



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 10:09 pm GMT

PDB ID : 2HQR  
Title : Structure of a Atypical Orphan Response Regulator Protein Revealed a New Phosphorylation-Independent Regulatory Mechanism  
Authors : Hong, E.; Lee, W.  
Deposited on : 2006-07-19

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

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  
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

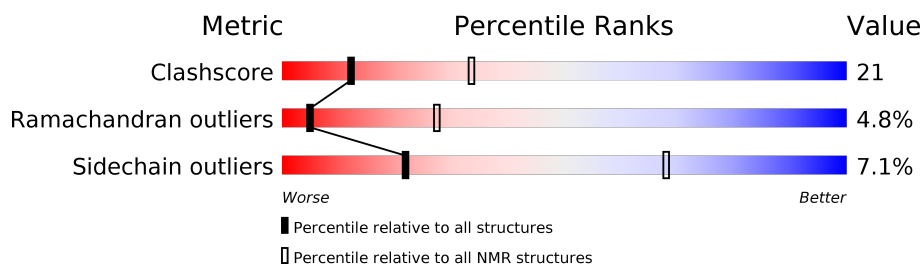
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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	223	 57% 35% • 6%
1	B	223	 64% 28% • 5%

## 2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:173, A:182-A:217, B:1-B:173, B:181-B:218 (420)	0.73	14

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 7196 atoms, of which 3622 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative TRANSCRIPTIONAL REGULATOR.

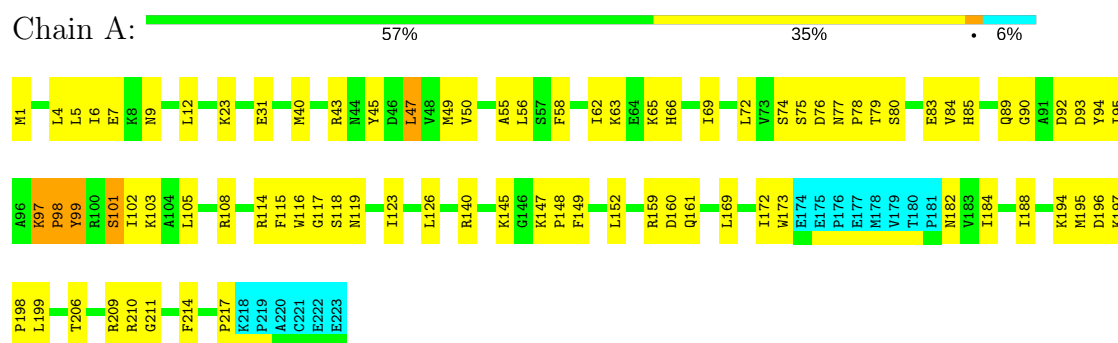
Mol	Chain	Residues	Atoms						Trace
1	A	223	Total	C	H	N	O	S	0
			3598	1128	1811	307	344	8	
1	B	223	Total	C	H	N	O	S	0
			3598	1128	1811	307	344	8	

## 4 Residue-property plots

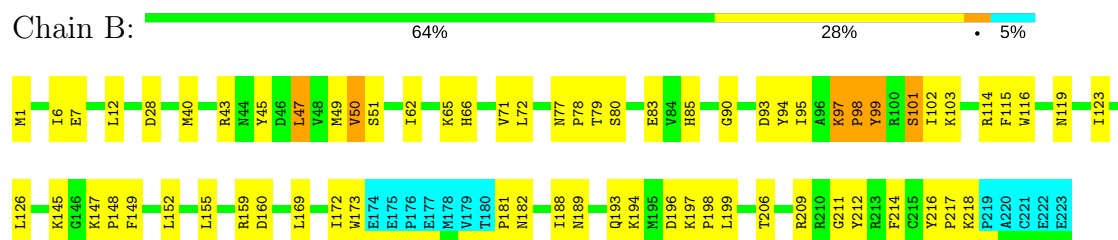
### 4.1 Average score per residue in the NMR ensemble

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: Putative TRANSCRIPTIONAL REGULATOR



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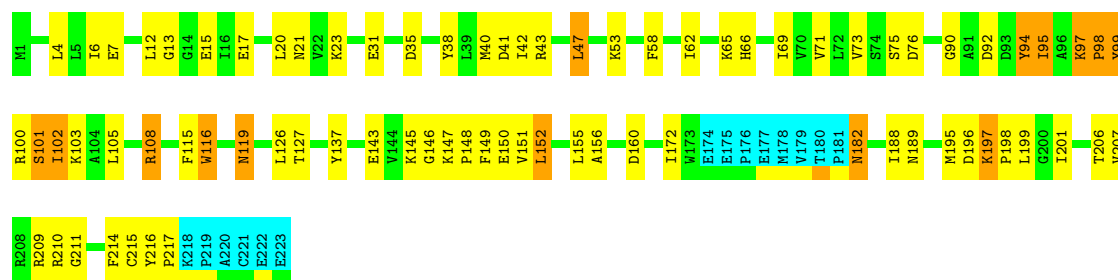
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

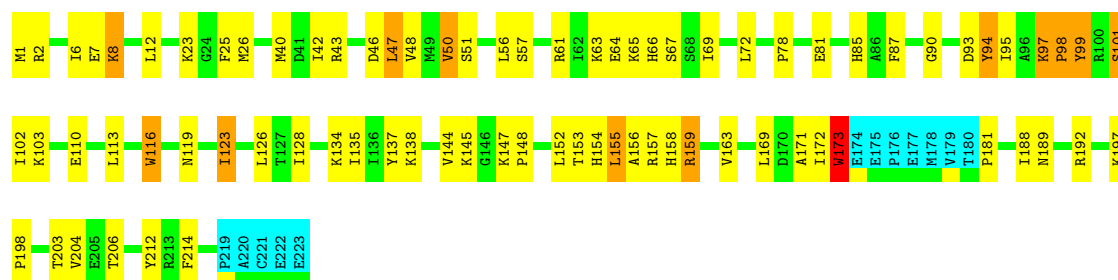
#### • Molecule 1: Putative TRANSCRIPTIONAL REGULATOR





• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

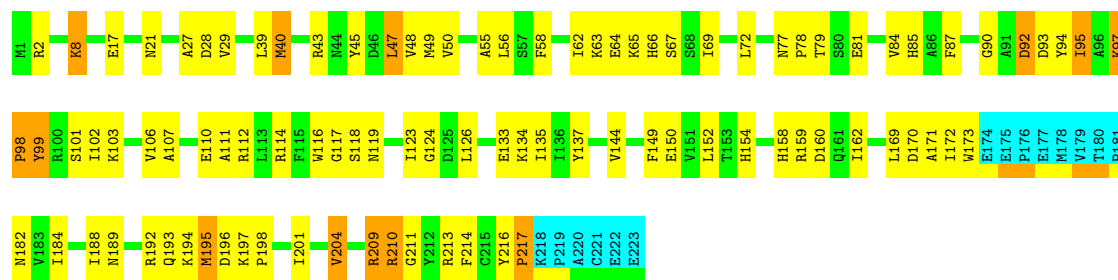
Chain B:



#### 4.2.2 Score per residue for model 2

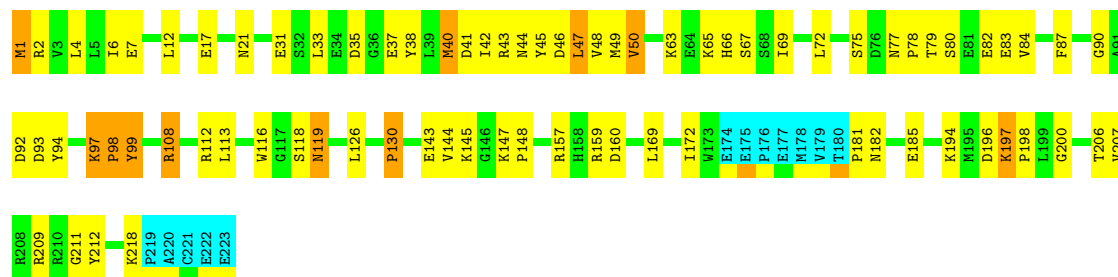
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:



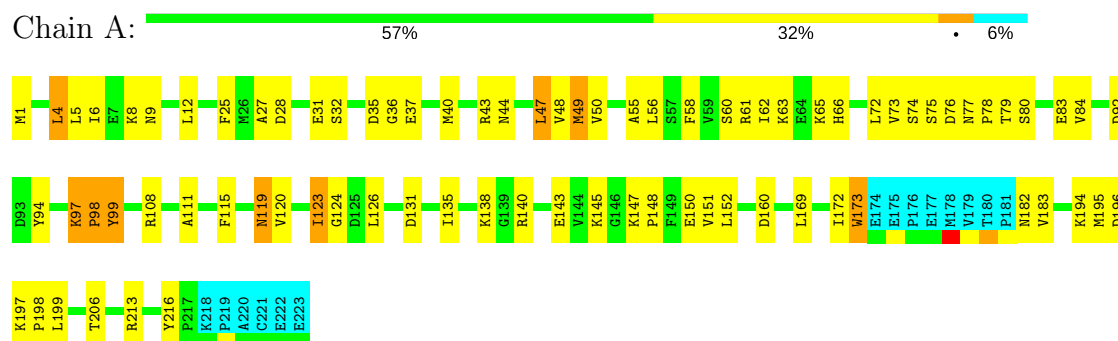
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain B:

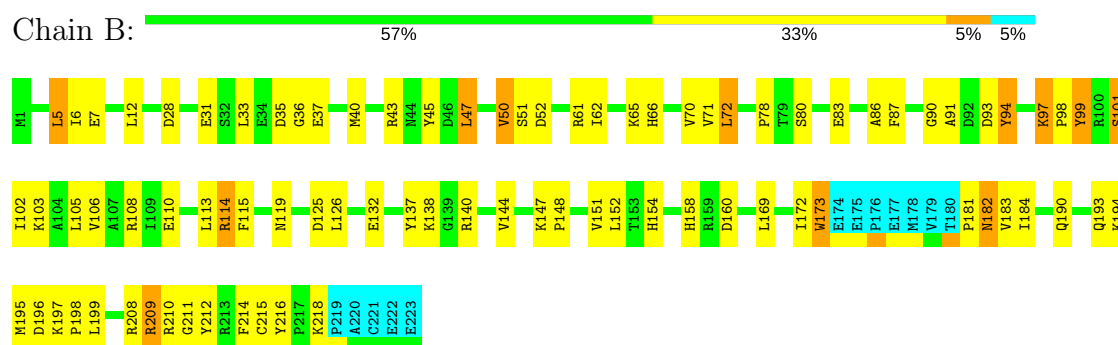


### 4.2.3 Score per residue for model 3

#### • Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

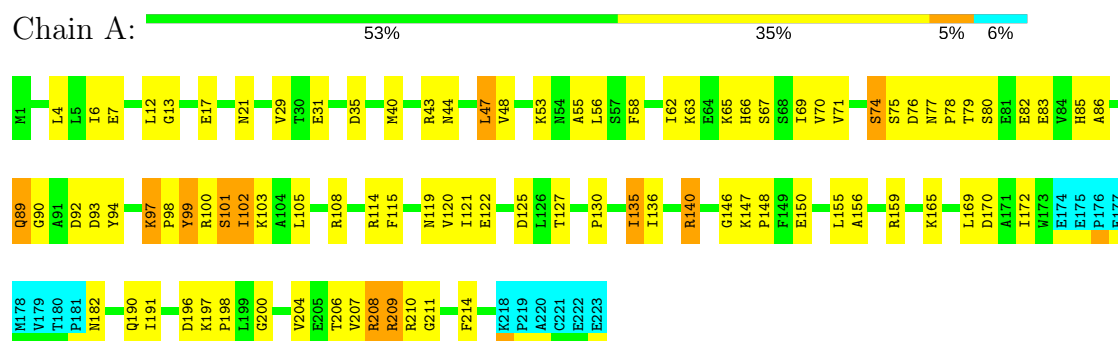


#### • Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

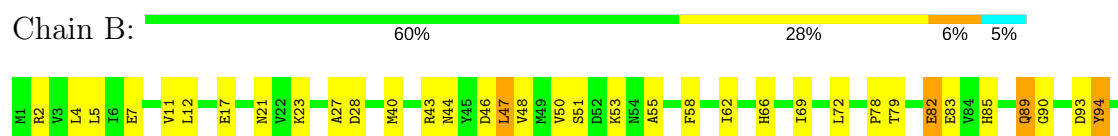


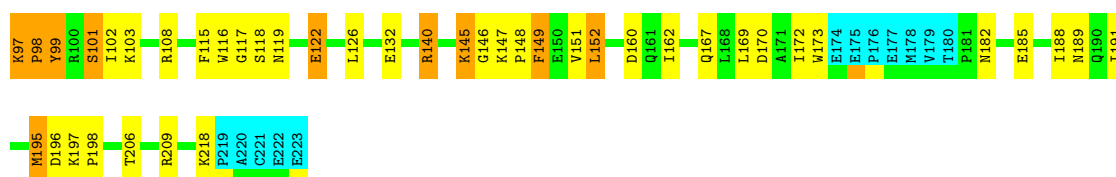
### 4.2.4 Score per residue for model 4

#### • Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



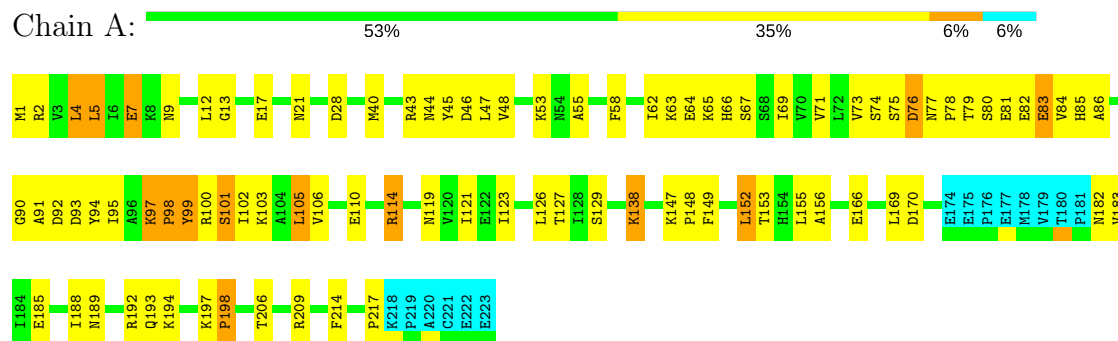
#### • Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



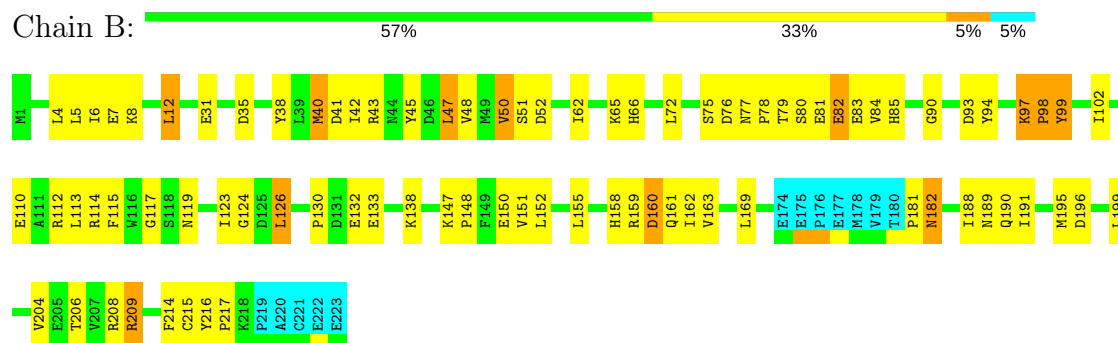


#### 4.2.5 Score per residue for model 5

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

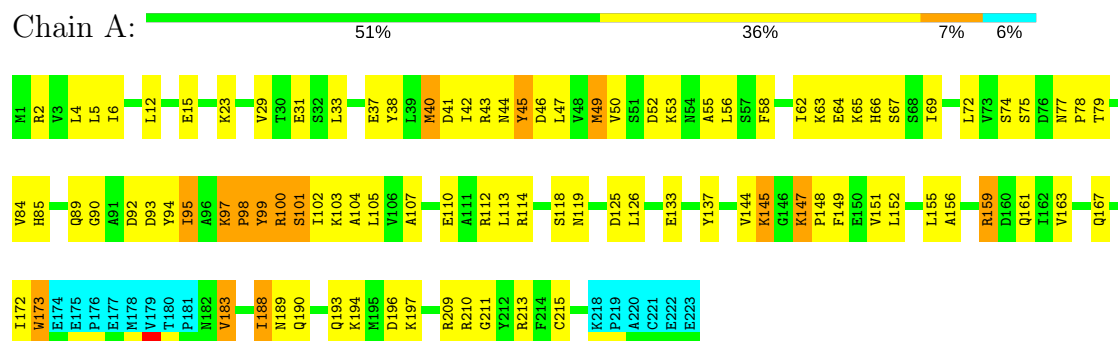


- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

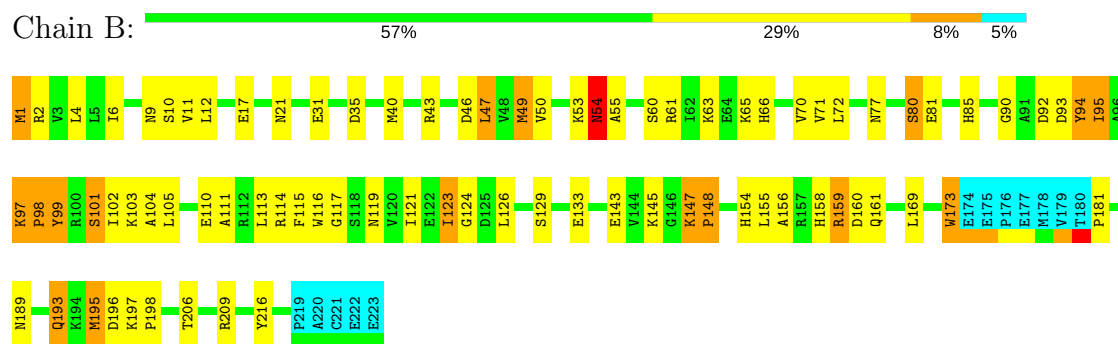


#### 4.2.6 Score per residue for model 6

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

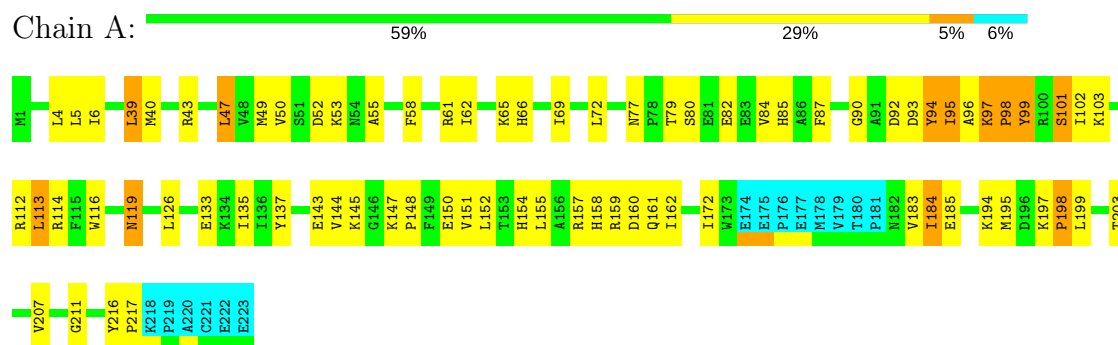


- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

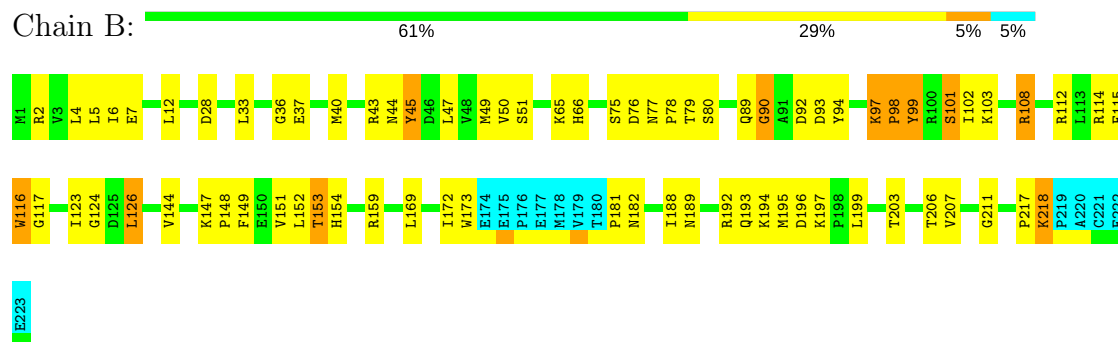


#### 4.2.7 Score per residue for model 7

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

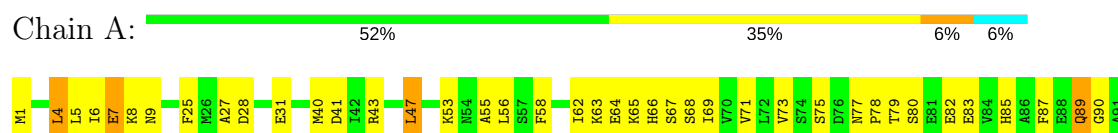


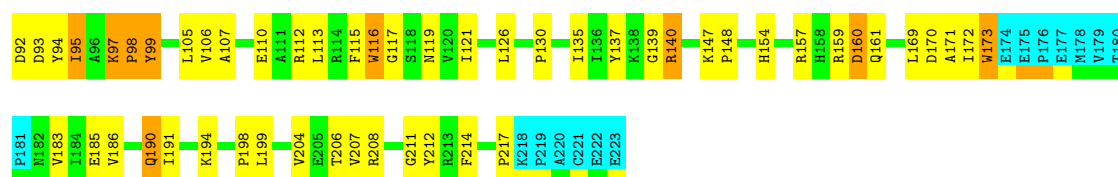
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



#### 4.2.8 Score per residue for model 8

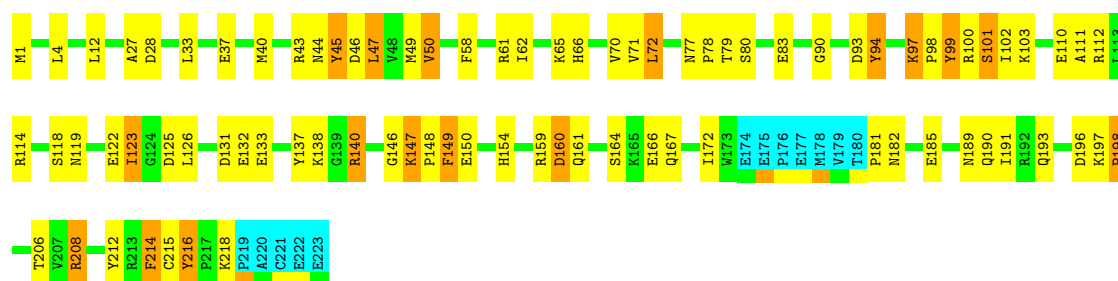
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR





### • Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

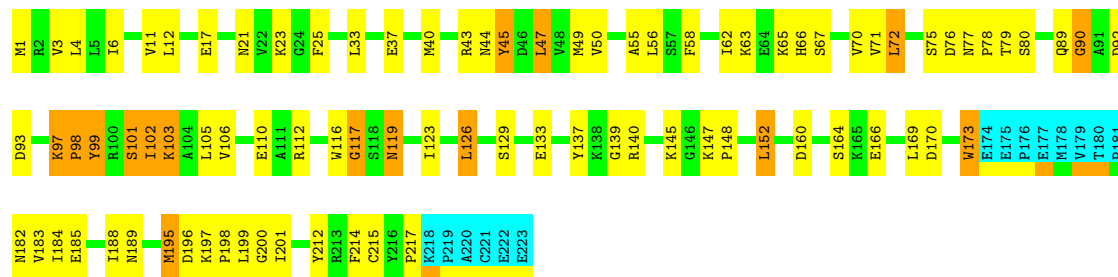
Chain B: 57% 30% 8% 5%



## 4.2.9 Score per residue for model 9

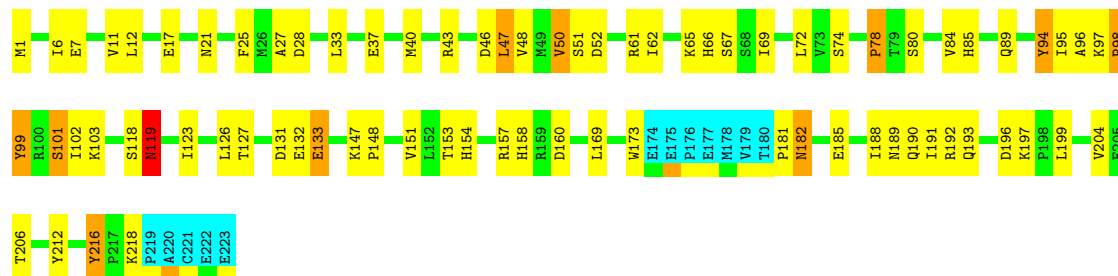
### • Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A: 55% 32% 7% 6%



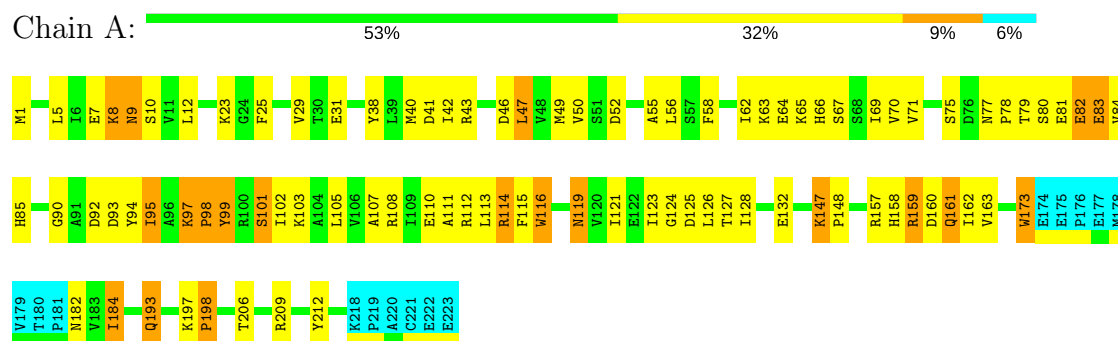
### • Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain B: 60% 30% 5%

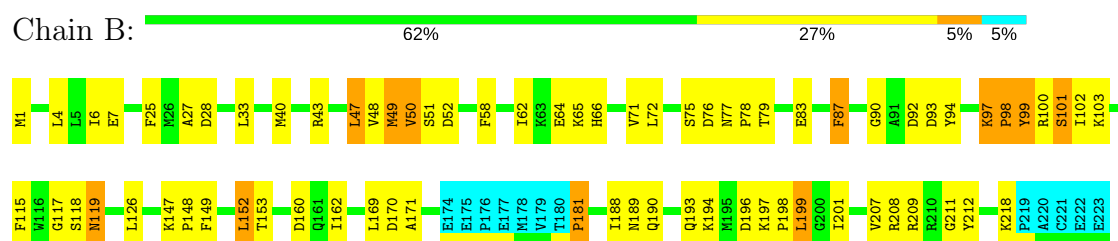


## 4.2.10 Score per residue for model 10

### • Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

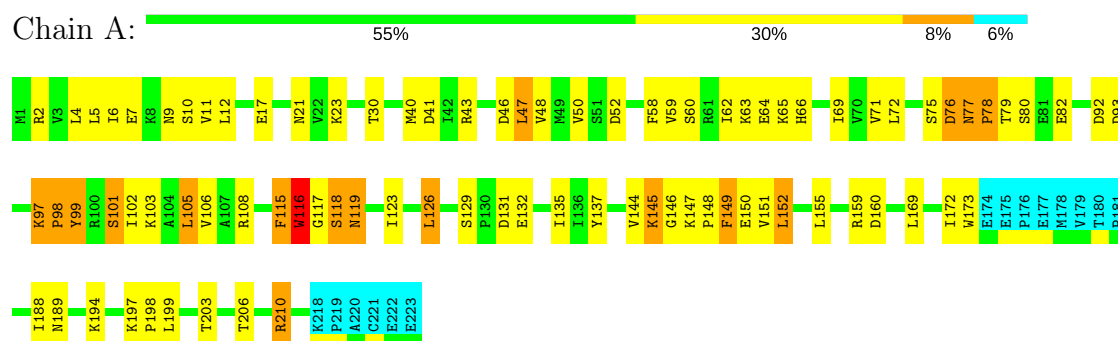


### • Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

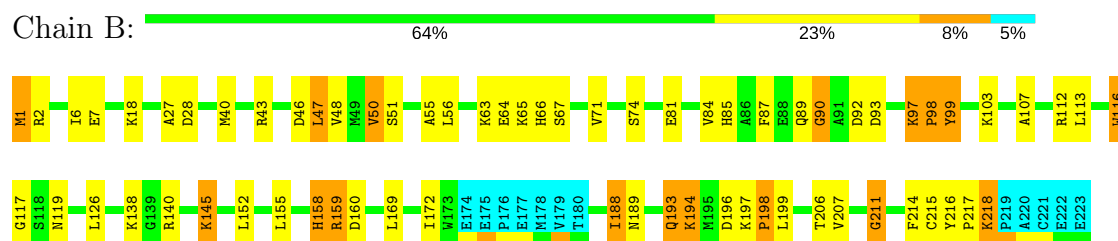


## 4.2.11 Score per residue for model 11

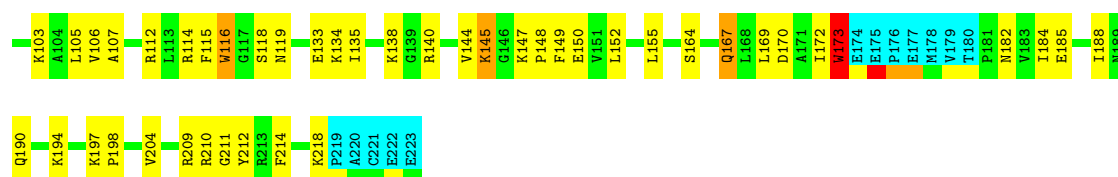
### • Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



### • Molecule 1: Putative TRANSCRIPTIONAL REGULATOR



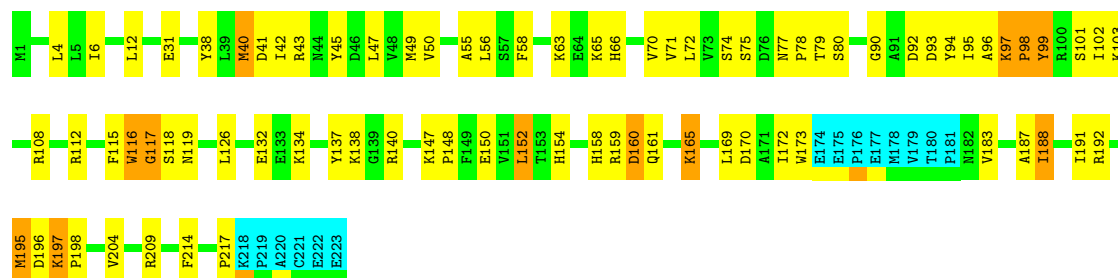




#### 4.2.14 Score per residue for model 14 (medoid)

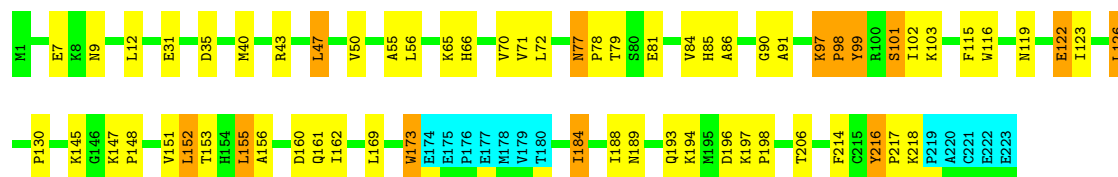
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A: 58% 30% 5% 6%



- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

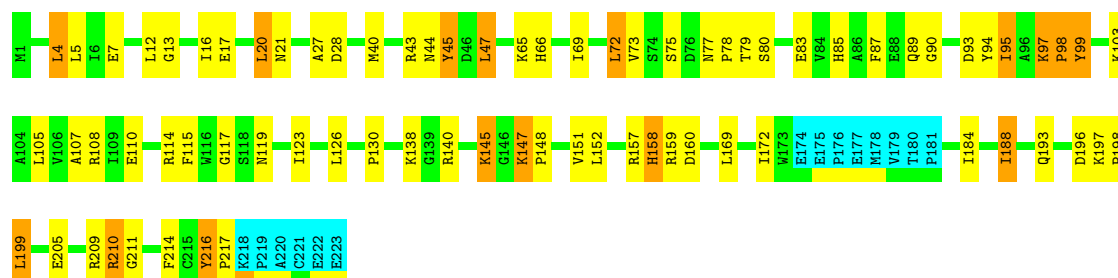
Chain B: 66% 23% 6% 5%



#### 4.2.15 Score per residue for model 15

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

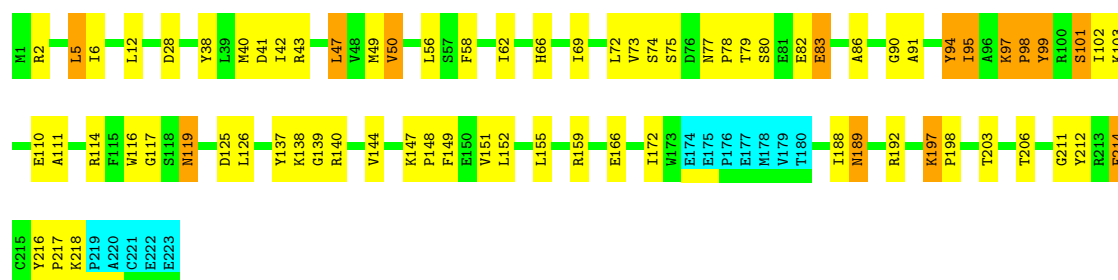
Chain A: 60% 27% 7% 6%



- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain B: 61% 27% 6% 5%

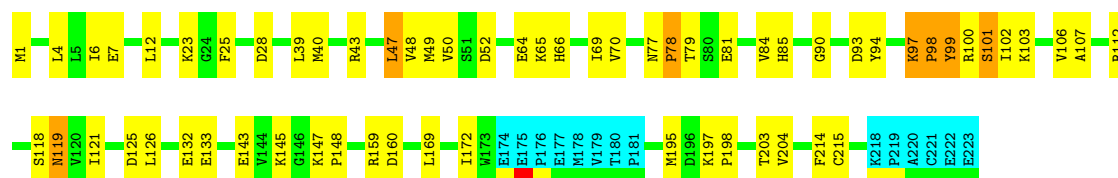




#### 4.2.16 Score per residue for model 16

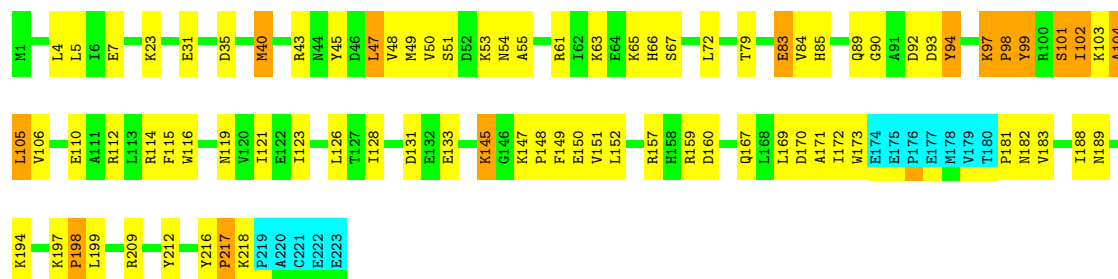
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A: 66% 25% 6%



- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

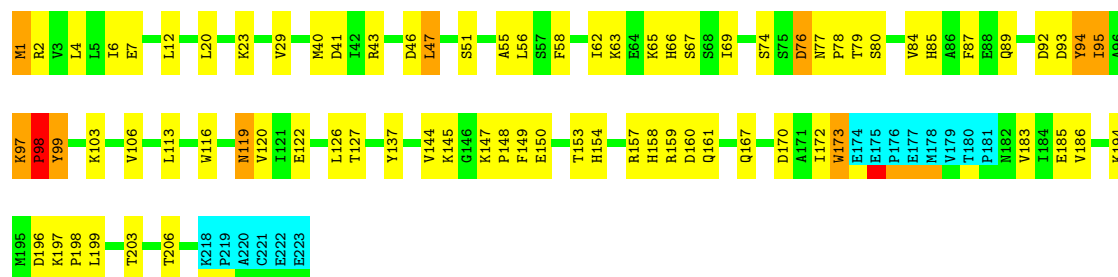
Chain B: 57% 31% 6% 5%



#### 4.2.17 Score per residue for model 17

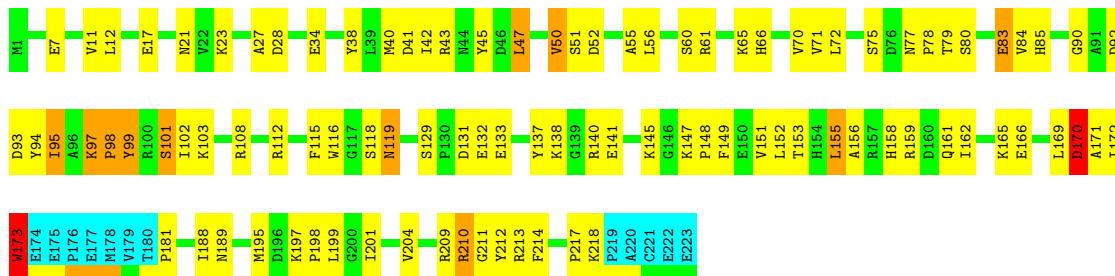
- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A: 59% 30% 6%



● Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

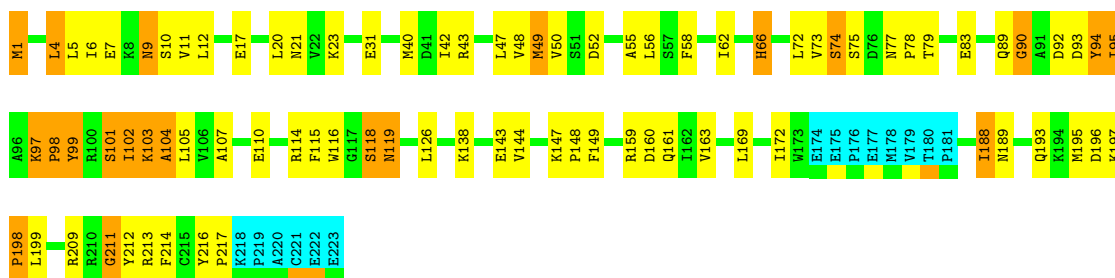
Chain B:  51% 38% 5% • 5%



#### 4.2.18 Score per residue for model 18

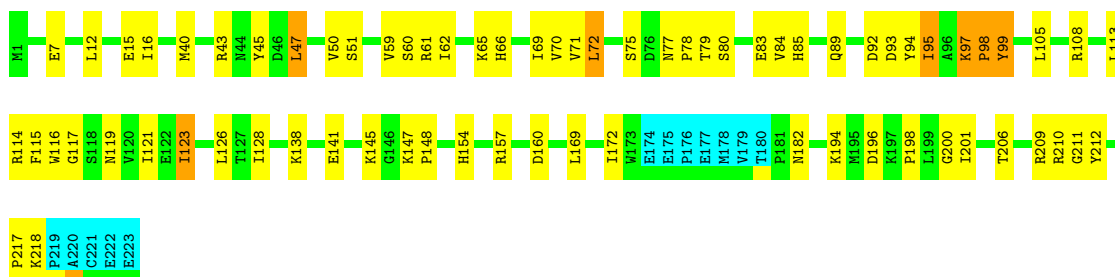
● Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:  56% 28% 9% 6%



● Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

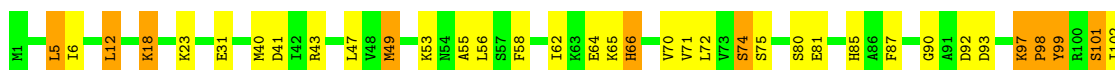
Chain B:  63% 29% 5%

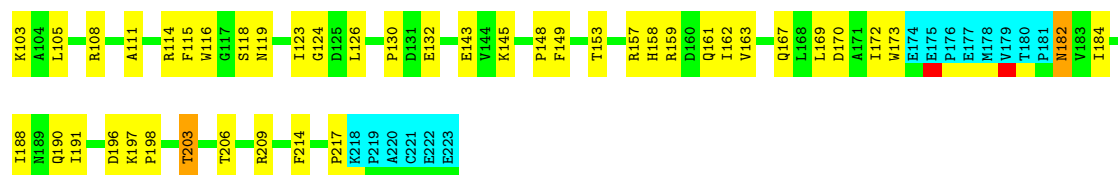


#### 4.2.19 Score per residue for model 19

- Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:  58% 30% 5% 6%





• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

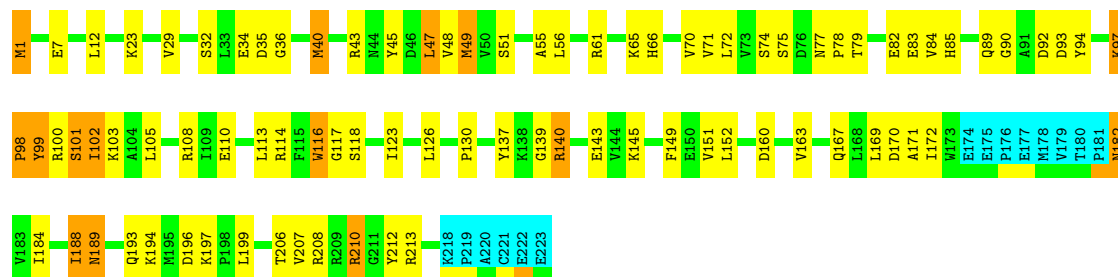
Chain B: 56% 32% 7% 5%



#### 4.2.20 Score per residue for model 20

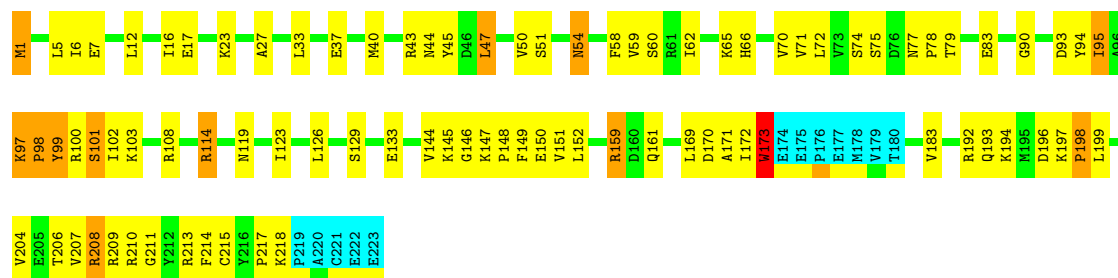
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A: 55% 32% 7% 6%



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain B: 55% 34% 5% 5%



## 5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
Cyana	structure solution	2.1
Cyana	refinement	2.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1678	1712	1708	76±13
1	B	1694	1732	1728	73±12
All	All	67440	68880	68718	2926

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:159:ARG:HH21	1:B:216:TYR:CA	1.52	1.18	16	1
1:B:192:ARG:HH12	1:B:204:VAL:CG2	1.43	1.25	1	1
1:A:145:LYS:HA	1:A:149:PHE:CE2	1.42	1.50	11	1
1:B:159:ARG:NH2	1:B:216:TYR:HA	1.38	1.05	16	1
1:A:161:GLN:NE2	1:A:162:ILE:O	1.36	1.58	19	4
1:B:192:ARG:NH1	1:B:204:VAL:CG2	1.35	1.90	1	1
1:A:149:PHE:CE1	1:A:150:GLU:HG3	1.34	1.56	11	1
1:B:192:ARG:HH12	1:B:204:VAL:CB	1.32	1.34	1	1
1:B:147:LYS:NZ	1:B:172:ILE:O	1.32	1.56	8	1
1:B:192:ARG:NH1	1:B:204:VAL:HG21	1.30	1.39	1	1
1:A:145:LYS:N	1:A:149:PHE:CD2	1.28	2.01	11	1
1:A:133:GLU:HB3	1:A:149:PHE:CZ	1.23	1.67	6	1
1:A:108:ARG:HB3	1:A:112:ARG:NH1	1.22	1.48	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:2:ARG:CZ	1:B:43:ARG:NH2	1.22	2.02	6	1
1:A:145:LYS:CA	1:A:149:PHE:CD2	1.21	2.23	11	1
1:A:163:VAL:HB	1:A:214:PHE:CE1	1.19	1.72	18	1
1:B:159:ARG:CB	1:B:159:ARG:HH11	1.17	1.52	20	1
1:A:145:LYS:CA	1:A:149:PHE:CE2	1.13	2.31	11	1
1:A:146:GLY:O	1:A:149:PHE:CD1	1.11	2.03	11	2
1:A:195:MET:HE1	1:A:204:VAL:HG11	1.11	1.19	16	1
1:B:147:LYS:HG3	1:B:172:ILE:CG2	1.08	1.78	8	1
1:B:159:ARG:HB2	1:B:159:ARG:NH1	1.07	1.63	20	1
1:A:133:GLU:CB	1:A:149:PHE:CZ	1.07	2.37	6	1
1:A:1:MET:CE	1:A:115:PHE:HA	1.06	1.80	10	1
1:B:154:HIS:CE1	1:B:158:HIS:CE1	1.03	2.46	9	3
1:A:145:LYS:HA	1:A:149:PHE:CG	1.02	1.89	6	1
1:A:116:TRP:CZ2	1:A:132:GLU:OE1	1.01	2.13	10	1
1:A:149:PHE:CD1	1:A:150:GLU:N	1.01	2.28	11	2
1:B:192:ARG:NH1	1:B:204:VAL:CB	1.00	2.16	1	1
1:B:165:LYS:NZ	1:B:185:GLU:HA	1.00	1.71	19	1
1:A:149:PHE:CZ	1:A:150:GLU:HG3	0.99	1.91	11	1
1:A:157:ARG:HG3	1:A:158:HIS:ND1	0.99	1.71	17	1
1:A:149:PHE:CE1	1:A:150:GLU:CG	0.99	2.44	11	1
1:A:182:ASN:ND2	1:A:185:GLU:OE1	0.99	1.94	5	1
1:A:209:ARG:NH2	1:A:213:ARG:NH1	0.98	2.12	18	1
1:A:116:TRP:CH2	1:A:132:GLU:OE1	0.97	2.17	10	1
1:B:2:ARG:NE	1:B:43:ARG:HH21	0.97	1.57	6	1
1:A:144:VAL:C	1:A:149:PHE:HD2	0.96	1.64	11	1
1:B:137:TYR:CE1	1:B:140:ARG:CB	0.96	2.48	8	1
1:A:145:LYS:HA	1:A:149:PHE:CD2	0.96	1.90	11	2
1:B:2:ARG:NH2	1:B:43:ARG:HH22	0.95	1.59	6	1
1:A:44:ASN:CG	1:A:143:GLU:OE2	0.95	2.04	3	1
1:B:123:ILE:HD12	1:B:159:ARG:CD	0.95	1.91	19	1
1:B:122:GLU:O	1:B:122:GLU:OE1	0.95	1.84	14	1
1:A:138:LYS:HB3	1:A:138:LYS:NZ	0.95	1.77	5	1
1:B:159:ARG:HB2	1:B:159:ARG:HH11	0.94	0.79	20	1
1:A:108:ARG:CB	1:A:112:ARG:NH1	0.94	2.30	10	1
1:A:195:MET:HE2	1:A:199:LEU:HD22	0.94	1.39	3	1
1:B:160:ASP:OD2	1:B:216:TYR:CE2	0.93	2.21	6	1
1:B:147:LYS:CE	1:B:172:ILE:O	0.93	2.16	8	1
1:B:118:SER:N	1:B:132:GLU:OE2	0.93	2.02	8	2
1:A:209:ARG:HH21	1:A:213:ARG:NH2	0.92	1.61	2	1
1:A:145:LYS:N	1:A:149:PHE:HD2	0.91	1.51	11	1
1:A:44:ASN:CB	1:A:143:GLU:OE2	0.91	2.18	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:163:VAL:HB	1:A:214:PHE:HE1	0.91	1.14	18	1
1:B:161:GLN:NE2	1:B:162:ILE:O	0.91	2.03	14	1
1:B:123:ILE:CD1	1:B:159:ARG:CZ	0.91	2.49	16	1
1:B:146:GLY:O	1:B:150:GLU:HG3	0.90	1.66	20	1
1:B:147:LYS:CG	1:B:172:ILE:CG2	0.90	2.50	8	1
1:B:155:LEU:HD13	1:B:156:ALA:N	0.90	1.81	19	4
1:B:137:TYR:CE1	1:B:140:ARG:HB2	0.90	2.02	8	1
1:A:116:TRP:CE2	1:A:132:GLU:OE1	0.90	2.25	10	1
1:B:2:ARG:NH2	1:B:43:ARG:NH2	0.89	2.17	6	1
1:A:131:ASP:OD1	1:A:132:GLU:OE2	0.88	1.91	11	1
1:A:216:TYR:CE2	1:A:217:PRO:O	0.88	2.25	18	1
1:B:165:LYS:HZ1	1:B:185:GLU:HA	0.88	1.21	19	1
1:A:209:ARG:NH2	1:A:213:ARG:HH22	0.88	1.66	2	1
1:A:195:MET:CE	1:A:204:VAL:HG11	0.88	1.99	16	1
1:A:209:ARG:HH21	1:A:213:ARG:HH22	0.88	0.91	2	1
1:B:123:ILE:HD11	1:B:159:ARG:NH2	0.87	1.83	16	1
1:A:138:LYS:HB3	1:A:138:LYS:HZ3	0.87	1.30	5	1
1:A:133:GLU:CB	1:A:149:PHE:HZ	0.87	1.82	6	1
1:B:192:ARG:NH1	1:B:204:VAL:HB	0.87	1.84	1	1
1:A:163:VAL:CB	1:A:214:PHE:CE1	0.87	2.57	18	1
1:A:157:ARG:CD	1:A:158:HIS:CE1	0.87	2.58	17	1
1:B:195:MET:CE	1:B:203:THR:OG1	0.86	2.23	7	1
1:A:161:GLN:OE1	1:B:216:TYR:OH	0.84	1.95	8	1
1:A:101:SER:O	1:A:103:LYS:N	0.84	2.10	16	16
1:A:160:ASP:HB2	1:A:216:TYR:HE1	0.84	1.28	15	1
1:B:199:LEU:HD23	1:B:201:ILE:O	0.84	1.73	17	1
1:B:2:ARG:CZ	1:B:43:ARG:HH22	0.83	1.81	6	1
1:B:195:MET:HE2	1:B:203:THR:OG1	0.83	1.74	7	1
1:A:195:MET:HE2	1:A:199:LEU:CD2	0.83	2.04	3	1
1:B:95:ILE:H	1:B:95:ILE:HD12	0.83	1.33	18	4
1:A:123:ILE:HG13	1:A:159:ARG:NE	0.82	1.89	15	1
1:A:195:MET:CE	1:A:199:LEU:CD2	0.82	2.57	3	1
1:A:154:HIS:O	1:A:158:HIS:ND1	0.82	2.13	17	1
1:A:146:GLY:O	1:A:149:PHE:CE1	0.82	2.32	11	2
1:A:157:ARG:HG3	1:A:158:HIS:CE1	0.81	2.10	17	1
1:B:192:ARG:HH11	1:B:204:VAL:HG21	0.81	1.35	1	1
1:B:148:PRO:O	1:B:152:LEU:HD13	0.81	1.74	16	1
1:B:182:ASN:OD1	1:B:185:GLU:OE2	0.81	1.99	13	1
1:B:125:ASP:OD2	1:B:138:LYS:HD3	0.81	1.76	8	1
1:A:116:TRP:CZ3	1:A:132:GLU:OE1	0.81	2.33	10	1
1:B:147:LYS:NZ	1:B:172:ILE:C	0.80	2.35	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:MET:HE1	1:A:115:PHE:HA	0.80	1.52	10	1
1:A:123:ILE:HG21	1:A:159:ARG:NH1	0.80	1.91	2	1
1:B:155:LEU:HD23	1:B:214:PHE:CE2	0.80	2.11	1	1
1:B:145:LYS:O	1:B:149:PHE:HE2	0.80	1.59	4	1
1:B:154:HIS:CE1	1:B:158:HIS:HE1	0.80	1.94	9	1
1:B:2:ARG:CZ	1:B:43:ARG:HH21	0.80	1.82	6	1
1:B:159:ARG:CB	1:B:159:ARG:NH1	0.80	2.33	20	1
1:B:154:HIS:HE1	1:B:158:HIS:CE1	0.80	1.89	9	1
1:B:2:ARG:NE	1:B:43:ARG:NH2	0.79	2.26	6	1
1:B:199:LEU:HD21	1:B:201:ILE:O	0.79	1.77	10	1
1:B:137:TYR:CE1	1:B:140:ARG:HB3	0.79	2.11	8	1
1:B:131:ASP:O	1:B:133:GLU:OE2	0.79	2.00	9	2
1:A:123:ILE:HG13	1:A:159:ARG:CZ	0.79	2.08	15	1
1:B:170:ASP:OD1	1:B:170:ASP:N	0.79	2.16	17	1
1:B:192:ARG:NH2	1:B:204:VAL:HB	0.79	1.92	1	1
1:A:146:GLY:O	1:A:149:PHE:HD1	0.78	1.60	1	1
1:A:209:ARG:NH2	1:A:213:ARG:HH12	0.78	1.77	18	1
1:B:138:LYS:CE	1:B:198:PRO:O	0.78	2.32	1	1
1:B:101:SER:O	1:B:103:LYS:N	0.78	2.17	10	15
1:B:145:LYS:O	1:B:149:PHE:CE2	0.78	2.36	4	1
1:A:159:ARG:HG3	1:A:214:PHE:CE1	0.78	2.14	15	1
1:B:160:ASP:OD2	1:B:216:TYR:CE1	0.77	2.37	8	1
1:A:95:ILE:H	1:A:95:ILE:HD12	0.77	1.39	18	7
1:A:157:ARG:HD3	1:A:158:HIS:HE1	0.77	1.40	17	1
1:B:159:ARG:HH22	1:B:217:PRO:HD3	0.77	1.39	16	1
1:A:216:TYR:N	1:A:216:TYR:CD1	0.76	2.47	15	1
1:A:118:SER:HB3	1:A:132:GLU:OE2	0.76	1.81	19	1
1:B:116:TRP:CE3	1:B:117:GLY:O	0.76	2.39	7	1
1:B:138:LYS:NZ	1:B:198:PRO:O	0.76	2.18	1	2
1:B:199:LEU:HD23	1:B:199:LEU:O	0.75	1.81	10	1
1:B:95:ILE:HD12	1:B:95:ILE:N	0.75	1.97	17	2
1:A:44:ASN:CG	1:A:143:GLU:CD	0.75	2.45	3	1
1:A:95:ILE:HD12	1:A:95:ILE:N	0.75	1.97	17	4
1:A:46:ASP:OD2	1:A:116:TRP:CH2	0.74	2.40	10	1
1:B:95:ILE:N	1:B:95:ILE:HD12	0.74	1.96	15	4
1:A:195:MET:CE	1:A:199:LEU:HD22	0.74	2.12	3	1
1:A:95:ILE:N	1:A:95:ILE:HD12	0.74	1.97	2	4
1:A:157:ARG:CG	1:A:158:HIS:CE1	0.74	2.70	17	1
1:B:192:ARG:CZ	1:B:204:VAL:HB	0.74	2.12	1	1
1:B:125:ASP:OD2	1:B:138:LYS:NZ	0.74	2.18	8	1
1:A:123:ILE:CG2	1:A:159:ARG:NH1	0.73	2.51	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:159:ARG:HG2	1:B:160:ASP:OD1	0.73	1.84	16	1
1:B:145:LYS:C	1:B:149:PHE:CD2	0.73	2.61	4	1
1:B:145:LYS:C	1:B:149:PHE:CE2	0.73	2.62	4	1
1:A:116:TRP:CD2	1:A:132:GLU:OE1	0.73	2.42	10	1
1:A:71:VAL:N	1:A:92:ASP:OD2	0.72	2.22	10	5
1:A:209:ARG:HH22	1:A:213:ARG:HH12	0.72	1.24	18	1
1:B:122:GLU:C	1:B:122:GLU:OE1	0.72	2.27	14	1
1:B:192:ARG:HH22	1:B:204:VAL:HB	0.72	1.43	1	1
1:A:44:ASN:HB3	1:A:143:GLU:OE2	0.72	1.82	3	1
1:B:166:GLU:O	1:B:170:ASP:OD1	0.72	2.07	17	1
1:B:159:ARG:O	1:B:161:GLN:N	0.72	2.23	5	3
1:A:46:ASP:OD2	1:A:116:TRP:CZ3	0.72	2.42	10	1
1:B:123:ILE:HD12	1:B:159:ARG:NE	0.72	2.00	19	1
1:A:145:LYS:HA	1:A:149:PHE:CB	0.72	2.14	6	1
1:A:108:ARG:HB3	1:A:112:ARG:HH12	0.72	1.44	10	1
1:A:209:ARG:HH22	1:A:213:ARG:NH1	0.72	1.79	18	1
1:A:216:TYR:CD2	1:A:217:PRO:O	0.72	2.42	18	1
1:B:162:ILE:HD12	1:B:162:ILE:N	0.71	1.98	4	3
1:B:147:LYS:HZ2	1:B:172:ILE:C	0.71	1.79	8	1
1:A:4:LEU:HD12	1:A:5:LEU:N	0.71	2.00	3	5
1:A:108:ARG:O	1:A:112:ARG:HG3	0.71	1.86	10	1
1:B:147:LYS:HE3	1:B:172:ILE:HG22	0.71	1.63	8	1
1:A:97:LYS:O	1:A:99:TYR:N	0.70	2.23	5	20
1:B:23:LYS:HZ2	1:B:106:VAL:HG12	0.70	1.45	16	1
1:B:155:LEU:HD13	1:B:214:PHE:CE2	0.70	2.20	13	1
1:A:195:MET:HE1	1:A:204:VAL:CG1	0.70	2.10	16	1
1:A:172:ILE:N	1:A:172:ILE:HD12	0.70	2.01	16	5
1:B:146:GLY:N	1:B:149:PHE:CD2	0.70	2.59	4	2
1:A:102:ILE:HD12	1:A:102:ILE:N	0.70	2.01	18	1
1:B:123:ILE:HD11	1:B:159:ARG:CZ	0.70	2.11	16	1
1:B:97:LYS:O	1:B:99:TYR:N	0.69	2.25	1	20
1:B:159:ARG:NH2	1:B:216:TYR:CA	0.69	2.01	16	1
1:B:165:LYS:NZ	1:B:185:GLU:CA	0.69	2.54	19	1
1:A:149:PHE:CG	1:A:150:GLU:N	0.69	2.59	1	2
1:A:116:TRP:CE3	1:A:132:GLU:OE1	0.69	2.45	10	1
1:B:160:ASP:OD2	1:B:216:TYR:HE2	0.69	1.68	6	1
1:A:144:VAL:C	1:A:149:PHE:CD2	0.69	2.52	11	1
1:A:123:ILE:HG13	1:A:159:ARG:NH2	0.68	2.02	15	1
1:A:201:ILE:N	1:A:201:ILE:HD12	0.68	2.02	2	2
1:A:201:ILE:HD12	1:A:201:ILE:N	0.68	2.03	13	1
1:B:162:ILE:N	1:B:162:ILE:HD12	0.68	2.04	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:155:LEU:O	1:B:155:LEU:HD22	0.68	1.88	19	2
1:B:147:LYS:CE	1:B:172:ILE:HG22	0.68	2.17	8	1
1:B:146:GLY:N	1:B:149:PHE:HD2	0.68	1.86	4	2
1:B:172:ILE:N	1:B:172:ILE:HD12	0.67	2.04	15	4
1:A:184:ILE:HD12	1:A:184:ILE:H	0.67	1.49	2	2
1:B:147:LYS:CG	1:B:172:ILE:HG22	0.67	2.18	8	1
1:A:172:ILE:HD12	1:A:172:ILE:N	0.67	2.03	19	8
1:B:172:ILE:HD12	1:B:172:ILE:N	0.67	2.05	19	4
1:A:155:LEU:HD12	1:A:156:ALA:N	0.67	2.05	5	4
1:B:155:LEU:C	1:B:155:LEU:HD22	0.66	2.11	12	2
1:A:149:PHE:CZ	1:A:150:GLU:CG	0.66	2.71	11	1
1:A:25:PHE:CE1	1:A:115:PHE:CE2	0.66	2.83	10	1
1:A:157:ARG:HD3	1:A:158:HIS:CE1	0.66	2.21	17	1
1:A:118:SER:N	1:A:132:GLU:OE2	0.66	2.29	19	1
1:B:123:ILE:CD1	1:B:159:ARG:CD	0.66	2.73	19	1
1:A:157:ARG:CG	1:A:158:HIS:ND1	0.65	2.58	17	1
1:A:108:ARG:O	1:A:112:ARG:CG	0.65	2.45	10	1
1:B:201:ILE:HD12	1:B:201:ILE:N	0.65	2.06	19	1
1:B:201:ILE:N	1:B:201:ILE:HD12	0.65	2.06	18	1
1:A:182:ASN:CG	1:A:185:GLU:OE1	0.65	2.34	5	1
1:A:133:GLU:CG	1:A:149:PHE:CZ	0.65	2.80	6	1
1:B:160:ASP:OD2	1:B:216:TYR:HE1	0.65	1.73	8	1
1:A:148:PRO:HG2	1:A:149:PHE:CE1	0.65	2.27	19	1
1:B:155:LEU:HD23	1:B:214:PHE:CD1	0.65	2.26	19	1
1:B:155:LEU:HD22	1:B:155:LEU:C	0.64	2.13	1	2
1:B:216:TYR:CD1	1:B:216:TYR:N	0.64	2.65	9	1
1:B:118:SER:CB	1:B:132:GLU:OE2	0.64	2.44	4	1
1:A:112:ARG:O	1:A:113:LEU:HD23	0.64	1.92	10	1
1:A:158:HIS:N	1:A:158:HIS:ND1	0.64	2.43	15	2
1:B:147:LYS:HG3	1:B:172:ILE:HG23	0.64	1.63	8	1
1:B:160:ASP:CG	1:B:216:TYR:CE1	0.64	2.71	8	1
1:B:105:LEU:C	1:B:105:LEU:HD13	0.63	2.14	13	2
1:A:147:LYS:N	1:A:148:PRO:CD	0.63	2.61	7	17
1:B:154:HIS:ND1	1:B:158:HIS:CE1	0.63	2.67	9	1
1:B:147:LYS:N	1:B:148:PRO:CD	0.63	2.61	5	19
1:A:105:LEU:HD13	1:A:106:VAL:N	0.63	2.08	5	3
1:A:105:LEU:C	1:A:105:LEU:HD13	0.63	2.14	8	2
1:A:195:MET:CE	1:A:199:LEU:HD21	0.63	2.22	3	1
1:A:123:ILE:O	1:A:123:ILE:HG23	0.63	1.93	5	2
1:B:123:ILE:HG23	1:B:123:ILE:O	0.63	1.92	14	3
1:A:145:LYS:HA	1:A:149:PHE:HE2	0.63	1.37	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:ARG:CB	1:A:112:ARG:HH12	0.63	2.05	10	1
1:A:193:GLN:NE2	1:A:193:GLN:N	0.63	2.47	10	1
1:A:133:GLU:CG	1:A:149:PHE:HZ	0.63	2.06	6	1
1:A:197:LYS:N	1:A:198:PRO:CD	0.63	2.62	10	6
1:A:148:PRO:HA	1:A:151:VAL:HB	0.63	1.69	3	1
1:B:212:TYR:N	1:B:213:ARG:NH2	0.63	2.46	12	1
1:A:102:ILE:N	1:A:102:ILE:HD12	0.63	2.09	9	1
1:A:159:ARG:NH1	1:A:160:ASP:OD2	0.63	2.31	18	1
1:A:173:TRP:CD1	1:A:173:TRP:O	0.63	2.52	8	1
1:B:85:HIS:CE1	1:B:89:GLN:NE2	0.62	2.67	16	1
1:A:159:ARG:HH12	1:B:161:GLN:NE2	0.62	1.91	6	1
1:B:208:ARG:NE	1:B:208:ARG:H	0.62	1.92	8	1
1:A:133:GLU:OE1	1:A:149:PHE:CE2	0.62	2.53	6	1
1:A:44:ASN:OD1	1:A:143:GLU:CD	0.62	2.37	3	1
1:A:85:HIS:CE1	1:A:89:GLN:NE2	0.62	2.68	13	1
1:B:137:TYR:CZ	1:B:140:ARG:CB	0.62	2.83	8	1
1:B:123:ILE:H	1:B:123:ILE:HD13	0.62	1.54	18	2
1:A:105:LEU:HD13	1:A:105:LEU:C	0.62	2.15	9	3
1:B:152:LEU:HD23	1:B:195:MET:SD	0.62	2.34	19	1
1:B:193:GLN:N	1:B:193:GLN:NE2	0.62	2.47	11	1
1:B:160:ASP:OD1	1:B:216:TYR:CE1	0.62	2.53	8	1
1:A:87:PHE:CZ	1:B:108:ARG:NH1	0.61	2.68	17	1
1:A:161:GLN:CD	1:A:162:ILE:O	0.61	2.36	19	1
1:A:123:ILE:HB	1:A:159:ARG:HH12	0.61	1.54	2	1
1:B:144:VAL:H	1:B:145:LYS:HZ2	0.61	1.39	13	1
1:A:1:MET:HE2	1:A:115:PHE:HA	0.61	1.69	10	1
1:A:61:ARG:NH2	1:A:65:LYS:NZ	0.61	2.48	3	3
1:B:119:ASN:ND2	1:B:119:ASN:N	0.61	2.49	9	1
1:B:118:SER:HB3	1:B:132:GLU:OE2	0.61	1.95	4	1
1:B:195:MET:SD	1:B:195:MET:N	0.61	2.73	6	2
1:A:121:ILE:CG2	1:A:159:ARG:HH21	0.61	2.09	12	1
1:B:155:LEU:HD23	1:B:214:PHE:CZ	0.61	2.30	1	1
1:A:199:LEU:HD22	1:A:199:LEU:N	0.61	2.10	17	2
1:A:195:MET:CE	1:A:204:VAL:CG1	0.61	2.77	16	1
1:B:2:ARG:NH1	1:B:43:ARG:NE	0.60	2.49	15	1
1:B:147:LYS:HZ3	1:B:172:ILE:HG23	0.60	1.56	8	1
1:A:138:LYS:CB	1:A:138:LYS:NZ	0.60	2.51	5	1
1:A:93:ASP:CG	1:A:112:ARG:HH21	0.60	1.99	10	3
1:B:195:MET:CE	1:B:203:THR:HG1	0.60	2.09	7	1
1:B:123:ILE:N	1:B:123:ILE:HD13	0.60	2.10	8	2
1:B:155:LEU:HD13	1:B:156:ALA:H	0.60	1.55	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:VAL:HG23	1:A:92:ASP:OD2	0.60	1.96	10	1
1:A:162:ILE:N	1:A:162:ILE:HD12	0.60	2.10	19	1
1:B:97:LYS:N	1:B:98:PRO:CD	0.60	2.64	16	4
1:A:160:ASP:HB2	1:A:216:TYR:CE1	0.60	2.21	15	1
1:A:160:ASP:CB	1:A:216:TYR:HE1	0.60	2.08	15	1
1:A:102:ILE:HD12	1:A:102:ILE:H	0.60	1.56	18	1
1:A:208:ARG:NE	1:A:210:ARG:NH2	0.60	2.50	20	1
1:B:169:LEU:C	1:B:169:LEU:HD13	0.60	2.16	11	1
1:A:147:LYS:NZ	1:A:173:TRP:HE1	0.60	1.94	14	1
1:B:134:LYS:C	1:B:135:ILE:HD12	0.60	2.17	13	2
1:A:119:ASN:ND2	1:A:119:ASN:N	0.59	2.50	3	1
1:A:48:VAL:HG23	1:A:48:VAL:O	0.59	1.97	18	1
1:B:197:LYS:N	1:B:198:PRO:CD	0.59	2.65	20	5
1:B:155:LEU:HD22	1:B:155:LEU:O	0.59	1.98	12	2
1:B:213:ARG:HH12	1:B:215:CYS:CB	0.59	2.11	20	1
1:B:1:MET:SD	1:B:1:MET:N	0.59	2.76	11	2
1:B:154:HIS:CE1	1:B:171:ALA:CB	0.59	2.86	1	1
1:A:1:MET:SD	1:A:25:PHE:CE2	0.59	2.96	8	4
1:B:1:MET:SD	1:B:25:PHE:CE2	0.59	2.96	1	2
1:A:49:MET:SD	1:A:50:VAL:N	0.59	2.76	9	4
1:B:45:TYR:N	1:B:45:TYR:CD1	0.59	2.70	2	4
1:B:173:TRP:O	1:B:173:TRP:CE3	0.59	2.55	3	2
1:A:208:ARG:HE	1:A:210:ARG:NH2	0.59	1.95	20	1
1:A:147:LYS:NZ	1:A:173:TRP:NE1	0.58	2.51	14	1
1:A:160:ASP:N	1:A:161:GLN:HE22	0.58	1.95	14	1
1:B:147:LYS:HG3	1:B:172:ILE:HG21	0.58	1.70	8	1
1:B:195:MET:HE3	1:B:203:THR:OG1	0.58	1.98	7	1
1:A:39:LEU:HD23	1:A:39:LEU:C	0.58	2.18	2	1
1:B:147:LYS:HZ3	1:B:172:ILE:CG2	0.58	2.11	8	1
1:B:160:ASP:HB3	1:B:216:TYR:HE1	0.58	1.58	9	1
1:A:157:ARG:HG3	1:A:158:HIS:HD1	0.58	1.57	17	1
1:A:1:MET:HE1	1:A:115:PHE:CA	0.58	2.28	10	1
1:B:158:HIS:O	1:B:158:HIS:CG	0.58	2.57	1	1
1:B:159:ARG:NH1	1:B:214:PHE:CZ	0.58	2.72	15	1
1:A:184:ILE:N	1:A:184:ILE:HD12	0.58	2.13	13	1
1:A:169:LEU:C	1:A:169:LEU:HD13	0.58	2.18	5	1
1:B:116:TRP:CG	1:B:117:GLY:N	0.58	2.72	7	1
1:B:184:ILE:H	1:B:184:ILE:HD12	0.58	1.58	19	1
1:A:58:PHE:CZ	1:A:62:ILE:HD11	0.58	2.32	10	11
1:B:159:ARG:CG	1:B:159:ARG:HH11	0.58	2.12	20	1
1:A:58:PHE:CE2	1:A:62:ILE:HD11	0.58	2.32	12	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:ARG:NE	1:A:158:HIS:CE1	0.58	2.71	17	1
1:B:215:CYS:SG	1:B:216:TYR:N	0.58	2.76	3	3
1:A:105:LEU:N	1:A:105:LEU:HD23	0.58	2.14	6	1
1:A:149:PHE:CZ	1:A:153:THR:CG2	0.58	2.87	17	2
1:B:169:LEU:O	1:B:171:ALA:N	0.58	2.37	20	2
1:B:137:TYR:CD1	1:B:140:ARG:HB2	0.58	2.32	8	1
1:A:25:PHE:CE1	1:A:115:PHE:CZ	0.57	2.93	10	1
1:A:123:ILE:HG13	1:A:159:ARG:HE	0.57	1.59	15	1
1:A:135:ILE:HD13	1:A:136:ILE:N	0.57	2.13	4	1
1:A:207:VAL:CG1	1:A:213:ARG:NH1	0.57	2.67	20	1
1:B:33:LEU:HD12	1:B:58:PHE:CG	0.57	2.34	10	1
1:B:159:ARG:NH1	1:B:214:PHE:CE1	0.57	2.73	15	1
1:A:2:ARG:NH2	1:A:28:ASP:CB	0.57	2.68	5	1
1:A:209:ARG:O	1:A:211:GLY:N	0.57	2.37	15	6
1:A:89:GLN:N	1:A:89:GLN:NE2	0.57	2.53	4	1
1:A:61:ARG:HH21	1:A:65:LYS:NZ	0.57	1.97	20	3
1:B:61:ARG:NH2	1:B:65:LYS:HZ3	0.57	1.97	3	1
1:A:97:LYS:C	1:A:99:TYR:H	0.57	2.03	14	19
1:B:172:ILE:O	1:B:173:TRP:CG	0.57	2.57	1	1
1:A:85:HIS:ND1	1:A:86:ALA:N	0.57	2.52	4	1
1:B:195:MET:HE2	1:B:203:THR:HG1	0.57	1.59	7	1
1:A:87:PHE:CE2	1:B:108:ARG:CZ	0.57	2.88	2	1
1:A:73:VAL:O	1:A:95:ILE:HD12	0.57	1.99	1	3
1:A:154:HIS:ND1	1:A:157:ARG:NH2	0.57	2.53	8	1
1:A:195:MET:SD	1:A:196:ASP:N	0.57	2.78	1	2
1:B:151:VAL:HG13	1:B:152:LEU:HD22	0.57	1.77	20	1
1:A:160:ASP:N	1:A:161:GLN:NE2	0.57	2.52	14	1
1:B:125:ASP:CG	1:B:138:LYS:HZ2	0.57	2.03	8	1
1:B:1:MET:SD	1:B:25:PHE:CZ	0.57	2.98	1	1
1:B:1:MET:N	1:B:1:MET:SD	0.57	2.77	6	3
1:A:45:TYR:CD1	1:A:45:TYR:N	0.56	2.73	6	3
1:A:63:LYS:HZ3	1:A:92:ASP:CG	0.56	2.03	9	2
1:A:4:LEU:HD12	1:A:4:LEU:C	0.56	2.20	3	4
1:A:40:MET:SD	1:A:45:TYR:CE1	0.56	2.99	6	1
1:B:144:VAL:H	1:B:145:LYS:NZ	0.56	1.97	13	1
1:A:161:GLN:OE1	1:A:163:VAL:CG1	0.56	2.53	19	1
1:A:133:GLU:CA	1:A:149:PHE:CZ	0.56	2.89	6	1
1:B:162:ILE:CD1	1:B:162:ILE:N	0.56	2.68	4	2
1:A:162:ILE:HD12	1:A:162:ILE:N	0.56	2.15	2	1
1:B:123:ILE:CD1	1:B:159:ARG:HD2	0.56	2.30	19	1
1:B:194:LYS:O	1:B:199:LEU:HD13	0.56	2.01	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:TYR:N	1:A:45:TYR:CD1	0.56	2.73	14	2
1:B:172:ILE:N	1:B:172:ILE:CD1	0.56	2.68	15	6
1:B:95:ILE:N	1:B:95:ILE:CD1	0.56	2.66	18	2
1:A:184:ILE:H	1:A:184:ILE:HD12	0.56	1.61	9	3
1:B:125:ASP:OD2	1:B:138:LYS:CD	0.56	2.52	8	1
1:A:12:LEU:N	1:A:12:LEU:HD22	0.56	2.16	6	4
1:B:97:LYS:NZ	1:B:99:TYR:CE2	0.56	2.73	13	1
1:B:12:LEU:HD12	1:B:97:LYS:NZ	0.56	2.16	7	3
1:A:172:ILE:N	1:A:172:ILE:CD1	0.56	2.68	16	5
1:A:119:ASN:HD21	1:A:128:ILE:N	0.55	1.98	10	1
1:B:196:ASP:OD1	1:B:197:LYS:N	0.55	2.39	14	8
1:B:66:HIS:O	1:B:69:ILE:HG22	0.55	2.01	19	6
1:A:95:ILE:N	1:A:95:ILE:CD1	0.55	2.68	18	6
1:B:1:MET:N	1:B:25:PHE:CD2	0.55	2.75	9	1
1:A:121:ILE:HG21	1:A:159:ARG:HH21	0.55	1.60	12	1
1:B:94:TYR:CD1	1:B:94:TYR:O	0.55	2.59	8	4
1:B:123:ILE:CD1	1:B:123:ILE:N	0.55	2.70	18	2
1:B:154:HIS:CE1	1:B:157:ARG:NH2	0.55	2.74	18	1
1:B:105:LEU:CD2	1:B:108:ARG:NH2	0.55	2.69	3	1
1:B:215:CYS:SG	1:B:216:TYR:CE1	0.55	3.00	3	1
1:A:159:ARG:O	1:A:161:GLN:N	0.55	2.40	10	3
1:B:41:ASP:OD1	1:B:42:ILE:N	0.55	2.40	15	4
1:A:119:ASN:ND2	1:A:121:ILE:O	0.55	2.40	10	3
1:B:169:LEU:HD13	1:B:169:LEU:C	0.55	2.22	7	4
1:B:184:ILE:O	1:B:184:ILE:HD13	0.55	2.02	14	1
1:B:126:LEU:HD13	1:B:199:LEU:HD13	0.55	1.78	9	1
1:A:201:ILE:CD1	1:A:201:ILE:N	0.55	2.69	13	2
1:A:12:LEU:HD22	1:A:12:LEU:N	0.55	2.17	15	5
1:A:1:MET:N	1:A:1:MET:SD	0.55	2.75	20	3
1:B:162:ILE:N	1:B:162:ILE:CD1	0.55	2.70	10	2
1:B:105:LEU:H	1:B:105:LEU:HD23	0.55	1.61	6	2
1:A:66:HIS:O	1:A:69:ILE:HG22	0.55	2.02	2	12
1:B:97:LYS:C	1:B:99:TYR:H	0.55	2.06	9	19
1:A:119:ASN:N	1:A:119:ASN:ND2	0.55	2.55	7	1
1:B:147:LYS:CE	1:B:172:ILE:C	0.55	2.75	8	1
1:B:199:LEU:N	1:B:199:LEU:HD22	0.55	2.16	11	1
1:A:107:ALA:HB1	1:B:87:PHE:CE2	0.54	2.37	10	1
1:B:66:HIS:CE1	1:B:145:LYS:NZ	0.54	2.75	20	1
1:B:154:HIS:CD2	1:B:158:HIS:ND1	0.54	2.75	1	2
1:A:35:ASP:OD1	1:A:36:GLY:N	0.54	2.40	20	2
1:A:102:ILE:N	1:A:102:ILE:CD1	0.54	2.68	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:158:HIS:CD2	1:B:158:HIS:O	0.54	2.61	1	1
1:B:151:VAL:HG13	1:B:152:LEU:HD12	0.54	1.79	16	1
1:B:155:LEU:O	1:B:159:ARG:N	0.54	2.41	5	1
1:A:123:ILE:O	1:A:125:ASP:N	0.54	2.41	10	1
1:A:41:ASP:OD1	1:A:42:ILE:N	0.54	2.40	1	4
1:A:173:TRP:O	1:A:173:TRP:CG	0.54	2.59	3	1
1:B:1:MET:N	1:B:2:ARG:CZ	0.54	2.71	19	1
1:A:199:LEU:N	1:A:199:LEU:CD2	0.54	2.70	17	2
1:B:199:LEU:HD23	1:B:199:LEU:C	0.54	2.22	10	1
1:A:12:LEU:N	1:A:12:LEU:HD12	0.54	2.18	3	2
1:A:115:PHE:CD1	1:A:116:TRP:N	0.54	2.75	11	1
1:A:94:TYR:CD1	1:A:95:ILE:N	0.54	2.75	17	3
1:B:209:ARG:O	1:B:211:GLY:N	0.54	2.41	3	4
1:A:62:ILE:O	1:A:66:HIS:N	0.54	2.41	1	6
1:A:159:ARG:CG	1:A:214:PHE:CE1	0.54	2.91	15	1
1:B:110:GLU:O	1:B:114:ARG:N	0.54	2.41	19	5
1:B:213:ARG:NH1	1:B:215:CYS:HB2	0.54	2.18	20	1
1:B:208:ARG:NE	1:B:208:ARG:N	0.54	2.56	8	1
1:A:40:MET:SD	1:A:45:TYR:CE2	0.54	3.00	5	1
1:A:196:ASP:OD1	1:A:197:LYS:N	0.54	2.41	20	6
1:B:105:LEU:HD13	1:B:106:VAL:N	0.54	2.17	3	2
1:B:159:ARG:HH22	1:B:217:PRO:CD	0.54	2.11	16	1
1:A:118:SER:O	1:A:129:SER:OG	0.54	2.24	11	1
1:A:135:ILE:N	1:A:135:ILE:HD12	0.54	2.17	7	1
1:A:105:LEU:HD23	1:A:105:LEU:H	0.54	1.63	18	1
1:B:173:TRP:CG	1:B:173:TRP:O	0.54	2.60	12	3
1:A:118:SER:CB	1:A:132:GLU:OE2	0.54	2.54	19	1
1:A:16:ILE:O	1:A:20:LEU:HD23	0.54	2.03	15	2
1:B:83:GLU:OE1	1:B:94:TYR:CD1	0.54	2.61	8	1
1:A:7:GLU:OE2	1:A:97:LYS:NZ	0.54	2.41	16	1
1:A:145:LYS:C	1:A:149:PHE:CD2	0.54	2.81	11	1
1:A:82:GLU:O	1:A:85:HIS:ND1	0.53	2.42	4	1
1:B:82:GLU:OE1	1:B:82:GLU:N	0.53	2.41	4	2
1:B:53:LYS:O	1:B:55:ALA:N	0.53	2.41	6	4
1:A:123:ILE:HD13	1:A:124:GLY:N	0.53	2.18	3	1
1:A:192:ARG:HE	1:A:204:VAL:CG2	0.53	2.16	14	1
1:B:170:ASP:O	1:B:173:TRP:CH2	0.53	2.61	16	1
1:B:190:GLN:HB3	1:B:194:LYS:NZ	0.53	2.18	13	1
1:A:12:LEU:N	1:A:12:LEU:CD2	0.53	2.71	15	8
1:B:93:ASP:N	1:B:93:ASP:OD1	0.53	2.40	1	1
1:A:172:ILE:CD1	1:A:172:ILE:N	0.53	2.71	19	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:58:PHE:CE2	1:B:62:ILE:HD11	0.53	2.38	8	4
1:A:47:LEU:HD13	1:A:48:VAL:N	0.53	2.18	3	8
1:B:169:LEU:O	1:B:172:ILE:N	0.53	2.41	17	1
1:B:2:ARG:NH1	1:B:26:MET:SD	0.53	2.82	1	1
1:B:115:PHE:O	1:B:117:GLY:N	0.53	2.41	4	4
1:A:93:ASP:OD2	1:A:112:ARG:NH2	0.53	2.42	12	3
1:A:23:LYS:NZ	1:A:103:LYS:NZ	0.53	2.56	16	1
1:A:63:LYS:O	1:A:67:SER:N	0.53	2.42	8	9
1:B:83:GLU:OE1	1:B:94:TYR:CG	0.53	2.62	8	2
1:B:94:TYR:O	1:B:94:TYR:CD1	0.53	2.61	3	2
1:B:108:ARG:NE	1:B:108:ARG:O	0.53	2.40	7	1
1:B:2:ARG:NH2	1:B:28:ASP:OD2	0.53	2.42	7	1
1:A:75:SER:O	1:A:77:ASN:N	0.53	2.41	9	3
1:A:115:PHE:O	1:A:117:GLY:N	0.53	2.41	14	2
1:A:40:MET:SD	1:A:45:TYR:CZ	0.53	3.01	6	2
1:B:85:HIS:CE1	1:B:89:GLN:HE21	0.53	2.21	9	1
1:B:205:GLU:OE2	1:B:205:GLU:N	0.53	2.42	12	1
1:B:83:GLU:OE1	1:B:83:GLU:N	0.53	2.41	15	2
1:B:93:ASP:OD1	1:B:94:TYR:N	0.53	2.42	10	7
1:A:155:LEU:O	1:A:159:ARG:N	0.53	2.41	7	2
1:B:12:LEU:HD22	1:B:12:LEU:N	0.53	2.18	8	5
1:B:105:LEU:HD23	1:B:105:LEU:N	0.53	2.19	18	1
1:A:66:HIS:ND1	1:A:66:HIS:N	0.53	2.56	19	2
1:B:137:TYR:CG	1:B:137:TYR:O	0.53	2.61	8	1
1:A:44:ASN:N	1:A:44:ASN:HD22	0.53	1.99	12	1
1:A:108:ARG:NH1	1:B:87:PHE:CZ	0.53	2.76	11	1
1:B:162:ILE:H	1:B:162:ILE:HD12	0.53	1.62	17	1
1:B:160:ASP:N	1:B:214:PHE:O	0.53	2.41	11	3
1:A:169:LEU:O	1:A:171:ALA:N	0.53	2.42	2	2
1:A:204:VAL:CG1	1:A:214:PHE:CE2	0.53	2.92	2	2
1:A:140:ARG:CD	1:A:140:ARG:N	0.53	2.72	9	2
1:A:115:PHE:CD2	1:A:116:TRP:O	0.53	2.62	8	1
1:B:85:HIS:ND1	1:B:89:GLN:NE2	0.53	2.57	16	1
1:A:100:ARG:NE	1:B:94:TYR:OH	0.53	2.41	16	1
1:B:138:LYS:O	1:B:140:ARG:NH1	0.53	2.42	3	4
1:B:65:LYS:O	1:B:66:HIS:CG	0.53	2.62	18	12
1:B:62:ILE:O	1:B:66:HIS:N	0.53	2.41	3	10
1:A:115:PHE:O	1:A:116:TRP:CG	0.53	2.61	14	1
1:B:114:ARG:O	1:B:116:TRP:N	0.53	2.42	12	1
1:A:95:ILE:HD12	1:A:95:ILE:H	0.53	1.64	10	1
1:A:17:GLU:O	1:A:21:ASN:ND2	0.53	2.42	15	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:LYS:O	1:A:66:HIS:ND1	0.53	2.42	13	6
1:B:159:ARG:NH1	1:B:159:ARG:CG	0.53	2.68	20	1
1:B:145:LYS:N	1:B:145:LYS:CD	0.53	2.72	16	1
1:A:71:VAL:N	1:A:92:ASP:OD1	0.53	2.42	9	1
1:A:108:ARG:NE	1:B:83:GLU:OE2	0.53	2.42	13	2
1:A:93:ASP:OD1	1:A:94:TYR:N	0.53	2.42	16	5
1:A:114:ARG:O	1:A:115:PHE:CG	0.53	2.62	13	5
1:B:172:ILE:O	1:B:173:TRP:CB	0.53	2.57	1	1
1:B:116:TRP:O	1:B:116:TRP:CD2	0.53	2.62	15	1
1:A:100:ARG:NH1	1:B:83:GLU:OE2	0.53	2.42	4	1
1:A:12:LEU:CD2	1:A:12:LEU:N	0.53	2.72	4	1
1:B:94:TYR:O	1:B:94:TYR:CG	0.53	2.62	16	3
1:B:83:GLU:OE2	1:B:94:TYR:CE1	0.53	2.62	8	2
1:A:196:ASP:O	1:A:200:GLY:N	0.53	2.42	12	3
1:A:158:HIS:O	1:A:161:GLN:NE2	0.53	2.42	14	1
1:A:2:ARG:HE	1:A:43:ARG:HH21	0.53	1.46	17	1
1:B:115:PHE:O	1:B:116:TRP:CG	0.53	2.62	14	2
1:A:150:GLU:O	1:A:154:HIS:ND1	0.53	2.42	7	3
1:B:17:GLU:O	1:B:21:ASN:ND2	0.53	2.42	6	8
1:A:108:ARG:NE	1:A:108:ARG:O	0.53	2.41	1	1
1:A:100:ARG:NH2	1:B:94:TYR:OH	0.53	2.42	16	1
1:A:83:GLU:OE1	1:A:94:TYR:CD2	0.53	2.62	12	1
1:B:71:VAL:N	1:B:92:ASP:OD2	0.52	2.42	17	2
1:B:77:ASN:O	1:B:79:THR:N	0.52	2.42	18	11
1:A:138:LYS:O	1:A:140:ARG:NH1	0.52	2.42	14	2
1:A:83:GLU:OE2	1:B:108:ARG:NH2	0.52	2.42	4	1
1:B:2:ARG:N	1:B:46:ASP:OD2	0.52	2.43	4	1
1:B:71:VAL:N	1:B:92:ASP:OD1	0.52	2.42	18	2
1:B:160:ASP:CB	1:B:216:TYR:HE1	0.52	2.17	9	1
1:A:92:ASP:OD2	1:A:112:ARG:NH1	0.52	2.42	6	1
1:B:93:ASP:OD2	1:B:112:ARG:NH1	0.52	2.42	11	1
1:B:116:TRP:CD1	1:B:117:GLY:N	0.52	2.78	11	1
1:A:65:LYS:O	1:A:66:HIS:CG	0.52	2.63	14	14
1:A:105:LEU:CD1	1:A:108:ARG:HH22	0.52	2.17	15	1
1:B:173:TRP:CE3	1:B:173:TRP:O	0.52	2.62	14	1
1:A:121:ILE:CD1	1:A:121:ILE:N	0.52	2.72	8	1
1:B:159:ARG:NH2	1:B:217:PRO:CD	0.52	2.73	16	1
1:B:95:ILE:CD1	1:B:95:ILE:N	0.52	2.71	20	4
1:A:82:GLU:OE1	1:A:82:GLU:N	0.52	2.42	10	1
1:A:83:GLU:N	1:A:83:GLU:OE1	0.52	2.42	10	1
1:A:83:GLU:OE1	1:A:94:TYR:CD1	0.52	2.62	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:LYS:NZ	1:A:92:ASP:OD2	0.52	2.42	3	4
1:A:100:ARG:NE	1:B:83:GLU:OE2	0.52	2.42	5	2
1:B:92:ASP:OD1	1:B:112:ARG:NH1	0.52	2.42	11	1
1:A:65:LYS:O	1:A:145:LYS:NZ	0.52	2.42	17	1
1:B:93:ASP:OD2	1:B:112:ARG:NH2	0.52	2.42	17	1
1:A:63:LYS:NZ	1:A:92:ASP:OD1	0.52	2.42	4	6
1:A:77:ASN:O	1:A:79:THR:N	0.52	2.42	9	17
1:A:23:LYS:N	1:A:23:LYS:CD	0.52	2.72	6	4
1:B:154:HIS:CE1	1:B:158:HIS:ND1	0.52	2.78	3	2
1:A:123:ILE:CB	1:A:159:ARG:HH12	0.52	2.17	2	1
1:B:95:ILE:CG2	1:B:108:ARG:NH2	0.52	2.73	18	1
1:A:76:ASP:N	1:A:76:ASP:OD1	0.52	2.42	5	1
1:A:23:LYS:NZ	1:A:110:GLU:OE1	0.52	2.42	9	1
1:B:113:LEU:O	1:B:115:PHE:CD2	0.52	2.62	12	1
1:A:52:ASP:N	1:A:52:ASP:OD1	0.52	2.42	6	1
1:B:63:LYS:NZ	1:B:92:ASP:OD1	0.52	2.42	13	1
1:B:155:LEU:HD13	1:B:155:LEU:C	0.52	2.25	19	1
1:A:108:ARG:NH2	1:B:83:GLU:OE1	0.52	2.42	19	1
1:A:159:ARG:NH1	1:A:203:THR:OG1	0.52	2.42	17	1
1:B:50:VAL:HG22	1:B:52:ASP:H	0.52	1.65	3	7
1:B:188:ILE:HG23	1:B:189:ASN:N	0.52	2.20	1	7
1:A:173:TRP:O	1:A:173:TRP:CD2	0.52	2.62	3	1
1:B:123:ILE:HD11	1:B:216:TYR:HB3	0.52	1.80	9	1
1:B:192:ARG:NH2	1:B:212:TYR:CD1	0.52	2.78	9	1
1:B:65:LYS:O	1:B:66:HIS:ND1	0.52	2.43	18	10
1:B:81:GLU:O	1:B:85:HIS:ND1	0.52	2.42	19	6
1:B:159:ARG:NH2	1:B:203:THR:OG1	0.52	2.43	7	1
1:B:172:ILE:CD1	1:B:172:ILE:N	0.52	2.73	19	3
1:B:116:TRP:NE1	1:B:141:GLU:OE2	0.52	2.42	18	1
1:B:83:GLU:N	1:B:83:GLU:OE1	0.52	2.42	16	1
1:B:149:PHE:CE1	1:B:153:THR:HG21	0.52	2.39	17	1
1:B:188:ILE:HD12	1:B:212:TYR:CZ	0.52	2.38	10	2
1:A:119:ASN:ND2	1:A:128:ILE:O	0.52	2.42	13	2
1:B:49:MET:SD	1:B:72:LEU:O	0.52	2.68	12	6
1:A:85:HIS:NE2	1:A:89:GLN:OE1	0.52	2.42	15	1
1:B:72:LEU:HD23	1:B:72:LEU:C	0.52	2.25	16	4
1:B:76:ASP:OD1	1:B:77:ASN:N	0.52	2.42	10	3
1:B:135:ILE:HD12	1:B:135:ILE:N	0.52	2.19	1	1
1:B:44:ASN:C	1:B:45:TYR:CD1	0.52	2.83	7	1
1:A:2:ARG:NH2	1:A:28:ASP:OD2	0.52	2.42	2	1
1:B:155:LEU:HD12	1:B:156:ALA:N	0.52	2.20	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:160:ASP:OD2	1:B:161:GLN:NE2	0.52	2.43	12	1
1:A:95:ILE:CD1	1:A:95:ILE:N	0.52	2.66	17	4
1:A:7:GLU:OE2	1:A:9:ASN:ND2	0.52	2.42	18	2
1:A:102:ILE:O	1:A:105:LEU:N	0.52	2.42	4	3
1:B:40:MET:SD	1:B:45:TYR:CE1	0.52	3.03	3	2
1:A:105:LEU:HD23	1:A:105:LEU:N	0.52	2.19	18	1
1:A:53:LYS:NZ	1:A:77:ASN:OD1	0.52	2.43	6	1
1:B:164:SER:OG	1:B:167:GLN:NE2	0.52	2.43	13	1
1:A:143:GLU:N	1:A:143:GLU:OE1	0.52	2.43	7	3
1:A:85:HIS:CD2	1:A:89:GLN:OE1	0.52	2.62	4	2
1:A:155:LEU:C	1:A:155:LEU:HD12	0.52	2.26	4	2
1:A:49:MET:SD	1:A:72:LEU:O	0.52	2.68	19	7
1:A:108:ARG:O	1:A:112:ARG:NH1	0.52	2.43	14	1
1:A:116:TRP:N	1:A:116:TRP:CD1	0.52	2.77	11	1
1:A:160:ASP:O	1:A:161:GLN:NE2	0.51	2.43	17	1
1:A:110:GLU:O	1:A:114:ARG:N	0.51	2.43	5	3
1:A:146:GLY:O	1:A:150:GLU:HB2	0.51	2.05	4	1
1:B:146:GLY:HA3	1:B:149:PHE:CE2	0.51	2.40	4	1
1:B:12:LEU:CD2	1:B:12:LEU:N	0.51	2.73	7	4
1:B:158:HIS:C	1:B:160:ASP:N	0.51	2.62	5	1
1:A:76:ASP:OD1	1:A:76:ASP:N	0.51	2.42	17	1
1:A:5:LEU:HD12	1:A:49:MET:SD	0.51	2.45	10	3
1:A:7:GLU:OE1	1:A:13:GLY:N	0.51	2.42	15	4
1:A:93:ASP:OD2	1:A:108:ARG:NE	0.51	2.42	15	1
1:B:83:GLU:OE1	1:B:84:VAL:N	0.51	2.43	18	2
1:B:161:GLN:NE2	1:B:162:ILE:N	0.51	2.58	14	1
1:A:7:GLU:OE1	1:A:9:ASN:N	0.51	2.41	8	1
1:B:45:TYR:CD1	1:B:45:TYR:N	0.51	2.78	16	2
1:A:173:TRP:O	1:A:173:TRP:CE3	0.51	2.63	10	1
1:A:155:LEU:HD12	1:A:155:LEU:C	0.51	2.26	6	2
1:B:116:TRP:O	1:B:116:TRP:CE3	0.51	2.63	15	1
1:B:12:LEU:N	1:B:12:LEU:CD2	0.51	2.73	3	4
1:A:87:PHE:CE2	1:B:108:ARG:NH1	0.51	2.79	2	1
1:B:218:LYS:CB	1:B:218:LYS:NZ	0.51	2.74	2	1
1:A:163:VAL:CG2	1:A:214:PHE:CE1	0.51	2.93	18	1
1:B:201:ILE:CD1	1:B:201:ILE:N	0.51	2.74	18	1
1:B:93:ASP:OD1	1:B:112:ARG:NH2	0.51	2.43	16	2
1:B:151:VAL:HG22	1:B:191:ILE:HG21	0.51	1.82	9	1
1:A:83:GLU:OE2	1:B:100:ARG:NH1	0.51	2.41	10	2
1:B:140:ARG:CD	1:B:140:ARG:N	0.51	2.74	15	2
1:A:81:GLU:O	1:A:85:HIS:ND1	0.51	2.43	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ILE:O	1:A:104:ALA:N	0.51	2.43	18	1
1:B:213:ARG:NH1	1:B:215:CYS:SG	0.51	2.83	20	1
1:A:2:ARG:N	1:A:46:ASP:OD1	0.51	2.42	17	1
1:A:169:LEU:HD23	1:A:169:LEU:C	0.51	2.26	15	5
1:B:182:ASN:ND2	1:B:185:GLU:OE2	0.51	2.43	4	1
1:A:195:MET:SD	1:A:195:MET:O	0.51	2.69	18	1
1:B:158:HIS:C	1:B:160:ASP:H	0.51	2.07	5	1
1:B:119:ASN:ND2	1:B:121:ILE:O	0.51	2.42	6	1
1:B:138:LYS:NZ	1:B:140:ARG:HE	0.51	2.02	13	1
1:B:135:ILE:CG2	1:B:137:TYR:CE2	0.51	2.93	1	1
1:B:123:ILE:CG2	1:B:123:ILE:O	0.51	2.58	14	3
1:B:194:LYS:O	1:B:198:PRO:CD	0.51	2.58	13	4
1:A:160:ASP:N	1:A:214:PHE:O	0.51	2.42	14	2
1:B:137:TYR:CZ	1:B:140:ARG:HB2	0.51	2.40	8	1
1:A:210:ARG:NE	1:A:210:ARG:N	0.51	2.58	11	1
1:B:167:GLN:OE1	1:B:167:GLN:N	0.51	2.43	13	1
1:B:70:VAL:HG12	1:B:71:VAL:N	0.51	2.21	8	9
1:A:12:LEU:HD13	1:A:15:GLU:OE2	0.51	2.06	6	2
1:A:47:LEU:C	1:A:47:LEU:HD13	0.51	2.25	5	6
1:B:154:HIS:CE1	1:B:158:HIS:HD1	0.51	2.24	3	1
1:B:211:GLY:H	1:B:213:ARG:HH12	0.51	1.47	12	1
1:A:113:LEU:O	1:A:116:TRP:CE2	0.51	2.64	17	1
1:A:97:LYS:C	1:A:99:TYR:N	0.51	2.63	16	19
1:A:87:PHE:CE1	1:B:108:ARG:NH1	0.51	2.78	7	1
1:B:151:VAL:CG2	1:B:191:ILE:HG21	0.51	2.35	9	1
1:A:184:ILE:HD12	1:A:184:ILE:N	0.51	2.21	12	1
1:A:145:LYS:C	1:A:149:PHE:CE2	0.51	2.84	11	1
1:B:95:ILE:HD12	1:B:95:ILE:H	0.51	1.66	17	1
1:A:184:ILE:O	1:A:184:ILE:HD13	0.51	2.06	10	2
1:A:12:LEU:CD2	1:A:97:LYS:NZ	0.51	2.74	3	1
1:B:93:ASP:OD2	1:B:112:ARG:NE	0.51	2.44	16	2
1:A:113:LEU:O	1:A:115:PHE:N	0.51	2.43	12	1
1:A:145:LYS:CA	1:A:149:PHE:CB	0.51	2.89	6	1
1:B:119:ASN:ND2	1:B:121:ILE:N	0.51	2.59	6	1
1:B:131:ASP:HB2	1:B:132:GLU:OE2	0.51	2.06	17	1
1:B:84:VAL:HG23	1:B:85:HIS:N	0.51	2.20	18	7
1:B:144:VAL:CG2	1:B:149:PHE:CG	0.51	2.94	15	1
1:A:155:LEU:HD13	1:A:214:PHE:CE2	0.51	2.41	4	2
1:B:140:ARG:N	1:B:140:ARG:CD	0.51	2.74	4	2
1:A:169:LEU:C	1:A:169:LEU:HD23	0.51	2.27	18	4
1:A:119:ASN:ND2	1:A:129:SER:OG	0.51	2.42	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:188:ILE:O	1:A:188:ILE:HD13	0.50	2.06	14	3
1:A:161:GLN:NE2	1:A:162:ILE:N	0.50	2.58	7	2
1:A:10:SER:OG	1:A:11:VAL:N	0.50	2.45	18	1
1:A:137:TYR:CE2	1:A:138:LYS:CD	0.50	2.94	14	1
1:A:121:ILE:N	1:A:121:ILE:HD12	0.50	2.20	8	1
1:B:169:LEU:O	1:B:169:LEU:HD23	0.50	2.05	16	1
1:B:12:LEU:HD12	1:B:12:LEU:N	0.50	2.21	13	1
1:A:173:TRP:CD2	1:A:173:TRP:C	0.50	2.84	17	3
1:A:108:ARG:O	1:A:112:ARG:HD2	0.50	2.05	10	1
1:A:67:SER:O	1:A:69:ILE:N	0.50	2.42	8	2
1:A:135:ILE:HD12	1:A:135:ILE:N	0.50	2.21	2	2
1:A:161:GLN:N	1:A:161:GLN:NE2	0.50	2.58	14	1
1:A:135:ILE:CD1	1:A:135:ILE:N	0.50	2.74	8	1
1:A:173:TRP:CE3	1:A:173:TRP:O	0.50	2.64	9	1
1:B:165:LYS:NZ	1:B:212:TYR:CZ	0.50	2.79	17	1
1:B:119:ASN:N	1:B:119:ASN:OD1	0.50	2.44	15	1
1:B:93:ASP:OD1	1:B:93:ASP:N	0.50	2.42	4	1
1:B:185:GLU:H	1:B:185:GLU:CD	0.50	2.10	2	1
1:B:89:GLN:NE2	1:B:89:GLN:N	0.50	2.60	19	1
1:B:160:ASP:O	1:B:163:VAL:HG13	0.50	2.07	5	1
1:B:12:LEU:CD1	1:B:12:LEU:N	0.50	2.74	13	1
1:B:158:HIS:CG	1:B:161:GLN:NE2	0.50	2.80	17	1
1:B:11:VAL:HG13	1:B:12:LEU:N	0.50	2.21	4	4
1:A:135:ILE:N	1:A:135:ILE:CD1	0.50	2.75	7	1
1:B:44:ASN:OD1	1:B:45:TYR:N	0.50	2.45	7	2
1:A:138:LYS:O	1:A:138:LYS:CG	0.50	2.60	3	1
1:B:132:GLU:N	1:B:132:GLU:OE1	0.50	2.45	3	1
1:A:115:PHE:CD2	1:A:115:PHE:O	0.50	2.64	14	2
1:B:196:ASP:O	1:B:200:GLY:N	0.50	2.43	2	3
1:B:185:GLU:CD	1:B:185:GLU:H	0.50	2.09	13	1
1:B:75:SER:CB	1:B:94:TYR:OH	0.50	2.60	20	8
1:B:161:GLN:CD	1:B:162:ILE:N	0.50	2.65	14	1
1:B:12:LEU:HD13	1:B:15:GLU:OE2	0.50	2.05	12	1
1:A:7:GLU:N	1:A:7:GLU:CD	0.50	2.65	13	1
1:A:140:ARG:N	1:A:140:ARG:CD	0.50	2.74	3	5
1:B:169:LEU:HD23	1:B:169:LEU:C	0.50	2.27	2	1
1:B:16:ILE:HD11	1:B:99:TYR:CZ	0.50	2.41	20	1
1:A:9:ASN:OD1	1:A:10:SER:N	0.50	2.44	11	2
1:A:50:VAL:HG22	1:A:52:ASP:H	0.50	1.67	10	5
1:B:157:ARG:O	1:B:159:ARG:N	0.50	2.41	1	1
1:B:94:TYR:CD1	1:B:94:TYR:C	0.50	2.85	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:TYR:CD1	1:A:94:TYR:C	0.50	2.84	7	2
1:B:94:TYR:CG	1:B:94:TYR:O	0.50	2.64	3	1
1:B:97:LYS:O	1:B:99:TYR:CD2	0.50	2.65	3	5
1:A:184:ILE:CD1	1:A:184:ILE:H	0.50	2.20	2	1
1:A:201:ILE:N	1:A:201:ILE:CD1	0.50	2.74	2	1
1:B:130:PRO:CB	1:B:157:ARG:HE	0.50	2.20	2	1
1:A:199:LEU:N	1:A:199:LEU:HD12	0.50	2.22	20	3
1:A:185:GLU:CD	1:A:185:GLU:H	0.50	2.09	9	1
1:B:160:ASP:OD1	1:B:160:ASP:N	0.50	2.44	9	1
1:B:63:LYS:NZ	1:B:92:ASP:OD2	0.50	2.42	12	1
1:A:119:ASN:N	1:A:119:ASN:OD1	0.50	2.45	9	1
1:B:199:LEU:N	1:B:199:LEU:CD2	0.50	2.74	11	1
1:B:135:ILE:N	1:B:135:ILE:HD12	0.50	2.22	13	1
1:A:173:TRP:CG	1:A:173:TRP:O	0.49	2.65	17	2
1:B:169:LEU:CB	1:B:173:TRP:CZ3	0.49	2.95	17	1
1:A:40:MET:SD	1:A:41:ASP:OD1	0.49	2.70	11	4
1:A:194:LYS:O	1:A:198:PRO:CG	0.49	2.60	7	4
1:B:7:GLU:CD	1:B:51:SER:HG	0.49	2.09	11	2
1:A:12:LEU:N	1:A:12:LEU:CD1	0.49	2.75	14	2
1:A:116:TRP:CG	1:A:117:GLY:N	0.49	2.78	8	2
1:B:115:PHE:O	1:B:116:TRP:CD1	0.49	2.65	14	2
1:A:83:GLU:OE1	1:A:94:TYR:CE1	0.49	2.65	10	1
1:A:44:ASN:ND2	1:A:145:LYS:NZ	0.49	2.60	15	1
1:A:72:LEU:C	1:A:72:LEU:HD23	0.49	2.28	6	3
1:B:184:ILE:O	1:B:188:ILE:HG22	0.49	2.07	13	1
1:B:204:VAL:HG12	1:B:214:PHE:CE2	0.49	2.41	17	1
1:B:97:LYS:C	1:B:99:TYR:N	0.49	2.64	9	19
1:A:205:GLU:CD	1:A:205:GLU:N	0.49	2.65	15	1
1:A:122:GLU:H	1:A:159:ARG:HH12	0.49	1.49	4	1
1:A:83:GLU:OE1	1:A:84:VAL:N	0.49	2.45	3	1
1:A:207:VAL:HG22	1:A:208:ARG:N	0.49	2.22	20	1
1:B:173:TRP:O	1:B:173:TRP:CD2	0.49	2.66	12	2
1:B:173:TRP:CE3	1:B:173:TRP:C	0.49	2.85	12	2
1:B:72:LEU:HG	1:B:95:ILE:HD11	0.49	1.84	17	4
1:A:169:LEU:HD13	1:A:169:LEU:C	0.49	2.28	4	1
1:A:132:GLU:N	1:A:132:GLU:OE1	0.49	2.45	14	1
1:A:1:MET:SD	1:A:116:TRP:NE1	0.49	2.86	8	1
1:B:160:ASP:OD2	1:B:216:TYR:CZ	0.49	2.64	6	1
1:B:160:ASP:N	1:B:160:ASP:OD1	0.49	2.44	12	1
1:B:152:LEU:O	1:B:155:LEU:CD1	0.49	2.60	1	3
1:B:151:VAL:HG13	1:B:152:LEU:N	0.49	2.22	15	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:LEU:HD23	1:A:72:LEU:C	0.49	2.28	20	2
1:A:40:MET:SD	1:A:45:TYR:OH	0.49	2.70	2	3
1:A:11:VAL:HG13	1:A:12:LEU:N	0.49	2.21	11	3
1:B:194:LYS:O	1:B:198:PRO:CG	0.49	2.61	16	3
1:B:119:ASN:ND2	1:B:129:SER:OG	0.49	2.46	12	1
1:B:155:LEU:HD23	1:B:214:PHE:CD2	0.49	2.43	17	1
1:B:188:ILE:HD12	1:B:212:TYR:CE2	0.49	2.42	17	2
1:B:2:ARG:NH1	1:B:43:ARG:HE	0.49	2.04	7	1
1:B:89:GLN:CG	1:B:90:GLY:N	0.49	2.76	11	2
1:A:2:ARG:NE	1:A:28:ASP:OD2	0.49	2.42	2	1
1:B:12:LEU:N	1:B:12:LEU:HD22	0.49	2.22	2	3
1:A:89:GLN:CG	1:A:90:GLY:N	0.49	2.74	18	2
1:B:119:ASN:ND2	1:B:128:ILE:O	0.49	2.46	12	1
1:A:119:ASN:OD1	1:A:120:VAL:N	0.49	2.46	13	1
1:B:172:ILE:O	1:B:173:TRP:CD2	0.49	2.65	1	1
1:A:169:LEU:HD21	1:A:184:ILE:CG1	0.49	2.37	2	1
1:A:1:MET:CE	1:A:116:TRP:HE1	0.49	2.21	8	1
1:A:89:GLN:NE2	1:A:89:GLN:N	0.49	2.60	8	1
1:A:108:ARG:CA	1:A:112:ARG:NH1	0.49	2.76	10	1
1:B:40:MET:SD	1:B:45:TYR:OH	0.49	2.69	2	2
1:A:115:PHE:C	1:A:116:TRP:CG	0.49	2.86	11	2
1:B:185:GLU:O	1:B:189:ASN:ND2	0.49	2.46	8	1
1:B:1:MET:SD	1:B:46:ASP:OD2	0.49	2.70	8	2
1:B:83:GLU:CD	1:B:94:TYR:CE2	0.49	2.87	15	1
1:A:37:GLU:OE2	1:A:61:ARG:NH2	0.49	2.45	3	1
1:A:147:LYS:HZ2	1:A:173:TRP:HE1	0.49	1.50	14	1
1:B:7:GLU:OE1	1:B:9:ASN:N	0.49	2.46	14	1
1:A:115:PHE:C	1:A:116:TRP:CD1	0.49	2.86	11	2
1:B:201:ILE:N	1:B:201:ILE:CD1	0.49	2.76	19	1
1:A:44:ASN:O	1:A:45:TYR:O	0.48	2.31	15	2
1:B:4:LEU:HD11	1:B:6:ILE:CG1	0.48	2.38	19	5
1:A:8:LYS:NZ	1:A:32:SER:OG	0.48	2.44	3	1
1:A:6:ILE:CG2	1:A:31:GLU:O	0.48	2.60	6	8
1:B:2:ARG:NH2	1:B:43:ARG:C	0.48	2.66	2	1
1:B:154:HIS:O	1:B:158:HIS:ND1	0.48	2.46	6	1
1:A:2:ARG:N	1:A:46:ASP:OD2	0.48	2.46	11	2
1:B:34:GLU:CD	1:B:34:GLU:H	0.48	2.12	17	1
1:B:97:LYS:HD2	1:B:97:LYS:O	0.48	2.08	4	3
1:B:6:ILE:HD12	1:B:50:VAL:HB	0.48	1.85	9	8
1:B:72:LEU:C	1:B:72:LEU:HD23	0.48	2.29	2	2
1:A:75:SER:CB	1:A:94:TYR:OH	0.48	2.61	13	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:53:LYS:C	1:B:55:ALA:N	0.48	2.67	16	4
1:A:161:GLN:CD	1:A:162:ILE:N	0.48	2.67	13	3
1:B:208:ARG:O	1:B:210:ARG:N	0.48	2.46	20	1
1:B:173:TRP:C	1:B:173:TRP:CD2	0.48	2.86	12	4
1:A:135:ILE:C	1:A:136:ILE:HD13	0.48	2.28	12	1
1:B:67:SER:O	1:B:69:ILE:N	0.48	2.43	9	4
1:B:97:LYS:O	1:B:97:LYS:HD2	0.48	2.09	2	1
1:B:114:ARG:O	1:B:115:PHE:CG	0.48	2.65	18	1
1:B:195:MET:SD	1:B:196:ASP:OD1	0.48	2.71	5	1
1:B:143:GLU:CD	1:B:143:GLU:H	0.48	2.12	6	1
1:A:210:ARG:NE	1:A:210:ARG:H	0.48	2.05	11	1
1:B:63:LYS:NZ	1:B:71:VAL:CG2	0.48	2.76	11	1
1:A:165:LYS:NZ	1:A:165:LYS:CB	0.48	2.77	4	2
1:A:70:VAL:HG12	1:A:71:VAL:N	0.48	2.24	9	5
1:A:154:HIS:CD2	1:A:158:HIS:CE1	0.48	3.02	2	1
1:A:102:ILE:C	1:A:104:ALA:N	0.48	2.66	18	1
1:A:114:ARG:O	1:A:116:TRP:N	0.48	2.46	20	1
1:A:161:GLN:CD	1:A:161:GLN:N	0.48	2.67	14	1
1:B:161:GLN:NE2	1:B:162:ILE:C	0.48	2.65	14	1
1:B:94:TYR:C	1:B:94:TYR:CD1	0.48	2.86	12	1
1:B:158:HIS:O	1:B:159:ARG:O	0.48	2.31	11	1
1:B:211:GLY:C	1:B:212:TYR:CD1	0.48	2.87	3	2
1:A:147:LYS:N	1:A:148:PRO:HD2	0.48	2.23	4	2
1:B:72:LEU:CD1	1:B:108:ARG:HH22	0.48	2.21	3	1
1:A:212:TYR:N	1:A:212:TYR:CD1	0.48	2.82	20	4
1:A:72:LEU:CD1	1:A:108:ARG:HH22	0.48	2.20	20	1
1:A:182:ASN:OD1	1:A:184:ILE:CD1	0.48	2.62	9	1
1:A:72:LEU:HD13	1:A:72:LEU:C	0.48	2.29	11	1
1:B:87:PHE:CD1	1:B:87:PHE:C	0.48	2.87	10	1
1:B:169:LEU:C	1:B:169:LEU:HD23	0.48	2.28	4	6
1:B:116:TRP:O	1:B:116:TRP:CG	0.48	2.67	15	1
1:B:33:LEU:O	1:B:37:GLU:N	0.48	2.44	7	6
1:A:85:HIS:CE1	1:A:89:GLN:HE21	0.48	2.27	20	2
1:B:199:LEU:N	1:B:199:LEU:HD12	0.48	2.23	20	4
1:A:123:ILE:CG2	1:A:123:ILE:O	0.48	2.61	5	1
1:A:138:LYS:CB	1:A:138:LYS:HZ2	0.48	2.20	5	1
1:A:89:GLN:CD	1:A:90:GLY:N	0.48	2.67	9	1
1:B:102:ILE:O	1:B:104:ALA:N	0.48	2.47	12	1
1:A:119:ASN:HA	1:A:129:SER:OG	0.48	2.08	11	1
1:B:64:GLU:CG	1:B:65:LYS:N	0.48	2.77	1	4
1:B:31:GLU:CG	1:B:35:ASP:OD2	0.48	2.62	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:ARG:O	1:A:160:ASP:CB	0.48	2.61	14	1
1:B:158:HIS:ND1	1:B:158:HIS:O	0.48	2.46	5	1
1:A:123:ILE:HG12	1:A:159:ARG:CZ	0.48	2.38	12	1
1:B:65:LYS:C	1:B:66:HIS:CG	0.48	2.87	17	11
1:B:152:LEU:O	1:B:152:LEU:HD13	0.48	2.08	4	2
1:B:2:ARG:NH2	1:B:44:ASN:C	0.48	2.67	4	1
1:B:61:ARG:HH21	1:B:65:LYS:HZ3	0.48	1.52	3	1
1:B:7:GLU:CD	1:B:7:GLU:N	0.48	2.67	2	1
1:A:115:PHE:CD1	1:A:115:PHE:N	0.48	2.80	18	1
1:A:199:LEU:CD1	1:A:199:LEU:N	0.48	2.75	20	1
1:B:132:GLU:O	1:B:133:GLU:C	0.48	2.52	9	2
1:A:47:LEU:HD13	1:A:47:LEU:C	0.48	2.29	18	5
1:A:65:LYS:C	1:A:66:HIS:CG	0.48	2.87	20	10
1:B:118:SER:N	1:B:132:GLU:OE1	0.48	2.43	4	1
1:A:8:LYS:HZ3	1:A:31:GLU:C	0.48	2.11	3	1
1:B:215:CYS:SG	1:B:216:TYR:CD1	0.48	3.07	3	1
1:B:152:LEU:HD13	1:B:152:LEU:O	0.48	2.09	14	2
1:A:118:SER:O	1:A:119:ASN:ND2	0.48	2.47	12	1
1:A:2:ARG:NE	1:A:43:ARG:HH21	0.48	2.07	17	1
1:B:158:HIS:ND1	1:B:161:GLN:NE2	0.48	2.61	17	1
1:A:7:GLU:OE1	1:A:51:SER:CB	0.48	2.62	20	3
1:A:119:ASN:OD1	1:A:119:ASN:N	0.48	2.46	1	1
1:B:5:LEU:HD22	1:B:49:MET:HG3	0.48	1.85	15	1
1:B:83:GLU:OE2	1:B:94:TYR:CZ	0.48	2.67	4	1
1:A:100:ARG:CZ	1:B:94:TYR:OH	0.48	2.62	4	1
1:B:44:ASN:O	1:B:45:TYR:CG	0.48	2.67	7	1
1:A:83:GLU:OE2	1:B:100:ARG:CZ	0.48	2.62	8	1
1:B:28:ASP:OD2	1:B:43:ARG:NH1	0.48	2.46	8	1
1:B:63:LYS:NZ	1:B:90:GLY:O	0.48	2.41	6	1
1:A:31:GLU:N	1:A:35:ASP:OD2	0.47	2.43	3	1
1:A:61:ARG:HH21	1:A:65:LYS:HZ2	0.47	1.52	20	1
1:A:12:LEU:HD13	1:A:97:LYS:NZ	0.47	2.23	16	1
1:B:150:GLU:CG	1:B:151:VAL:N	0.47	2.77	5	1
1:A:160:ASP:OD1	1:A:160:ASP:N	0.47	2.47	12	1
1:A:80:SER:CB	1:B:101:SER:OG	0.47	2.62	12	1
1:A:119:ASN:ND2	1:A:127:THR:CG2	0.47	2.77	17	1
1:A:122:GLU:CD	1:A:122:GLU:N	0.47	2.67	17	1
1:A:85:HIS:NE2	1:A:89:GLN:NE2	0.47	2.62	17	1
1:A:84:VAL:HG23	1:A:85:HIS:N	0.47	2.24	20	10
1:A:188:ILE:HG23	1:A:189:ASN:N	0.47	2.24	9	3
1:B:159:ARG:NH2	1:B:203:THR:O	0.47	2.43	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:102:ILE:C	1:B:104:ALA:N	0.47	2.68	12	2
1:A:213:ARG:NH1	1:A:215:CYS:SG	0.47	2.86	6	1
1:A:116:TRP:CD1	1:A:116:TRP:N	0.47	2.82	19	1
1:A:5:LEU:HD22	1:A:49:MET:CG	0.47	2.39	19	1
1:A:194:LYS:O	1:A:198:PRO:CD	0.47	2.62	5	7
1:A:97:LYS:O	1:A:99:TYR:CD2	0.47	2.67	3	8
1:A:123:ILE:CG1	1:A:159:ARG:NE	0.47	2.71	15	1
1:A:161:GLN:NE2	1:B:160:ASP:OD2	0.47	2.47	18	1
1:B:85:HIS:CE1	1:B:89:GLN:CD	0.47	2.88	16	1
1:A:3:VAL:HG13	1:A:47:LEU:HB3	0.47	1.85	9	1
1:B:119:ASN:HD21	1:B:121:ILE:C	0.47	2.11	6	1
1:A:94:TYR:C	1:A:94:TYR:CD1	0.47	2.87	1	2
1:A:119:ASN:CG	1:A:120:VAL:N	0.47	2.67	13	3
1:A:56:LEU:HD13	1:A:85:HIS:NE2	0.47	2.25	4	1
1:B:40:MET:CE	1:B:45:TYR:OH	0.47	2.62	2	1
1:A:162:ILE:N	1:A:162:ILE:CD1	0.47	2.77	19	2
1:B:213:ARG:HH12	1:B:215:CYS:HB2	0.47	1.67	20	1
1:A:113:LEU:N	1:A:113:LEU:HD12	0.47	2.25	6	1
1:B:118:SER:C	1:B:119:ASN:ND2	0.47	2.68	17	3
1:A:108:ARG:O	1:A:112:ARG:CD	0.47	2.63	10	1
1:B:6:ILE:CG2	1:B:31:GLU:O	0.47	2.62	3	1
1:A:106:VAL:HG13	1:A:107:ALA:N	0.47	2.25	8	2
1:B:93:ASP:OD2	1:B:112:ARG:CD	0.47	2.62	8	1
1:B:83:GLU:CD	1:B:94:TYR:CD1	0.47	2.88	8	1
1:B:93:ASP:OD2	1:B:112:ARG:CZ	0.47	2.62	11	1
1:B:103:LYS:O	1:B:107:ALA:HB2	0.47	2.10	13	2
1:B:93:ASP:CG	1:B:112:ARG:NH2	0.47	2.68	17	1
1:A:4:LEU:HD11	1:A:6:ILE:CG1	0.47	2.39	9	7
1:A:123:ILE:CB	1:A:159:ARG:NH1	0.47	2.78	2	1
1:B:159:ARG:O	1:B:214:PHE:HB3	0.47	2.09	20	1
1:A:143:GLU:CD	1:A:143:GLU:H	0.47	2.12	19	1
1:A:114:ARG:O	1:A:115:PHE:CD2	0.47	2.67	10	1
1:A:63:LYS:NZ	1:A:92:ASP:CG	0.47	2.68	10	4
1:B:33:LEU:N	1:B:33:LEU:CD2	0.47	2.78	10	1
1:A:114:ARG:O	1:A:115:PHE:CD1	0.47	2.68	4	1
1:B:144:VAL:HG21	1:B:149:PHE:CZ	0.47	2.45	7	1
1:B:44:ASN:C	1:B:45:TYR:CG	0.47	2.88	7	1
1:B:63:LYS:O	1:B:67:SER:N	0.47	2.47	2	3
1:B:78:PRO:CB	1:B:94:TYR:OH	0.47	2.63	9	1
1:A:12:LEU:HD12	1:A:99:TYR:CE2	0.47	2.44	12	1
1:A:152:LEU:HD12	1:A:155:LEU:HD21	0.47	1.86	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:123:ILE:HD13	1:B:124:GLY:N	0.47	2.24	6	1
1:A:173:TRP:CE3	1:A:173:TRP:C	0.47	2.88	17	1
1:B:169:LEU:HB3	1:B:173:TRP:CZ3	0.47	2.44	17	1
1:B:208:ARG:CD	1:B:208:ARG:N	0.47	2.78	10	1
1:A:189:ASN:ND2	1:A:193:GLN:OE1	0.47	2.48	2	1
1:A:211:GLY:C	1:A:212:TYR:CD1	0.47	2.88	18	1
1:A:110:GLU:O	1:A:113:LEU:N	0.47	2.46	8	1
1:A:160:ASP:OD1	1:A:215:CYS:SG	0.47	2.71	9	1
1:B:144:VAL:N	1:B:145:LYS:HZ2	0.47	2.07	13	1
1:A:55:ALA:O	1:A:58:PHE:N	0.47	2.48	6	12
1:A:182:ASN:OD1	1:A:182:ASN:N	0.47	2.45	10	2
1:B:47:LEU:HD13	1:B:47:LEU:C	0.47	2.30	8	10
1:B:23:LYS:NZ	1:B:110:GLU:OE1	0.47	2.42	16	2
1:B:110:GLU:O	1:B:114:ARG:CA	0.47	2.63	15	1
1:B:166:GLU:CD	1:B:166:GLU:H	0.47	2.11	15	2
1:B:192:ARG:HH21	1:B:204:VAL:HG23	0.47	1.69	20	1
1:B:97:LYS:CE	1:B:97:LYS:O	0.47	2.63	4	3
1:A:151:VAL:HG13	1:A:152:LEU:N	0.47	2.25	6	5
1:B:5:LEU:HD22	1:B:49:MET:CG	0.47	2.40	15	1
1:A:101:SER:OG	1:A:101:SER:O	0.47	2.33	18	1
1:B:110:GLU:O	1:B:114:ARG:CG	0.47	2.63	8	1
1:B:147:LYS:H	1:B:148:PRO:CD	0.47	2.23	16	1
1:B:105:LEU:N	1:B:105:LEU:HD23	0.47	2.25	6	1
1:B:114:ARG:O	1:B:116:TRP:CE3	0.47	2.68	6	1
1:B:54:ASN:C	1:B:54:ASN:ND2	0.47	2.68	6	1
1:A:149:PHE:CD1	1:A:150:GLU:HG3	0.47	2.31	11	1
1:B:113:LEU:C	1:B:115:PHE:H	0.47	2.13	19	1
1:B:12:LEU:HD13	1:B:97:LYS:NZ	0.46	2.25	1	1
1:B:122:GLU:CD	1:B:122:GLU:N	0.46	2.68	4	1
1:B:144:VAL:O	1:B:144:VAL:HG23	0.46	2.09	3	2
1:A:83:GLU:OE2	1:B:108:ARG:NE	0.46	2.49	18	1
1:B:170:ASP:O	1:B:173:TRP:CZ3	0.46	2.68	16	1
1:B:154:HIS:HA	1:B:157:ARG:NH1	0.46	2.25	9	1
1:B:56:LEU:HD12	1:B:56:LEU:N	0.46	2.25	1	1
1:B:49:MET:SD	1:B:50:VAL:N	0.46	2.88	8	2
1:A:173:TRP:C	1:A:173:TRP:CE3	0.46	2.88	3	1
1:B:105:LEU:H	1:B:105:LEU:HD12	0.46	1.70	16	1
1:A:152:LEU:HD13	1:A:152:LEU:O	0.46	2.10	5	2
1:A:53:LYS:C	1:A:55:ALA:N	0.46	2.69	5	1
1:A:93:ASP:CG	1:A:112:ARG:NH2	0.46	2.68	12	1
1:B:141:GLU:N	1:B:141:GLU:CD	0.46	2.68	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:207:VAL:N	1:B:211:GLY:O	0.46	2.43	10	1
1:B:217:PRO:O	1:B:218:LYS:O	0.46	2.34	7	2
1:A:216:TYR:CD1	1:A:217:PRO:O	0.46	2.68	2	1
1:A:20:LEU:HD23	1:A:20:LEU:N	0.46	2.25	18	1
1:B:192:ARG:NE	1:B:204:VAL:HG21	0.46	2.24	20	1
1:B:163:VAL:O	1:B:212:TYR:O	0.46	2.34	19	2
1:A:188:ILE:CG2	1:A:189:ASN:N	0.46	2.78	6	7
1:B:151:VAL:CG1	1:B:152:LEU:N	0.46	2.78	15	4
1:A:100:ARG:NH1	1:B:83:GLU:CD	0.46	2.69	4	1
1:A:73:VAL:HG22	1:A:74:SER:N	0.46	2.26	3	2
1:A:169:LEU:C	1:A:171:ALA:N	0.46	2.69	8	2
1:B:61:ARG:O	1:B:65:LYS:N	0.46	2.41	18	3
1:A:44:ASN:N	1:A:44:ASN:ND2	0.46	2.64	12	1
1:B:47:LEU:HD13	1:B:48:VAL:N	0.46	2.24	10	8
1:B:194:LYS:NZ	1:B:194:LYS:CB	0.46	2.78	2	1
1:B:147:LYS:CE	1:B:172:ILE:CG2	0.46	2.92	8	1
1:B:190:GLN:CG	1:B:191:ILE:N	0.46	2.77	8	3
1:B:149:PHE:CG	1:B:150:GLU:N	0.46	2.83	16	2
1:A:108:ARG:C	1:A:112:ARG:NH1	0.46	2.69	12	1
1:B:81:GLU:N	1:B:81:GLU:OE1	0.46	2.45	11	1
1:A:81:GLU:OE1	1:A:81:GLU:N	0.46	2.44	10	1
1:A:31:GLU:CG	1:A:35:ASP:OD2	0.46	2.63	4	2
1:A:23:LYS:CD	1:A:23:LYS:N	0.46	2.78	13	4
1:B:129:SER:O	1:B:133:GLU:N	0.46	2.49	20	2
1:B:208:ARG:N	1:B:208:ARG:CD	0.46	2.78	8	1
1:B:75:SER:O	1:B:97:LYS:N	0.46	2.42	13	1
1:B:47:LEU:C	1:B:47:LEU:HD13	0.46	2.31	17	6
1:A:8:LYS:NZ	1:A:8:LYS:CB	0.46	2.78	10	1
1:B:33:LEU:N	1:B:33:LEU:HD22	0.46	2.26	10	1
1:B:46:ASP:OD2	1:B:116:TRP:NE1	0.46	2.49	1	1
1:B:128:ILE:HG21	1:B:156:ALA:HB1	0.46	1.87	1	1
1:B:192:ARG:HH22	1:B:204:VAL:CB	0.46	2.17	1	1
1:B:72:LEU:HD23	1:B:95:ILE:HD11	0.46	1.88	18	1
1:B:194:LYS:CB	1:B:194:LYS:NZ	0.46	2.78	20	1
1:A:169:LEU:O	1:A:173:TRP:O	0.46	2.34	11	3
1:A:44:ASN:ND2	1:A:45:TYR:N	0.46	2.64	6	1
1:B:188:ILE:CG2	1:B:189:ASN:N	0.46	2.78	10	8
1:B:4:LEU:O	1:B:49:MET:O	0.46	2.34	2	6
1:A:87:PHE:CD2	1:B:108:ARG:CZ	0.46	2.99	2	1
1:A:8:LYS:H	1:A:8:LYS:CD	0.46	2.24	2	1
1:B:143:GLU:N	1:B:143:GLU:CD	0.46	2.69	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:152:LEU:O	1:B:156:ALA:HB2	0.46	2.10	14	1
1:B:131:ASP:O	1:B:133:GLU:CD	0.46	2.52	9	1
1:B:133:GLU:N	1:B:133:GLU:CD	0.46	2.69	9	1
1:A:161:GLN:OE1	1:A:163:VAL:HG12	0.46	2.09	19	1
1:B:40:MET:O	1:B:43:ARG:O	0.46	2.33	2	19
1:A:108:ARG:NH1	1:B:87:PHE:CE1	0.46	2.83	1	1
1:A:92:ASP:HB3	1:A:112:ARG:HH21	0.46	1.71	7	1
1:B:196:ASP:OD1	1:B:196:ASP:N	0.46	2.49	7	1
1:A:209:ARG:NH2	1:A:213:ARG:NH2	0.46	2.42	2	1
1:B:114:ARG:HE	1:B:114:ARG:CA	0.46	2.24	20	1
1:A:40:MET:SD	1:A:41:ASP:N	0.46	2.89	14	2
1:A:133:GLU:HA	1:A:149:PHE:CZ	0.46	2.46	6	1
1:A:135:ILE:HG21	1:A:137:TYR:CE2	0.46	2.45	11	1
1:A:79:THR:HG23	1:A:82:GLU:H	0.46	1.71	11	1
1:A:160:ASP:OD1	1:A:216:TYR:CD2	0.46	2.69	1	1
1:B:123:ILE:O	1:B:123:ILE:HG23	0.46	2.11	7	3
1:A:32:SER:O	1:A:35:ASP:OD1	0.46	2.34	3	2
1:A:144:VAL:CG2	1:A:149:PHE:CG	0.46	2.98	18	1
1:A:75:SER:O	1:A:97:LYS:N	0.46	2.42	14	1
1:A:133:GLU:CA	1:A:149:PHE:HZ	0.46	2.23	6	1
1:A:184:ILE:N	1:A:184:ILE:CD1	0.46	2.78	13	1
1:B:138:LYS:CG	1:B:138:LYS:O	0.46	2.63	13	1
1:B:155:LEU:HD13	1:B:214:PHE:HE2	0.46	1.69	13	1
1:B:16:ILE:HD11	1:B:99:TYR:CD1	0.46	2.46	13	1
1:B:169:LEU:C	1:B:171:ALA:N	0.45	2.68	20	2
1:B:70:VAL:CG1	1:B:71:VAL:N	0.45	2.79	8	4
1:B:203:THR:O	1:B:214:PHE:CE1	0.45	2.69	15	1
1:B:189:ASN:OD1	1:B:192:ARG:NH2	0.45	2.50	7	1
1:A:152:LEU:HD11	1:A:195:MET:SD	0.45	2.51	2	1
1:A:40:MET:CE	1:A:45:TYR:OH	0.45	2.64	2	1
1:B:143:GLU:OE1	1:B:143:GLU:N	0.45	2.48	2	1
1:A:137:TYR:O	1:A:139:GLY:N	0.45	2.49	20	2
1:B:147:LYS:NZ	1:B:172:ILE:CG2	0.45	2.79	8	1
1:A:40:MET:O	1:A:43:ARG:O	0.45	2.34	5	20
1:A:70:VAL:HG21	1:A:113:LEU:HD11	0.45	1.87	10	1
1:A:195:MET:C	1:A:195:MET:SD	0.45	2.95	14	2
1:A:74:SER:O	1:A:75:SER:OG	0.45	2.34	19	5
1:A:133:GLU:HA	1:A:149:PHE:HZ	0.45	1.70	2	1
1:A:137:TYR:C	1:A:139:GLY:N	0.45	2.69	20	3
1:B:199:LEU:CD1	1:B:199:LEU:N	0.45	2.79	20	1
1:B:123:ILE:CD1	1:B:159:ARG:NH1	0.45	2.78	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:190:GLN:HB3	1:B:194:LYS:HZ3	0.45	1.71	13	1
1:A:97:LYS:N	1:A:98:PRO:HD2	0.45	2.26	3	18
1:B:38:TYR:O	1:B:41:ASP:OD1	0.45	2.34	15	4
1:B:40:MET:C	1:B:40:MET:SD	0.45	2.94	2	9
1:A:190:GLN:CG	1:A:191:ILE:N	0.45	2.80	8	3
1:A:165:LYS:CD	1:A:165:LYS:H	0.45	2.23	14	1
1:A:118:SER:C	1:A:119:ASN:ND2	0.45	2.69	16	1
1:B:113:LEU:O	1:B:116:TRP:CD1	0.45	2.69	11	2
1:B:188:ILE:HD13	1:B:188:ILE:O	0.45	2.11	11	1
1:B:18:LYS:CD	1:B:18:LYS:N	0.45	2.79	11	1
1:A:40:MET:SD	1:A:40:MET:C	0.45	2.95	14	9
1:B:118:SER:O	1:B:119:ASN:ND2	0.45	2.50	10	2
1:A:49:MET:C	1:A:49:MET:SD	0.45	2.95	7	4
1:A:143:GLU:N	1:A:143:GLU:CD	0.45	2.70	16	3
1:A:197:LYS:CB	1:A:198:PRO:CD	0.45	2.95	9	10
1:A:159:ARG:NH2	1:A:203:THR:OG1	0.45	2.49	7	1
1:A:188:ILE:HD13	1:A:188:ILE:O	0.45	2.11	20	2
1:B:213:ARG:NH1	1:B:215:CYS:CB	0.45	2.76	20	1
1:B:191:ILE:O	1:B:195:MET:CG	0.45	2.65	5	1
1:A:102:ILE:CD1	1:A:102:ILE:N	0.45	2.78	9	1
1:A:149:PHE:CE2	1:A:153:THR:CG2	0.45	2.99	12	1
1:A:150:GLU:O	1:A:153:THR:OG1	0.45	2.34	12	1
1:A:12:LEU:O	1:A:12:LEU:HD13	0.45	2.11	19	1
1:B:133:GLU:HA	1:B:149:PHE:CE1	0.45	2.46	17	1
1:B:11:VAL:CG1	1:B:12:LEU:N	0.45	2.80	4	3
1:A:79:THR:O	1:A:83:GLU:OE2	0.45	2.35	10	2
1:B:193:GLN:O	1:B:196:ASP:OD1	0.45	2.35	14	7
1:B:82:GLU:OE1	1:B:82:GLU:CA	0.45	2.65	5	2
1:A:189:ASN:OD1	1:A:193:GLN:NE2	0.45	2.50	5	2
1:A:207:VAL:O	1:A:208:ARG:CB	0.45	2.62	20	1
1:A:75:SER:CB	1:A:82:GLU:OE2	0.45	2.64	8	1
1:A:216:TYR:O	1:A:217:PRO:O	0.45	2.34	13	1
1:B:114:ARG:O	1:B:115:PHE:CB	0.45	2.65	13	1
1:A:20:LEU:N	1:A:20:LEU:HD23	0.45	2.26	17	2
1:B:197:LYS:CB	1:B:198:PRO:CD	0.45	2.95	2	11
1:A:110:GLU:CG	1:A:111:ALA:N	0.45	2.79	10	1
1:A:157:ARG:O	1:A:159:ARG:N	0.45	2.47	10	2
1:A:161:GLN:OE1	1:A:162:ILE:N	0.45	2.46	10	2
1:B:40:MET:SD	1:B:40:MET:C	0.45	2.95	4	6
1:A:103:LYS:O	1:A:107:ALA:HB2	0.45	2.11	15	2
1:A:40:MET:C	1:A:40:MET:SD	0.45	2.95	19	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:115:PHE:C	1:B:117:GLY:N	0.45	2.70	6	2
1:B:66:HIS:CE1	1:B:145:LYS:HZ3	0.45	2.29	20	1
1:B:138:LYS:O	1:B:138:LYS:CG	0.45	2.63	19	2
1:B:185:GLU:CG	1:B:186:VAL:N	0.45	2.79	12	1
1:B:65:LYS:NZ	1:B:65:LYS:CB	0.45	2.80	12	1
1:B:129:SER:HB3	1:B:132:GLU:OE1	0.45	2.12	17	1
1:B:23:LYS:N	1:B:23:LYS:CD	0.45	2.80	4	3
1:B:137:TYR:C	1:B:139:GLY:N	0.45	2.70	15	1
1:B:137:TYR:CZ	1:B:198:PRO:O	0.45	2.70	15	1
1:B:73:VAL:O	1:B:73:VAL:HG13	0.45	2.12	15	1
1:A:161:GLN:NE2	1:A:162:ILE:H	0.45	2.09	7	1
1:B:193:GLN:HG3	1:B:197:LYS:CE	0.45	2.41	7	1
1:A:8:LYS:HZ3	1:A:32:SER:N	0.45	2.10	3	1
1:B:105:LEU:CD2	1:B:108:ARG:HH21	0.45	2.24	3	1
1:B:59:VAL:HG23	1:B:60:SER:N	0.45	2.27	20	2
1:A:93:ASP:OD2	1:A:112:ARG:CZ	0.45	2.65	14	1
1:A:23:LYS:NZ	1:A:103:LYS:HZ2	0.45	2.09	16	1
1:B:158:HIS:ND1	1:B:158:HIS:N	0.45	2.65	12	1
1:A:38:TYR:O	1:A:41:ASP:OD1	0.45	2.35	10	4
1:B:97:LYS:N	1:B:98:PRO:HD2	0.45	2.27	6	12
1:A:72:LEU:HG	1:A:95:ILE:HD11	0.45	1.89	15	1
1:B:36:GLY:O	1:B:40:MET:CG	0.45	2.65	3	2
1:A:115:PHE:O	1:A:115:PHE:CD2	0.45	2.70	18	1
1:B:83:GLU:CD	1:B:94:TYR:CE1	0.45	2.90	8	1
1:B:12:LEU:HD13	1:B:12:LEU:O	0.45	2.11	5	1
1:A:118:SER:H	1:A:132:GLU:CD	0.45	2.14	19	1
1:A:185:GLU:CG	1:A:186:VAL:N	0.45	2.80	17	2
1:B:2:ARG:NH1	1:B:43:ARG:CZ	0.45	2.80	15	1
1:B:207:VAL:O	1:B:211:GLY:O	0.45	2.34	7	4
1:A:115:PHE:C	1:A:117:GLY:N	0.45	2.70	14	1
1:A:46:ASP:OD1	1:A:113:LEU:CD2	0.45	2.65	6	1
1:B:189:ASN:O	1:B:193:GLN:OE1	0.45	2.35	6	2
1:B:1:MET:H2	1:B:2:ARG:CZ	0.45	2.25	19	1
1:B:40:MET:CE	1:B:45:TYR:CZ	0.45	3.00	3	2
1:A:158:HIS:O	1:A:159:ARG:O	0.45	2.35	12	2
1:A:130:PRO:CB	1:A:157:ARG:HE	0.45	2.25	15	1
1:B:28:ASP:OD2	1:B:43:ARG:NH2	0.45	2.50	3	1
1:A:106:VAL:HG23	1:A:107:ALA:N	0.45	2.27	2	1
1:A:11:VAL:CG1	1:A:12:LEU:N	0.45	2.80	11	3
1:A:105:LEU:C	1:A:105:LEU:CD1	0.45	2.85	8	1
1:A:1:MET:SD	1:A:46:ASP:OD2	0.45	2.75	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:94:TYR:CD1	1:B:95:ILE:N	0.44	2.86	1	2
1:A:111:ALA:CB	1:B:87:PHE:CZ	0.44	3.00	3	1
1:A:111:ALA:HB1	1:B:87:PHE:CE1	0.44	2.46	2	1
1:A:23:LYS:NZ	1:A:110:GLU:CD	0.44	2.71	9	1
1:A:195:MET:SD	1:A:195:MET:C	0.44	2.96	9	1
1:B:206:THR:HG23	1:B:206:THR:O	0.44	2.12	9	1
1:B:2:ARG:O	1:B:46:ASP:OD1	0.44	2.35	6	2
1:B:195:MET:SD	1:B:195:MET:C	0.44	2.96	17	1
1:A:64:GLU:CG	1:A:65:LYS:N	0.44	2.80	10	9
1:B:192:ARG:CZ	1:B:204:VAL:CB	0.44	2.83	1	1
1:A:169:LEU:O	1:A:169:LEU:HD13	0.44	2.11	5	2
1:B:46:ASP:OD2	1:B:116:TRP:CD1	0.44	2.70	2	1
1:B:207:VAL:O	1:B:208:ARG:O	0.44	2.36	20	1
1:B:54:ASN:H	1:B:54:ASN:HD22	0.44	1.55	20	1
1:B:77:ASN:H	1:B:77:ASN:ND2	0.44	2.10	14	1
1:B:8:LYS:NZ	1:B:52:ASP:OD1	0.44	2.50	5	1
1:B:211:GLY:C	1:B:213:ARG:NH2	0.44	2.71	12	1
1:B:169:LEU:C	1:B:169:LEU:CD1	0.44	2.85	11	1
1:B:115:PHE:CD2	1:B:116:TRP:N	0.44	2.86	19	1
1:A:5:LEU:CD1	1:A:49:MET:SD	0.44	3.05	10	1
1:A:214:PHE:O	1:A:215:CYS:SG	0.44	2.72	1	2
1:A:123:ILE:O	1:A:123:ILE:CG2	0.44	2.65	3	1
1:A:114:ARG:C	1:A:116:TRP:N	0.44	2.70	20	1
1:B:50:VAL:CG2	1:B:52:ASP:H	0.44	2.26	17	6
1:A:167:GLN:O	1:A:170:ASP:OD1	0.44	2.36	19	3
1:A:163:VAL:O	1:A:212:TYR:O	0.44	2.36	10	2
1:A:98:PRO:O	1:A:99:TYR:O	0.44	2.34	14	10
1:B:169:LEU:O	1:B:173:TRP:O	0.44	2.35	4	2
1:B:191:ILE:O	1:B:195:MET:SD	0.44	2.75	4	1
1:A:89:GLN:N	1:A:89:GLN:CD	0.44	2.71	8	2
1:B:115:PHE:O	1:B:116:TRP:O	0.44	2.36	7	1
1:A:160:ASP:OD1	1:A:216:TYR:CE2	0.44	2.70	3	1
1:B:84:VAL:CG2	1:B:85:HIS:N	0.44	2.79	18	2
1:A:116:TRP:CD2	1:A:117:GLY:N	0.44	2.85	8	1
1:B:55:ALA:O	1:B:58:PHE:N	0.44	2.51	19	1
1:B:188:ILE:HD12	1:B:212:TYR:CE1	0.44	2.47	10	1
1:A:115:PHE:O	1:A:116:TRP:O	0.44	2.36	1	3
1:A:87:PHE:CE1	1:B:111:ALA:HB1	0.44	2.47	15	1
1:B:16:ILE:HD11	1:B:99:TYR:CE2	0.44	2.48	20	1
1:A:7:GLU:OE1	1:A:8:LYS:N	0.44	2.50	8	1
1:B:160:ASP:CG	1:B:216:TYR:HE1	0.44	2.07	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:169:LEU:CD1	1:A:169:LEU:C	0.44	2.86	5	1
1:A:137:TYR:CE2	1:A:198:PRO:O	0.44	2.71	17	2
1:A:173:TRP:CD2	1:A:173:TRP:O	0.44	2.71	17	1
1:B:79:THR:O	1:B:83:GLU:OE2	0.44	2.36	15	3
1:A:102:ILE:O	1:A:103:LYS:C	0.44	2.56	4	1
1:A:207:VAL:O	1:A:208:ARG:O	0.44	2.35	4	1
1:B:44:ASN:O	1:B:45:TYR:O	0.44	2.34	7	2
1:B:110:GLU:O	1:B:113:LEU:N	0.44	2.51	3	1
1:A:124:GLY:C	1:A:126:LEU:H	0.44	2.16	2	1
1:A:159:ARG:C	1:A:161:GLN:HE22	0.44	2.14	14	1
1:A:169:LEU:O	1:A:170:ASP:C	0.44	2.56	9	1
1:B:113:LEU:O	1:B:115:PHE:N	0.44	2.51	19	1
1:A:100:ARG:O	1:A:101:SER:OG	0.44	2.32	1	1
1:B:85:HIS:O	1:B:89:GLN:OE1	0.44	2.36	4	2
1:A:47:LEU:HD23	1:A:113:LEU:HD21	0.44	1.90	7	1
1:A:61:ARG:HH21	1:A:65:LYS:HZ3	0.44	1.56	3	1
1:B:5:LEU:N	1:B:5:LEU:HD23	0.44	2.27	3	1
1:B:173:TRP:C	1:B:173:TRP:CE3	0.44	2.91	20	1
1:A:94:TYR:CE1	1:A:95:ILE:O	0.44	2.70	5	1
1:A:126:LEU:N	1:A:126:LEU:HD23	0.44	2.28	11	1
1:B:92:ASP:CG	1:B:112:ARG:NH1	0.44	2.71	11	1
1:A:62:ILE:O	1:A:66:HIS:O	0.44	2.36	19	1
1:B:182:ASN:HD21	1:B:185:GLU:CD	0.44	2.16	4	1
1:B:154:HIS:ND1	1:B:157:ARG:NH2	0.44	2.66	18	1
1:B:93:ASP:OD2	1:B:108:ARG:NH2	0.44	2.50	20	1
1:A:12:LEU:HD13	1:A:97:LYS:HZ1	0.44	1.72	16	1
1:B:61:ARG:HE	1:B:65:LYS:NZ	0.44	2.11	16	1
1:B:123:ILE:HD11	1:B:216:TYR:CD1	0.44	2.48	9	1
1:B:147:LYS:CB	1:B:147:LYS:NZ	0.44	2.81	6	1
1:A:149:PHE:HD1	1:A:149:PHE:H	0.44	1.56	11	1
1:A:158:HIS:CD2	1:A:158:HIS:N	0.44	2.82	19	1
1:A:159:ARG:O	1:A:214:PHE:O	0.44	2.35	19	1
1:A:2:ARG:O	1:A:46:ASP:OD1	0.44	2.36	17	1
1:A:85:HIS:NE2	1:A:89:GLN:CD	0.44	2.71	17	1
1:B:98:PRO:O	1:B:99:TYR:O	0.44	2.36	1	9
1:A:70:VAL:CG2	1:A:113:LEU:HD11	0.44	2.42	10	1
1:A:31:GLU:OE2	1:A:35:ASP:OD2	0.44	2.36	1	2
1:A:132:GLU:O	1:A:133:GLU:C	0.44	2.55	16	1
1:B:105:LEU:H	1:B:105:LEU:CD1	0.44	2.26	16	1
1:A:8:LYS:O	1:A:9:ASN:O	0.44	2.36	12	1
1:B:147:LYS:CB	1:B:147:LYS:HZ2	0.44	2.26	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:154:HIS:CD2	1:B:158:HIS:HD1	0.44	2.31	6	1
1:B:153:THR:CG2	1:B:157:ARG:NH2	0.44	2.81	19	1
1:A:20:LEU:H	1:A:20:LEU:HD23	0.43	1.73	17	1
1:A:47:LEU:C	1:A:47:LEU:CD1	0.43	2.86	5	6
1:A:53:LYS:NZ	1:A:76:ASP:H	0.43	2.11	4	1
1:A:85:HIS:O	1:A:89:GLN:OE1	0.43	2.36	4	2
1:B:95:ILE:CG2	1:B:108:ARG:HH22	0.43	2.25	18	1
1:B:164:SER:N	1:B:167:GLN:OE1	0.43	2.42	8	1
1:B:8:LYS:NZ	1:B:52:ASP:CG	0.43	2.72	5	1
1:B:110:GLU:CG	1:B:111:ALA:N	0.43	2.80	6	2
1:B:210:ARG:NH1	1:B:213:ARG:HH21	0.43	2.11	17	1
1:B:7:GLU:OE1	1:B:51:SER:OG	0.43	2.36	10	11
1:A:207:VAL:O	1:A:211:GLY:O	0.43	2.36	1	4
1:B:57:SER:O	1:B:61:ARG:NH1	0.43	2.51	1	1
1:B:7:GLU:OE2	1:B:51:SER:OG	0.43	2.36	11	3
1:A:199:LEU:HD13	1:A:199:LEU:O	0.43	2.12	15	1
1:A:4:LEU:C	1:A:4:LEU:HD12	0.43	2.32	15	1
1:B:86:ALA:O	1:B:91:ALA:HB3	0.43	2.12	14	3
1:A:214:PHE:N	1:A:214:PHE:CD1	0.43	2.86	18	1
1:B:5:LEU:HD23	1:B:6:ILE:N	0.43	2.27	19	3
1:A:116:TRP:O	1:A:118:SER:N	0.43	2.51	14	1
1:A:49:MET:CE	1:A:99:TYR:OH	0.43	2.66	16	1
1:B:159:ARG:CG	1:B:160:ASP:N	0.43	2.81	16	1
1:B:100:ARG:O	1:B:101:SER:OG	0.43	2.32	12	1
1:B:211:GLY:CA	1:B:213:ARG:HH22	0.43	2.26	12	1
1:A:161:GLN:HE22	1:A:163:VAL:CG2	0.43	2.26	6	1
1:B:143:GLU:CD	1:B:143:GLU:N	0.43	2.72	6	1
1:A:5:LEU:HD23	1:A:6:ILE:N	0.43	2.28	11	1
1:A:203:THR:O	1:A:203:THR:OG1	0.43	2.34	19	1
1:A:27:ALA:O	1:A:28:ASP:OD1	0.43	2.37	15	4
1:B:56:LEU:N	1:B:56:LEU:HD12	0.43	2.28	15	1
1:A:44:ASN:OD1	1:A:69:ILE:HD11	0.43	2.13	4	1
1:A:85:HIS:CG	1:A:86:ALA:N	0.43	2.86	4	1
1:B:182:ASN:ND2	1:B:185:GLU:CD	0.43	2.71	4	1
1:A:137:TYR:C	1:A:139:GLY:H	0.43	2.16	20	3
1:A:33:LEU:O	1:A:37:GLU:N	0.43	2.43	6	2
1:A:149:PHE:CD1	1:A:149:PHE:N	0.43	2.86	19	2
1:B:133:GLU:OE1	1:B:149:PHE:CD2	0.43	2.71	13	1
1:A:61:ARG:NH2	1:A:65:LYS:HZ3	0.43	2.10	3	1
1:B:181:PRO:O	1:B:185:GLU:OE1	0.43	2.37	2	1
1:A:92:ASP:O	1:A:93:ASP:OD1	0.43	2.37	5	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:69:ILE:HG22	1:B:70:VAL:N	0.43	2.28	18	1
1:A:160:ASP:OD2	1:B:161:GLN:OE1	0.43	2.36	20	1
1:A:166:GLU:O	1:A:170:ASP:OD2	0.43	2.37	5	1
1:B:204:VAL:HG12	1:B:214:PHE:CD2	0.43	2.48	5	1
1:B:27:ALA:O	1:B:28:ASP:OD1	0.43	2.37	11	7
1:A:79:THR:OG1	1:A:82:GLU:OE2	0.43	2.36	10	1
1:B:160:ASP:OD2	1:B:160:ASP:O	0.43	2.36	2	2
1:A:193:GLN:O	1:A:196:ASP:OD1	0.43	2.36	18	4
1:B:92:ASP:CG	1:B:112:ARG:HH21	0.43	2.17	7	1
1:A:120:VAL:HG21	1:A:131:ASP:OD1	0.43	2.13	3	1
1:B:195:MET:C	1:B:195:MET:SD	0.43	2.96	3	1
1:B:208:ARG:O	1:B:209:ARG:O	0.43	2.37	12	3
1:A:23:LYS:HZ1	1:A:103:LYS:NZ	0.43	2.10	16	1
1:A:197:LYS:H	1:A:198:PRO:CD	0.43	2.26	5	1
1:A:121:ILE:HG21	1:A:159:ARG:NH2	0.43	2.28	12	1
1:A:133:GLU:CD	1:A:149:PHE:CE2	0.43	2.92	6	1
1:A:137:TYR:CD1	1:A:137:TYR:N	0.43	2.86	6	1
1:A:47:LEU:CD1	1:A:47:LEU:C	0.43	2.87	18	6
1:B:79:THR:OG1	1:B:82:GLU:OE2	0.43	2.36	4	1
1:A:137:TYR:OH	1:A:199:LEU:O	0.43	2.35	7	1
1:A:150:GLU:OE1	1:A:172:ILE:O	0.43	2.36	3	1
1:A:4:LEU:HD11	1:A:6:ILE:HG12	0.43	1.89	3	2
1:B:113:LEU:O	1:B:116:TRP:N	0.43	2.51	6	2
1:A:48:VAL:CG2	1:A:48:VAL:O	0.43	2.65	18	1
1:B:51:SER:CB	1:B:74:SER:OG	0.43	2.67	20	1
1:B:7:GLU:OE1	1:B:9:ASN:O	0.43	2.36	14	1
1:B:214:PHE:C	1:B:215:CYS:SG	0.43	2.96	12	2
1:A:105:LEU:CD2	1:A:105:LEU:N	0.43	2.80	6	1
1:A:159:ARG:HH22	1:B:161:GLN:HE22	0.43	1.55	6	1
1:A:8:LYS:CD	1:A:8:LYS:H	0.43	2.26	13	1
1:A:93:ASP:OD1	1:A:112:ARG:NH2	0.43	2.44	10	1
1:A:53:LYS:NZ	1:A:76:ASP:OD1	0.43	2.45	1	1
1:A:160:ASP:O	1:A:160:ASP:OD1	0.43	2.37	13	3
1:A:135:ILE:HD12	1:A:152:LEU:CD2	0.43	2.43	3	1
1:B:121:ILE:O	1:B:128:ILE:O	0.43	2.37	16	2
1:A:143:GLU:CD	1:A:143:GLU:N	0.43	2.72	19	2
1:A:132:GLU:N	1:A:132:GLU:CD	0.43	2.71	14	1
1:A:4:LEU:O	1:A:49:MET:O	0.43	2.36	13	3
1:B:123:ILE:O	1:B:126:LEU:O	0.43	2.37	5	1
1:B:158:HIS:O	1:B:160:ASP:N	0.43	2.52	5	1
1:A:100:ARG:HE	1:B:80:SER:CB	0.43	2.27	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:152:LEU:HD23	1:B:152:LEU:C	0.43	2.34	13	1
1:A:55:ALA:O	1:A:56:LEU:C	0.43	2.57	20	13
1:B:60:SER:OG	1:B:61:ARG:N	0.43	2.52	6	2
1:B:75:SER:OG	1:B:82:GLU:OE1	0.43	2.36	15	2
1:B:160:ASP:OD1	1:B:160:ASP:O	0.43	2.37	4	1
1:A:53:LYS:C	1:A:55:ALA:H	0.43	2.17	5	3
1:B:72:LEU:CD2	1:B:108:ARG:NH2	0.43	2.81	3	1
1:B:150:GLU:O	1:B:154:HIS:CD2	0.43	2.72	8	1
1:A:145:LYS:CA	1:A:149:PHE:HB2	0.43	2.43	6	1
1:B:89:GLN:N	1:B:89:GLN:CD	0.43	2.72	19	1
1:B:132:GLU:CD	1:B:132:GLU:N	0.43	2.72	17	1
1:B:185:GLU:O	1:B:189:ASN:OD1	0.43	2.36	4	2
1:A:152:LEU:CD1	1:A:195:MET:SD	0.43	3.07	7	1
1:A:61:ARG:NH2	1:A:65:LYS:HZ2	0.43	2.10	3	1
1:B:113:LEU:O	1:B:114:ARG:O	0.43	2.36	3	2
1:B:92:ASP:O	1:B:93:ASP:OD1	0.43	2.37	16	3
1:A:143:GLU:CG	1:A:144:VAL:N	0.43	2.82	18	1
1:A:23:LYS:HZ3	1:A:103:LYS:HZ2	0.43	1.56	16	1
1:B:118:SER:O	1:B:119:ASN:O	0.43	2.36	9	1
1:A:190:GLN:O	1:A:194:LYS:CB	0.43	2.67	6	1
1:B:133:GLU:O	1:B:145:LYS:NZ	0.43	2.47	13	1
1:B:137:TYR:O	1:B:139:GLY:N	0.43	2.52	15	1
1:B:28:ASP:O	1:B:28:ASP:OD1	0.43	2.37	15	1
1:B:212:TYR:CD1	1:B:212:TYR:N	0.43	2.87	2	2
1:A:157:ARG:HE	1:A:158:HIS:CE1	0.43	2.30	7	1
1:B:149:PHE:O	1:B:153:THR:OG1	0.43	2.37	7	1
1:B:182:ASN:O	1:B:185:GLU:OE1	0.43	2.37	2	1
1:B:17:GLU:OE2	1:B:27:ALA:O	0.43	2.36	20	1
1:A:69:ILE:HG22	1:A:70:VAL:N	0.43	2.29	16	1
1:B:155:LEU:O	1:B:159:ARG:CA	0.43	2.67	5	1
1:A:123:ILE:O	1:A:126:LEU:O	0.43	2.36	9	2
1:B:212:TYR:O	1:B:213:ARG:NH2	0.43	2.52	12	1
1:B:75:SER:OG	1:B:94:TYR:OH	0.42	2.36	17	2
1:A:23:LYS:NZ	1:A:106:VAL:HG11	0.42	2.29	13	2
1:B:135:ILE:HD13	1:B:144:VAL:HG11	0.42	1.91	1	1
1:B:167:GLN:O	1:B:170:ASP:OD1	0.42	2.36	16	2
1:A:161:GLN:OE1	1:A:162:ILE:O	0.42	2.37	13	2
1:B:31:GLU:OE2	1:B:35:ASP:OD2	0.42	2.37	3	4
1:A:144:VAL:HG23	1:A:149:PHE:CD1	0.42	2.48	2	1
1:A:194:LYS:NZ	1:A:194:LYS:CB	0.42	2.81	20	2
1:A:207:VAL:CG1	1:A:213:ARG:HH11	0.42	2.26	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:SER:OG	1:B:101:SER:OG	0.42	2.36	12	1
1:A:7:GLU:O	1:A:30:THR:O	0.42	2.37	11	1
1:A:196:ASP:O	1:A:196:ASP:OD1	0.42	2.37	19	1
1:A:199:LEU:C	1:A:201:ILE:H	0.42	2.18	1	1
1:A:152:LEU:O	1:A:152:LEU:HD13	0.42	2.14	14	3
1:A:122:GLU:H	1:A:159:ARG:NH1	0.42	2.12	4	1
1:A:39:LEU:CD1	1:A:39:LEU:C	0.42	2.87	7	1
1:A:8:LYS:NZ	1:A:32:SER:N	0.42	2.67	3	1
1:A:110:GLU:O	1:A:114:ARG:CG	0.42	2.67	2	1
1:A:105:LEU:CD1	1:A:105:LEU:C	0.42	2.87	9	1
1:B:113:LEU:C	1:B:113:LEU:HD23	0.42	2.34	11	1
1:B:113:LEU:C	1:B:115:PHE:N	0.42	2.73	19	1
1:B:119:ASN:OD1	1:B:128:ILE:O	0.42	2.36	19	1
1:A:151:VAL:CG1	1:A:152:LEU:N	0.42	2.82	1	2
1:A:75:SER:OG	1:A:94:TYR:OH	0.42	2.36	8	3
1:A:73:VAL:HG13	1:A:73:VAL:O	0.42	2.14	15	1
1:B:89:GLN:N	1:B:89:GLN:NE2	0.42	2.66	4	1
1:A:77:ASN:O	1:A:82:GLU:OE1	0.42	2.37	7	1
1:A:108:ARG:NH1	1:B:83:GLU:OE2	0.42	2.53	3	1
1:A:83:GLU:CD	1:B:108:ARG:CZ	0.42	2.88	18	1
1:B:12:LEU:HD12	1:B:99:TYR:CE2	0.42	2.50	8	1
1:A:164:SER:OG	1:A:166:GLU:OE1	0.42	2.37	9	1
1:A:169:LEU:HD12	1:A:169:LEU:N	0.42	2.30	9	1
1:A:45:TYR:O	1:A:46:ASP:OD1	0.42	2.38	13	1
1:A:199:LEU:N	1:A:199:LEU:HD22	0.42	2.30	1	1
1:B:135:ILE:N	1:B:135:ILE:CD1	0.42	2.82	1	1
1:B:214:PHE:O	1:B:215:CYS:SG	0.42	2.78	20	1
1:A:82:GLU:OE1	1:A:94:TYR:OH	0.42	2.37	13	2
1:A:93:ASP:OD2	1:A:112:ARG:NE	0.42	2.52	8	1
1:A:59:VAL:HG23	1:A:60:SER:N	0.42	2.29	12	2
1:A:149:PHE:HD1	1:A:150:GLU:H	0.42	1.35	11	1
1:B:169:LEU:CD1	1:B:169:LEU:C	0.42	2.87	7	3
1:A:192:ARG:O	1:A:196:ASP:OD1	0.42	2.37	2	1
1:A:42:ILE:HD12	1:A:43:ARG:NH1	0.42	2.29	18	1
1:B:58:PHE:CZ	1:B:62:ILE:HD11	0.42	2.50	20	1
1:B:216:TYR:N	1:B:216:TYR:CD1	0.42	2.85	14	1
1:A:106:VAL:CG1	1:A:107:ALA:N	0.42	2.82	8	1
1:B:79:THR:OG1	1:B:81:GLU:OE1	0.42	2.37	5	1
1:A:44:ASN:ND2	1:A:45:TYR:H	0.42	2.12	6	1
1:A:85:HIS:CE1	1:A:89:GLN:CD	0.42	2.93	13	1
1:B:28:ASP:OD1	1:B:28:ASP:O	0.42	2.37	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:GLU:OE1	1:A:51:SER:OG	0.42	2.37	17	1
1:A:63:LYS:O	1:A:67:SER:CA	0.42	2.67	2	3
1:A:82:GLU:O	1:A:86:ALA:HB2	0.42	2.14	5	2
1:B:45:TYR:O	1:B:45:TYR:CD2	0.42	2.73	7	1
1:A:60:SER:OG	1:A:61:ARG:N	0.42	2.51	3	1
1:B:105:LEU:C	1:B:105:LEU:CD1	0.42	2.85	13	2
1:B:159:ARG:O	1:B:160:ASP:OD1	0.42	2.37	2	1
1:A:52:ASP:OD1	1:A:52:ASP:N	0.42	2.52	18	1
1:B:15:GLU:CG	1:B:16:ILE:N	0.42	2.82	18	1
1:A:32:SER:O	1:A:34:GLU:N	0.42	2.53	20	1
1:B:172:ILE:O	1:B:172:ILE:HG22	0.42	2.15	16	1
1:A:7:GLU:O	1:A:9:ASN:N	0.42	2.50	5	1
1:A:133:GLU:HB3	1:A:149:PHE:CE1	0.42	2.40	6	1
1:B:115:PHE:C	1:B:117:GLY:H	0.42	2.18	6	1
1:A:76:ASP:OD1	1:A:77:ASN:N	0.42	2.53	13	1
1:B:203:THR:OG1	1:B:214:PHE:CZ	0.42	2.71	1	1
1:B:125:ASP:OD1	1:B:125:ASP:N	0.42	2.51	15	1
1:A:148:PRO:O	1:A:151:VAL:HG12	0.42	2.14	7	1
1:B:199:LEU:HD12	1:B:199:LEU:N	0.42	2.29	3	1
1:A:163:VAL:HG23	1:A:214:PHE:CD1	0.42	2.49	18	1
1:A:115:PHE:O	1:A:116:TRP:C	0.42	2.58	11	2
1:A:23:LYS:HZ1	1:A:103:LYS:HZ1	0.42	1.58	16	1
1:A:70:VAL:HG22	1:A:112:ARG:NH2	0.42	2.29	9	1
1:A:115:PHE:C	1:A:115:PHE:CD1	0.42	2.92	11	1
1:B:75:SER:CB	1:B:94:TYR:HH	0.42	2.26	19	1
1:A:137:TYR:O	1:A:137:TYR:CD1	0.42	2.73	1	1
1:B:206:THR:O	1:B:206:THR:HG23	0.42	2.14	1	1
1:A:170:ASP:O	1:A:170:ASP:OD1	0.42	2.37	4	1
1:A:199:LEU:H	1:A:199:LEU:HD22	0.42	1.73	7	1
1:B:5:LEU:CD1	1:B:49:MET:SD	0.42	3.07	16	2
1:A:121:ILE:HG23	1:A:159:ARG:HH12	0.42	1.74	16	1
1:B:123:ILE:HD12	1:B:159:ARG:CZ	0.42	2.38	16	1
1:B:75:SER:CB	1:B:94:TYR:CZ	0.42	3.03	5	1
1:B:10:SER:OG	1:B:11:VAL:N	0.42	2.52	12	1
1:A:75:SER:OG	1:A:94:TYR:CE2	0.42	2.62	6	1
1:A:103:LYS:CD	1:A:103:LYS:N	0.42	2.83	17	1
1:B:47:LEU:C	1:B:47:LEU:CD1	0.42	2.88	17	4
1:A:106:VAL:CG2	1:A:107:ALA:N	0.42	2.83	2	1
1:A:138:LYS:CG	1:A:138:LYS:O	0.42	2.68	18	1
1:B:85:HIS:CD2	1:B:89:GLN:NE2	0.42	2.88	18	1
1:B:123:ILE:CG2	1:B:126:LEU:HB2	0.42	2.44	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:PHE:CZ	1:B:111:ALA:HB1	0.42	2.49	8	2
1:B:23:LYS:HZ2	1:B:106:VAL:CG1	0.42	2.21	16	1
1:A:159:ARG:HH21	1:A:203:THR:HG21	0.42	1.75	7	1
1:A:77:ASN:O	1:A:77:ASN:OD1	0.42	2.38	3	1
1:A:83:GLU:OE2	1:B:100:ARG:NE	0.42	2.53	20	1
1:B:144:VAL:HB	1:B:149:PHE:CD1	0.42	2.50	20	1
1:B:77:ASN:ND2	1:B:77:ASN:N	0.42	2.67	14	1
1:A:110:GLU:O	1:A:114:ARG:CA	0.42	2.68	5	1
1:B:123:ILE:O	1:B:124:GLY:C	0.42	2.58	5	1
1:B:162:ILE:HG23	1:B:213:ARG:NE	0.42	2.30	12	1
1:A:119:ASN:CB	1:A:129:SER:OG	0.42	2.68	11	1
1:A:112:ARG:C	1:A:113:LEU:HD23	0.41	2.35	10	1
1:A:75:SER:CB	1:A:94:TYR:CZ	0.41	3.03	15	2
1:B:12:LEU:CD1	1:B:97:LYS:NZ	0.41	2.83	15	1
1:B:146:GLY:CA	1:B:149:PHE:CE2	0.41	3.03	4	1
1:A:199:LEU:CD2	1:A:199:LEU:N	0.41	2.83	7	1
1:A:95:ILE:HG22	1:A:96:ALA:N	0.41	2.30	14	1
1:B:131:ASP:O	1:B:133:GLU:OE1	0.41	2.37	8	1
1:A:5:LEU:N	1:A:5:LEU:HD23	0.41	2.30	5	1
1:A:100:ARG:HE	1:B:80:SER:CA	0.41	2.27	6	1
1:B:190:GLN:O	1:B:194:LYS:CB	0.41	2.68	10	2
1:B:8:LYS:H	1:B:8:LYS:CD	0.41	2.27	1	1
1:B:137:TYR:C	1:B:139:GLY:H	0.41	2.18	15	1
1:B:182:ASN:C	1:B:184:ILE:H	0.41	2.19	3	1
1:B:31:GLU:OE2	1:B:35:ASP:OD1	0.41	2.38	14	1
1:A:86:ALA:O	1:A:91:ALA:HB3	0.41	2.15	5	1
1:B:77:ASN:N	1:B:78:PRO:CD	0.41	2.83	12	1
1:A:108:ARG:HE	1:B:83:GLU:CD	0.41	2.19	12	1
1:B:209:ARG:CD	1:B:209:ARG:N	0.41	2.83	10	1
1:A:169:LEU:C	1:A:169:LEU:CD2	0.41	2.89	15	1
1:B:97:LYS:CD	1:B:97:LYS:O	0.41	2.69	4	1
1:B:105:LEU:H	1:B:105:LEU:CD2	0.41	2.28	18	1
1:A:187:ALA:O	1:A:191:ILE:CG1	0.41	2.68	14	1
1:A:28:ASP:OD2	1:A:39:LEU:CD2	0.41	2.68	16	1
1:B:123:ILE:CD1	1:B:159:ARG:HH12	0.41	2.28	5	1
1:A:70:VAL:CG1	1:A:71:VAL:N	0.41	2.83	9	1
1:A:72:LEU:C	1:A:72:LEU:CD1	0.41	2.89	11	1
1:B:103:LYS:N	1:B:103:LYS:CD	0.41	2.83	13	1
1:A:103:LYS:N	1:A:103:LYS:CD	0.41	2.83	15	1
1:B:47:LEU:CD1	1:B:47:LEU:C	0.41	2.89	18	9
1:B:2:ARG:NH2	1:B:44:ASN:N	0.41	2.68	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:126:LEU:HD22	1:B:137:TYR:CD1	0.41	2.50	3	1
1:B:53:LYS:C	1:B:55:ALA:H	0.41	2.17	19	2
1:B:193:GLN:NE2	1:B:193:GLN:N	0.41	2.69	6	1
1:A:123:ILE:O	1:A:124:GLY:C	0.41	2.58	19	2
1:B:49:MET:CE	1:B:74:SER:OG	0.41	2.68	19	1
1:B:16:ILE:HD11	1:B:99:TYR:CE1	0.41	2.51	20	1
1:B:12:LEU:HD11	1:B:97:LYS:HZ2	0.41	1.75	14	1
1:A:81:GLU:CD	1:A:81:GLU:N	0.41	2.74	10	1
1:A:199:LEU:C	1:A:201:ILE:N	0.41	2.73	1	1
1:A:209:ARG:O	1:A:210:ARG:C	0.41	2.58	2	1
1:A:77:ASN:N	1:A:78:PRO:CD	0.41	2.82	11	2
1:B:119:ASN:CG	1:B:120:VAL:N	0.41	2.74	12	1
1:B:150:GLU:OE1	1:B:172:ILE:O	0.41	2.38	12	1
1:B:96:ALA:O	1:B:97:LYS:C	0.41	2.58	12	2
1:A:23:LYS:HZ2	1:A:110:GLU:CD	0.41	2.18	6	1
1:B:147:LYS:N	1:B:148:PRO:HD2	0.41	2.31	13	1
1:B:184:ILE:CD1	1:B:184:ILE:H	0.41	2.24	19	1
1:A:119:ASN:CG	1:A:120:VAL:H	0.41	2.18	17	1
1:B:149:PHE:CE2	1:B:153:THR:HG23	0.41	2.51	10	1
1:A:117:GLY:O	1:A:118:SER:OG	0.41	2.37	2	1
1:B:16:ILE:CD1	1:B:99:TYR:CZ	0.41	3.03	20	1
1:B:72:LEU:HD21	1:B:108:ARG:NH2	0.41	2.30	20	1
1:B:160:ASP:OD1	1:B:216:TYR:CD1	0.41	2.73	8	1
1:B:157:ARG:C	1:B:159:ARG:H	0.41	2.18	16	1
1:B:157:ARG:C	1:B:159:ARG:N	0.41	2.74	16	1
1:B:72:LEU:CD2	1:B:72:LEU:C	0.41	2.89	16	1
1:A:44:ASN:C	1:A:45:TYR:CD2	0.41	2.94	5	1
1:A:166:GLU:CD	1:A:166:GLU:H	0.41	2.19	9	1
1:B:155:LEU:C	1:B:155:LEU:CD2	0.41	2.82	12	1
1:A:23:LYS:NZ	1:A:106:VAL:CG1	0.41	2.84	17	1
1:B:83:GLU:OE2	1:B:94:TYR:OH	0.41	2.37	4	1
1:A:133:GLU:OE2	1:A:144:VAL:O	0.41	2.37	7	1
1:A:160:ASP:OD1	1:A:160:ASP:O	0.41	2.38	2	1
1:B:149:PHE:CD1	1:B:150:GLU:N	0.41	2.88	16	1
1:B:95:ILE:HG22	1:B:96:ALA:N	0.41	2.30	9	1
1:B:211:GLY:C	1:B:213:ARG:HH22	0.41	2.19	12	1
1:B:196:ASP:N	1:B:196:ASP:OD1	0.41	2.54	6	1
1:B:210:ARG:NH1	1:B:213:ARG:NH2	0.41	2.69	17	1
1:B:55:ALA:O	1:B:56:LEU:C	0.41	2.58	19	5
1:A:85:HIS:CG	1:A:89:GLN:OE1	0.41	2.74	4	1
1:B:4:LEU:HD12	1:B:5:LEU:N	0.41	2.31	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:SER:O	1:A:101:SER:OG	0.41	2.35	7	1
1:A:39:LEU:CD2	1:A:39:LEU:C	0.41	2.87	2	1
1:A:116:TRP:O	1:A:116:TRP:CG	0.41	2.73	2	1
1:B:82:GLU:OE1	1:B:94:TYR:OH	0.41	2.39	2	1
1:A:110:GLU:OE2	1:A:114:ARG:NH1	0.41	2.53	18	1
1:B:212:TYR:N	1:B:212:TYR:CD1	0.41	2.88	18	2
1:A:97:LYS:CD	1:A:97:LYS:C	0.41	2.89	14	1
1:B:122:GLU:CG	1:B:122:GLU:O	0.41	2.69	8	1
1:B:123:ILE:HD11	1:B:216:TYR:CB	0.41	2.46	9	1
1:B:119:ASN:HD21	1:B:128:ILE:C	0.41	2.18	12	1
1:B:77:ASN:OD1	1:B:77:ASN:N	0.41	2.54	6	1
1:A:76:ASP:OD1	1:A:76:ASP:O	0.41	2.38	11	1
1:A:5:LEU:HD22	1:A:49:MET:HG3	0.41	1.92	19	1
1:A:111:ALA:HB2	1:B:87:PHE:CZ	0.41	2.50	19	1
1:B:155:LEU:CD2	1:B:155:LEU:C	0.41	2.85	19	1
1:A:169:LEU:HD23	1:A:169:LEU:O	0.41	2.16	15	1
1:B:124:GLY:C	1:B:126:LEU:H	0.41	2.19	7	1
1:B:2:ARG:HH21	1:B:44:ASN:C	0.41	2.19	2	1
1:B:97:LYS:O	1:B:97:LYS:CD	0.41	2.69	2	1
1:A:32:SER:C	1:A:34:GLU:N	0.41	2.74	20	1
1:B:86:ALA:O	1:B:91:ALA:CB	0.41	2.69	14	1
1:A:149:PHE:CE2	1:A:153:THR:HG23	0.41	2.51	5	1
1:A:53:LYS:O	1:A:55:ALA:N	0.41	2.54	5	1
1:B:169:LEU:O	1:B:170:ASP:C	0.41	2.59	13	1
1:A:18:LYS:CD	1:A:18:LYS:N	0.41	2.84	19	1
1:B:137:TYR:CD1	1:B:137:TYR:N	0.40	2.89	17	1
1:B:123:ILE:HD13	1:B:123:ILE:N	0.40	2.31	1	1
1:A:135:ILE:CG2	1:A:135:ILE:O	0.40	2.69	4	1
1:A:206:THR:HG23	1:A:206:THR:O	0.40	2.16	3	1
1:A:134:LYS:C	1:A:135:ILE:HD12	0.40	2.37	2	1
1:B:137:TYR:CZ	1:B:140:ARG:HG2	0.40	2.51	8	1
1:B:147:LYS:HE3	1:B:172:ILE:C	0.40	2.36	8	1
1:B:205:GLU:N	1:B:205:GLU:CD	0.40	2.75	12	1
1:A:144:VAL:O	1:A:149:PHE:CD1	0.40	2.74	6	1
1:A:145:LYS:N	1:A:149:PHE:CG	0.40	2.76	11	1
1:A:122:GLU:OE1	1:A:122:GLU:N	0.40	2.54	17	1
1:B:115:PHE:CE2	1:B:116:TRP:CE3	0.40	3.10	17	1
1:B:189:ASN:ND2	1:B:189:ASN:C	0.40	2.74	15	1
1:A:56:LEU:HD22	1:A:85:HIS:NE2	0.40	2.31	4	1
1:A:12:LEU:CD2	1:A:97:LYS:HZ2	0.40	2.29	3	1
1:A:97:LYS:O	1:A:98:PRO:C	0.40	2.59	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:ASP:OD1	1:A:171:ALA:N	0.40	2.54	20	1
1:B:159:ARG:NH2	1:B:217:PRO:HD3	0.40	2.16	16	1
1:B:149:PHE:CE1	1:B:153:THR:CG2	0.40	3.05	12	1
1:B:158:HIS:CG	1:B:161:GLN:HE22	0.40	2.32	17	1
1:A:107:ALA:HB1	1:B:87:PHE:CD2	0.40	2.51	10	1
1:A:161:GLN:CD	1:A:162:ILE:H	0.40	2.20	10	1
1:B:199:LEU:CD2	1:B:199:LEU:C	0.40	2.88	10	1
1:B:42:ILE:HD12	1:B:43:ARG:NH1	0.40	2.32	1	1
1:B:189:ASN:HD22	1:B:189:ASN:C	0.40	2.17	15	1
1:A:72:LEU:CD2	1:A:72:LEU:C	0.40	2.90	20	1
1:B:12:LEU:HD11	1:B:97:LYS:NZ	0.40	2.32	14	1
1:B:72:LEU:C	1:B:72:LEU:CD2	0.40	2.90	5	2
1:A:125:ASP:OD1	1:A:125:ASP:N	0.40	2.55	6	1
1:B:214:PHE:N	1:B:214:PHE:CD1	0.40	2.89	11	1
1:A:184:ILE:O	1:A:188:ILE:HG22	0.40	2.17	19	1
1:A:144:VAL:CG2	1:A:149:PHE:CD1	0.40	3.04	17	1
1:A:71:VAL:CG2	1:A:92:ASP:OD2	0.40	2.69	10	1
1:B:170:ASP:O	1:B:171:ALA:C	0.40	2.60	10	1
1:A:195:MET:CG	1:A:196:ASP:N	0.40	2.85	1	1
1:A:84:VAL:CG2	1:A:85:HIS:N	0.40	2.85	7	1
1:B:169:LEU:CD2	1:B:169:LEU:C	0.40	2.89	2	1
1:A:118:SER:O	1:A:119:ASN:O	0.40	2.39	18	1
1:A:211:GLY:O	1:A:212:TYR:CD1	0.40	2.74	18	1
1:B:204:VAL:HG23	1:B:204:VAL:O	0.40	2.16	9	1
1:B:188:ILE:HD13	1:B:212:TYR:CE1	0.40	2.52	13	1
1:B:162:ILE:CD1	1:B:162:ILE:H	0.40	2.27	17	1
1:A:44:ASN:ND2	1:A:145:LYS:HZ1	0.40	2.14	15	1
1:A:184:ILE:CG2	1:A:185:GLU:N	0.40	2.84	7	1
1:A:96:ALA:O	1:A:97:LYS:C	0.40	2.60	7	1
1:B:124:GLY:C	1:B:126:LEU:N	0.40	2.75	7	1
1:B:59:VAL:CG2	1:B:60:SER:N	0.40	2.85	18	1
1:B:69:ILE:CG2	1:B:70:VAL:N	0.40	2.84	18	1
1:A:169:LEU:CD2	1:A:169:LEU:C	0.40	2.90	16	1
1:B:170:ASP:OD1	1:B:171:ALA:N	0.40	2.55	16	1
1:B:102:ILE:HD13	1:B:102:ILE:N	0.40	2.31	5	1
1:A:129:SER:O	1:A:133:GLU:N	0.40	2.55	9	1
1:A:49:MET:SD	1:A:49:MET:C	0.40	2.99	9	1
1:B:183:VAL:O	1:B:186:VAL:HG12	0.40	2.16	12	1
1:A:103:LYS:O	1:A:107:ALA:CB	0.40	2.70	6	1
1:B:159:ARG:O	1:B:160:ASP:C	0.40	2.59	11	1
1:A:170:ASP:C	1:A:170:ASP:OD1	0.40	2.60	19	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	208/223 (93%)	177±3 (85±1%)	21±3 (10±1%)	10±3 (5±1%)	5	27
1	B	210/223 (94%)	181±4 (86±2%)	18±3 (9±1%)	10±2 (5±1%)	5	27
All	All	8360/8920 (94%)	7163 (86%)	792 (9%)	405 (5%)	5	27

All 74 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	99	TYR	20
1	B	99	TYR	20
1	B	98	PRO	20
1	A	98	PRO	20
1	B	90	GLY	17
1	A	78	PRO	17
1	A	90	GLY	17
1	B	78	PRO	16
1	A	102	ILE	16
1	B	101	SER	15
1	B	102	ILE	15
1	A	101	SER	14
1	B	181	PRO	11
1	B	209	ARG	9
1	B	217	PRO	8
1	A	145	LYS	8
1	A	116	TRP	8
1	A	217	PRO	7
1	B	145	LYS	6
1	A	210	ARG	6
1	A	9	ASN	5
1	A	117	GLY	5
1	A	183	VAL	5
1	B	130	PRO	5
1	B	116	TRP	5
1	A	160	ASP	5

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Mol	Chain	Res	Type	Models (Total)
1	A	209	ARG	5
1	A	198	PRO	4
1	B	210	ARG	4
1	B	173	TRP	4
1	B	159	ARG	4
1	A	130	PRO	4
1	B	115	PHE	4
1	B	198	PRO	4
1	A	118	SER	3
1	B	160	ASP	3
1	A	76	ASP	3
1	B	114	ARG	3
1	A	115	PHE	3
1	A	182	ASN	3
1	B	182	ASN	3
1	B	119	ASN	2
1	B	183	VAL	2
1	A	159	ARG	2
1	A	199	LEU	2
1	B	54	ASN	2
1	B	104	ALA	2
1	A	114	ARG	2
1	A	104	ALA	2
1	B	9	ASN	2
1	A	170	ASP	2
1	A	45	TYR	2
1	B	117	GLY	2
1	B	45	TYR	2
1	B	10	SER	2
1	A	119	ASN	2
1	B	170	ASP	2
1	B	218	LYS	2
1	A	208	ARG	2
1	A	103	LYS	1
1	A	31	GLU	1
1	A	197	LYS	1
1	B	118	SER	1
1	A	68	SER	1
1	A	211	GLY	1
1	B	158	HIS	1
1	B	148	PRO	1
1	A	10	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	B	211	GLY	1
1	B	208	ARG	1
1	A	124	GLY	1
1	B	44	ASN	1
1	A	77	ASN	1
1	A	7	GLU	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	186/199 (93%)	173±3 (93±1%)	13±3 (7±1%)	21	67
1	B	188/199 (94%)	175±3 (93±1%)	13±3 (7±1%)	23	69
All	All	7480/7960 (94%)	6950 (93%)	530 (7%)	22	68

All 146 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	97	LYS	20
1	B	50	VAL	20
1	B	47	LEU	20
1	B	97	LYS	18
1	A	47	LEU	18
1	A	126	LEU	18
1	B	126	LEU	16
1	B	119	ASN	16
1	A	80	SER	14
1	A	119	ASN	14
1	B	206	THR	13
1	B	80	SER	13
1	A	206	THR	11
1	A	95	ILE	10
1	B	94	TYR	9
1	A	29	VAL	8
1	B	173	TRP	8
1	A	173	TRP	7

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Mol	Chain	Res	Type	Models (Total)
1	B	155	LEU	7
1	B	145	LYS	7
1	B	72	LEU	7
1	B	95	ILE	6
1	A	74	SER	6
1	A	49	MET	6
1	B	152	LEU	5
1	A	145	LYS	5
1	A	4	LEU	5
1	A	188	ILE	5
1	A	152	LEU	5
1	A	94	TYR	5
1	B	1	MET	5
1	B	74	SER	5
1	B	123	ILE	4
1	A	127	THR	4
1	B	153	THR	4
1	A	40	MET	4
1	B	216	TYR	4
1	A	1	MET	3
1	B	83	GLU	3
1	B	147	LYS	3
1	B	49	MET	3
1	A	105	LEU	3
1	B	40	MET	3
1	A	140	ARG	3
1	B	112	ARG	3
1	B	113	LEU	3
1	A	203	THR	3
1	A	195	MET	3
1	A	112	ARG	3
1	A	147	LYS	3
1	A	210	ARG	3
1	A	114	ARG	3
1	A	8	LYS	3
1	A	113	LEU	3
1	A	149	PHE	2
1	A	216	TYR	2
1	B	114	ARG	2
1	A	20	LEU	2
1	A	123	ILE	2
1	B	214	PHE	2

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Mol	Chain	Res	Type	Models (Total)
1	B	116	TRP	2
1	B	140	ARG	2
1	B	189	ASN	2
1	B	82	GLU	2
1	A	209	ARG	2
1	A	50	VAL	2
1	B	89	GLN	2
1	B	108	ARG	2
1	A	197	LYS	2
1	B	195	MET	2
1	A	108	ARG	2
1	B	149	PHE	2
1	A	83	GLU	2
1	A	204	VAL	2
1	B	5	LEU	2
1	B	159	ARG	2
1	A	89	GLN	2
1	A	72	LEU	2
1	B	54	ASN	2
1	A	76	ASP	2
1	B	193	GLN	2
1	A	161	GLN	2
1	A	66	HIS	2
1	B	197	LYS	2
1	B	122	GLU	2
1	B	8	LYS	2
1	A	5	LEU	2
1	A	184	ILE	2
1	A	7	GLU	2
1	A	53	LYS	1
1	A	125	ASP	1
1	B	77	ASN	1
1	A	158	HIS	1
1	A	138	LYS	1
1	B	12	LEU	1
1	A	189	ASN	1
1	B	133	GLU	1
1	B	169	LEU	1
1	A	45	TYR	1
1	A	103	LYS	1
1	B	63	LYS	1
1	A	135	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	B	204	VAL	1
1	A	165	LYS	1
1	B	167	GLN	1
1	A	110	GLU	1
1	B	199	LEU	1
1	B	157	ARG	1
1	B	188	ILE	1
1	B	87	PHE	1
1	A	159	ARG	1
1	B	125	ASP	1
1	B	184	ILE	1
1	B	127	THR	1
1	A	190	GLN	1
1	B	105	LEU	1
1	A	199	LEU	1
1	A	12	LEU	1
1	B	192	ARG	1
1	A	153	THR	1
1	A	79	THR	1
1	A	75	SER	1
1	A	18	LYS	1
1	A	23	LYS	1
1	B	194	LYS	1
1	A	160	ASP	1
1	B	208	ARG	1
1	B	154	HIS	1
1	A	193	GLN	1
1	A	82	GLU	1
1	A	100	ARG	1
1	A	129	SER	1
1	A	98	PRO	1
1	B	2	ARG	1
1	A	118	SER	1
1	A	213	ARG	1
1	A	167	GLN	1
1	A	116	TRP	1
1	B	170	ASP	1
1	A	92	ASP	1
1	A	192	ARG	1
1	A	134	LYS	1
1	A	39	LEU	1
1	B	218	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	136	ILE	1
1	A	48	VAL	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided