Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 01:49 PM EDT

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

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

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

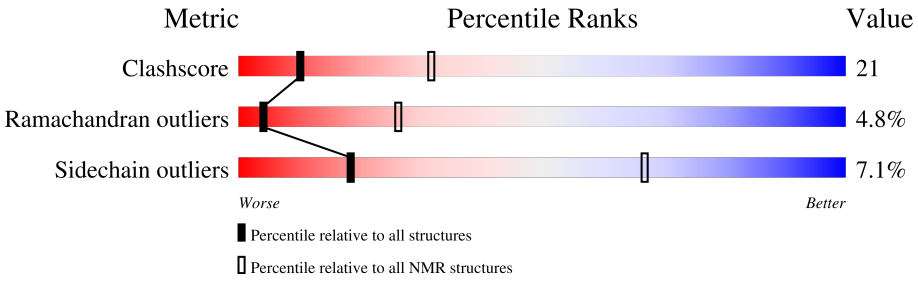
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment 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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	223	58% 34% · 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)	1.26	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	

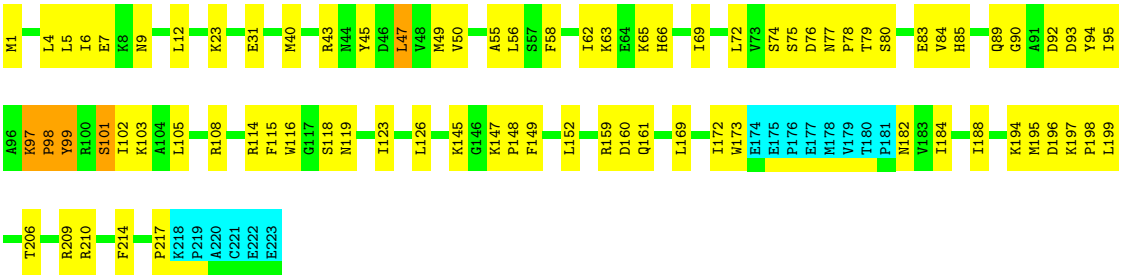
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

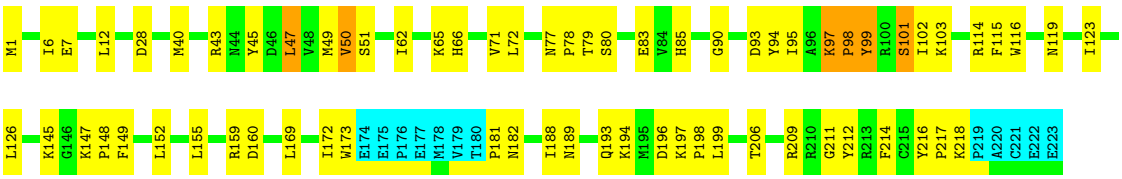
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain B:



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

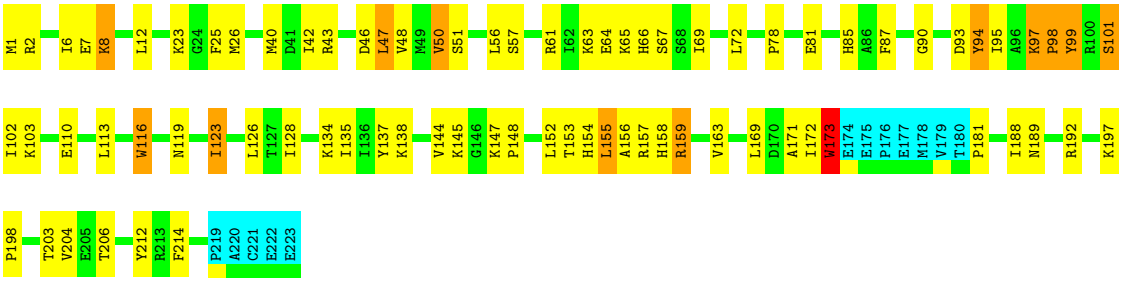
4.2.1 Score per residue for model 1

• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:

• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

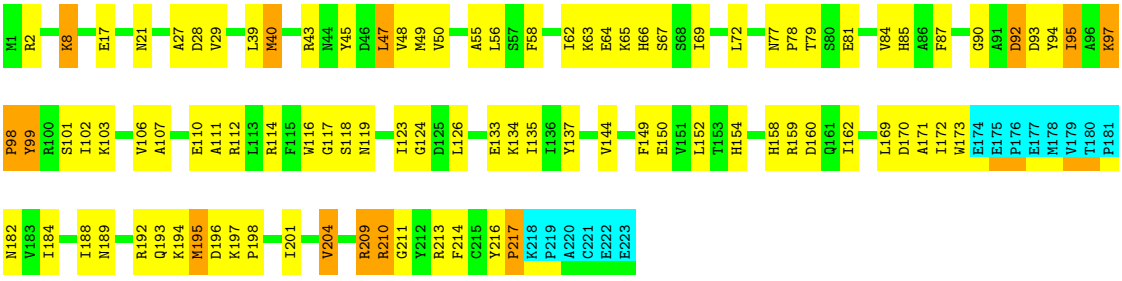
Chain B:



4.2.2 Score per residue for model 2

• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:



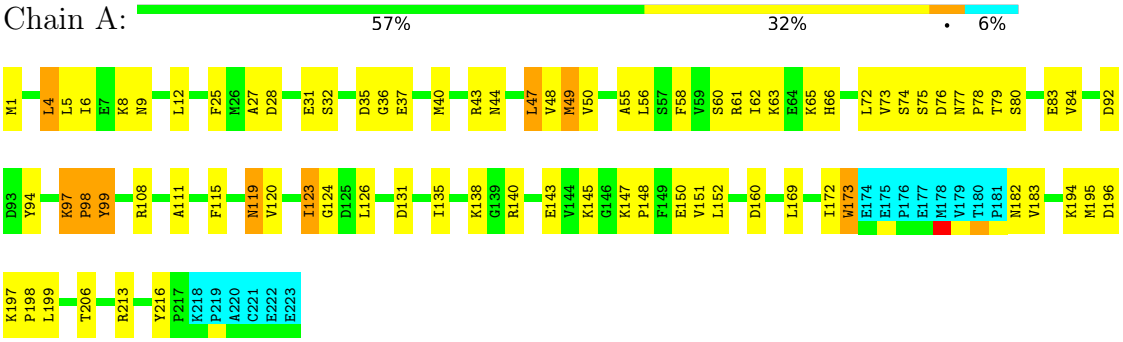
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain B:

4.2.3 Score per residue for model 3

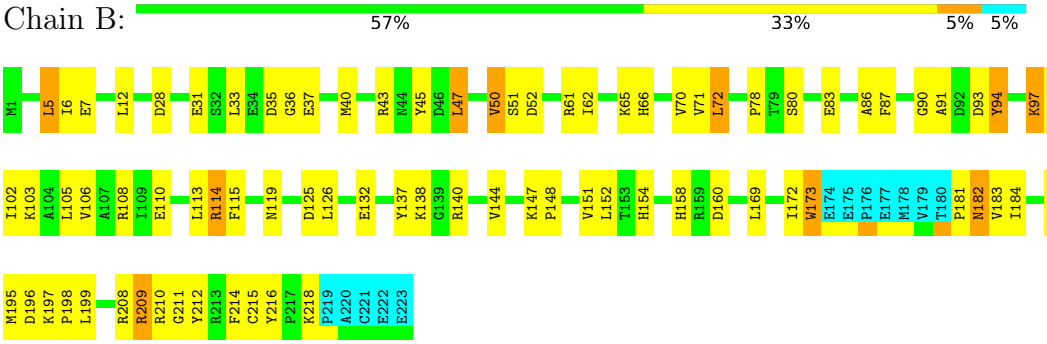
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

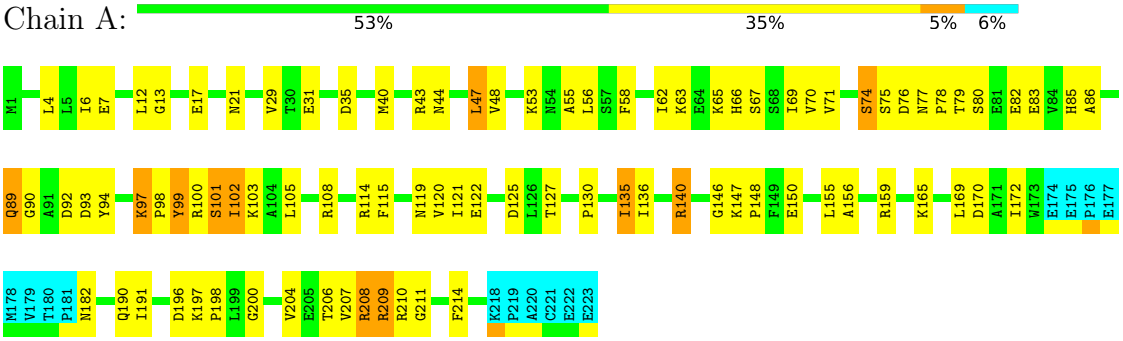
Chain B:



4.2.4 Score per residue for model 4

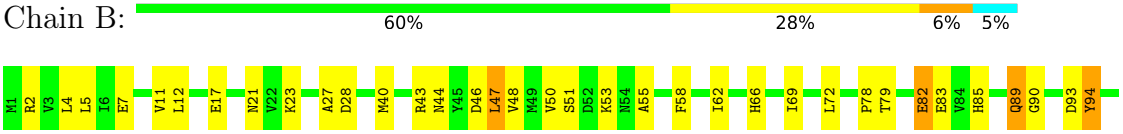
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

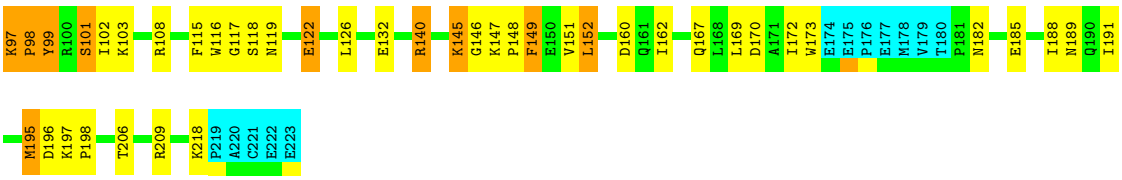
Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain B:

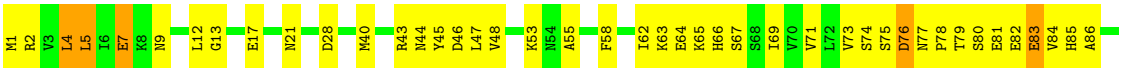




4.2.5 Score per residue for model 5

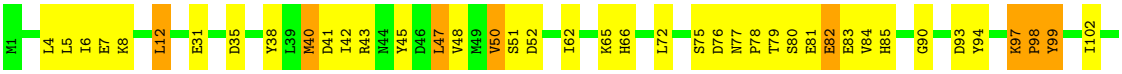
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

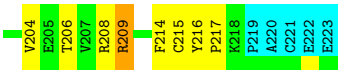
Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain B:

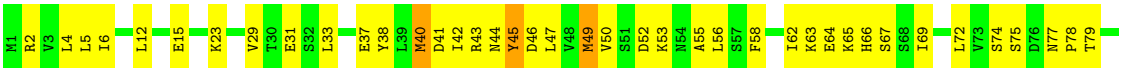


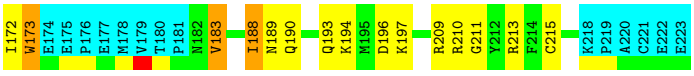


4.2.6 Score per residue for model 6

• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

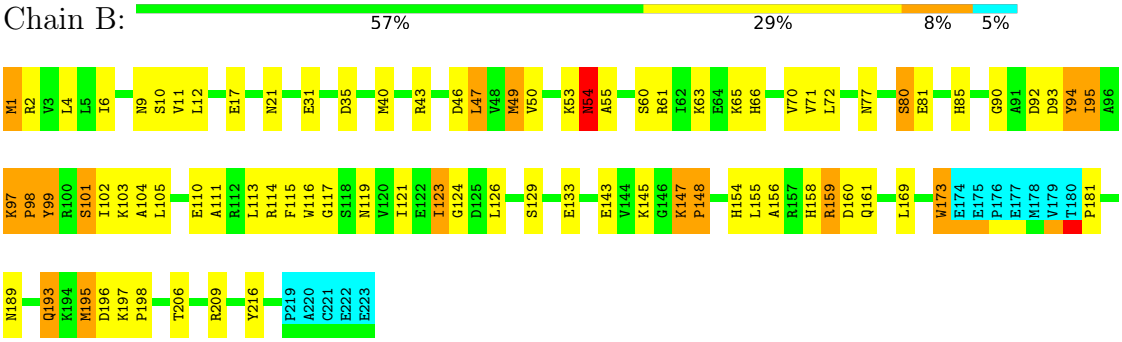
Chain A:





• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

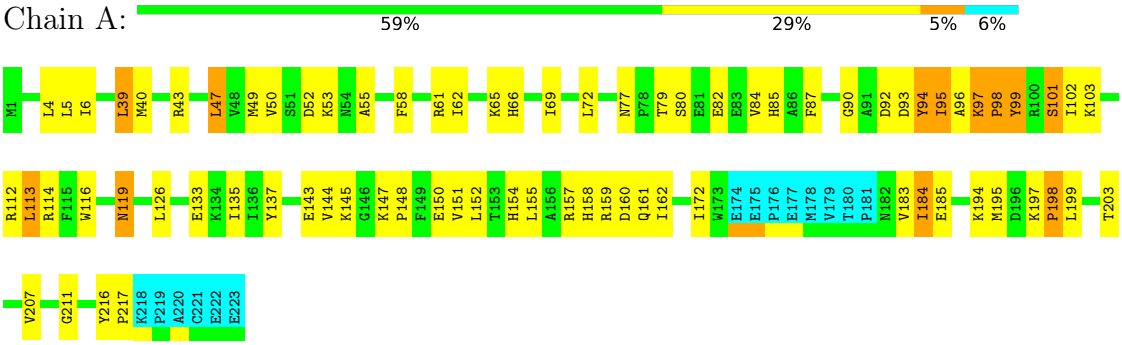
Chain B:



4.2.7 Score per residue for model 7

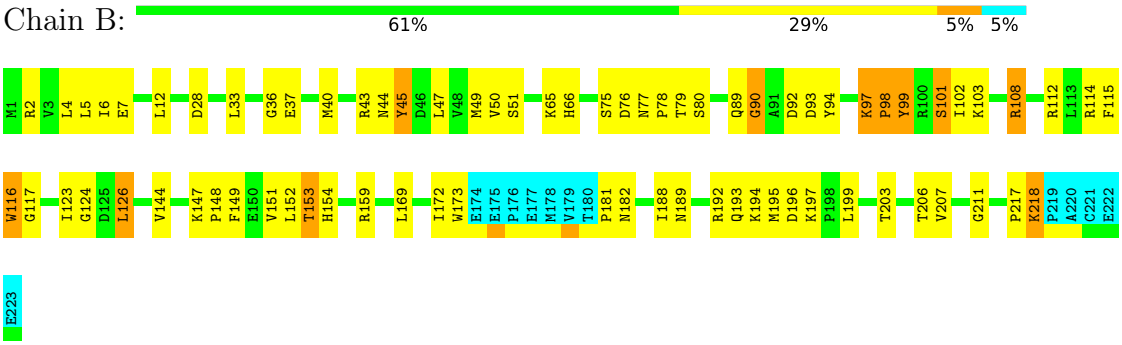
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

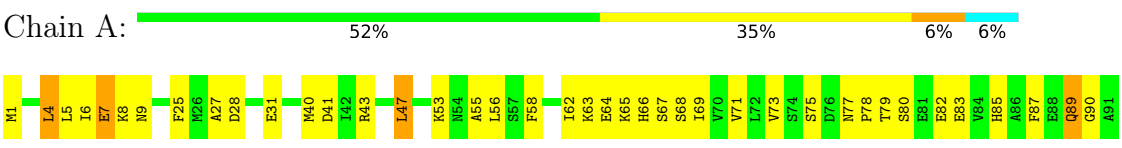
Chain B:

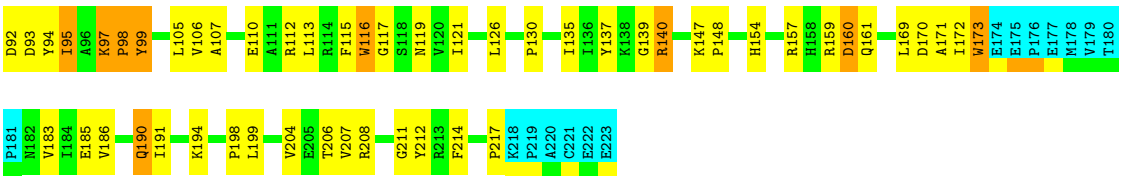


4.2.8 Score per residue for model 8

• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

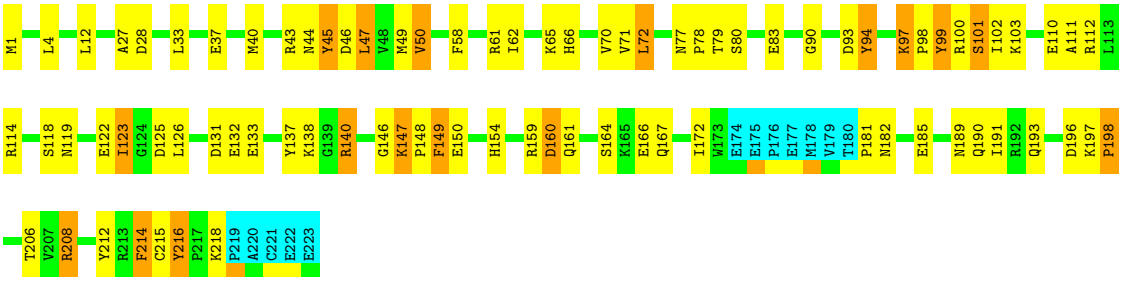
Chain A:





• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

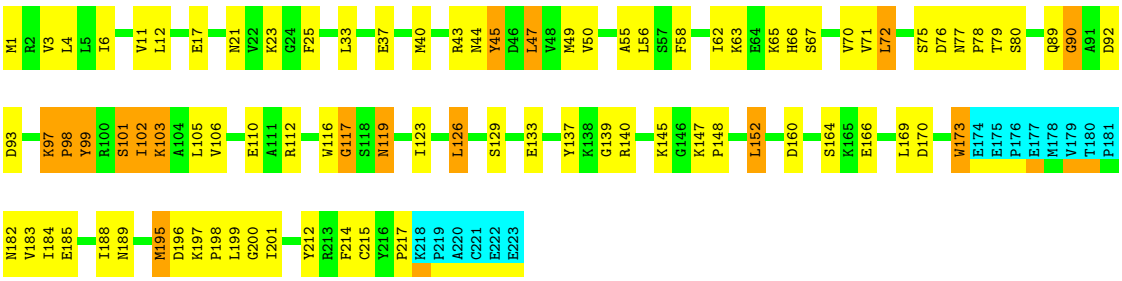
Chain B:



4.2.9 Score per residue for model 9

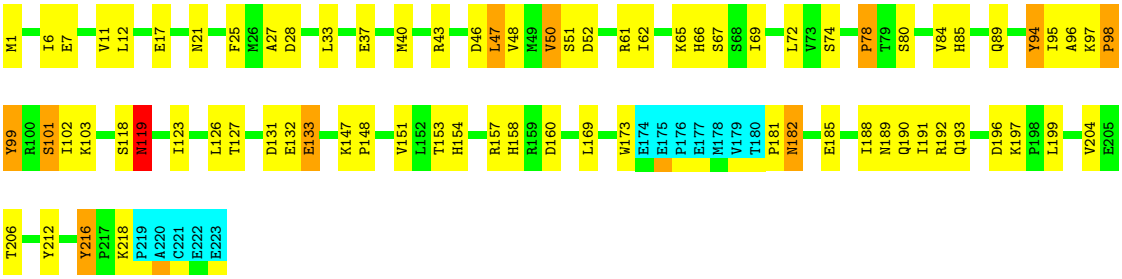
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

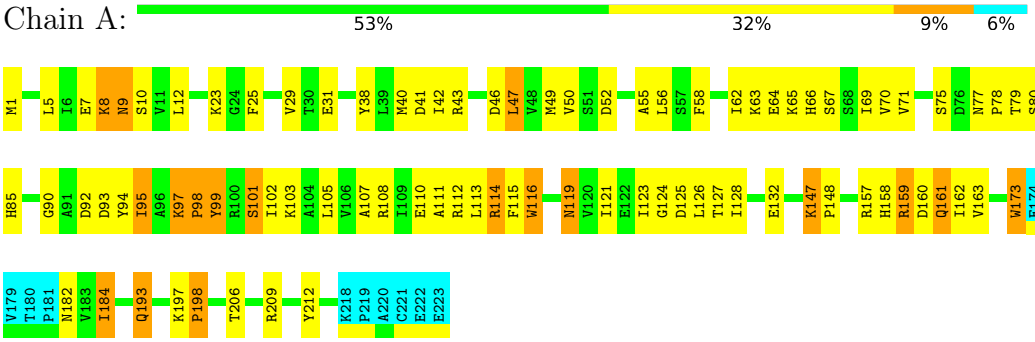
Chain B:



4.2.10 Score per residue for model 10

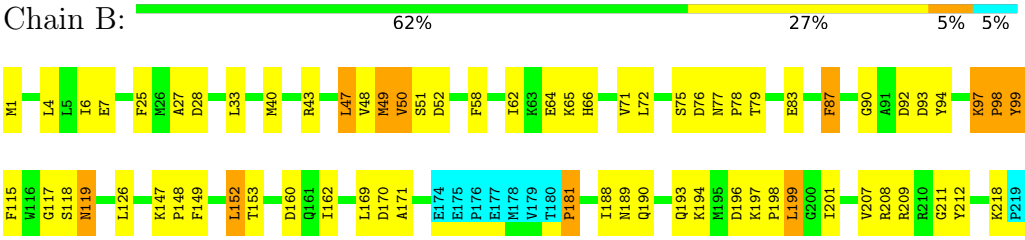
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

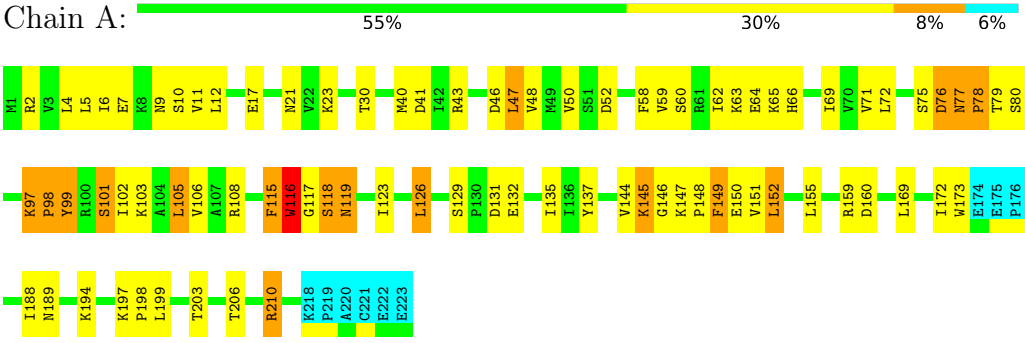
Chain B:



4.2.11 Score per residue for model 11

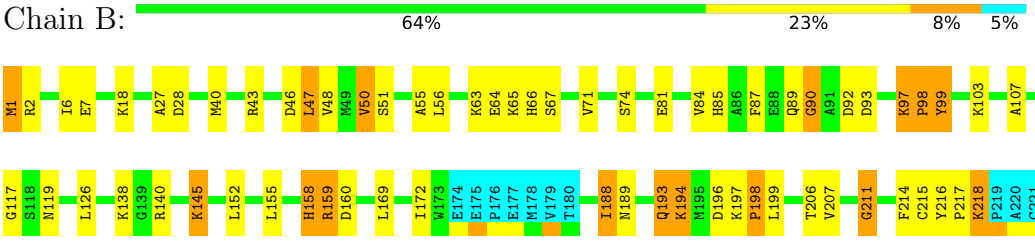
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

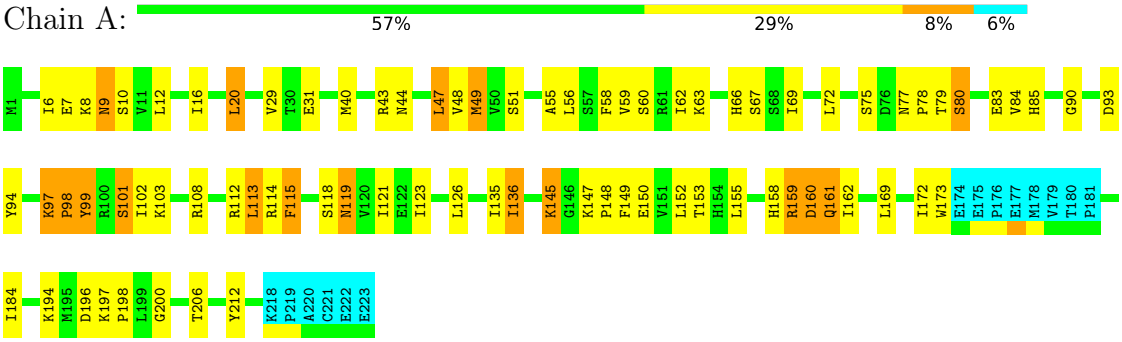
Chain B:



4.2.12 Score per residue for model 12

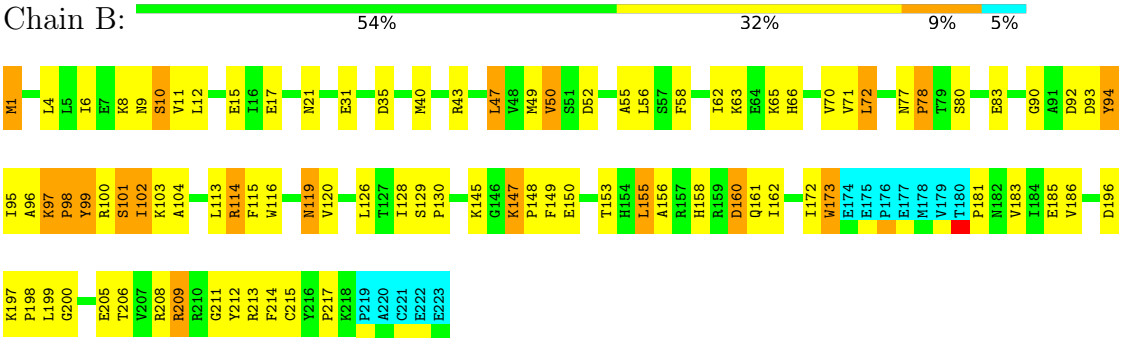
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

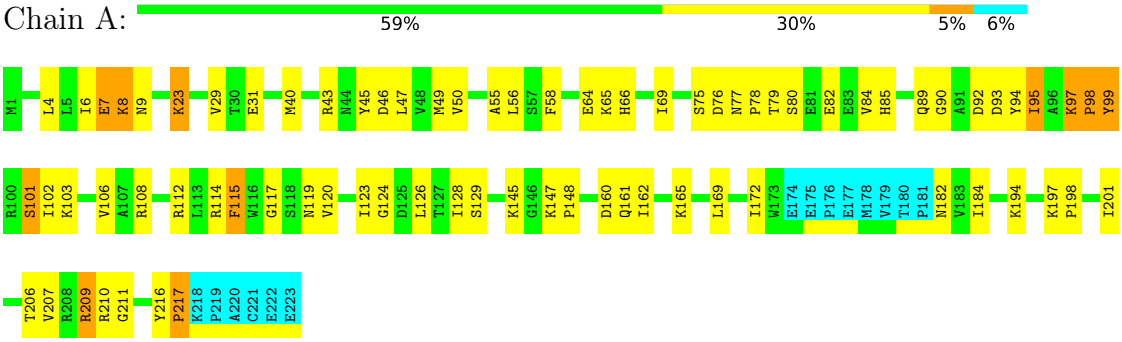
Chain B:



4.2.13 Score per residue for model 13

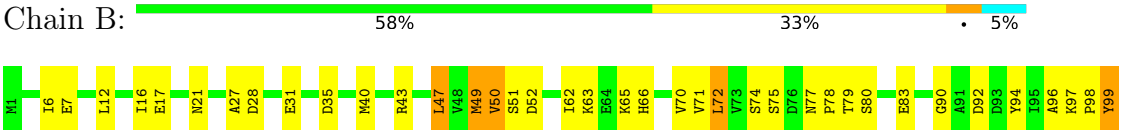
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

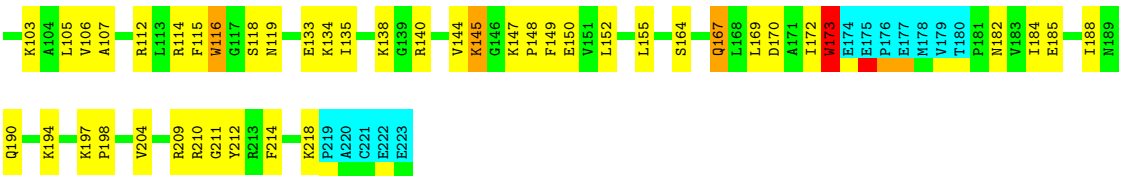
Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain B:

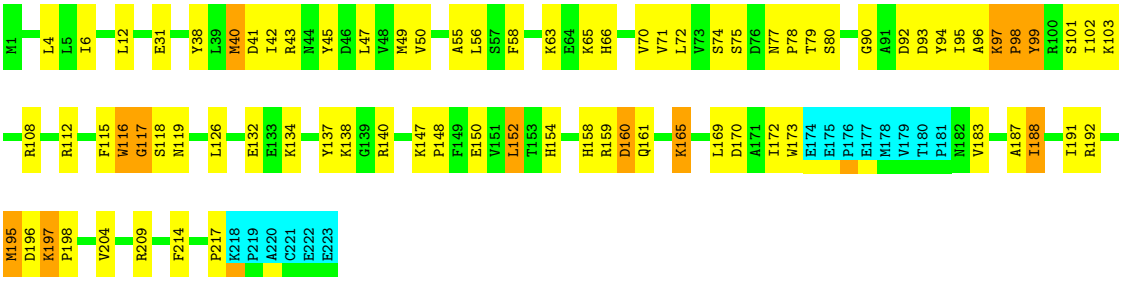




4.2.14 Score per residue for model 14 (medoid)

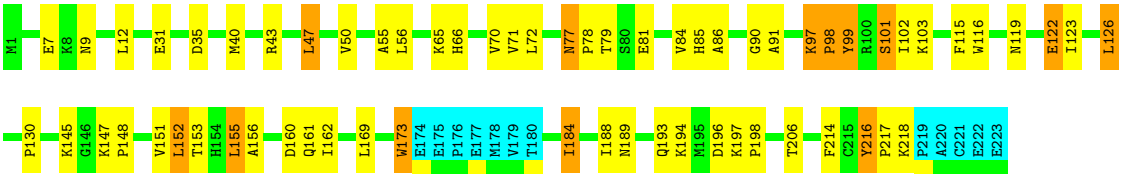
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

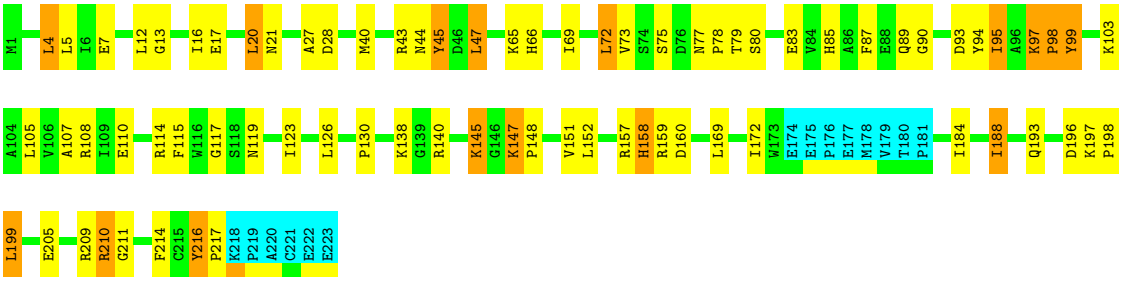
Chain B:



4.2.15 Score per residue for model 15

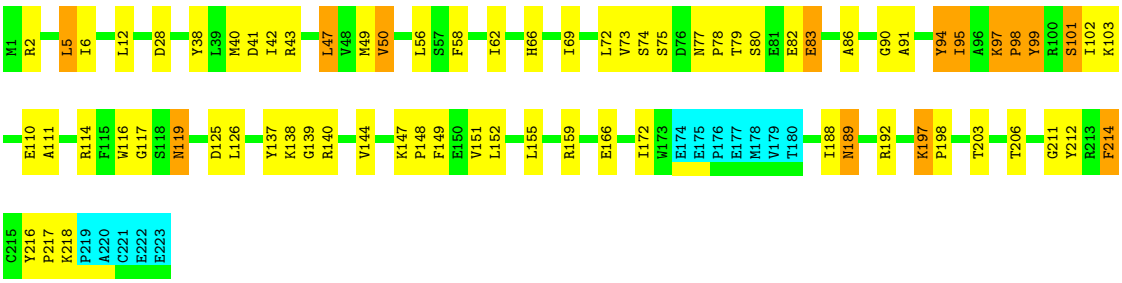
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

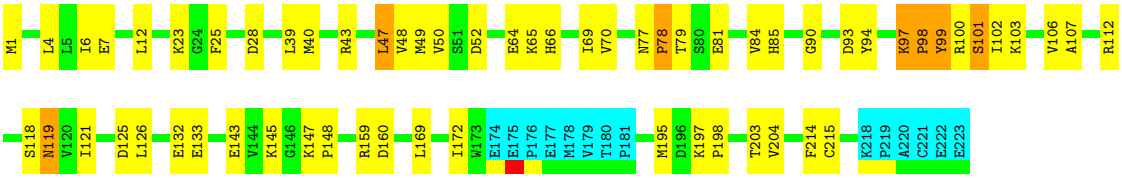
Chain B:



4.2.16 Score per residue for model 16

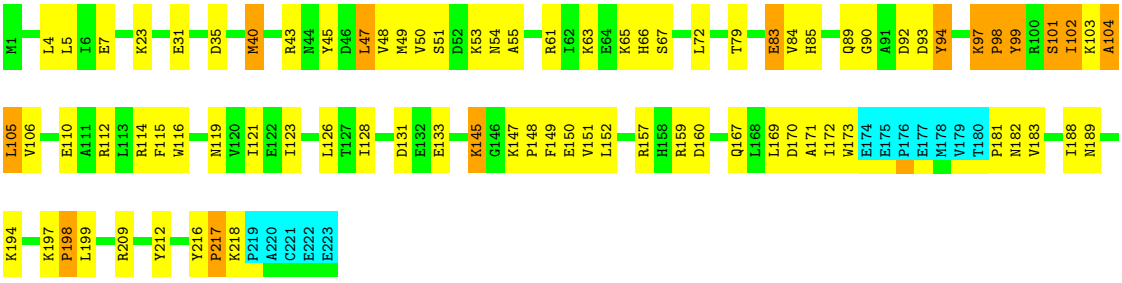
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain B:



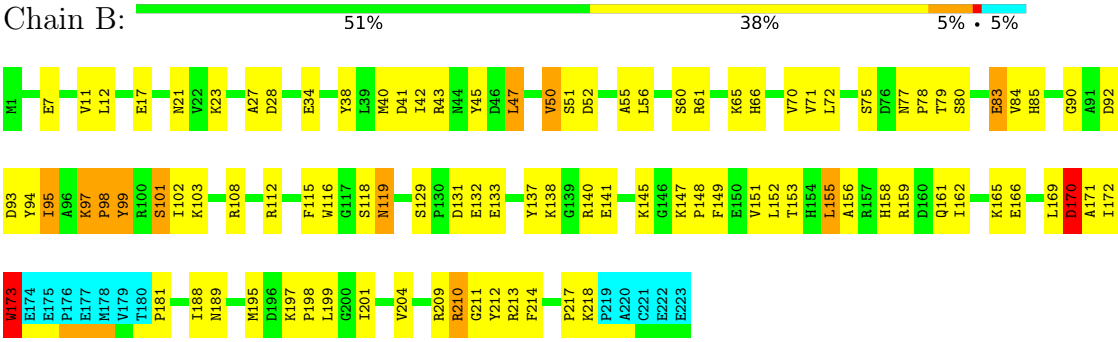
4.2.17 Score per residue for model 17

• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:

• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

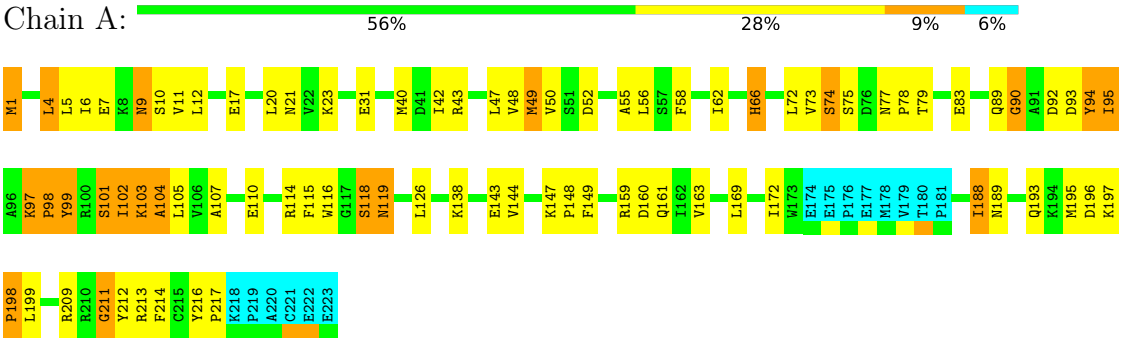
Chain B:



4.2.18 Score per residue for model 18

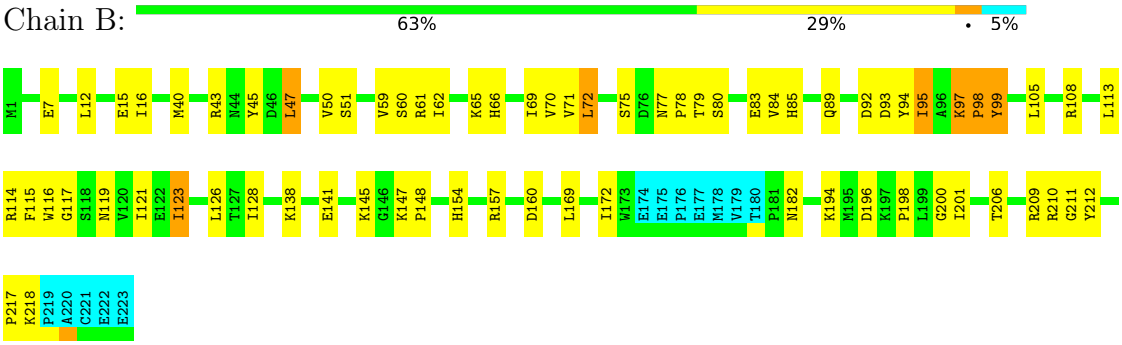
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

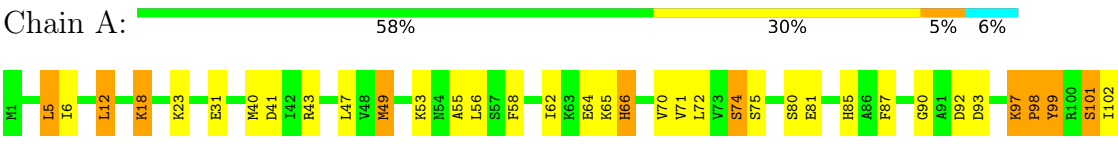
Chain B:



4.2.19 Score per residue for model 19

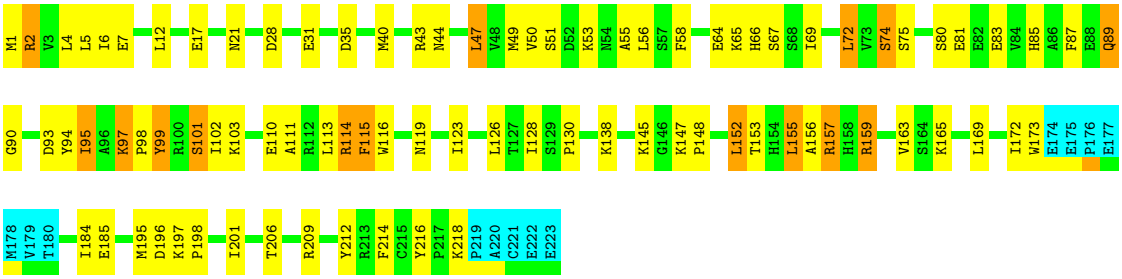
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

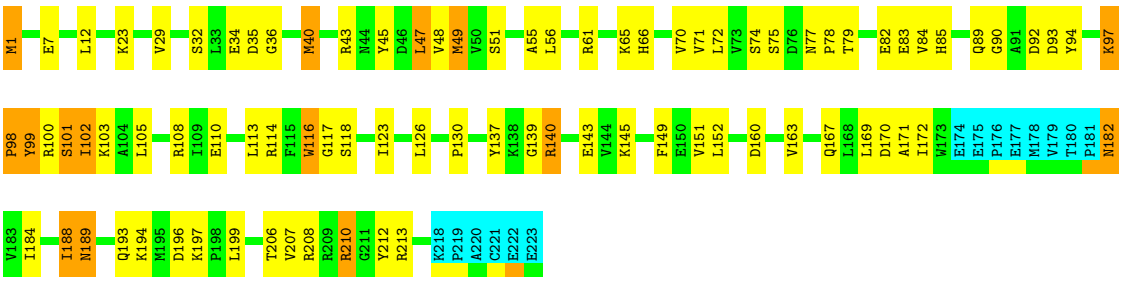
Chain B:



4.2.20 Score per residue for model 20

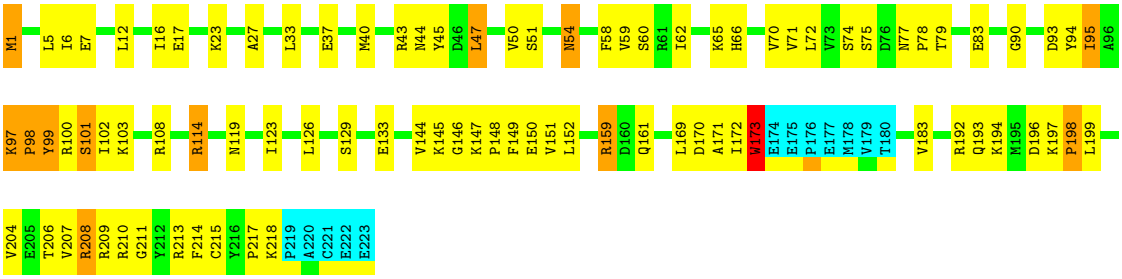
• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain A:



• Molecule 1: Putative TRANSCRIPTIONAL REGULATOR

Chain B:



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.

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:HH11	1:B:159:ARG:CB	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:A:133:GLU:CB	1:A:149:PHE:CZ	1.07	2.37	6	1
1:B:159:ARG:HB2	1:B:159:ARG:NH1	1.07	1.63	20	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:NZ	1:A:138:LYS:HB3	0.95	1.77	5	1
1:B:159:ARG:HH11	1:B:159:ARG:HB2	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:B:161:GLN:NE2	1:B:162:ILE:O	0.91	2.03	14	1
1:A:163:VAL:HB	1:A:214:PHE:HE1	0.91	1.14	18	1
1:B:123:ILE:CD1	1:B:159:ARG:CZ	0.91	2.49	16	1
1:B:147:LYS:CG	1:B:172:ILE:CG2	0.90	2.50	8	1
1:B:146:GLY:O	1:B:150:GLU:HG3	0.90	1.66	20	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:A:195:MET:HE2	1:A:199:LEU:CD2	0.83	2.04	3	1
1:B:195:MET:HE2	1:B:203:THR:OG1	0.83	1.74	7	1
1:B:95:ILE:HD12	1:B:95:ILE:H	0.83	1.33	18	5
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:B:192:ARG:HH11	1:B:204:VAL:HG21	0.81	1.35	1	1
1:B:182:ASN:OD1	1:B:185:GLU:OE2	0.81	1.99	13	1
1:B:148:PRO:O	1:B:152:LEU:HD13	0.81	1.74	16	1
1:A:157:ARG:HG3	1:A:158:HIS:CE1	0.81	2.10	17	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:123:ILE:HG21	1:A:159:ARG:NH1	0.80	1.91	2	1
1:A:1:MET:HE1	1:A:115:PHE:HA	0.80	1.52	10	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:2:ARG:CZ	1:B:43:ARG:HH21	0.80	1.82	6	1
1:B:154:HIS:CE1	1:B:158:HIS:HE1	0.80	1.94	9	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	4
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:CD1	1:A:216:TYR:N	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:O	1:B:199:LEU:HD23	0.75	1.81	10	1
1:A:44:ASN:CG	1:A:143:GLU:CD	0.75	2.45	3	1
1:B:95:ILE:N	1:B:95:ILE:HD12	0.75	1.97	17	5
1:A:95:ILE:HD12	1:A:95:ILE:N	0.75	1.97	17	8
1:A:195:MET:CE	1:A:199:LEU:HD22	0.74	2.12	3	1
1:A:46:ASP:OD2	1:A:116:TRP:CH2	0.74	2.40	10	1
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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:122:GLU:OE1	1:B:122:GLU:C	0.72	2.27	14	1
1:A:209:ARG:HH22	1:A:213:ARG:HH12	0.72	1.24	18	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:159:ARG:O	1:B:161:GLN:N	0.72	2.23	5	3
1:B:166:GLU:O	1:B:170:ASP:OD1	0.72	2.07	17	1
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	4
1:B:147:LYS:HZ2	1:B:172:ILE:C	0.71	1.79	8	1
1:B:95:ILE:HD12	1:B:95:ILE:N	0.71	2.00	18	1
1:A:4:LEU:HD12	1:A:5:LEU:N	0.71	2.00	3	5
1:B:147:LYS:HE3	1:B:172:ILE:HG22	0.71	1.63	8	1
1:A:108:ARG:O	1:A:112:ARG:HG3	0.71	1.86	10	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:HD12	1:A:172:ILE:N	0.70	2.01	16	12
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	2
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	3
1:B:155:LEU:HD22	1:B:155:LEU:O	0.68	1.88	19	4
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:184:ILE:H	1:A:184:ILE:HD12	0.67	1.49	2	4
1:B:172:ILE:HD12	1:B:172:ILE:N	0.67	2.04	15	8
1:B:147:LYS:CG	1:B:172:ILE:HG22	0.67	2.18	8	1
1:A:155:LEU:HD12	1:A:156:ALA:N	0.67	2.05	5	4
1:B:155:LEU:HD22	1:B:155:LEU:C	0.66	2.11	12	4
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:108:ARG:O	1:A:112:ARG:CG	0.65	2.45	10	1
1:A:157:ARG:CG	1:A:158:HIS:ND1	0.65	2.58	17	1
1:B:201:ILE:HD12	1:B:201:ILE:N	0.65	2.06	19	2
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:216:TYR:N	1:B:216:TYR:CD1	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:195:MET:CE	1:A:199:LEU:HD21	0.63	2.22	3	1
1:A:123:ILE:HG23	1:A:123:ILE:O	0.63	1.93	5	1
1:B:123:ILE:O	1:B:123:ILE:HG23	0.63	1.92	14	6
1:A:105:LEU:C	1:A:105:LEU:HD13	0.63	2.14	8	3
1:A:145:LYS:HA	1:A:149:PHE:HE2	0.63	1.37	11	1
1:A:133:GLU:CG	1:A:149:PHE:HZ	0.63	2.06	6	1
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:148:PRO:HA	1:A:151:VAL:HB	0.63	1.69	3	1
1:A:197:LYS:N	1:A:198:PRO:CD	0.63	2.62	10	6
1:B:212:TYR:N	1:B:213:ARG:NH2	0.63	2.46	12	1
1:A:173:TRP:CD1	1:A:173:TRP:O	0.63	2.52	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:ARG:NH1	1:A:160:ASP:OD2	0.63	2.31	18	1
1:A:159:ARG:HH12	1:B:161:GLN:NE2	0.62	1.91	6	1
1:B:85:HIS:CE1	1:B:89:GLN:NE2	0.62	2.67	16	1
1:B:208:ARG:H	1:B:208:ARG:NE	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:HD13	1:B:123:ILE:H	0.62	1.53	8	2
1:B:152:LEU:HD23	1:B:195:MET:SD	0.62	2.34	19	1
1:B:193:GLN:NE2	1:B:193:GLN:N	0.62	2.47	11	2
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:61:ARG:NH2	1:A:65:LYS:NZ	0.61	2.48	3	3
1:A:1:MET:HE2	1:A:115:PHE:HA	0.61	1.69	10	1
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:A:138:LYS:NZ	1:A:138:LYS:CB	0.60	2.51	5	1
1:B:147:LYS:HZ3	1:B:172:ILE:HG23	0.60	1.56	8	1
1:B:2:ARG:NH1	1:B:43:ARG:NE	0.60	2.49	15	1
1:B:123:ILE:HD13	1:B:123:ILE:N	0.60	2.10	8	3
1:B:195:MET:CE	1:B:203:THR:HG1	0.60	2.09	7	1
1:A:93:ASP:CG	1:A:112:ARG:HH21	0.60	1.99	10	3
1:B:155:LEU:HD13	1:B:156:ALA:H	0.60	1.55	1	4
1:A:162:ILE:HD12	1:A:162:ILE:N	0.60	2.10	19	2
1:A:71:VAL:HG23	1:A:92:ASP:OD2	0.60	1.96	10	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:B:169:LEU:C	1:B:169:LEU:HD13	0.60	2.16	11	5
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:A:147:LYS:NZ	1:A:173:TRP:HE1	0.60	1.94	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	2
1:B:197:LYS:N	1:B:198:PRO:CD	0.59	2.65	20	5
1:A:48:VAL:O	1:A:48:VAL:HG23	0.59	1.97	18	1
1:B:213:ARG:HH12	1:B:215:CYS:CB	0.59	2.11	20	1
1:B:1:MET:N	1:B:1:MET:SD	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:CD1	1:B:45:TYR:N	0.59	2.70	2	6
1:B:173:TRP:O	1:B:173:TRP:CE3	0.59	2.55	3	3
1:A:208:ARG:HE	1:A:210:ARG:NH2	0.59	1.95	20	1
1:B:147:LYS:HG3	1:B:172:ILE:HG21	0.58	1.70	8	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:A:39:LEU:C	1:A:39:LEU:HD23	0.58	2.18	2	1
1:B:195:MET:HE3	1:B:203:THR:OG1	0.58	1.98	7	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:1:MET:HE1	1:A:115:PHE:CA	0.58	2.28	10	1
1:A:157:ARG:HG3	1:A:158:HIS:HD1	0.58	1.57	17	1
1:B:158:HIS:CG	1:B:158:HIS:O	0.58	2.57	1	1
1:A:184:ILE:N	1:A:184:ILE:HD12	0.58	2.13	13	2
1:B:159:ARG:NH1	1:B:214:PHE:CZ	0.58	2.72	15	1
1:A:169:LEU:C	1:A:169:LEU:HD13	0.58	2.18	5	2
1:B:116:TRP:CG	1:B:117:GLY:N	0.58	2.72	7	1
1:B:184:ILE:HD12	1:B:184:ILE:H	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:HH11	1:B:159:ARG:CG	0.58	2.12	20	1
1:A:58:PHE:CE2	1:A:62:ILE:HD11	0.58	2.32	12	7
1:B:215:CYS:SG	1:B:216:TYR:N	0.58	2.76	3	3
1:A:105:LEU:HD23	1:A:105:LEU:N	0.58	2.14	6	2
1:A:157:ARG:NE	1:A:158:HIS:CE1	0.58	2.71	17	1
1:B:137:TYR:CD1	1:B:140:ARG:HB2	0.58	2.32	8	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:A:135:ILE:HD13	1:A:136:ILE:N	0.57	2.13	4	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:B:1:MET:SD	1:B:1:MET:N	0.57	2.75	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:207:VAL:CG1	1:A:213:ARG:NH1	0.57	2.67	20	1
1:A:2:ARG:NH2	1:A:28:ASP:CB	0.57	2.68	5	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:209:ARG:O	1:A:211:GLY:N	0.57	2.37	15	6
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:89:GLN:N	1:A:89:GLN:NE2	0.57	2.53	4	2
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:87:PHE:CE2	1:B:108:ARG:CZ	0.57	2.88	2	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: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:125:ASP:CG	1:B:138:LYS:HZ2	0.57	2.03	8	1
1:A:160:ASP:N	1:A:161:GLN:NE2	0.57	2.52	14	1
1:B:151:VAL:HG13	1:B:152:LEU:HD22	0.57	1.77	20	1
1:B:1:MET:SD	1:B:25:PHE:CZ	0.57	2.98	1	1
1:A:45:TYR:CD1	1:A:45:TYR:N	0.56	2.73	6	5
1:A:105:LEU:HD13	1:A:105:LEU:C	0.56	2.20	11	2
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	5
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:95:ILE:HD12	1:A:95:ILE:H	0.56	1.58	2	4
1:A:133:GLU:CA	1:A:149:PHE:CZ	0.56	2.89	6	1
1:B:162:ILE:N	1:B:162:ILE:CD1	0.56	2.68	4	4
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
1:B:172:ILE:N	1:B:172:ILE:CD1	0.56	2.68	15	9
1:B:95:ILE:N	1:B:95:ILE:CD1	0.56	2.66	18	6
1:B:125:ASP:OD2	1:B:138:LYS:CD	0.56	2.52	8	1
1:A:12:LEU:HD22	1:A:12:LEU:N	0.56	2.16	6	4
1:B:97:LYS:NZ	1:B:99:TYR:CE2	0.56	2.73	13	1
1:A:172:ILE:N	1:A:172:ILE:CD1	0.56	2.68	16	13
1:B:12:LEU:HD12	1:B:97:LYS:NZ	0.56	2.16	7	3
1:B:66:HIS:O	1:B:69:ILE:HG22	0.55	2.01	19	6
1:B:196:ASP:OD1	1:B:197:LYS:N	0.55	2.39	14	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:ASN:HD21	1:A:128:ILE:N	0.55	1.98	10	1
1:A:95:ILE:N	1:A:95:ILE:CD1	0.55	2.68	18	10
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	6
1:B:123:ILE:N	1:B:123:ILE:CD1	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:A:201:ILE:N	1:A:201:ILE:CD1	0.55	2.69	13	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:126:LEU:HD13	1:B:199:LEU:HD13	0.55	1.78	9	1
1:B:184:ILE:O	1:B:184:ILE:HD13	0.55	2.02	14	1
1:B:105:LEU:H	1:B:105:LEU:HD23	0.55	1.61	6	1
1:A:1:MET:SD	1:A:1:MET:N	0.55	2.75	20	3
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: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	2
1:B:158:HIS:O	1:B:158:HIS:CD2	0.54	2.61	1	1
1:B:155:LEU:O	1:B:159:ARG:N	0.54	2.41	5	1
1:B:151:VAL:HG13	1:B:152:LEU:HD12	0.54	1.79	16	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	3
1:A:123:ILE:O	1:A:125:ASP:N	0.54	2.41	10	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	3
1:A:12:LEU:N	1:A:12:LEU:HD12	0.54	2.18	3	2
1:B:199:LEU:HD23	1:B:199:LEU:C	0.54	2.22	10	1
1:A:115:PHE:CD1	1:A:116:TRP:N	0.54	2.75	11	1
1:A:62:ILE:O	1:A:66:HIS:N	0.54	2.41	1	6
1:A:94:TYR:CD1	1:A:95:ILE:N	0.54	2.75	17	3
1:B:110:GLU:O	1:B:114:ARG:N	0.54	2.41	19	5
1:B:209:ARG:O	1:B:211:GLY:N	0.54	2.41	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:MET:SD	1:A:45:TYR:CE2	0.54	3.00	5	1
1:B:208:ARG:NE	1:B:208:ARG:N	0.54	2.56	8	1
1:A:159:ARG:CG	1:A:214:PHE:CE1	0.54	2.91	15	1
1:B:213:ARG:NH1	1:B:215:CYS:HB2	0.54	2.18	20	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:A:118:SER:O	1:A:129:SER:OG	0.54	2.24	11	1
1:B:159:ARG:HH22	1:B:217:PRO:CD	0.54	2.11	16	1
1:A:135:ILE:N	1:A:135:ILE:HD12	0.54	2.17	7	3
1:B:173:TRP:O	1:B:173:TRP:CG	0.54	2.60	12	3
1:A:105:LEU:HD23	1:A:105:LEU:H	0.54	1.63	18	1
1:A:118:SER:CB	1:A:132:GLU:OE2	0.54	2.54	19	1
1:B:83:GLU:OE1	1:B:94:TYR:CD1	0.54	2.61	8	1
1:A:145:LYS:C	1:A:149:PHE:CD2	0.54	2.81	11	1
1:A:16:ILE:O	1:A:20:LEU:HD23	0.54	2.03	15	2
1:A:7:GLU:OE2	1:A:97:LYS:NZ	0.54	2.41	16	1
1:A:123:ILE:HD13	1:A:124:GLY:N	0.53	2.18	3	1
1:A:82:GLU:O	1:A:85:HIS:ND1	0.53	2.42	4	1
1:B:53:LYS:O	1:B:55:ALA:N	0.53	2.41	6	4
1:B:82:GLU:OE1	1:B:82:GLU:N	0.53	2.41	4	2
1:B:190:GLN:HB3	1:B:194:LYS:NZ	0.53	2.18	13	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:A:12:LEU:N	1:A:12:LEU:CD2	0.53	2.71	5	9
1:B:93:ASP:N	1:B:93:ASP:OD1	0.53	2.40	1	2
1:A:47:LEU:HD13	1:A:48:VAL:N	0.53	2.18	3	8
1:B:58:PHE:CE2	1:B:62:ILE:HD11	0.53	2.38	8	4
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:B:169:LEU:O	1:B:172:ILE:N	0.53	2.41	17	1
1:A:12:LEU:N	1:A:12:LEU:HD22	0.53	2.18	5	5
1:A:63:LYS:O	1:A:67:SER:N	0.53	2.42	8	9
1:A:75:SER:O	1:A:77:ASN:N	0.53	2.41	9	3
1:A:40:MET:SD	1:A:45:TYR:CZ	0.53	3.01	6	2
1:B:2:ARG:NH2	1:B:28:ASP:OD2	0.53	2.42	7	1
1:B:108:ARG:O	1:B:108:ARG:NE	0.53	2.40	7	1
1:B:83:GLU:OE1	1:B:94:TYR:CG	0.53	2.62	8	2
1:B:85:HIS:CE1	1:B:89:GLN:HE21	0.53	2.21	9	1
1:A:115:PHE:O	1:A:117:GLY:N	0.53	2.41	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:205:GLU:N	1:B:205:GLU:OE2	0.53	2.42	12	1
1:B:12:LEU:N	1:B:12:LEU:HD22	0.53	2.18	8	8
1:B:93:ASP:OD1	1:B:94:TYR:N	0.53	2.42	10	7
1:B:105:LEU:HD23	1:B:105:LEU:N	0.53	2.19	18	2
1:A:155:LEU:O	1:A:159:ARG:N	0.53	2.41	7	2
1:B:137:TYR:O	1:B:137:TYR:CG	0.53	2.61	8	1
1:A:108:ARG:NH1	1:B:87:PHE:CZ	0.53	2.76	11	1
1:A:44:ASN:HD22	1:A:44:ASN:N	0.53	1.99	12	1
1:B:83:GLU:N	1:B:83:GLU:OE1	0.53	2.41	15	3
1:A:66:HIS:ND1	1:A:66:HIS:N	0.53	2.56	19	2
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	6
1:B:160:ASP:N	1:B:214:PHE:O	0.53	2.41	11	3
1:A:115:PHE:CD2	1:A:116:TRP:O	0.53	2.62	8	1
1:A:100:ARG:NE	1:B:94:TYR:OH	0.53	2.41	16	1
1:B:85:HIS:ND1	1:B:89:GLN:NE2	0.53	2.57	16	1
1:B:162:ILE:HD12	1:B:162:ILE:H	0.53	1.62	17	1
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:B:138:LYS:O	1:B:140:ARG:NH1	0.53	2.42	3	4
1:B:114:ARG:O	1:B:116:TRP:N	0.53	2.42	12	1
1:A:115:PHE:O	1:A:116:TRP:CG	0.53	2.61	14	1
1:A:17:GLU:O	1:A:21:ASN:ND2	0.53	2.42	15	8
1:A:65:LYS:O	1:A:66:HIS:ND1	0.53	2.42	13	6
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:B:145:LYS:N	1:B:145:LYS:CD	0.53	2.72	16	1
1:B:159:ARG:NH1	1:B:159:ARG:CG	0.53	2.68	20	1
1:B:172:ILE:O	1:B:173:TRP:CB	0.53	2.57	1	1
1:B:94:TYR:O	1:B:94:TYR:CG	0.53	2.62	16	4
1:A:93:ASP:OD1	1:A:94:TYR:N	0.53	2.42	16	5
1:A:100:ARG:NH1	1:B:83:GLU:OE2	0.53	2.42	4	1
1:A:114:ARG:O	1:A:115:PHE:CG	0.53	2.62	13	5
1:A:196:ASP:O	1:A:200:GLY:N	0.53	2.42	12	3
1:B:83:GLU:OE2	1:B:94:TYR:CE1	0.53	2.62	8	2
1:A:158:HIS:O	1:A:161:GLN:NE2	0.53	2.42	14	1
1:B:116:TRP:CD2	1:B:116:TRP:O	0.53	2.62	15	1
1:A:108:ARG:O	1:A:108:ARG:NE	0.53	2.41	1	1
1:B:17:GLU:O	1:B:21:ASN:ND2	0.53	2.42	6	8
1:A:150:GLU:O	1:A:154:HIS:ND1	0.53	2.42	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:GLU:OE1	1:A:94:TYR:CD2	0.53	2.62	12	1
1:B:115:PHE:O	1:B:116:TRP:CG	0.53	2.62	14	2
1:A:100:ARG:NH2	1:B:94:TYR:OH	0.53	2.42	16	1
1:A:2:ARG:HE	1:A:43:ARG:HH21	0.53	1.46	17	1
1:B:77:ASN:O	1:B:79:THR:N	0.52	2.42	18	11
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:A:92:ASP:OD2	1:A:112:ARG:NH1	0.52	2.42	6	1
1:B:160:ASP:CB	1:B:216:TYR:HE1	0.52	2.17	9	1
1:B:71:VAL:N	1:B:92:ASP:OD2	0.52	2.42	17	2
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:B:71:VAL:N	1:B:92:ASP:OD1	0.52	2.42	18	2
1:A:138:LYS:O	1:A:140:ARG:NH1	0.52	2.42	14	2
1:A:65:LYS:O	1:A:66:HIS:CG	0.52	2.63	14	14
1:A:121:ILE:CD1	1:A:121:ILE:N	0.52	2.72	8	1
1:A:105:LEU:CD1	1:A:108:ARG:HH22	0.52	2.17	15	1
1:B:159:ARG:NH2	1:B:217:PRO:CD	0.52	2.73	16	1
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:A:82:GLU:N	1:A:82:GLU:OE1	0.52	2.42	10	1
1:A:83:GLU:OE1	1:A:83:GLU:N	0.52	2.42	10	1
1:B:92:ASP:OD1	1:B:112:ARG:NH1	0.52	2.42	11	1
1:A:83:GLU:OE1	1:A:94:TYR:CD1	0.52	2.62	15	1
1:A:23:LYS:N	1:A:23:LYS:CD	0.52	2.72	6	8
1:A:77:ASN:O	1:A:79:THR:N	0.52	2.42	9	17
1:A:123:ILE:CB	1:A:159:ARG:HH12	0.52	2.17	2	1
1:A:63:LYS:NZ	1:A:92:ASP:OD1	0.52	2.42	4	6
1:B:154:HIS:CE1	1:B:158:HIS:ND1	0.52	2.78	3	2
1:A:76:ASP:N	1:A:76:ASP:OD1	0.52	2.42	5	2
1:A:52:ASP:N	1:A:52:ASP:OD1	0.52	2.42	6	2
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:B:63:LYS:NZ	1:B:92:ASP:OD1	0.52	2.42	13	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:B:95:ILE:CG2	1:B:108:ARG:NH2	0.52	2.73	18	1
1:A:108:ARG:NH2	1:B:83:GLU:OE1	0.52	2.42	19	1
1:B:155:LEU:HD13	1:B:155:LEU:C	0.52	2.25	19	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:50:VAL:HG22	1:B:52:ASP:H	0.52	1.65	3	7
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:A:159:ARG:NH1	1:A:203:THR:OG1	0.52	2.42	17	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:116:TRP:NE1	1:B:141:GLU:OE2	0.52	2.42	18	1
1:B:72:LEU:C	1:B:72:LEU:HD23	0.52	2.25	16	6
1:B:49:MET:SD	1:B:72:LEU:O	0.52	2.68	12	6
1:A:119:ASN:ND2	1:A:128:ILE:O	0.52	2.42	13	2
1:B:188:ILE:HD12	1:B:212:TYR:CZ	0.52	2.38	10	2
1:A:85:HIS:NE2	1:A:89:GLN:OE1	0.52	2.42	15	1
1:B:149:PHE:CE1	1:B:153:THR:HG21	0.52	2.39	17	1
1:B:135:ILE:HD12	1:B:135:ILE:N	0.52	2.19	1	2
1:A:2:ARG:NH2	1:A:28:ASP:OD2	0.52	2.42	2	1
1:B:76:ASP:OD1	1:B:77:ASN:N	0.52	2.42	10	3
1:B:155:LEU:HD12	1:B:156:ALA:N	0.52	2.20	14	2
1:B:44:ASN:C	1:B:45:TYR:CD1	0.52	2.83	7	1
1:A:160:ASP:OD2	1:B:161:GLN:NE2	0.52	2.43	12	1
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:53:LYS:NZ	1:A:77:ASN:OD1	0.52	2.43	6	1
1:A:7:GLU:OE2	1:A:9:ASN:ND2	0.52	2.42	18	2
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:155:LEU:HD12	1:A:155:LEU:C	0.52	2.26	4	4
1:A:49:MET:SD	1:A:72:LEU:O	0.52	2.68	19	7
1:A:85:HIS:CD2	1:A:89:GLN:OE1	0.52	2.62	4	2
1:A:116:TRP:N	1:A:116:TRP:CD1	0.52	2.77	11	1
1:A:108:ARG:O	1:A:112:ARG:NH1	0.52	2.43	14	1
1:B:12:LEU:N	1:B:12:LEU:CD2	0.51	2.73	7	8
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:A:110:GLU:O	1:A:114:ARG:N	0.51	2.43	5	3
1:B:158:HIS:C	1:B:160:ASP:N	0.51	2.62	5	1
1:A:160:ASP:O	1:A:161:GLN:NE2	0.51	2.43	17	1
1:A:7:GLU:OE1	1:A:13:GLY:N	0.51	2.42	15	4
1:B:83:GLU:OE1	1:B:84:VAL:N	0.51	2.43	18	2
1:A:5:LEU:HD12	1:A:49:MET:SD	0.51	2.45	10	3
1:A:7:GLU:OE1	1:A:9:ASN:N	0.51	2.41	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:161:GLN:NE2	1:B:162:ILE:N	0.51	2.58	14	1
1:A:93:ASP:OD2	1:A:108:ARG:NE	0.51	2.42	15	1
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:173:TRP:CE3	1:A:173:TRP:O	0.51	2.63	10	2
1:B:151:VAL:HG22	1:B:191:ILE:HG21	0.51	1.82	9	1
1:B:93:ASP:OD1	1:B:112:ARG:NH2	0.51	2.43	16	2
1:B:116:TRP:O	1:B:116:TRP:CE3	0.51	2.63	15	1
1:A:163:VAL:CG2	1:A:214:PHE:CE1	0.51	2.93	18	1
1:B:201:ILE:N	1:B:201:ILE:CD1	0.51	2.74	18	2
1:A:81:GLU:O	1:A:85:HIS:ND1	0.51	2.43	16	4
1:B:140:ARG:N	1:B:140:ARG:CD	0.51	2.74	15	4
1:A:83:GLU:OE2	1:B:100:ARG:NH1	0.51	2.41	10	2
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:169:LEU:C	1:A:169:LEU:HD23	0.51	2.26	15	9
1:B:182:ASN:ND2	1:B:185:GLU:OE2	0.51	2.43	4	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:A:2:ARG:N	1:A:46:ASP:OD1	0.51	2.42	17	1
1:A:195:MET:O	1:A:195:MET:SD	0.51	2.69	18	1
1:B:135:ILE:CG2	1:B:137:TYR:CE2	0.51	2.93	1	1
1:B:194:LYS:O	1:B:198:PRO:CD	0.51	2.58	13	4
1:B:123:ILE:O	1:B:123:ILE:CG2	0.51	2.58	14	3
1:B:137:TYR:CZ	1:B:140:ARG:HB2	0.51	2.40	8	1
1:A:160:ASP:N	1:A:214:PHE:O	0.51	2.42	14	2
1:A:210:ARG:NE	1:A:210:ARG:N	0.51	2.58	11	1
1:B:167:GLN:N	1:B:167:GLN:OE1	0.51	2.43	13	1
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	9
1:B:70:VAL:HG12	1:B:71:VAL:N	0.51	2.21	8	9
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: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:145:LYS:C	1:A:149:PHE:CE2	0.51	2.84	11	1
1:A:113:LEU:O	1:A:116:TRP:CE2	0.51	2.64	17	1
1:A:12:LEU:CD2	1:A:97:LYS:NZ	0.51	2.74	3	1
1:A:145:LYS:CA	1:A:149:PHE:CB	0.51	2.89	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:119:ASN:ND2	1:B:121:ILE:N	0.51	2.59	6	1
1:A:184:ILE:O	1:A:184:ILE:HD13	0.51	2.06	10	2
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:155:LEU:HD13	1:A:214:PHE:CE2	0.51	2.41	4	2
1:B:84:VAL:HG23	1:B:85:HIS:N	0.51	2.20	18	7
1:A:119:ASN:ND2	1:A:129:SER:OG	0.51	2.42	13	1
1:B:144:VAL:CG2	1:B:149:PHE:CG	0.51	2.94	15	1
1:B:131:ASP:HB2	1:B:132:GLU:OE2	0.51	2.06	17	1
1:A:188:ILE:HD13	1:A:188:ILE:O	0.50	2.06	14	5
1:A:161:GLN:NE2	1:A:162:ILE:N	0.50	2.58	7	2
1:A:121:ILE:N	1:A:121:ILE:HD12	0.50	2.20	8	1
1:B:12:LEU:HD12	1:B:12:LEU:N	0.50	2.21	13	1
1:A:137:TYR:CE2	1:A:138:LYS:CD	0.50	2.94	14	1
1:B:169:LEU:HD23	1:B:169:LEU:O	0.50	2.05	16	1
1:A:10:SER:OG	1:A:11:VAL:N	0.50	2.45	18	1
1:A:173:TRP:C	1:A:173:TRP:CD2	0.50	2.84	17	2
1:A:67:SER:O	1:A:69:ILE:N	0.50	2.42	8	2
1:A:135:ILE:CD1	1:A:135:ILE:N	0.50	2.74	8	1
1:A:108:ARG:O	1:A:112:ARG:HD2	0.50	2.05	10	1
1:A:161:GLN:NE2	1:A:161:GLN:N	0.50	2.58	14	1
1:B:185:GLU:H	1:B:185:GLU:CD	0.50	2.10	2	2
1:B:89:GLN:NE2	1:B:89:GLN:N	0.50	2.60	19	2
1:B:119:ASN:OD1	1:B:119:ASN:N	0.50	2.44	15	1
1:B:165:LYS:NZ	1:B:212:TYR:CZ	0.50	2.79	17	1
1:B:160:ASP:O	1:B:163:VAL:HG13	0.50	2.07	5	1
1:B:12:LEU:N	1:B:12:LEU:CD1	0.50	2.74	13	1
1:B:196:ASP:O	1:B:200:GLY:N	0.50	2.43	2	3
1:A:138:LYS:O	1:A:138:LYS:CG	0.50	2.60	3	2
1:B:132:GLU:N	1:B:132:GLU:OE1	0.50	2.45	3	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:115:PHE:O	1:A:115:PHE:CD2	0.50	2.64	14	1
1:B:158:HIS:CG	1:B:161:GLN:NE2	0.50	2.80	17	1
1:B:75:SER:CB	1:B:94:TYR:OH	0.50	2.60	20	8
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:B:161:GLN:CD	1:B:162:ILE:N	0.50	2.65	14	1
1:B:169:LEU:C	1:B:169:LEU:HD23	0.50	2.27	2	6
1:A:9:ASN:OD1	1:A:10:SER:N	0.50	2.44	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:16:ILE:HD11	1:B:99:TYR:CZ	0.50	2.41	20	1
1:B:94:TYR:C	1:B:94:TYR:CD1	0.50	2.85	1	2
1:B:157:ARG:O	1:B:159:ARG:N	0.50	2.41	1	1
1:A:184:ILE:H	1:A:184:ILE:CD1	0.50	2.20	2	1
1:B:130:PRO:CB	1:B:157:ARG:HE	0.50	2.20	2	1
1:A:173:TRP:CD2	1:A:173:TRP:C	0.50	2.85	3	1
1:B:97:LYS:O	1:B:99:TYR:CD2	0.50	2.65	3	5
1:A:50:VAL:HG22	1:A:52:ASP:H	0.50	1.67	10	5
1:A:94:TYR:C	1:A:94:TYR:CD1	0.50	2.84	7	1
1:A:199:LEU:N	1:A:199:LEU:HD12	0.50	2.22	20	3
1:A:185:GLU:H	1:A:185:GLU:CD	0.50	2.09	9	1
1:B:160:ASP:N	1:B:160:ASP:OD1	0.50	2.44	9	2
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	2
1:B:199:LEU:N	1:B:199:LEU:CD2	0.50	2.74	11	1
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:40:MET:SD	1:A:41:ASP:OD1	0.49	2.70	11	4
1:A:116:TRP:CG	1:A:117:GLY:N	0.49	2.78	8	2
1:A:12:LEU:CD1	1:A:12:LEU:N	0.49	2.75	14	1
1:B:169:LEU:CB	1:B:173:TRP:CZ3	0.49	2.95	17	1
1:A:72:LEU:C	1:A:72:LEU:HD23	0.49	2.28	6	5
1:A:83:GLU:OE1	1:A:94:TYR:CE1	0.49	2.65	10	1
1:B:184:ILE:O	1:B:188:ILE:HG22	0.49	2.07	13	1
1:B:115:PHE:O	1:B:116:TRP:CD1	0.49	2.65	14	2
1:A:44:ASN:ND2	1:A:145:LYS:NZ	0.49	2.60	15	1
1:B:97:LYS:C	1:B:99:TYR:N	0.49	2.64	9	19
1:A:83:GLU:OE1	1:A:84:VAL:N	0.49	2.45	3	1
1:A:122:GLU:H	1:A:159:ARG:HH12	0.49	1.49	4	1
1:A:172:ILE:N	1:A:172:ILE:HD12	0.49	2.22	6	1
1:B:173:TRP:O	1:B:173:TRP:CD2	0.49	2.66	12	1
1:B:173:TRP:CE3	1:B:173:TRP:C	0.49	2.85	12	1
1:A:205:GLU:CD	1:A:205:GLU:N	0.49	2.65	15	1
1:B:204:VAL:HG12	1:B:214:PHE:CE2	0.49	2.41	17	1
1:A:207:VAL:HG22	1:A:208:ARG:N	0.49	2.22	20	1
1:B:160:ASP:OD2	1:B:216:TYR:CZ	0.49	2.64	6	1
1:A:1:MET:SD	1:A:116:TRP:NE1	0.49	2.86	8	1
1:A:132:GLU:OE1	1:A:132:GLU:N	0.49	2.45	14	1
1:B:72:LEU:HG	1:B:95:ILE:HD11	0.49	1.84	17	4
1:B:152:LEU:O	1:B:155:LEU:CD1	0.49	2.60	1	3
1:A:40:MET:SD	1:A:45:TYR:OH	0.49	2.70	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:151:VAL:HG13	1:B:152:LEU:N	0.49	2.22	15	8
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:A:2:ARG:NE	1:A:28:ASP:OD2	0.49	2.42	2	1
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: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:188:ILE:HD12	1:B:212:TYR:CE2	0.49	2.42	17	2
1:B:155:LEU:HD23	1:B:214:PHE:CD2	0.49	2.43	17	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:B:40:MET:SD	1:B:45:TYR:OH	0.49	2.69	2	2
1:B:1:MET:SD	1:B:46:ASP:OD2	0.49	2.70	8	2
1:B:185:GLU:O	1:B:189:ASN:ND2	0.49	2.46	8	1
1:A:108:ARG:CA	1:A:112:ARG:NH1	0.49	2.76	10	1
1:A:115:PHE:C	1:A:116:TRP:CG	0.49	2.86	11	2
1:A:37:GLU:OE2	1:A:61:ARG:NH2	0.49	2.45	3	1
1:A:115:PHE:C	1:A:116:TRP:CD1	0.49	2.86	11	2
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:B:83:GLU:CD	1:B:94:TYR:CE2	0.49	2.87	15	1
1:B:2:ARG:NH2	1:B:43:ARG:C	0.48	2.66	2	1
1:B:4:LEU:HD11	1:B:6:ILE:CG1	0.48	2.38	19	5
1:A:6:ILE:CG2	1:A:31:GLU:O	0.48	2.60	6	8
1:A:8:LYS:NZ	1:A:32:SER:OG	0.48	2.44	3	1
1:A:2:ARG:N	1:A:46:ASP:OD2	0.48	2.46	11	2
1:B:154:HIS:O	1:B:158:HIS:ND1	0.48	2.46	6	1
1:A:44:ASN:O	1:A:45:TYR:O	0.48	2.31	15	2
1:B:6:ILE:HD12	1:B:50:VAL:HB	0.48	1.85	9	8
1:B:97:LYS:O	1:B:97:LYS:HD2	0.48	2.08	4	4
1:A:75:SER:CB	1:A:94:TYR:OH	0.48	2.61	13	7
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:A:135:ILE:C	1:A:136:ILE:HD13	0.48	2.28	12	1
1:B:173:TRP:CD2	1:B:173:TRP:C	0.48	2.86	12	2
1:B:34:GLU:H	1:B:34:GLU:CD	0.48	2.12	17	1
1:B:208:ARG:O	1:B:210:ARG:N	0.48	2.46	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:67:SER:O	1:B:69:ILE:N	0.48	2.43	9	4
1:B:195:MET:SD	1:B:196:ASP:OD1	0.48	2.71	5	1
1:B:143:GLU:H	1:B:143:GLU:CD	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:B:114:ARG:O	1:B:115:PHE:CG	0.48	2.65	18	1
1:A:154:HIS:CD2	1:A:158:HIS:CE1	0.48	3.02	2	1
1:A:70:VAL:HG12	1:A:71:VAL:N	0.48	2.24	9	5
1:A:165:LYS:CB	1:A:165:LYS:NZ	0.48	2.77	4	2
1:B:158:HIS:O	1:B:159:ARG:O	0.48	2.31	11	1
1:A:161:GLN:N	1:A:161:GLN:CD	0.48	2.67	14	1
1:B:161:GLN:NE2	1:B:162:ILE:C	0.48	2.65	14	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: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:B:211:GLY:C	1:B:212:TYR:CD1	0.48	2.87	3	2
1:B:173:TRP:C	1:B:173:TRP:CD2	0.48	2.87	6	2
1:A:182:ASN:OD1	1:A:184:ILE:CD1	0.48	2.62	9	1
1:A:72:LEU:C	1:A:72:LEU:HD13	0.48	2.29	11	1
1:A:212:TYR:N	1:A:212:TYR:CD1	0.48	2.82	20	2
1:A:72:LEU:CD1	1:A:108:ARG:HH22	0.48	2.20	20	1
1:B:33:LEU:O	1:B:37:GLU:N	0.48	2.44	7	6
1:A:123:ILE:O	1:A:123:ILE:CG2	0.48	2.61	5	2
1:B:199:LEU:HD12	1:B:199:LEU:N	0.48	2.23	20	5
1:A:138:LYS:CB	1:A:138:LYS:HZ2	0.48	2.20	5	1
1:A:85:HIS:CE1	1:A:89:GLN:HE21	0.48	2.27	20	2
1:A:89:GLN:CD	1:A:90:GLY:N	0.48	2.67	9	1
1:B:87:PHE:C	1:B:87:PHE:CD1	0.48	2.87	10	1
1:A:119:ASN:HA	1:A:129:SER:OG	0.48	2.08	11	1
1:B:102:ILE:O	1:B:104:ALA:N	0.48	2.47	12	1
1:B:116:TRP:O	1:B:116:TRP:CG	0.48	2.67	15	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
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:A:159:ARG:O	1:A:160:ASP:CB	0.48	2.61	14	1
1:B:7:GLU:N	1:B:7:GLU:CD	0.48	2.67	2	1
1:B:61:ARG:HH21	1:B:65:LYS:HZ3	0.48	1.52	3	1
1:B:65:LYS:C	1:B:66:HIS:CG	0.48	2.87	17	11
1:B:2:ARG:NH2	1:B:44:ASN:C	0.48	2.67	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:152:LEU:HD13	1:B:152:LEU:O	0.48	2.08	4	4
1:B:132:GLU:O	1:B:133:GLU:C	0.48	2.52	9	2
1:A:115:PHE:CD1	1:A:115:PHE:N	0.48	2.80	18	1
1:A:199:LEU:N	1:A:199:LEU:CD1	0.48	2.75	20	1
1:A:8:LYS:HZ3	1:A:31:GLU:C	0.48	2.11	3	1
1:A:65:LYS:C	1:A:66:HIS:CG	0.48	2.87	20	10
1:B:215:CYS:SG	1:B:216:TYR:CD1	0.48	3.07	3	1
1:B:118:SER:N	1:B:132:GLU:OE1	0.48	2.43	4	1
1:A:118:SER:O	1:A:119:ASN:ND2	0.48	2.47	12	1
1:A:100:ARG:CZ	1:B:94:TYR:OH	0.48	2.62	4	1
1:B:83:GLU:OE2	1:B:94:TYR:CZ	0.48	2.67	4	1
1:B:63:LYS:NZ	1:B:90:GLY:O	0.48	2.41	6	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:A:7:GLU:OE1	1:A:51:SER:CB	0.48	2.62	20	3
1:B:5:LEU:HD22	1:B:49:MET:HG3	0.48	1.85	15	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:31:GLU:N	1:A:35:ASP:OD2	0.47	2.43	3	1
1:B:150:GLU:CG	1:B:151:VAL:N	0.47	2.77	5	1
1:A:80:SER:CB	1:B:101:SER:OG	0.47	2.62	12	1
1:A:160:ASP:N	1:A:160:ASP:OD1	0.47	2.47	12	1
1:A:12:LEU:HD13	1:A:97:LYS:NZ	0.47	2.23	16	1
1:A:61:ARG:HH21	1:A:65:LYS:HZ2	0.47	1.52	20	1
1:A:188:ILE:HG23	1:A:189:ASN:N	0.47	2.24	9	3
1:A:84:VAL:HG23	1:A:85:HIS:N	0.47	2.24	20	10
1:A:213:ARG:NH1	1:A:215:CYS:SG	0.47	2.86	6	1
1:B:159:ARG:NH2	1:B:203:THR:O	0.47	2.43	7	1
1:B:102:ILE:C	1:B:104:ALA:N	0.47	2.68	12	2
1:A:85:HIS:NE2	1:A:89:GLN:NE2	0.47	2.62	17	1
1:A:119:ASN:ND2	1:A:127:THR:CG2	0.47	2.77	17	1
1:A:122:GLU:N	1:A:122:GLU:CD	0.47	2.67	17	1
1:A:5:LEU:HD22	1:A:49:MET:CG	0.47	2.39	19	1
1:A:116:TRP:CD1	1:A:116:TRP:N	0.47	2.82	19	1
1:A:97:LYS:O	1:A:99:TYR:CD2	0.47	2.67	3	8
1:A:194:LYS:O	1:A:198:PRO:CD	0.47	2.62	5	7
1:B:119:ASN:HD21	1:B:121:ILE:C	0.47	2.11	6	1
1:A:3:VAL:HG13	1:A:47:LEU:HB3	0.47	1.85	9	1
1:A:123:ILE:CG1	1:A:159:ARG:NE	0.47	2.71	15	1
1:B:85:HIS:CE1	1:B:89:GLN:CD	0.47	2.88	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:161:GLN:NE2	1:B:160:ASP:OD2	0.47	2.47	18	1
1:A:94:TYR:CD1	1:A:94:TYR:C	0.47	2.87	1	3
1:A:162:ILE:N	1:A:162:ILE:CD1	0.47	2.77	19	2
1:B:40:MET:CE	1:B:45:TYR:OH	0.47	2.62	2	1
1:A:56:LEU:HD13	1:A:85:HIS:NE2	0.47	2.25	4	1
1:A:119:ASN:CG	1:A:120:VAL:N	0.47	2.67	13	3
1:A:113:LEU:HD12	1:A:113:LEU:N	0.47	2.25	6	1
1:B:173:TRP:C	1:B:173:TRP:CE3	0.47	2.88	13	2
1:B:213:ARG:HH12	1:B:215:CYS:HB2	0.47	1.67	20	1
1:B:118:SER:C	1:B:119:ASN:ND2	0.47	2.68	17	3
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:83:GLU:CD	1:B:94:TYR:CD1	0.47	2.88	8	1
1:B:93:ASP:OD2	1:B:112:ARG:CD	0.47	2.62	8	1
1:A:108:ARG:O	1:A:112:ARG:CD	0.47	2.63	10	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: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:93:ASP:CG	1:B:112:ARG:NH2	0.47	2.68	17	1
1:A:143:GLU:CD	1:A:143:GLU:H	0.47	2.12	19	1
1:B:159:ARG:O	1:B:214:PHE:HB3	0.47	2.09	20	1
1:B:63:LYS:O	1:B:67:SER:N	0.47	2.47	2	3
1:A:63:LYS:NZ	1:A:92:ASP:CG	0.47	2.68	10	4
1:A:114:ARG:O	1:A:115:PHE:CD1	0.47	2.68	4	1
1:B:123:ILE:HD13	1:B:124:GLY:N	0.47	2.24	6	1
1:B:44:ASN:C	1:B:45:TYR:CG	0.47	2.88	7	1
1:B:144:VAL:HG21	1:B:149:PHE:CZ	0.47	2.45	7	1
1:B:78:PRO:CB	1:B:94:TYR:OH	0.47	2.63	9	1
1:A:114:ARG:O	1:A:115:PHE:CD2	0.47	2.67	10	1
1:B:33:LEU:CD2	1:B:33:LEU:N	0.47	2.78	10	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
1:A:189:ASN:ND2	1:A:193:GLN:OE1	0.47	2.48	2	1
1:A:173:TRP:C	1:A:173:TRP:CE3	0.47	2.88	17	2
1:A:110:GLU:O	1:A:113:LEU:N	0.47	2.46	8	1
1:B:208:ARG:N	1:B:208:ARG:CD	0.47	2.78	10	2
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:B:169:LEU:HB3	1:B:173:TRP:CZ3	0.47	2.44	17	1
1:A:211:GLY:C	1:A:212:TYR:CD1	0.47	2.88	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:23:LYS:NZ	1:B:110:GLU:OE1	0.47	2.42	16	2
1:A:55:ALA:O	1:A:58:PHE:N	0.47	2.48	6	12
1:B:47:LEU:C	1:B:47:LEU:HD13	0.47	2.30	8	11
1:B:166:GLU:H	1:B:166:GLU:CD	0.47	2.11	15	2
1:A:182:ASN:N	1:A:182:ASN:OD1	0.47	2.45	10	2
1:B:110:GLU:O	1:B:114:ARG:CA	0.47	2.63	15	1
1:B:192:ARG:HH21	1:B:204:VAL:HG23	0.47	1.69	20	1
1:A:151:VAL:HG13	1:A:152:LEU:N	0.47	2.25	6	5
1:B:97:LYS:O	1:B:97:LYS:CE	0.47	2.63	4	3
1:B:54:ASN:C	1:B:54:ASN:ND2	0.47	2.68	6	1
1:B:114:ARG:O	1:B:116:TRP:CE3	0.47	2.68	6	1
1:A:101:SER:O	1:A:101:SER:OG	0.47	2.33	18	2
1:B:110:GLU:O	1:B:114:ARG:CG	0.47	2.63	8	1
1:A:149:PHE:CD1	1:A:150:GLU:HG3	0.47	2.31	11	1
1:B:5:LEU:HD22	1:B:49:MET:CG	0.47	2.40	15	1
1:B:147:LYS:H	1:B:148:PRO:CD	0.47	2.23	16	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:144:VAL:O	1:B:144:VAL:HG23	0.46	2.09	3	2
1:B:122:GLU:CD	1:B:122:GLU:N	0.46	2.68	4	1
1:B:154:HIS:HA	1:B:157:ARG:NH1	0.46	2.25	9	1
1:B:170:ASP:O	1:B:173:TRP:CZ3	0.46	2.68	16	1
1:A:83:GLU:OE2	1:B:108:ARG:NE	0.46	2.49	18	1
1:A:152:LEU:HD13	1:A:152:LEU:O	0.46	2.10	5	5
1:B:56:LEU:HD12	1:B:56:LEU:N	0.46	2.25	1	2
1:A:53:LYS:C	1:A:55:ALA:N	0.46	2.69	5	1
1:B:49:MET:SD	1:B:50:VAL:N	0.46	2.88	8	2
1:A:93:ASP:CG	1:A:112:ARG:NH2	0.46	2.68	12	1
1:B:105:LEU:HD12	1:B:105:LEU:H	0.46	1.70	16	1
1:A:20:LEU:N	1:A:20:LEU:HD23	0.46	2.25	18	3
1:A:216:TYR:CD1	1:A:217:PRO:O	0.46	2.68	2	1
1:B:217:PRO:O	1:B:218:LYS:O	0.46	2.34	7	2
1:B:207:VAL:N	1:B:211:GLY:O	0.46	2.43	10	1
1:B:141:GLU:N	1:B:141:GLU:CD	0.46	2.68	17	1
1:B:192:ARG:NE	1:B:204:VAL:HG21	0.46	2.24	20	1
1:A:188:ILE:CG2	1:A:189:ASN:N	0.46	2.78	6	7
1:B:163:VAL:O	1:B:212:TYR:O	0.46	2.34	19	2
1:A:169:LEU:C	1:A:171:ALA:N	0.46	2.69	8	2
1:A:73:VAL:HG22	1:A:74:SER:N	0.46	2.26	3	2
1:A:100:ARG:NH1	1:B:83:GLU:CD	0.46	2.69	4	1
1:B:151:VAL:CG1	1:B:152:LEU:N	0.46	2.78	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	2
1:B:190:GLN:CG	1:B:191:ILE:N	0.46	2.77	8	3
1:B:147:LYS:CE	1:B:172:ILE:CG2	0.46	2.92	8	1
1:B:81:GLU:OE1	1:B:81:GLU:N	0.46	2.45	11	1
1:A:108:ARG:C	1:A:112:ARG:NH1	0.46	2.69	12	1
1:B:149:PHE:CG	1:B:150:GLU:N	0.46	2.83	16	2
1:A:31:GLU:CG	1:A:35:ASP:OD2	0.46	2.63	4	2
1:B:129:SER:O	1:B:133:GLU:N	0.46	2.49	6	2
1:A:81:GLU:OE1	1:A:81:GLU:N	0.46	2.44	10	1
1:B:75:SER:O	1:B:97:LYS:N	0.46	2.42	13	1
1:B:105:LEU:HD23	1:B:105:LEU:H	0.46	1.69	18	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:A:44:ASN:ND2	1:A:45:TYR:N	0.46	2.64	6	1
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:A:169:LEU:O	1:A:173:TRP:O	0.46	2.34	11	3
1:B:72:LEU:HD23	1:B:95:ILE:HD11	0.46	1.88	18	1
1:B:188:ILE:CG2	1:B:189:ASN:N	0.46	2.78	10	8
1:A:8:LYS:H	1:A:8:LYS:CD	0.46	2.24	2	1
1:A:87:PHE:CD2	1:B:108:ARG:CZ	0.46	2.99	2	1
1:B:4:LEU:O	1:B:49:MET:O	0.46	2.34	2	6
1:B:143:GLU:CD	1:B:143:GLU:N	0.46	2.69	2	2
1:A:115:PHE:CD2	1:A:115:PHE:O	0.46	2.69	3	2
1:B:131:ASP:O	1:B:133:GLU:CD	0.46	2.52	9	1
1:B:133:GLU:CD	1:B:133:GLU:N	0.46	2.69	9	1
1:B:152:LEU:O	1:B:156:ALA:HB2	0.46	2.10	14	1
1:A:161:GLN:OE1	1:A:163:VAL:HG12	0.46	2.09	19	1
1:A:108:ARG:NH1	1:B:87:PHE:CE1	0.46	2.83	1	1
1:B:40:MET:O	1:B:43:ARG:O	0.46	2.33	2	19
1:A:209:ARG:NH2	1:A:213:ARG:NH2	0.46	2.42	2	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:92:ASP:HB3	1:A:112:ARG:HH21	0.46	1.71	7	1
1:B:196:ASP:N	1:B:196:ASP:OD1	0.46	2.49	7	1
1:A:79:THR:HG23	1:A:82:GLU:H	0.46	1.71	11	1
1:A:135:ILE:HG21	1:A:137:TYR:CE2	0.46	2.45	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:114:ARG:CA	1:B:114:ARG:HE	0.46	2.24	20	1
1:A:160:ASP:OD1	1:A:216:TYR:CD2	0.46	2.69	1	1
1:A:32:SER:O	1:A:35:ASP:OD1	0.46	2.34	3	2
1:B:138:LYS:O	1:B:138:LYS:CG	0.46	2.63	13	3
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:16:ILE:HD11	1:B:99:TYR:CD1	0.46	2.46	13	1
1:B:155:LEU:HD13	1:B:214:PHE:HE2	0.46	1.69	13	1
1:A:75:SER:O	1:A:97:LYS:N	0.46	2.42	14	1
1:A:144:VAL:CG2	1:A:149:PHE:CG	0.46	2.98	18	1
1:A:40:MET:CE	1:A:45:TYR:OH	0.45	2.64	2	1
1:A:152:LEU:HD11	1:A:195:MET:SD	0.45	2.51	2	1
1:B:143:GLU:N	1:B:143:GLU:OE1	0.45	2.48	2	1
1:B:70:VAL:CG1	1:B:71:VAL:N	0.45	2.79	8	4
1:B:189:ASN:OD1	1:B:192:ARG:NH2	0.45	2.50	7	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:B:203:THR:O	1:B:214:PHE:CE1	0.45	2.69	15	1
1:B:169:LEU:C	1:B:171:ALA:N	0.45	2.68	20	2
1:A:40:MET:O	1:A:43:ARG:O	0.45	2.34	5	20
1:A:195:MET:SD	1:A:195:MET:C	0.45	2.95	14	2
1:A:133:GLU:HA	1:A:149:PHE:HZ	0.45	1.70	2	1
1:A:74:SER:O	1:A:75:SER:OG	0.45	2.34	19	5
1:A:137:TYR:C	1:A:139:GLY:N	0.45	2.69	20	3
1:A:70:VAL:HG21	1:A:113:LEU:HD11	0.45	1.87	10	1
1:B:190:GLN:HB3	1:B:194:LYS:HZ3	0.45	1.71	13	1
1:B:123:ILE:CD1	1:B:159:ARG:NH1	0.45	2.78	16	1
1:B:199:LEU:N	1:B:199:LEU:CD1	0.45	2.79	20	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:SD	1:B:40:MET:C	0.45	2.94	2	2
1:A:190:GLN:CG	1:A:191:ILE:N	0.45	2.80	8	3
1:B:113:LEU:O	1:B:116:TRP:CD1	0.45	2.69	11	2
1:B:18:LYS:N	1:B:18:LYS:CD	0.45	2.79	11	1
1:B:188:ILE:HD13	1:B:188:ILE:O	0.45	2.11	11	1
1:A:165:LYS:H	1:A:165:LYS:CD	0.45	2.23	14	1
1:A:118:SER:C	1:A:119:ASN:ND2	0.45	2.69	16	1
1:A:197:LYS:CB	1:A:198:PRO:CD	0.45	2.95	9	10
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:B:191:ILE:O	1:B:195:MET:CG	0.45	2.65	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:MET:SD	1:A:49:MET:C	0.45	2.95	7	5
1:A:159:ARG:NH2	1:A:203:THR:OG1	0.45	2.49	7	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:143:GLU:CD	1:A:143:GLU:N	0.45	2.70	16	2
1:A:12:LEU:O	1:A:12:LEU:HD13	0.45	2.11	19	1
1:B:213:ARG:NH1	1:B:215:CYS:CB	0.45	2.76	20	1
1:B:193:GLN:O	1:B:196:ASP:OD1	0.45	2.35	14	7
1:B:11:VAL:CG1	1:B:12:LEU:N	0.45	2.80	4	3
1:B:82:GLU:OE1	1:B:82:GLU:CA	0.45	2.65	5	2
1:A:79:THR:O	1:A:83:GLU:OE2	0.45	2.35	10	2
1:A:189:ASN:OD1	1:A:193:GLN:NE2	0.45	2.50	5	2
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:B:133:GLU:HA	1:B:149:PHE:CE1	0.45	2.46	17	1
1:A:207:VAL:O	1:A:208:ARG:CB	0.45	2.62	20	1
1:B:40:MET:C	1:B:40:MET:SD	0.45	2.95	4	13
1:B:197:LYS:CB	1:B:198:PRO:CD	0.45	2.95	2	11
1:B:115:PHE:C	1:B:117:GLY:N	0.45	2.70	6	2
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:65:LYS:CB	1:B:65:LYS:NZ	0.45	2.80	12	1
1:B:185:GLU:CG	1:B:186:VAL:N	0.45	2.79	12	1
1:A:103:LYS:O	1:A:107:ALA:HB2	0.45	2.11	15	2
1:B:66:HIS:CE1	1:B:145:LYS:HZ3	0.45	2.29	20	1
1:A:40:MET:C	1:A:40:MET:SD	0.45	2.95	9	9
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:23:LYS:N	1:B:23:LYS:CD	0.45	2.80	4	3
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:B:158:HIS:ND1	1:B:158:HIS:N	0.45	2.65	12	1
1:A:93:ASP:OD2	1:A:112:ARG:CZ	0.45	2.65	14	1
1:B:73:VAL:O	1:B:73:VAL:HG13	0.45	2.12	15	1
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:A:23:LYS:NZ	1:A:103:LYS:HZ2	0.45	2.09	16	1
1:B:129:SER:HB3	1:B:132:GLU:OE1	0.45	2.12	17	1
1:B:59:VAL:HG23	1:B:60:SER:N	0.45	2.27	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:TYR:O	1:A:41:ASP:OD1	0.45	2.35	10	4
1:B:47:LEU:HD13	1:B:47:LEU:C	0.45	2.32	10	5
1:B:97:LYS:N	1:B:98:PRO:HD2	0.45	2.27	6	12
1:B:36:GLY:O	1:B:40:MET:CG	0.45	2.65	3	2
1:B:12:LEU:O	1:B:12:LEU:HD13	0.45	2.11	5	1
1:B:83:GLU:CD	1:B:94:TYR:CE1	0.45	2.90	8	1
1:A:72:LEU:HG	1:A:95:ILE:HD11	0.45	1.89	15	1
1:A:118:SER:H	1:A:132:GLU:CD	0.45	2.14	19	1
1:B:207:VAL:O	1:B:211:GLY:O	0.45	2.34	7	4
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:A:185:GLU:CG	1:A:186:VAL:N	0.45	2.80	17	2
1:A:115:PHE:C	1:A:117:GLY:N	0.45	2.70	14	1
1:B:2:ARG:NH1	1:B:43:ARG:CZ	0.45	2.80	15	1
1:B:1:MET:H2	1:B:2:ARG:CZ	0.45	2.25	19	1
1:A:106:VAL:HG23	1:A:107:ALA:N	0.45	2.27	2	1
1:B:28:ASP:OD2	1:B:43:ARG:NH2	0.45	2.50	3	1
1:B:40:MET:CE	1:B:45:TYR:CZ	0.45	3.00	3	2
1:A:1:MET:SD	1:A:46:ASP:OD2	0.45	2.75	5	1
1:A:105:LEU:C	1:A:105:LEU:CD1	0.45	2.85	8	2
1:A:11:VAL:CG1	1:A:12:LEU:N	0.45	2.80	11	3
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:94:TYR:CD1	1:B:95:ILE:N	0.44	2.86	1	2
1:B:206:THR:HG23	1:B:206:THR:O	0.44	2.12	9	2
1:A:111:ALA:HB1	1:B:87:PHE:CE1	0.44	2.46	2	1
1:A:111:ALA:CB	1:B:87:PHE:CZ	0.44	3.00	3	1
1:B:2:ARG:O	1:B:46:ASP:OD1	0.44	2.35	6	2
1:A:23:LYS:NZ	1:A:110:GLU:CD	0.44	2.71	9	1
1:A:195:MET:C	1:A:195:MET:SD	0.44	2.96	9	1
1:B:192:ARG:CZ	1:B:204:VAL:CB	0.44	2.83	1	1
1:A:64:GLU:CG	1:A:65:LYS:N	0.44	2.80	10	9
1:B:46:ASP:OD2	1:B:116:TRP:CD1	0.44	2.70	2	1
1:B:169:LEU:C	1:B:169:LEU:CD1	0.44	2.85	11	4
1:B:195:MET:SD	1:B:195:MET:C	0.44	2.96	17	2
1:A:169:LEU:HD13	1:A:169:LEU:O	0.44	2.11	5	2
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:77:ASN:ND2	1:B:77:ASN:H	0.44	2.10	14	1
1:B:115:PHE:CD2	1:B:116:TRP:N	0.44	2.86	19	1
1:B:54:ASN:H	1:B:54:ASN:HD22	0.44	1.55	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:207:VAL:O	1:B:208:ARG:O	0.44	2.36	20	1
1:A:214:PHE:O	1:A:215:CYS:SG	0.44	2.72	1	2
1:A:5:LEU:CD1	1:A:49:MET:SD	0.44	3.05	10	1
1:A:114:ARG:C	1:A:116:TRP:N	0.44	2.70	20	1
1:A:98:PRO:O	1:A:99:TYR:O	0.44	2.34	14	10
1:A:160:ASP:OD1	1:A:216:TYR:CE2	0.44	2.70	3	1
1:B:50:VAL:CG2	1:B:52:ASP:H	0.44	2.26	17	6
1:A:89:GLN:N	1:A:89:GLN:CD	0.44	2.71	8	2
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:B:115:PHE:O	1:B:116:TRP:O	0.44	2.36	7	1
1:A:116:TRP:CD2	1:A:117:GLY:N	0.44	2.85	8	1
1:A:163:VAL:O	1:A:212:TYR:O	0.44	2.36	10	2
1:B:173:TRP:CD2	1:B:173:TRP:O	0.44	2.69	13	1
1:B:84:VAL:CG2	1:B:85:HIS:N	0.44	2.79	18	2
1:A:167:GLN:O	1:A:170:ASP:OD1	0.44	2.36	19	3
1:B:55:ALA:O	1:B:58:PHE:N	0.44	2.51	19	1
1:A:115:PHE:O	1:A:116:TRP:O	0.44	2.36	1	3
1:A:12:LEU:N	1:A:12:LEU:CD1	0.44	2.81	3	1
1:A:169:LEU:C	1:A:169:LEU:CD1	0.44	2.86	5	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
1:B:188:ILE:HD12	1:B:212:TYR:CE1	0.44	2.47	10	1
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:124:GLY:C	1:A:126:LEU:H	0.44	2.16	2	1
1:A:137:TYR:CE2	1:A:198:PRO:O	0.44	2.71	17	2
1:B:110:GLU:O	1:B:113:LEU:N	0.44	2.51	3	1
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:A:169:LEU:O	1:A:170:ASP:C	0.44	2.56	9	1
1:A:159:ARG:C	1:A:161:GLN:HE22	0.44	2.14	14	1
1:B:79:THR:O	1:B:83:GLU:OE2	0.44	2.36	15	3
1:A:173:TRP:CD2	1:A:173:TRP:O	0.44	2.71	17	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:A:61:ARG:HH21	1:A:65:LYS:HZ3	0.44	1.56	3	1
1:B:5:LEU:HD23	1:B:5:LEU:N	0.44	2.27	3	1
1:B:85:HIS:O	1:B:89:GLN:OE1	0.44	2.36	4	2
1:A:94:TYR:CE1	1:A:95:ILE:O	0.44	2.70	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LEU:HD23	1:A:113:LEU:HD21	0.44	1.90	7	1
1:A:126:LEU:HD23	1:A:126:LEU:N	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:147:LYS:CB	1:B:147:LYS:NZ	0.44	2.81	6	1
1:B:123:ILE:HD11	1:B:216:TYR:CD1	0.44	2.48	9	1
1:A:149:PHE:HD1	1:A:149:PHE:H	0.44	1.56	11	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:154:HIS:ND1	1:B:157:ARG:NH2	0.44	2.66	18	1
1:A:158:HIS:N	1:A:158:HIS:CD2	0.44	2.82	19	1
1:A:159:ARG:O	1:A:214:PHE:O	0.44	2.35	19	1
1:B:93:ASP:OD2	1:B:108:ARG:NH2	0.44	2.50	20	1
1:A:31:GLU:OE2	1:A:35:ASP:OD2	0.44	2.36	1	2
1:B:98:PRO:O	1:B:99:TYR:O	0.44	2.36	1	9
1:B:147:LYS:CB	1:B:147:LYS:HZ2	0.44	2.26	6	1
1:B:154:HIS:CD2	1:B:158:HIS:HD1	0.44	2.31	6	1
1:A:70:VAL:CG2	1:A:113:LEU:HD11	0.44	2.42	10	1
1:A:8:LYS:O	1:A:9:ASN:O	0.44	2.36	12	1
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: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:153:THR:CG2	1:B:157:ARG:NH2	0.44	2.81	19	1
1:A:47:LEU:C	1:A:47:LEU:CD1	0.43	2.86	5	11
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: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:164:SER:N	1:B:167:GLN:OE1	0.43	2.42	8	1
1:A:20:LEU:HD23	1:A:20:LEU:H	0.43	1.73	17	1
1:B:95:ILE:CG2	1:B:108:ARG:HH22	0.43	2.25	18	1
1:A:207:VAL:O	1:A:211:GLY:O	0.43	2.36	1	4
1:B:7:GLU:OE2	1:B:51:SER:OG	0.43	2.36	11	3
1:B:57:SER:O	1:B:61:ARG:NH1	0.43	2.51	1	1
1:B:7:GLU:OE1	1:B:51:SER:OG	0.43	2.36	10	11
1:B:86:ALA:O	1:B:91:ALA:HB3	0.43	2.12	14	3
1:B:5:LEU:HD23	1:B:6:ILE:N	0.43	2.27	19	3
1:A:161:GLN:HE22	1:A:163:VAL:CG2	0.43	2.26	6	1
1:A:5:LEU:HD23	1:A:6:ILE:N	0.43	2.28	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:116:TRP:O	1:A:118:SER:N	0.43	2.51	14	1
1:A:199:LEU:O	1:A:199:LEU:HD13	0.43	2.12	15	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:210:ARG:NH1	1:B:213:ARG:HH21	0.43	2.11	17	1
1:A:214:PHE:CD1	1:A:214:PHE:N	0.43	2.86	18	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:A:47:LEU:HD13	1:A:47:LEU:C	0.43	2.33	4	2
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:33:LEU:O	1:A:37:GLU:N	0.43	2.43	6	2
1:A:137:TYR:C	1:A:139:GLY:H	0.43	2.16	20	3
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:92:ASP:O	1:A:93:ASP:OD1	0.43	2.37	5	11
1:B:181:PRO:O	1:B:185:GLU:OE1	0.43	2.37	2	1
1:A:61:ARG:NH2	1:A:65:LYS:HZ3	0.43	2.10	3	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: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:B:160:ASP:O	1:B:160:ASP:OD2	0.43	2.36	2	2
1:A:120:VAL:HG21	1:A:131:ASP:OD1	0.43	2.13	3	1
1:B:208:ARG:O	1:B:209:ARG:O	0.43	2.37	12	3
1:B:27:ALA:O	1:B:28:ASP:OD1	0.43	2.37	11	7
1:A:197:LYS:H	1:A:198:PRO:CD	0.43	2.26	5	1
1:A:133:GLU:CD	1:A:149:PHE:CE2	0.43	2.92	6	1
1:A:137:TYR:N	1:A:137:TYR:CD1	0.43	2.86	6	1
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:79:THR:OG1	1:A:82:GLU:OE2	0.43	2.36	10	1
1:A:121:ILE:HG21	1:A:159:ARG:NH2	0.43	2.28	12	1
1:A:23:LYS:HZ1	1:A:103:LYS:NZ	0.43	2.10	16	1
1:A:143:GLU:N	1:A:143:GLU:CD	0.43	2.72	7	3
1:B:113:LEU:O	1:B:116:TRP:N	0.43	2.51	6	2
1:A:4:LEU:HD11	1:A:6:ILE:HG12	0.43	1.89	3	2
1:A:150:GLU:OE1	1:A:172:ILE:O	0.43	2.36	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:79:THR:OG1	1:B:82:GLU:OE2	0.43	2.36	4	1
1:A:105:LEU:N	1:A:105:LEU:CD2	0.43	2.80	6	1
1:A:159:ARG:HH22	1:B:161:GLN:HE22	0.43	1.55	6	1
1:A:137:TYR:OH	1:A:199:LEU:O	0.43	2.35	7	1
1:B:214:PHE:C	1:B:215:CYS:SG	0.43	2.96	12	2
1:A:8:LYS:CD	1:A:8:LYS:H	0.43	2.26	13	1
1:B:7:GLU:OE1	1:B:9:ASN:O	0.43	2.36	14	1
1:A:48:VAL:O	1:A:48:VAL:CG2	0.43	2.65	18	1
1:B:51:SER:CB	1:B:74:SER:OG	0.43	2.67	20	1
1:A:53:LYS:NZ	1:A:76:ASP:OD1	0.43	2.45	1	1
1:A:135:ILE:HD12	1:A:152:LEU:CD2	0.43	2.43	3	1
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:4:LEU:O	1:A:49:MET:O	0.43	2.36	13	3
1:A:100:ARG:HE	1:B:80:SER:CB	0.43	2.27	6	1
1:A:160:ASP:OD1	1:A:160:ASP:O	0.43	2.37	13	3
1:A:93:ASP:OD1	1:A:112:ARG:NH2	0.43	2.44	10	1
1:B:152:LEU:C	1:B:152:LEU:HD23	0.43	2.34	13	1
1:A:132:GLU:N	1:A:132:GLU:CD	0.43	2.71	14	1
1:B:121:ILE:O	1:B:128:ILE:O	0.43	2.37	16	2
1:A:55:ALA:O	1:A:56:LEU:C	0.43	2.57	9	13
1:B:75:SER:OG	1:B:82:GLU:OE1	0.43	2.36	15	2
1:B:72:LEU:CD2	1:B:108:ARG:NH2	0.43	2.81	3	1
1:B:160:ASP:O	1:B:160:ASP:OD1	0.43	2.37	4	1
1:A:53:LYS:C	1:A:55:ALA:H	0.43	2.17	5	3
1:A:145:LYS:CA	1:A:149:PHE:HB2	0.43	2.43	6	1
1:B:60:SER:OG	1:B:61:ARG:N	0.43	2.52	6	2
1:B:150:GLU:O	1:B:154:HIS:CD2	0.43	2.72	8	1
1:B:89:GLN:N	1:B:89:GLN:CD	0.43	2.72	19	1
1:B:92:ASP:O	1:B:93:ASP:OD1	0.43	2.37	16	3
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:185:GLU:O	1:B:189:ASN:OD1	0.43	2.36	4	2
1:A:190:GLN:O	1:A:194:LYS:CB	0.43	2.67	6	1
1:A:152:LEU:CD1	1:A:195:MET:SD	0.43	3.07	7	1
1:B:118:SER:O	1:B:119:ASN:O	0.43	2.36	9	1
1:B:133:GLU:O	1:B:145:LYS:NZ	0.43	2.47	13	1
1:A:23:LYS:HZ3	1:A:103:LYS:HZ2	0.43	1.56	16	1
1:B:132:GLU:CD	1:B:132:GLU:N	0.43	2.72	17	1
1:A:143:GLU:CG	1:A:144:VAL:N	0.43	2.82	18	1
1:B:182:ASN:O	1:B:185:GLU:OE1	0.43	2.37	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:212:TYR:CD1	1:B:212:TYR:N	0.43	2.87	2	4
1:B:155:LEU:O	1:B:159:ARG:CA	0.43	2.67	5	1
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: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:28:ASP:O	1:B:28:ASP:OD1	0.43	2.37	15	2
1:B:137:TYR:O	1:B:139:GLY:N	0.43	2.52	15	1
1:A:69:ILE:HG22	1:A:70:VAL:N	0.43	2.29	16	1
1:B:17:GLU:OE2	1:B:27:ALA:O	0.43	2.36	20	1
1:B:135:ILE:HD13	1:B:144:VAL:HG11	0.42	1.91	1	1
1:A:144:VAL:HG23	1:A:149:PHE:CD1	0.42	2.48	2	1
1:B:31:GLU:OE2	1:B:35:ASP:OD2	0.42	2.37	3	4
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:A:7:GLU:O	1:A:30:THR:O	0.42	2.37	11	1
1:A:194:LYS:CB	1:A:194:LYS:NZ	0.42	2.81	20	2
1:A:80:SER:OG	1:B:101:SER:OG	0.42	2.36	12	1
1:A:23:LYS:NZ	1:A:106:VAL:HG11	0.42	2.29	13	2
1:B:75:SER:OG	1:B:94:TYR:OH	0.42	2.36	17	2
1:A:196:ASP:O	1:A:196:ASP:OD1	0.42	2.37	19	1
1:A:207:VAL:CG1	1:A:213:ARG:HH11	0.42	2.26	20	1
1:A:199:LEU:C	1:A:201:ILE:H	0.42	2.18	1	1
1:A:110:GLU:O	1:A:114:ARG:CG	0.42	2.67	2	1
1:A:8:LYS:NZ	1:A:32:SER:N	0.42	2.67	3	1
1:A:123:ILE:O	1:A:123:ILE:HG23	0.42	2.14	3	1
1:A:122:GLU:H	1:A:159:ARG:NH1	0.42	2.12	4	1
1:A:39:LEU:C	1:A:39:LEU:CD1	0.42	2.87	7	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:75:SER:OG	1:A:94:TYR:OH	0.42	2.36	8	3
1:A:151:VAL:CG1	1:A:152:LEU:N	0.42	2.82	1	2
1:A:108:ARG:NH1	1:B:83:GLU:OE2	0.42	2.53	3	1
1:A:77:ASN:O	1:A:82:GLU:OE1	0.42	2.37	7	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:N	1:A:169:LEU:HD12	0.42	2.30	9	1
1:A:184:ILE:HD12	1:A:184:ILE:H	0.42	1.73	12	1
1:A:45:TYR:O	1:A:46:ASP:OD1	0.42	2.38	13	1
1:A:73:VAL:HG13	1:A:73:VAL:O	0.42	2.14	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:GLU:CD	1:B:108:ARG:CZ	0.42	2.88	18	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: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:A:82:GLU:OE1	1:A:94:TYR:OH	0.42	2.37	13	2
1:B:214:PHE:O	1:B:215:CYS:SG	0.42	2.78	20	1
1:A:192:ARG:O	1:A:196:ASP:OD1	0.42	2.37	2	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:106:VAL:CG1	1:A:107:ALA:N	0.42	2.82	8	1
1:A:85:HIS:CE1	1:A:89:GLN:CD	0.42	2.93	13	1
1:B:216:TYR:CD1	1:B:216:TYR:N	0.42	2.85	14	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:A:63:LYS:O	1:A:67:SER:CA	0.42	2.67	2	3
1:B:159:ARG:O	1:B:160:ASP:OD1	0.42	2.37	2	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:A:82:GLU:O	1:A:86:ALA:HB2	0.42	2.14	5	2
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:B:45:TYR:O	1:B:45:TYR:CD2	0.42	2.73	7	1
1:A:76:ASP:OD1	1:A:77:ASN:N	0.42	2.53	13	1
1:B:172:ILE:HG22	1:B:172:ILE:O	0.42	2.15	16	1
1:A:7:GLU:OE1	1:A:51:SER:OG	0.42	2.37	17	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:203:THR:OG1	1:B:214:PHE:CZ	0.42	2.71	1	1
1:A:148:PRO:O	1:A:151:VAL:HG12	0.42	2.14	7	1
1:A:70:VAL:HG22	1:A:112:ARG:NH2	0.42	2.29	9	1
1:A:115:PHE:CD1	1:A:115:PHE:C	0.42	2.92	11	1
1:A:115:PHE:O	1:A:116:TRP:C	0.42	2.58	11	2
1:B:125:ASP:OD1	1:B:125:ASP:N	0.42	2.51	15	1
1:A:23:LYS:HZ1	1:A:103:LYS:HZ1	0.42	1.58	16	1
1:A:163:VAL:HG23	1:A:214:PHE:CD1	0.42	2.49	18	1
1:B:75:SER:CB	1:B:94:TYR:HH	0.42	2.26	19	1
1:A:137:TYR:CD1	1:A:137:TYR:O	0.42	2.73	1	1
1:A:170:ASP:OD1	1:A:170:ASP:O	0.42	2.37	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:75:SER:CB	1:B:94:TYR:CZ	0.42	3.03	5	1
1:A:75:SER:OG	1:A:94:TYR:CE2	0.42	2.62	6	1
1:A:199:LEU:HD22	1:A:199:LEU:H	0.42	1.73	7	1
1:B:5:LEU:CD1	1:B:49:MET:SD	0.42	3.07	16	2
1:B:10:SER:OG	1:B:11:VAL:N	0.42	2.52	12	1
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:A:106:VAL:CG2	1:A:107:ALA:N	0.42	2.83	2	1
1:B:47:LEU:C	1:B:47:LEU:CD1	0.42	2.88	17	13
1:A:87:PHE:CZ	1:B:111:ALA:HB1	0.42	2.49	8	2
1:B:123:ILE:CG2	1:B:126:LEU:HB2	0.42	2.44	14	1
1:A:103:LYS:N	1:A:103:LYS:CD	0.42	2.83	17	2
1:B:23:LYS:HZ2	1:B:106:VAL:CG1	0.42	2.21	16	1
1:B:85:HIS:CD2	1:B:89:GLN:NE2	0.42	2.88	18	1
1:A:77:ASN:O	1:A:77:ASN:OD1	0.42	2.38	3	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:A:159:ARG:HH21	1:A:203:THR:HG21	0.42	1.75	7	1
1:A:119:ASN:CB	1:A:129:SER:OG	0.42	2.68	11	1
1:B:162:ILE:HG23	1:B:213:ARG:NE	0.42	2.30	12	1
1:B:77:ASN:ND2	1:B:77:ASN:N	0.42	2.67	14	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:146:GLY:CA	1:B:149:PHE:CE2	0.41	3.03	4	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:131:ASP:O	1:B:133:GLU:OE1	0.41	2.37	8	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:A:95:ILE:HG22	1:A:96:ALA:N	0.41	2.30	14	1
1:B:12:LEU:CD1	1:B:97:LYS:NZ	0.41	2.83	15	1
1:B:8:LYS:CD	1:B:8:LYS:H	0.41	2.27	1	1
1:B:182:ASN:C	1:B:184:ILE:H	0.41	2.19	3	1
1:B:190:GLN:O	1:B:194:LYS:CB	0.41	2.68	10	2
1:A:86:ALA:O	1:A:91:ALA:HB3	0.41	2.15	5	1
1:A:108:ARG:HE	1:B:83:GLU:CD	0.41	2.19	12	1
1:B:77:ASN:N	1:B:78:PRO:CD	0.41	2.83	12	1
1:B:31:GLU:OE2	1:B:35:ASP:OD1	0.41	2.38	14	1
1:B:137:TYR:C	1:B:139:GLY:H	0.41	2.18	15	1
1:B:97:LYS:O	1:B:97:LYS:CD	0.41	2.69	4	2
1:B:123:ILE:CD1	1:B:159:ARG:HH12	0.41	2.28	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:VAL:CG1	1:A:71:VAL:N	0.41	2.83	9	1
1:B:209:ARG:N	1:B:209:ARG:CD	0.41	2.83	10	1
1:A:72:LEU:C	1:A:72:LEU:CD1	0.41	2.89	11	1
1:B:103:LYS:CD	1:B:103:LYS:N	0.41	2.83	13	1
1:A:187:ALA:O	1:A:191:ILE:CG1	0.41	2.68	14	1
1:A:169:LEU:C	1:A:169:LEU:CD2	0.41	2.89	15	2
1:A:28:ASP:OD2	1:A:39:LEU:CD2	0.41	2.68	16	1
1:B:105:LEU:H	1:B:105:LEU:CD2	0.41	2.28	18	1
1:B:126:LEU:HD22	1:B:137:TYR:CD1	0.41	2.50	3	1
1:B:2:ARG:NH2	1:B:44:ASN:N	0.41	2.68	4	1
1:A:123:ILE:O	1:A:124:GLY:C	0.41	2.58	19	2
1:B:53:LYS:C	1:B:55:ALA:H	0.41	2.17	19	2
1:B:49:MET:CE	1:B:74:SER:OG	0.41	2.68	19	1
1:A:212:TYR:CD1	1:A:212:TYR:N	0.41	2.89	8	2
1:B:12:LEU:HD11	1:B:97:LYS:HZ2	0.41	1.75	14	1
1:B:16:ILE:HD11	1:B:99:TYR:CE1	0.41	2.51	20	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:23:LYS:HZ2	1:A:110:GLU:CD	0.41	2.18	6	1
1:A:81:GLU:N	1:A:81:GLU:CD	0.41	2.74	10	1
1:A:77:ASN:N	1:A:78:PRO:CD	0.41	2.82	11	2
1:B:96:ALA:O	1:B:97:LYS:C	0.41	2.58	12	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:147:LYS:N	1:B:148:PRO:HD2	0.41	2.31	13	1
1:B:184:ILE:H	1:B:184:ILE:CD1	0.41	2.24	19	1
1:A:117:GLY:O	1:A:118:SER:OG	0.41	2.37	2	1
1:A:44:ASN:C	1:A:45:TYR:CD2	0.41	2.94	5	1
1:B:72:LEU:C	1:B:72:LEU:CD2	0.41	2.89	16	3
1:B:160:ASP:OD1	1:B:216:TYR:CD1	0.41	2.73	8	1
1:A:166:GLU:H	1:A:166:GLU:CD	0.41	2.19	9	1
1:B:149:PHE:CE2	1:B:153:THR:HG23	0.41	2.51	10	1
1:B:155:LEU:C	1:B:155:LEU:CD2	0.41	2.82	12	2
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:A:119:ASN:CG	1:A:120:VAL:H	0.41	2.18	17	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:A:160:ASP:O	1:A:160:ASP:OD1	0.41	2.38	2	1
1:B:83:GLU:OE2	1:B:94:TYR:OH	0.41	2.37	4	1
1:B:196:ASP:OD1	1:B:196:ASP:N	0.41	2.54	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:GLU:OE2	1:A:144:VAL:O	0.41	2.37	7	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:149:PHE:CD1	1:B:150:GLU:N	0.41	2.88	16	1
1:A:23:LYS:NZ	1:A:106:VAL:CG1	0.41	2.84	17	1
1:B:169:LEU:HD23	1:B:169:LEU:C	0.41	2.36	19	1
1:A:39:LEU:C	1:A:39:LEU:CD2	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: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
1:B:77:ASN:OD1	1:B:77:ASN:N	0.41	2.54	6	1
1:B:122:GLU:O	1:B:122:GLU:CG	0.41	2.69	8	1
1:B:123:ILE:HD11	1:B:216:TYR:CB	0.41	2.46	9	1
1:A:76:ASP:O	1:A:76:ASP:OD1	0.41	2.38	11	1
1:B:55:ALA:O	1:B:56:LEU:C	0.41	2.58	19	5
1:B:119:ASN:HD21	1:B:128:ILE:C	0.41	2.18	12	1
1:A:97:LYS:C	1:A:97:LYS:CD	0.41	2.89	14	1
1:B:210:ARG:NH1	1:B:213:ARG:NH2	0.41	2.69	17	1
1:A:110:GLU:OE2	1:A:114:ARG:NH1	0.41	2.53	18	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:2:ARG:HH21	1:B:44:ASN:C	0.41	2.19	2	1
1:A:53:LYS:O	1:A:55:ALA:N	0.41	2.54	5	1
1:A:149:PHE:CE2	1:A:153:THR:HG23	0.41	2.51	5	1
1:B:124:GLY:C	1:B:126:LEU:H	0.41	2.19	7	1
1:B:169:LEU:O	1:B:170:ASP:C	0.41	2.59	13	1
1:B:86:ALA:O	1:B:91:ALA:CB	0.41	2.69	14	1
1:A:169:LEU:HD23	1:A:169:LEU:O	0.41	2.16	15	1
1:A:18:LYS:CD	1:A:18:LYS:N	0.41	2.84	19	1
1:A:32:SER:C	1:A:34:GLU:N	0.41	2.74	20	1
1:A:134:LYS:C	1:A:135:ILE:HD12	0.40	2.37	2	1
1:A:206:THR:HG23	1:A:206:THR:O	0.40	2.16	3	1
1:A:135:ILE:O	1:A:135:ILE:CG2	0.40	2.69	4	1
1:A:144:VAL:O	1:A:149:PHE:CD1	0.40	2.74	6	1
1:A:140:ARG:N	1:A:140:ARG:CD	0.40	2.84	8	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:A:145:LYS:N	1:A:149:PHE:CG	0.40	2.76	11	1
1:B:205:GLU:N	1:B:205:GLU:CD	0.40	2.75	12	1
1:B:137:TYR:CD1	1:B:137:TYR:N	0.40	2.89	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:56:LEU:HD22	1:A:85:HIS:NE2	0.40	2.31	4	1
1:B:149:PHE:CE1	1:B:153:THR:CG2	0.40	3.05	12	1
1:B:189:ASN:C	1:B:189:ASN:ND2	0.40	2.74	15	1
1:B:159:ARG:NH2	1:B:217:PRO:HD3	0.40	2.16	16	1
1:A:122:GLU:N	1:A:122:GLU:OE1	0.40	2.54	17	1
1:B:115:PHE:CE2	1:B:116:TRP:CE3	0.40	3.10	17	1
1:A:170:ASP:OD1	1:A:171:ALA:N	0.40	2.54	20	1
1:B:42:ILE:HD12	1:B:43:ARG:NH1	0.40	2.32	1	1
1:A:125:ASP:OD1	1:A:125:ASP:N	0.40	2.55	6	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:C	1:B:199:LEU:CD2	0.40	2.88	10	1
1:B:214:PHE:CD1	1:B:214:PHE:N	0.40	2.89	11	1
1:B:12:LEU:HD11	1:B:97:LYS:NZ	0.40	2.32	14	1
1:B:189:ASN:C	1:B:189:ASN:HD22	0.40	2.17	15	1
1:B:158:HIS:CG	1:B:161:GLN:HE22	0.40	2.32	17	1
1:A:184:ILE:O	1:A:188:ILE:HG22	0.40	2.17	19	1
1:A:72:LEU:C	1:A:72:LEU:CD2	0.40	2.90	20	1
1:A:195:MET:CG	1:A:196:ASP:N	0.40	2.85	1	1
1:B:169:LEU:C	1:B:169:LEU:CD2	0.40	2.89	2	1
1:A:84:VAL:CG2	1:A:85:HIS:N	0.40	2.85	7	1
1:B:204:VAL:HG23	1:B:204:VAL:O	0.40	2.16	9	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:B:188:ILE:HD13	1:B:212:TYR:CE1	0.40	2.52	13	1
1:A:144:VAL:CG2	1:A:149:PHE:CD1	0.40	3.04	17	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:102:ILE:N	1:B:102:ILE:HD13	0.40	2.31	5	1
1:A:103:LYS:O	1:A:107:ALA:CB	0.40	2.70	6	1
1:A:96:ALA:O	1:A:97:LYS:C	0.40	2.60	7	1
1:A:184:ILE:CG2	1:A:185:GLU:N	0.40	2.84	7	1
1:B:124:GLY:C	1:B:126:LEU:N	0.40	2.75	7	1
1:A:129:SER:O	1:A:133:GLU:N	0.40	2.55	9	1
1:A:47:LEU:CD1	1:A:47:LEU:C	0.40	2.89	11	1
1:B:159:ARG:O	1:B:160:ASP:C	0.40	2.59	11	1
1:B:183:VAL:O	1:B:186:VAL:HG12	0.40	2.16	12	1
1:A:44:ASN:ND2	1:A:145:LYS:HZ1	0.40	2.14	15	1
1:B:170:ASP:OD1	1:B:171:ALA:N	0.40	2.55	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:162:ILE:H	1:B:162:ILE:CD1	0.40	2.27	17	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:170:ASP:OD1	1:A:170:ASP:C	0.40	2.60	19	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	208/223 (93%)	177±3 (85±1%)	21±3 (10±1%)	10±3 (5±1%)	4	26
1	B	210/223 (94%)	181±4 (86±2%)	18±3 (9±1%)	10±2 (5±1%)	4	26
All	All	8360/8920 (94%)	7163 (86%)	792 (9%)	405 (5%)	4	26

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	98	PRO	20
1	A	99	TYR	20
1	B	98	PRO	20
1	B	99	TYR	20
1	A	90	GLY	17
1	B	90	GLY	17
1	A	78	PRO	17
1	A	102	ILE	16
1	B	78	PRO	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	A	116	TRP	8
1	A	145	LYS	8
1	B	217	PRO	8

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Mol	Chain	Res	Type	Models (Total)
1	A	217	PRO	7
1	A	210	ARG	6
1	B	145	LYS	6
1	B	116	TRP	5
1	B	130	PRO	5
1	A	9	ASN	5
1	A	183	VAL	5
1	A	209	ARG	5
1	A	160	ASP	5
1	A	117	GLY	5
1	B	173	TRP	4
1	B	115	PHE	4
1	B	210	ARG	4
1	A	130	PRO	4
1	A	198	PRO	4
1	B	159	ARG	4
1	B	198	PRO	4
1	A	182	ASN	3
1	A	76	ASP	3
1	B	114	ARG	3
1	B	182	ASN	3
1	B	160	ASP	3
1	A	118	SER	3
1	A	115	PHE	3
1	A	170	ASP	2
1	B	183	VAL	2
1	A	208	ARG	2
1	A	104	ALA	2
1	B	9	ASN	2
1	B	10	SER	2
1	B	54	ASN	2
1	B	104	ALA	2
1	B	45	TYR	2
1	B	218	LYS	2
1	A	45	TYR	2
1	B	119	ASN	2
1	A	114	ARG	2
1	A	159	ARG	2
1	B	117	GLY	2
1	A	199	LEU	2
1	A	119	ASN	2
1	B	170	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	197	LYS	1
1	A	7	GLU	1
1	B	148	PRO	1
1	A	68	SER	1
1	A	10	SER	1
1	A	31	GLU	1
1	A	124	GLY	1
1	A	77	ASN	1
1	B	158	HIS	1
1	B	211	GLY	1
1	B	118	SER	1
1	A	103	LYS	1
1	A	211	GLY	1
1	B	44	ASN	1
1	B	208	ARG	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/199 (93%)	173±3 (93±1%)	13±3 (7±1%)	18	66
1	B	188/199 (94%)	175±3 (93±1%)	13±3 (7±1%)	19	68
All	All	7480/7960 (94%)	6950 (93%)	530 (7%)	18	67

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	47	LEU	20
1	B	50	VAL	20
1	A	47	LEU	18
1	A	126	LEU	18
1	B	97	LYS	18
1	B	119	ASN	16
1	B	126	LEU	16
1	A	119	ASN	14

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Mol	Chain	Res	Type	Models (Total)
1	A	80	SER	14
1	B	80	SER	13
1	B	206	THR	13
1	A	206	THR	11
1	A	95	ILE	10
1	B	94	TYR	9
1	B	173	TRP	8
1	A	29	VAL	8
1	B	155	LEU	7
1	A	173	TRP	7
1	B	145	LYS	7
1	B	72	LEU	7
1	A	49	MET	6
1	A	74	SER	6
1	B	95	ILE	6
1	A	94	TYR	5
1	A	145	LYS	5
1	A	152	LEU	5
1	B	1	MET	5
1	A	4	LEU	5
1	B	152	LEU	5
1	A	188	ILE	5
1	B	74	SER	5
1	A	127	THR	4
1	B	123	ILE	4
1	B	153	THR	4
1	A	40	MET	4
1	B	216	TYR	4
1	B	113	LEU	3
1	A	8	LYS	3
1	A	112	ARG	3
1	A	195	MET	3
1	B	40	MET	3
1	B	112	ARG	3
1	A	140	ARG	3
1	A	105	LEU	3
1	A	114	ARG	3
1	A	147	LYS	3
1	B	49	MET	3
1	B	147	LYS	3
1	A	113	LEU	3
1	A	203	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	210	ARG	3
1	B	83	GLU	3
1	A	1	MET	3
1	A	108	ARG	2
1	A	197	LYS	2
1	B	8	LYS	2
1	B	159	ARG	2
1	A	204	VAL	2
1	A	209	ARG	2
1	B	108	ARG	2
1	B	197	LYS	2
1	A	123	ILE	2
1	B	5	LEU	2
1	A	89	GLN	2
1	B	82	GLU	2
1	B	89	GLN	2
1	B	122	GLU	2
1	B	140	ARG	2
1	B	149	PHE	2
1	B	195	MET	2
1	A	5	LEU	2
1	A	76	ASP	2
1	A	83	GLU	2
1	B	54	ASN	2
1	B	193	GLN	2
1	A	184	ILE	2
1	A	216	TYR	2
1	B	114	ARG	2
1	A	7	GLU	2
1	B	214	PHE	2
1	A	72	LEU	2
1	A	161	GLN	2
1	A	149	PHE	2
1	B	116	TRP	2
1	A	20	LEU	2
1	A	50	VAL	2
1	B	189	ASN	2
1	A	66	HIS	2
1	B	63	LYS	1
1	B	169	LEU	1
1	A	92	ASP	1
1	A	213	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	B	125	ASP	1
1	A	135	ILE	1
1	A	48	VAL	1
1	A	129	SER	1
1	A	138	LYS	1
1	A	192	ARG	1
1	B	12	LEU	1
1	A	45	TYR	1
1	A	100	ARG	1
1	A	159	ARG	1
1	A	167	GLN	1
1	A	39	LEU	1
1	A	79	THR	1
1	B	154	HIS	1
1	A	190	GLN	1
1	B	208	ARG	1
1	A	103	LYS	1
1	B	127	THR	1
1	B	133	GLU	1
1	A	75	SER	1
1	A	82	GLU	1
1	A	193	GLN	1
1	B	87	PHE	1
1	B	199	LEU	1
1	A	116	TRP	1
1	A	118	SER	1
1	A	160	ASP	1
1	B	188	ILE	1
1	B	194	LYS	1
1	A	136	ILE	1
1	A	23	LYS	1
1	B	167	GLN	1
1	B	204	VAL	1
1	A	134	LYS	1
1	A	165	LYS	1
1	B	77	ASN	1
1	B	184	ILE	1
1	A	158	HIS	1
1	A	199	LEU	1
1	B	192	ARG	1
1	A	125	ASP	1
1	B	105	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	98	PRO	1
1	B	170	ASP	1
1	A	12	LEU	1
1	A	18	LYS	1
1	A	53	LYS	1
1	A	153	THR	1
1	B	2	ARG	1
1	B	157	ARG	1
1	A	110	GLU	1
1	A	189	ASN	1
1	B	218	LYS	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided