	HG21	1.177	0.011	1
UNMAPPED	20	VAL	HA	3.743	0.013	1
UNMAPPED	27	MET	CE	17.2	0.05	1
UNMAPPED	6	PRO	CB	32.22	0.09	1
UNMAPPED	30	GLN	HB3	2.138	0.017	1
UNMAPPED	35	LEU	HD11	0.744	0.01	2
UNMAPPED	46	LYS	HD3	1.706	0.008	1
UNMAPPED	6	PRO	CD	50.05	0.05	1
UNMAPPED	44	GLU	N	122.49	0.08	1
UNMAPPED	14	HIS	HB3	2.551	0.02	2
UNMAPPED	13	ILE	CA	59.89	0.05	1
UNMAPPED	14	HIS	N	125.58	0.01	1
UNMAPPED	4	SER	HA	4.544	0.004	1
UNMAPPED	29	GLU	N	127.11	0.04	1
UNMAPPED	13	ILE	HD11	0.755	0.015	1
UNMAPPED	12	THR	HG21	1.09	0.018	1
UNMAPPED	9	PHE	N	116.56	0.05	1
UNMAPPED	39	ASN	ND2	112.18	0.02	1
UNMAPPED	24	PHE	HB2	3.145	0.019	2
UNMAPPED	30	GLN	CB	27.8	0.02	1
UNMAPPED	10	GLU	HA	4.201	0.014	1
UNMAPPED	40	ILE	HD13	0.902	0.014	1
UNMAPPED	43	SER	HA	4.514	0.025	1
UNMAPPED	21	THR	H	7.363	0.016	1
UNMAPPED	30	GLN	N	115.8	0.06	1
UNMAPPED	17	PHE	CA	57.19	0.1	1
UNMAPPED	36	GLN	HG3	2.514	0.012	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	17	PHE	HE2	6.935	0.002	1
UNMAPPED	31	TRP	HZ3	6.042	0.01	1
UNMAPPED	24	PHE	HE2	7.302	0.011	1
UNMAPPED	40	ILE	CG2	17.34	0.05	1
UNMAPPED	10	GLU	CB	33.41	0.05	1
UNMAPPED	46	LYS	HG3	1.427	0.004	1
UNMAPPED	34	LEU	N	119.6	0.04	1
UNMAPPED	11	HIS	HD2	7.018	0.021	1
UNMAPPED	26	GLY	H	8.786	0.01	1
UNMAPPED	28	PRO	HD3	3.022	0.013	2
UNMAPPED	14	HIS	CE1	137.57	0.03	1
UNMAPPED	1	GLY	HA3	3.836	0.031	2
UNMAPPED	24	PHE	HA	5.477	0.009	1
UNMAPPED	45	GLN	HG3	2.387	0.019	1
UNMAPPED	9	PHE	HE1	7.015	0.009	1
UNMAPPED	28	PRO	HG2	1.32	0.018	2
UNMAPPED	15	VAL	HG13	1.018	0.016	2
UNMAPPED	36	GLN	CG	33.67	0.02	1
UNMAPPED	11	HIS	CA	51.74	0.01	1
UNMAPPED	18	ASP	CB	41.73	0.05	1
UNMAPPED	24	PHE	CD2	131.99	0.01	1
UNMAPPED	3	ILE	CD1	13.65	0.05	1
UNMAPPED	37	THR	HA	4.418	0.028	1
UNMAPPED	19	ALA	H	8.571	0.014	1
UNMAPPED	21	THR	HB	4.251	0.027	1
UNMAPPED	17	PHE	CD2	131.47	0.02	1
UNMAPPED	33	ARG	HB3	1.95	0.015	1
UNMAPPED	34	LEU	CD1	22.64	0.06	2
UNMAPPED	25	THR	H	8.977	0.015	1
UNMAPPED	44	GLU	HG2	2.31	0.012	1
UNMAPPED	3	ILE	HG13	0.923	0.002	2
UNMAPPED	39	ASN	N	120.37	0.02	1
UNMAPPED	22	GLY	HA2	4.022	0.013	2
UNMAPPED	28	PRO	CA	62.76	0.08	1
UNMAPPED	40	ILE	HG12	1.511	0.016	2
UNMAPPED	29	GLU	CB	29.11	0.03	1
UNMAPPED	24	PHE	CE1	131.13	0.1	1
UNMAPPED	42	LYS	HE3	3.048	0.018	1
UNMAPPED	24	PHE	H	8.79	0.012	1
UNMAPPED	3	ILE	N	124.45	0.06	1
UNMAPPED	25	THR	HG21	1.135	0.013	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	11	HIS	H	8.998	0.014	1
UNMAPPED	43	SER	H	8.417	0.016	1
UNMAPPED	20	VAL	HG12	0.926	0.014	2
UNMAPPED	38	SER	CA	58.46	0.02	1
UNMAPPED	25	THR	CG2	21.05	0.05	1
UNMAPPED	31	TRP	H	7.279	0.013	1
UNMAPPED	31	TRP	HH2	5.415	0.017	1
UNMAPPED	40	ILE	HG22	0.956	0.012	1
UNMAPPED	28	PRO	HB3	1.028	0.02	2
UNMAPPED	36	GLN	HE21	6.942	0.003	2
UNMAPPED	39	ASN	HB2	2.912	0.009	2
UNMAPPED	3	ILE	HB	1.616	0.011	1
UNMAPPED	8	ASP	HA	4.337	0.008	1
UNMAPPED	24	PHE	HD1	7.502	0.012	1
UNMAPPED	1	GLY	CA	43.19	0.07	1
UNMAPPED	45	GLN	NE2	112.58	0.01	1
UNMAPPED	31	TRP	CE3	119.8	0.06	1
UNMAPPED	11	HIS	HE1	8.667	0.0	1
UNMAPPED	25	THR	HA	4.69	0.008	1
UNMAPPED	36	GLN	HE22	7.574	0.011	2
UNMAPPED	14	HIS	CD2	120.17	0.1	1
UNMAPPED	37	THR	HG22	1.306	0.018	1
UNMAPPED	9	PHE	HD2	6.91	0.011	1
UNMAPPED	43	SER	CA	58.25	0.07	1
UNMAPPED	9	PHE	H	8.117	0.013	1
UNMAPPED	10	GLU	HB2	1.859	0.015	2
UNMAPPED	42	LYS	HD2	1.729	0.018	1
UNMAPPED	21	THR	CB	69.9	0.02	1
UNMAPPED	42	LYS	HG3	1.454	0.015	2
UNMAPPED	21	THR	N	107.33	0.06	1
UNMAPPED	2	SER	N	115.49	0.04	1
UNMAPPED	2	SER	CB	63.58	0.09	1
UNMAPPED	27	MET	N	118.09	0.04	1
UNMAPPED	35	LEU	HD12	0.744	0.01	2
UNMAPPED	13	ILE	N	117.85	0.05	1
UNMAPPED	29	GLU	HG2	2.385	0.008	2
UNMAPPED	14	HIS	HB2	3.025	0.022	2
UNMAPPED	45	GLN	HB2	2.157	0.007	2
UNMAPPED	2	SER	HA	4.54	0.012	1
UNMAPPED	11	HIS	HA	5.061	0.016	1
UNMAPPED	42	LYS	CG	24.47	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	18	ASP	H	7.982	0.015	1
UNMAPPED	10	GLU	HG2	2.211	0.016	2
UNMAPPED	27	MET	HB3	1.946	0.02	2
UNMAPPED	36	GLN	HG2	2.577	0.015	2
UNMAPPED	10	GLU	CG	35.5	0.05	1
UNMAPPED	25	THR	CB	70.21	0.03	1
UNMAPPED	16	GLY	H	8.647	0.014	1
UNMAPPED	10	GLU	CA	54.62	0.06	1
UNMAPPED	12	THR	HA	4.013	0.019	1
UNMAPPED	34	LEU	CG	26.79	0.15	1
UNMAPPED	17	PHE	HB3	2.818	0.016	2
UNMAPPED	28	PRO	HD2	3.607	0.017	2
UNMAPPED	1	GLY	HA2	3.944	0.016	2
UNMAPPED	45	GLN	HG2	2.387	0.019	1
UNMAPPED	28	PRO	HG3	0.464	0.027	2
UNMAPPED	11	HIS	N	124.38	0.15	1
UNMAPPED	9	PHE	HZ	6.834	0.011	1
UNMAPPED	9	PHE	CD2	131.27	0.02	1
UNMAPPED	14	HIS	HD2	7.128	0.014	1
UNMAPPED	5	LEU	HD22	1.133	0.002	2
UNMAPPED	20	VAL	HG23	1.034	0.01	2
UNMAPPED	32	ALA	H	8.128	0.013	1
UNMAPPED	29	GLU	H	9.063	0.016	1
UNMAPPED	40	ILE	CA	61.28	0.06	1
UNMAPPED	45	GLN	HE22	7.678	0.001	2
UNMAPPED	5	LEU	CB	40.85	0.05	1
UNMAPPED	45	GLN	H	8.402	0.013	1
UNMAPPED	40	ILE	CD1	12.84	0.04	1
UNMAPPED	20	VAL	CB	31.13	0.04	1
UNMAPPED	28	PRO	HA	4.251	0.011	1
UNMAPPED	5	LEU	HD12	1.06	0.003	2
UNMAPPED	46	LYS	CA	57.3	0.08	1
UNMAPPED	22	GLY	CA	45.95	0.09	1
UNMAPPED	3	ILE	HG12	1.643	0.01	2
UNMAPPED	27	MET	HE2	1.656	0.015	1
UNMAPPED	29	GLU	CA	59.83	0.05	1
UNMAPPED	4	SER	H	8.932	0.018	1
UNMAPPED	46	LYS	HB2	1.867	0.009	2
UNMAPPED	34	LEU	HB3	1.54	0.017	2
UNMAPPED	40	ILE	HD11	0.902	0.014	1
UNMAPPED	38	SER	HB2	3.971	0.015	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	46	LYS	HG2	1.427	0.004	1
UNMAPPED	46	LYS	HB3	1.743	0.011	2
UNMAPPED	20	VAL	HG13	0.926	0.014	2
UNMAPPED	46	LYS	CD	28.83	0.0	1
UNMAPPED	8	ASP	HB3	2.879	0.017	1
UNMAPPED	41	THR	HA	4.38	0.011	1
UNMAPPED	19	ALA	N	126.35	0.02	1
UNMAPPED	33	ARG	HG3	1.731	0.009	2
UNMAPPED	40	ILE	HG23	0.956	0.012	1
UNMAPPED	28	PRO	HB2	2.037	0.022	2
UNMAPPED	7	SER	HB2	3.932	0.013	2
UNMAPPED	33	ARG	HD2	3.27	0.015	1
UNMAPPED	44	GLU	HB2	2.119	0.007	2
UNMAPPED	2	SER	H	8.751	0.015	1
UNMAPPED	3	ILE	HA	4.801	0.011	1
UNMAPPED	22	GLY	H	8.407	0.013	1
UNMAPPED	35	LEU	CG	26.48	0.01	1
UNMAPPED	3	ILE	HD12	0.84	0.013	1
UNMAPPED	45	GLN	HA	4.366	0.012	1
UNMAPPED	33	ARG	CD	43.14	0.05	1
UNMAPPED	11	HIS	HB2	3.525	0.022	2
UNMAPPED	3	ILE	H	8.5	0.012	1
UNMAPPED	12	THR	CA	64.64	0.03	1
UNMAPPED	37	THR	HG23	1.306	0.018	1
UNMAPPED	4	SER	HB3	4.002	0.01	1
UNMAPPED	26	GLY	HA3	3.755	0.013	2

## 7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	46	$0.00 \pm 0.00$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	42	$0.00 \pm 0.00$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	43	$0.00 \pm 0.00$	None needed ( $< 0.5$ ppm)

## 7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical

shift out of a possible 2752. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	0/1104 (0%)	0/438 (0%)	0/456 (0%)	0/210 (0%)
Sidechain	0/1430 (0%)	0/839 (0%)	0/541 (0%)	0/50 (0%)
Aromatic	0/218 (0%)	0/114 (0%)	0/92 (0%)	0/12 (0%)
Overall	0/2752 (0%)	0/1391 (0%)	0/1089 (0%)	0/272 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 2752. 0 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	0/1104 (0%)	0/438 (0%)	0/456 (0%)	0/210 (0%)
Sidechain	0/1430 (0%)	0/839 (0%)	0/541 (0%)	0/50 (0%)
Aromatic	0/218 (0%)	0/114 (0%)	0/92 (0%)	0/12 (0%)
Overall	0/2752 (0%)	0/1391 (0%)	0/1089 (0%)	0/272 (0%)

## 7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned\_chem\_shift\_list\_2). RCI is only applicable to proteins.