Full wwPDB NMR Structure Validation Report (i)

Feb 10, 2022 – 11:44 AM EST

PDB ID	:	1F3C
Title	:	REFINED SOLUTION STRUCTURE OF 8KDA DYNEIN LIGHT CHAIN (DLC8)
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Deposited on	:	2000-06-02

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

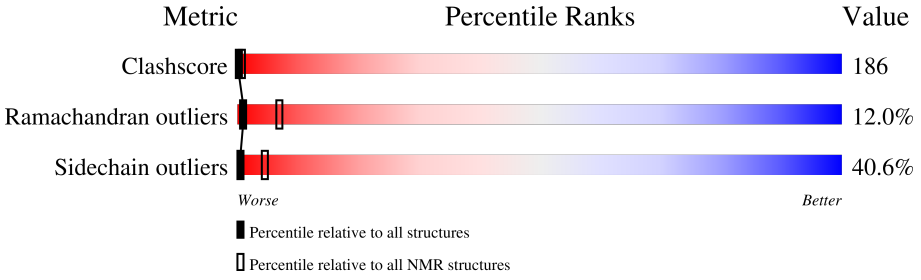
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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

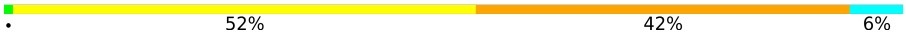
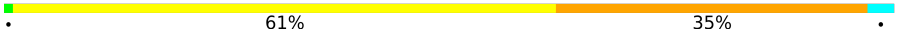
The overall completeness of chemical shifts assignment was not calculated.

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	89	
1	B	89	

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 2 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:5-A:88, B:4-B:89 (170)	0.42	3

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 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2892 atoms, of which 1436 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DYNEIN.

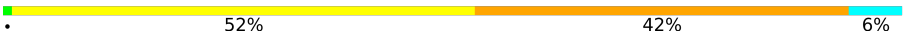
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	89	1446	465	718	122	135	6	0
1	B	89	1446	465	718	122	135	6	0

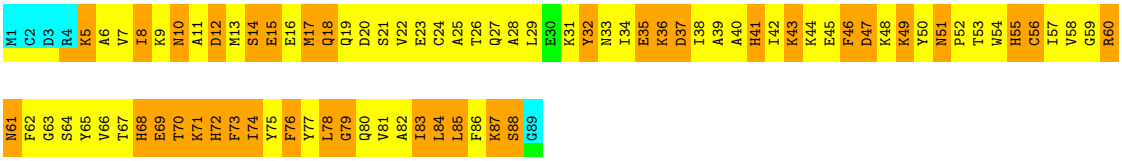
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

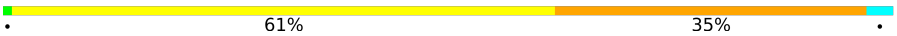
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for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

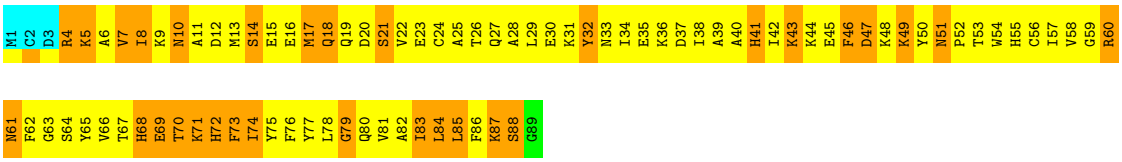
• Molecule 1: DYNEIN

Chain A: 



• Molecule 1: DYNEIN

Chain B: 

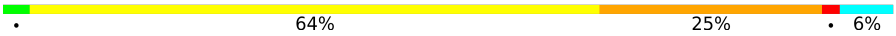


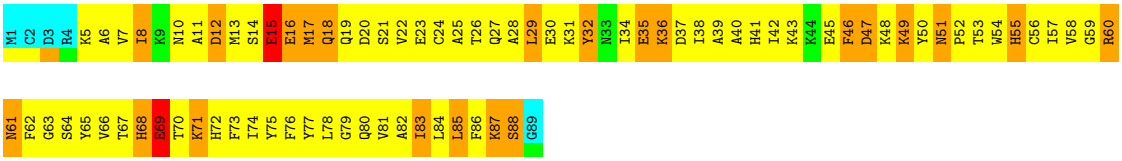
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: DYNEIN

Chain A: 



• Molecule 1: DYNEIN

Chain B: • 60% 33% • •

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

4.2.2 Score per residue for model 2

• Molecule 1: DYNEIN

Chain A: 7% 53% 34% • 6%

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

• Molecule 1: DYNEIN

Chain B: • 56% 37% • •

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: DYNEIN

Chain A: • 53% 33% • 6%

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

• Molecule 1: DYNEIN

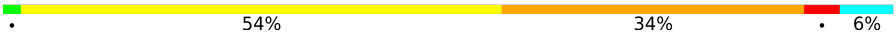
Chain B: • 60% 28% 6% •

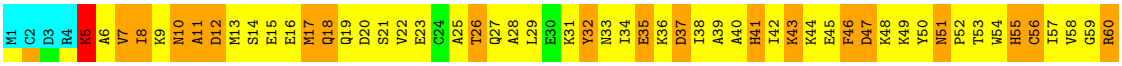
M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

4.2.4 Score per residue for model 4

- Molecule 1: DYNEIN

Chain A:





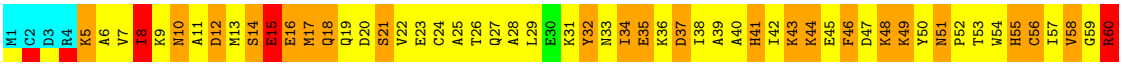
- Molecule 1: DYNEIN

Chain B:

4.2.5 Score per residue for model 5

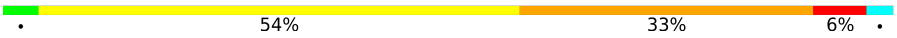
- Molecule 1: DYNEIN

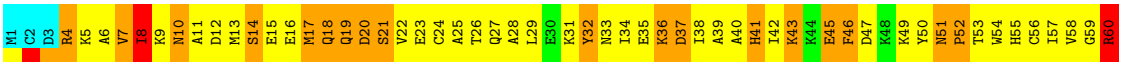
Chain A:



- Molecule 1: DYNEIN

Chain B:





4.2.6 Score per residue for model 6

- Molecule 1: DYNEIN

Chain A: • 46% 37% 8% 6%

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

• Molecule 1: DYNEIN

Chain B: 8% 62% 22% • •

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60 N61

F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

4.2.7 Score per residue for model 7

• Molecule 1: DYNEIN

Chain A: 6% 49% 36% • 6%

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

• Molecule 1: DYNEIN

Chain B: • 53% 38% • •

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

4.2.8 Score per residue for model 8

• Molecule 1: DYNEIN

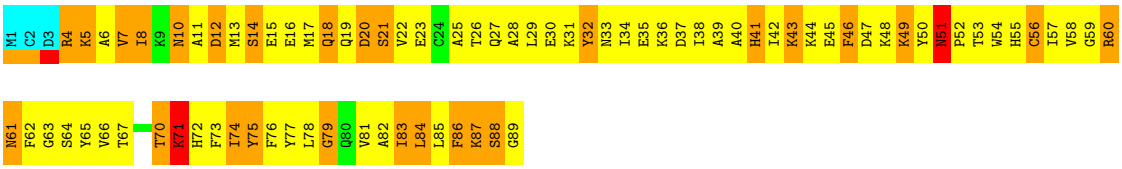
Chain A: • 58% 28% 6% 6%

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

- Molecule 1: DYNEIN

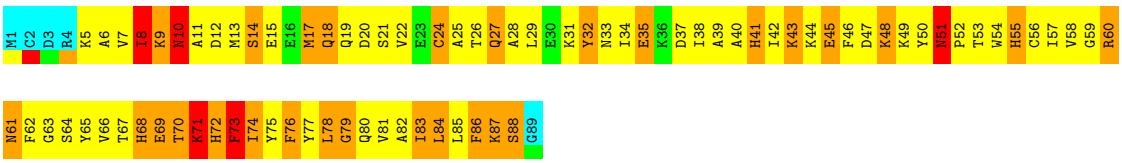
Chain B: 6% 58% 30%



4.2.9 Score per residue for model 9

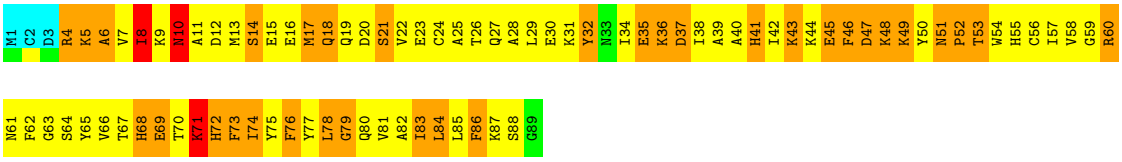
- Molecule 1: DYNEIN

Chain A: 53% 31% 6% 6%



- Molecule 1: DYNEIN

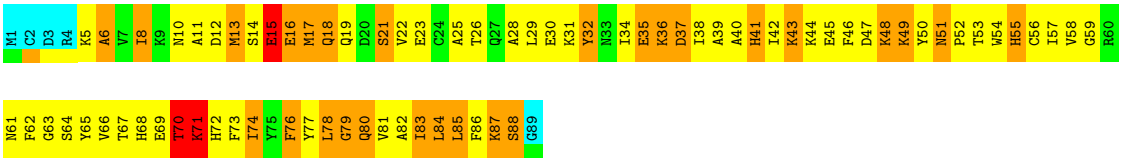
Chain B: 54% 37%



4.2.10 Score per residue for model 10

- Molecule 1: DYNEIN

Chain A: 9% 52% 30% 6%



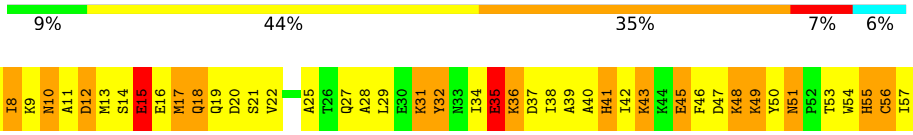
- Molecule 1: DYNEIN

Chain B: 65% 27%

4.2.11 Score per residue for model 11

- Molecule 1: DYNEIN

Chain A:



- Molecule 1: DYNEIN

Chain B:

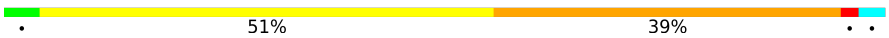
4.2.12 Score per residue for model 12

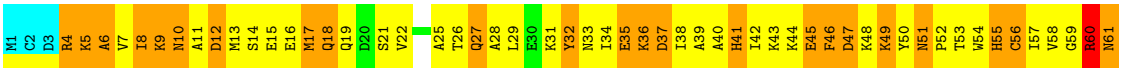
- Molecule 1: DYNEIN

Chain A:

- Molecule 1: DYNEIN

Chain B:





4.2.13 Score per residue for model 13

- Molecule 1: DYNEIN

Chain A: 55% 33% 6%

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

- Molecule 1: DYNEIN

Chain B: 7% 53% 31% 6%

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

4.2.14 Score per residue for model 14

- Molecule 1: DYNEIN

Chain A: 6% 56% 33% 6%

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60 N61

F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

- Molecule 1: DYNEIN

Chain B: 49% 39%

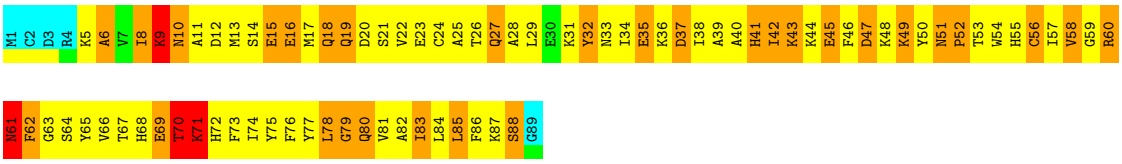
M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

4.2.15 Score per residue for model 15

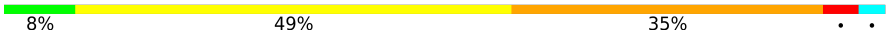
- Molecule 1: DYNEIN

Chain A: 54% 34% 6%



• Molecule 1: DYNEIN

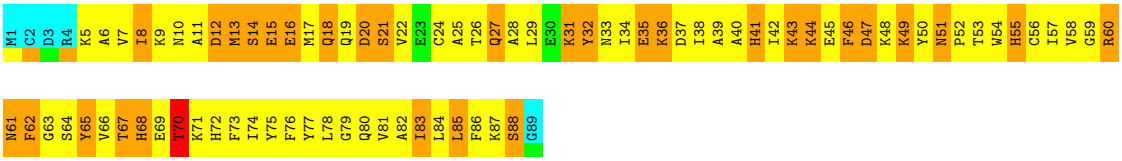
Chain B:



4.2.16 Score per residue for model 16

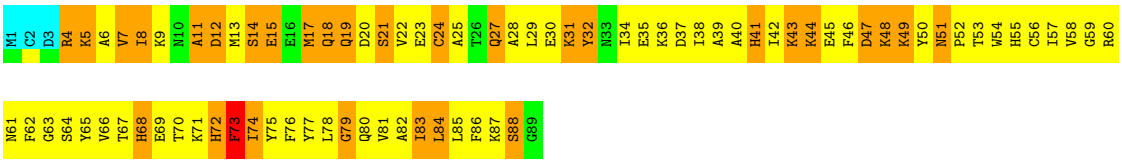
• Molecule 1: DYNEIN

Chain A:



• Molecule 1: DYNEIN

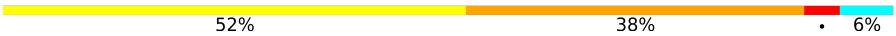
Chain B:

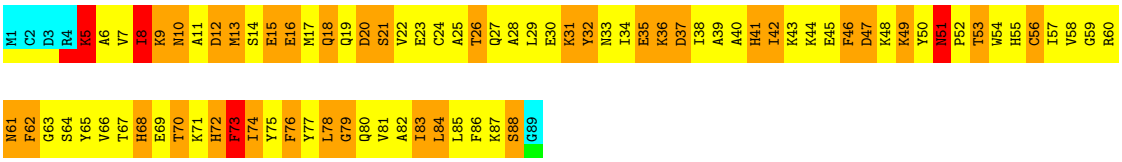


4.2.17 Score per residue for model 17

• Molecule 1: DYNEIN

Chain A:





• Molecule 1: DYNEIN

Chain B: • 51% 35% 7% •

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

4.2.18 Score per residue for model 18

- Molecule 1: DYNEIN

Chain A: • 54% 33% • 6%

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

- Molecule 1: DYNEIN

Chain B: 6% 56% 33% • •

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

4.2.19 Score per residue for model 19

- Molecule 1: DYNEIN

Chain A: • 49% 38% • 6%

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

- Molecule 1: DYNEIN

Chain B: 10% 46% 36% • •

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60 N61

F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

4.2.20 Score per residue for model 20

- Molecule 1: DYNEIN

Chain A: 58% 30% 6%

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

- Molecule 1: DYNEIN

Chain B: 6% 51% 36%

M1 C2 D3 R4 K5 A6 V7 I8 K9 N10 A11 D12 M13 S14 E15 E16 M17 Q18 Q19 D20 S21 V22 E23 C24 A25 T26 Q27 A28 L29 E30 K31 Y32 N33 I34 E35 K36 D37 I38 A39 A40 H41 I42 K43 K44 E45 F46 D47 K48 K49 Y50 N51 P52 T53 W54 H55 C56 I57 V58 G59 R60

N61 F62 G63 S64 Y65 V66 T67 H68 E69 T70 K71 H72 F73 I74 Y75 F76 Y77 L78 G79 Q80 V81 A82 I83 L84 L85 F86 K87 S88 G89

5 Refinement protocol and experimental data overview (i)

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR	structure solution	3.8
X-PLOR	refinement	3.8

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (i)

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	690	682	678	298±16
1	B	706	698	694	298±14
All	All	27920	27600	27440	10322

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 186.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:VAL:HG13	1:B:57:ILE:HD11	1.11	1.20	15	14
1:A:29:LEU:HD21	1:A:81:VAL:HG11	1.03	1.31	11	10
1:B:57:ILE:HG13	1:B:84:LEU:HD23	1.02	1.30	7	6
1:B:39:ALA:HB2	1:B:58:VAL:HG12	1.01	1.29	8	20
1:A:39:ALA:HB2	1:A:58:VAL:HG12	1.01	1.27	16	20
1:A:57:ILE:HG13	1:A:84:LEU:HD23	1.01	1.32	5	7
1:A:6:ALA:HA	1:A:78:LEU:HA	1.00	1.33	7	20
1:A:64:SER:HB2	1:B:57:ILE:HD12	0.99	1.33	17	10
1:A:57:ILE:HD12	1:B:64:SER:HB2	0.99	1.33	12	9
1:A:57:ILE:HG21	1:B:57:ILE:HG21	0.98	1.35	1	7
1:B:29:LEU:HD21	1:B:81:VAL:HG11	0.97	1.33	1	7
1:B:70:THR:HG23	1:B:71:LYS:HG2	0.96	1.37	5	1
1:B:6:ALA:HA	1:B:78:LEU:HA	0.96	1.35	8	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:56:CYS:HB3	1:B:85:LEU:HD12	0.94	1.34	1	8
1:B:56:CYS:HB2	1:B:85:LEU:HD12	0.94	1.40	12	6
1:B:28:ALA:HB1	1:B:38:ILE:HA	0.94	1.35	7	20
1:A:64:SER:HB2	1:A:84:LEU:HD22	0.93	1.38	17	13
1:A:11:ALA:HB1	1:A:18:GLN:NE2	0.93	1.78	12	11
1:A:34:ILE:HB	1:A:37:ASP:HB2	0.93	1.41	4	18
1:A:33:ASN:HA	1:A:38:ILE:HD11	0.92	1.41	14	7
1:A:72:HIS:HB2	1:A:87:LYS:HB2	0.92	1.42	7	3
1:A:67:THR:HG22	1:B:55:HIS:CE1	0.91	1.99	16	7
1:A:72:HIS:HB2	1:A:87:LYS:HG3	0.91	1.43	15	2
1:A:11:ALA:HA	1:A:74:ILE:HA	0.91	1.42	7	14
1:B:54:TRP:HA	1:B:87:LYS:HB3	0.91	1.43	18	4
1:A:62:PHE:HB3	1:B:62:PHE:HB3	0.91	1.42	17	19
1:B:18:GLN:HB3	1:B:74:ILE:HG13	0.90	1.43	17	9
1:B:42:ILE:HG21	1:B:85:LEU:HD11	0.90	1.42	19	10
1:A:67:THR:HG21	1:B:53:THR:HG21	0.90	1.41	10	12
1:B:82:ALA:O	1:B:83:ILE:HD13	0.90	1.67	15	11
1:A:56:CYS:HB2	1:A:85:LEU:HD12	0.89	1.40	20	14
1:A:68:HIS:HB2	1:A:72:HIS:HA	0.89	1.42	9	6
1:A:18:GLN:HA	1:A:74:ILE:HD12	0.89	1.42	17	19
1:B:34:ILE:HB	1:B:37:ASP:HB2	0.89	1.42	1	19
1:B:18:GLN:HA	1:B:74:ILE:HD12	0.89	1.44	8	18
1:B:22:VAL:HG22	1:B:76:PHE:CD2	0.89	2.02	18	18
1:A:57:ILE:HD11	1:B:66:VAL:HG13	0.89	1.45	2	18
1:A:56:CYS:HB3	1:A:85:LEU:HD12	0.89	1.43	19	6
1:B:38:ILE:HB	1:B:58:VAL:HG11	0.89	1.42	19	16
1:A:57:ILE:HD12	1:B:64:SER:HA	0.88	1.44	7	18
1:B:56:CYS:O	1:B:57:ILE:HD13	0.88	1.68	9	10
1:B:57:ILE:CG1	1:B:84:LEU:HD23	0.88	1.99	6	16
1:A:82:ALA:O	1:A:83:ILE:HD13	0.88	1.69	15	15
1:B:72:HIS:HB2	1:B:87:LYS:HB2	0.88	1.46	12	3
1:A:57:ILE:CG1	1:A:84:LEU:HD23	0.88	1.98	1	19
1:A:57:ILE:HD12	1:B:64:SER:CB	0.88	1.99	19	18
1:A:64:SER:CB	1:B:57:ILE:HD12	0.88	1.99	17	14
1:A:14:SER:HB2	1:A:17:MET:HG3	0.88	1.46	7	4
1:A:8:ILE:HG13	1:A:76:PHE:HB3	0.88	1.45	2	16
1:B:66:VAL:HG21	1:B:86:PHE:CE1	0.87	2.04	13	12
1:A:34:ILE:HB	1:A:37:ASP:HB3	0.87	1.43	17	2
1:A:57:ILE:HB	1:A:84:LEU:HB3	0.87	1.46	15	14
1:A:53:THR:HG21	1:B:67:THR:HG21	0.87	1.42	9	9
1:B:66:VAL:HG21	1:B:86:PHE:CZ	0.87	2.05	11	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ILE:HG13	1:B:57:ILE:HD12	0.86	1.46	2	2
1:B:28:ALA:HB3	1:B:38:ILE:HG23	0.86	1.47	7	18
1:B:75:TYR:CZ	1:B:84:LEU:HD13	0.86	2.05	20	1
1:A:35:GLU:HA	1:A:38:ILE:HD12	0.86	1.48	20	4
1:B:57:ILE:HD12	1:B:84:LEU:HD23	0.86	1.48	18	2
1:A:57:ILE:HD12	1:B:64:SER:CA	0.86	2.01	9	18
1:B:35:GLU:HG3	1:B:59:GLY:HA2	0.86	1.44	13	3
1:A:18:GLN:O	1:A:22:VAL:HG23	0.86	1.71	18	18
1:B:66:VAL:HG21	1:B:86:PHE:CE2	0.86	2.06	8	7
1:A:29:LEU:HD13	1:A:78:LEU:HG	0.85	1.46	17	8
1:B:18:GLN:O	1:B:22:VAL:HG23	0.85	1.70	3	15
1:A:6:ALA:HB2	1:A:78:LEU:HD13	0.85	1.49	4	12
1:A:74:ILE:HD13	1:A:76:PHE:CE1	0.85	2.05	8	13
1:B:25:ALA:O	1:B:29:LEU:HD12	0.85	1.71	15	19
1:B:9:LYS:HE2	1:B:9:LYS:HA	0.85	1.47	18	3
1:B:57:ILE:HG12	1:B:84:LEU:HD23	0.85	1.46	9	12
1:A:28:ALA:HB3	1:A:38:ILE:HG23	0.84	1.45	16	18
1:A:74:ILE:HD13	1:A:76:PHE:CD1	0.84	2.07	8	7
1:A:25:ALA:HA	1:A:42:ILE:HG12	0.84	1.48	20	13
1:A:57:ILE:HG12	1:A:84:LEU:HD23	0.84	1.45	2	14
1:B:18:GLN:CA	1:B:74:ILE:HD12	0.84	2.02	11	20
1:A:21:SER:HB2	1:A:85:LEU:HD22	0.84	1.48	4	4
1:A:22:VAL:HG22	1:A:76:PHE:CD2	0.84	2.07	19	16
1:B:11:ALA:HA	1:B:74:ILE:HA	0.84	1.47	7	19
1:A:66:VAL:HG21	1:A:86:PHE:CD1	0.84	2.07	19	2
1:A:56:CYS:O	1:A:57:ILE:HD13	0.84	1.72	13	15
1:A:18:GLN:CA	1:A:74:ILE:HD12	0.84	2.02	15	19
1:A:66:VAL:HG21	1:A:86:PHE:CD2	0.84	2.07	9	3
1:A:21:SER:OG	1:A:85:LEU:HD22	0.83	1.73	8	7
1:B:64:SER:CB	1:B:84:LEU:HD22	0.83	2.03	6	15
1:A:22:VAL:HG13	1:A:76:PHE:CE2	0.83	2.08	2	5
1:A:64:SER:HA	1:B:57:ILE:HG23	0.83	1.50	2	16
1:B:13:MET:HB2	1:B:72:HIS:HA	0.83	1.48	13	5
1:A:28:ALA:HB2	1:A:41:HIS:CD2	0.83	2.09	20	8
1:A:42:ILE:HG21	1:A:85:LEU:HD11	0.83	1.48	15	16
1:A:59:GLY:O	1:A:81:VAL:HG13	0.83	1.73	12	15
1:A:28:ALA:HB1	1:A:38:ILE:HA	0.82	1.49	19	20
1:A:13:MET:SD	1:A:17:MET:HB3	0.82	2.14	12	16
1:B:59:GLY:O	1:B:81:VAL:HG13	0.82	1.73	11	18
1:B:13:MET:SD	1:B:17:MET:HB3	0.82	2.15	2	16
1:B:29:LEU:HD11	1:B:78:LEU:HG	0.82	1.48	9	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:13:MET:SD	1:B:71:LYS:HG3	0.82	2.14	11	1
1:A:57:ILE:HG23	1:B:64:SER:HA	0.82	1.47	11	18
1:B:8:ILE:HG13	1:B:76:PHE:HB3	0.82	1.48	19	15
1:B:8:ILE:HA	1:B:76:PHE:HA	0.82	1.49	9	20
1:B:64:SER:OG	1:B:84:LEU:HD13	0.82	1.75	9	4
1:A:24:CYS:SG	1:A:42:ILE:HG23	0.82	2.13	8	3
1:A:55:HIS:NE2	1:A:88:SER:HB2	0.82	1.88	15	12
1:B:13:MET:SD	1:B:17:MET:HE2	0.81	2.15	1	6
1:A:57:ILE:HG12	1:B:64:SER:HA	0.81	1.52	4	2
1:A:67:THR:HG21	1:B:53:THR:CG2	0.81	2.05	1	2
1:B:48:LYS:HE3	1:B:48:LYS:HA	0.81	1.50	15	2
1:B:21:SER:OG	1:B:85:LEU:HD22	0.81	1.75	1	1
1:A:69:GLU:HG3	1:A:88:SER:HA	0.81	1.52	17	7
1:A:77:TYR:HD1	1:A:82:ALA:HB2	0.81	1.34	17	2
1:A:73:PHE:HA	1:A:86:PHE:HA	0.81	1.50	18	2
1:A:57:ILE:HG13	1:B:57:ILE:HG13	0.81	1.49	9	3
1:B:28:ALA:HB2	1:B:41:HIS:CD2	0.81	2.10	4	11
1:B:13:MET:HG2	1:B:14:SER:N	0.81	1.90	15	5
1:A:5:LYS:O	1:A:22:VAL:HG11	0.81	1.73	17	1
1:A:13:MET:SD	1:A:72:HIS:HA	0.81	2.15	7	7
1:A:35:GLU:HB3	1:B:63:GLY:N	0.81	1.90	10	13
1:B:70:THR:HG21	1:B:87:LYS:NZ	0.81	1.91	4	1
1:A:64:SER:CA	1:B:57:ILE:HD12	0.81	2.06	3	14
1:A:25:ALA:O	1:A:29:LEU:HD12	0.80	1.76	19	20
1:B:64:SER:HB2	1:B:84:LEU:HD22	0.80	1.50	20	11
1:A:64:SER:HA	1:B:57:ILE:HG12	0.80	1.51	13	6
1:A:48:LYS:HE3	1:A:48:LYS:HA	0.80	1.53	19	3
1:A:63:GLY:N	1:B:35:GLU:HB3	0.80	1.92	5	18
1:A:6:ALA:HB2	1:A:78:LEU:CD1	0.80	2.06	4	12
1:A:64:SER:CB	1:A:84:LEU:HD22	0.80	2.06	17	13
1:A:28:ALA:CB	1:A:38:ILE:HG23	0.80	2.05	16	17
1:A:8:ILE:HD11	1:A:74:ILE:HD11	0.80	1.50	5	13
1:A:18:GLN:HB3	1:A:74:ILE:HG13	0.80	1.54	8	5
1:A:13:MET:HG2	1:A:14:SER:N	0.80	1.90	3	7
1:A:13:MET:SD	1:A:74:ILE:HB	0.80	2.16	16	2
1:B:54:TRP:NE1	1:B:87:LYS:HE3	0.79	1.92	3	2
1:A:58:VAL:HG23	1:A:83:ILE:HD13	0.79	1.51	4	9
1:B:54:TRP:HA	1:B:87:LYS:HG3	0.79	1.50	12	3
1:B:26:THR:HA	1:B:29:LEU:HD12	0.79	1.51	18	13
1:B:42:ILE:CG2	1:B:85:LEU:HD11	0.79	2.07	19	7
1:B:66:VAL:HG21	1:B:86:PHE:CD2	0.79	2.13	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ILE:HG22	1:A:42:ILE:HD11	0.79	1.54	9	16
1:A:67:THR:CG2	1:B:53:THR:HG21	0.79	2.07	13	7
1:A:38:ILE:HB	1:A:58:VAL:HG11	0.78	1.54	20	18
1:B:47:ASP:HB2	1:B:52:PRO:HB3	0.78	1.54	6	7
1:A:74:ILE:HG23	1:A:76:PHE:HE1	0.78	1.38	12	13
1:B:74:ILE:HD13	1:B:76:PHE:CE1	0.78	2.12	17	15
1:B:21:SER:OG	1:B:74:ILE:HG21	0.78	1.79	11	10
1:B:12:ASP:HB2	1:B:72:HIS:HB3	0.78	1.53	11	4
1:A:13:MET:HB2	1:A:73:PHE:N	0.78	1.92	13	6
1:A:55:HIS:HB3	1:B:66:VAL:HB	0.78	1.56	18	13
1:A:66:VAL:CG1	1:B:57:ILE:HD11	0.78	2.08	4	8
1:B:18:GLN:HG2	1:B:74:ILE:HG13	0.78	1.54	11	1
1:A:58:VAL:HG23	1:A:83:ILE:CD1	0.78	2.09	13	13
1:A:65:TYR:H	1:B:57:ILE:HD13	0.78	1.37	7	12
1:A:53:THR:CG2	1:B:67:THR:HG21	0.78	2.09	19	4
1:A:64:SER:HA	1:B:57:ILE:HD12	0.77	1.55	7	13
1:B:54:TRP:CE2	1:B:87:LYS:HD2	0.77	2.14	6	20
1:A:8:ILE:HA	1:A:76:PHE:HA	0.77	1.56	8	20
1:B:13:MET:SD	1:B:72:HIS:HA	0.77	2.18	1	7
1:A:65:TYR:CE1	1:B:40:ALA:HB2	0.77	2.13	19	7
1:B:11:ALA:HB1	1:B:18:GLN:NE2	0.77	1.95	12	13
1:A:34:ILE:HG22	1:A:36:LYS:HD3	0.77	1.55	2	1
1:A:43:LYS:HE3	1:A:56:CYS:HB3	0.77	1.54	5	1
1:A:66:VAL:HG12	1:B:55:HIS:HB3	0.77	1.55	20	12
1:A:16:GLU:HA	1:A:19:GLN:HG2	0.77	1.57	15	2
1:A:36:LYS:HB2	1:A:36:LYS:NZ	0.77	1.95	2	1
1:A:55:HIS:HE2	1:A:88:SER:HB2	0.77	1.40	4	6
1:A:56:CYS:SG	1:A:85:LEU:HD12	0.77	2.19	11	4
1:A:28:ALA:HB2	1:A:41:HIS:CG	0.76	2.16	15	8
1:A:26:THR:HA	1:A:29:LEU:HD12	0.76	1.55	10	11
1:A:54:TRP:CE2	1:A:87:LYS:HD2	0.76	2.15	4	18
1:B:35:GLU:HA	1:B:38:ILE:HD12	0.76	1.57	17	7
1:B:57:ILE:HB	1:B:84:LEU:HD23	0.76	1.56	5	9
1:B:4:ARG:HD2	1:B:4:ARG:N	0.76	1.96	4	1
1:B:8:ILE:HD11	1:B:74:ILE:HD11	0.76	1.57	1	10
1:A:29:LEU:HD11	1:A:78:LEU:HG	0.76	1.57	16	5
1:B:27:GLN:HB3	1:B:41:HIS:NE2	0.76	1.95	7	2
1:A:6:ALA:CB	1:A:78:LEU:HD22	0.76	2.10	14	19
1:A:6:ALA:HB2	1:A:78:LEU:HD22	0.76	1.57	17	14
1:A:29:LEU:HG	1:A:38:ILE:HG21	0.76	1.57	11	5
1:B:22:VAL:HG13	1:B:76:PHE:CE2	0.75	2.17	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:34:ILE:HG22	1:B:36:LYS:HE3	0.75	1.57	14	1
1:A:65:TYR:HB2	1:B:39:ALA:HB1	0.75	1.57	14	6
1:B:10:ASN:HB3	1:B:75:TYR:HB3	0.75	1.55	2	1
1:B:21:SER:HA	1:B:46:PHE:CZ	0.75	2.16	1	20
1:B:74:ILE:HG23	1:B:76:PHE:HE1	0.75	1.40	17	15
1:B:43:LYS:HB2	1:B:56:CYS:SG	0.75	2.22	16	5
1:A:66:VAL:HG21	1:A:86:PHE:CE1	0.75	2.16	17	8
1:B:7:VAL:HG12	1:B:9:LYS:HE2	0.75	1.59	3	7
1:B:31:LYS:HB2	1:B:32:TYR:CE1	0.75	2.17	3	8
1:A:66:VAL:HG21	1:A:86:PHE:CE2	0.75	2.17	15	3
1:A:57:ILE:HD11	1:B:66:VAL:CG1	0.75	2.11	13	13
1:B:29:LEU:CD2	1:B:81:VAL:HG21	0.74	2.11	8	6
1:A:66:VAL:HG12	1:B:55:HIS:CB	0.74	2.11	20	3
1:B:6:ALA:HB2	1:B:78:LEU:HD13	0.74	1.59	18	10
1:B:15:GLU:HA	1:B:18:GLN:HG3	0.74	1.57	15	4
1:A:22:VAL:HG13	1:A:76:PHE:CD2	0.74	2.17	2	4
1:A:67:THR:HB	1:B:53:THR:HG21	0.74	1.58	8	2
1:A:29:LEU:CD2	1:A:81:VAL:HG21	0.74	2.12	17	4
1:A:13:MET:CG	1:A:17:MET:HG2	0.74	2.13	10	1
1:A:39:ALA:HB1	1:B:65:TYR:HB2	0.74	1.57	1	9
1:A:59:GLY:HA3	1:B:62:PHE:HB2	0.74	1.58	20	9
1:B:22:VAL:HA	1:B:76:PHE:CZ	0.74	2.18	5	9
1:A:27:GLN:HG3	1:A:28:ALA:N	0.74	1.97	16	2
1:B:21:SER:HA	1:B:46:PHE:CE2	0.74	2.18	19	5
1:B:55:HIS:NE2	1:B:88:SER:HB2	0.74	1.96	15	8
1:B:21:SER:HA	1:B:46:PHE:CE1	0.74	2.18	9	15
1:A:66:VAL:HB	1:B:55:HIS:HB3	0.74	1.57	1	9
1:B:64:SER:HB3	1:B:84:LEU:HD22	0.74	1.59	19	8
1:A:38:ILE:HG22	1:A:42:ILE:CD1	0.74	2.12	5	11
1:A:39:ALA:CB	1:A:58:VAL:HG12	0.74	2.11	3	15
1:A:21:SER:OG	1:A:74:ILE:HG21	0.74	1.82	14	11
1:A:55:HIS:CE1	1:B:67:THR:HG22	0.74	2.18	14	5
1:B:43:LYS:NZ	1:B:53:THR:HG23	0.74	1.97	7	1
1:B:57:ILE:CB	1:B:84:LEU:HD23	0.73	2.13	5	9
1:A:55:HIS:HB2	1:A:86:PHE:CE2	0.73	2.18	7	2
1:B:32:TYR:CB	1:B:34:ILE:HD13	0.73	2.13	7	1
1:A:72:HIS:HB2	1:A:87:LYS:HD3	0.73	1.60	16	3
1:B:13:MET:CG	1:B:17:MET:HG2	0.73	2.12	13	1
1:B:28:ALA:CB	1:B:38:ILE:HG23	0.73	2.13	3	17
1:A:77:TYR:CD1	1:A:82:ALA:HB2	0.73	2.18	17	2
1:A:22:VAL:HA	1:A:76:PHE:CE2	0.73	2.19	8	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:13:MET:HB3	1:B:18:GLN:NE2	0.73	1.98	1	2
1:A:56:CYS:HA	1:A:84:LEU:O	0.73	1.84	8	18
1:A:13:MET:CG	1:A:72:HIS:HA	0.73	2.14	16	5
1:A:21:SER:HA	1:A:46:PHE:CZ	0.73	2.19	20	20
1:A:21:SER:HA	1:A:46:PHE:CE1	0.73	2.19	20	16
1:A:55:HIS:HB2	1:A:86:PHE:CE1	0.73	2.19	19	9
1:B:58:VAL:HG23	1:B:81:VAL:HG11	0.73	1.61	7	2
1:A:68:HIS:HB3	1:A:86:PHE:HB2	0.73	1.60	12	1
1:A:15:GLU:HA	1:A:18:GLN:HG3	0.73	1.61	20	9
1:B:13:MET:SD	1:B:17:MET:SD	0.73	2.87	9	5
1:B:6:ALA:CB	1:B:78:LEU:HD22	0.72	2.14	15	20
1:B:25:ALA:HA	1:B:42:ILE:HG12	0.72	1.59	15	8
1:A:84:LEU:HD21	1:A:86:PHE:HE2	0.72	1.43	4	1
1:B:47:ASP:O	1:B:52:PRO:HD3	0.72	1.84	20	20
1:A:21:SER:HA	1:A:46:PHE:CE2	0.72	2.19	13	4
1:A:22:VAL:HA	1:A:76:PHE:CZ	0.72	2.20	13	10
1:B:22:VAL:HA	1:B:76:PHE:CE2	0.72	2.19	9	20
1:A:7:VAL:HG12	1:A:9:LYS:HE3	0.72	1.59	5	1
1:A:31:LYS:HB2	1:A:32:TYR:CE1	0.72	2.19	2	4
1:B:73:PHE:HB2	1:B:85:LEU:O	0.72	1.85	20	9
1:A:76:PHE:CE2	1:A:78:LEU:HD21	0.72	2.19	20	9
1:B:4:ARG:HH21	1:B:8:ILE:HD13	0.72	1.45	17	1
1:A:53:THR:O	1:A:87:LYS:HB3	0.72	1.85	15	7
1:B:21:SER:HG	1:B:85:LEU:HD22	0.72	1.43	1	1
1:B:72:HIS:O	1:B:73:PHE:HB3	0.72	1.85	18	10
1:A:61:ASN:HB3	1:B:60:ARG:CZ	0.72	2.14	19	1
1:A:82:ALA:C	1:A:83:ILE:HD13	0.72	2.05	12	15
1:A:53:THR:HG22	1:A:55:HIS:CE1	0.72	2.18	18	4
1:A:42:ILE:CG2	1:A:85:LEU:HD11	0.72	2.15	4	14
1:B:6:ALA:HB2	1:B:78:LEU:CD1	0.72	2.14	18	11
1:A:27:GLN:HB3	1:A:41:HIS:NE2	0.72	2.00	12	2
1:B:56:CYS:CB	1:B:85:LEU:HD12	0.72	2.14	1	11
1:B:76:PHE:CE2	1:B:83:ILE:HG13	0.72	2.19	6	18
1:A:27:GLN:O	1:A:31:LYS:HG2	0.72	1.84	15	5
1:B:68:HIS:CE1	1:B:87:LYS:HG3	0.72	2.19	4	1
1:B:17:MET:SD	1:B:71:LYS:HD3	0.72	2.25	16	1
1:B:27:GLN:HG3	1:B:28:ALA:N	0.72	1.98	18	1
1:A:65:TYR:CD2	1:B:40:ALA:HA	0.72	2.20	9	16
1:B:82:ALA:C	1:B:83:ILE:HD13	0.71	2.04	17	12
1:B:53:THR:O	1:B:87:LYS:HB3	0.71	1.84	13	6
1:B:11:ALA:HB1	1:B:18:GLN:HE21	0.71	1.44	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:34:ILE:HD12	1:B:34:ILE:N	0.71	2.00	7	1
1:A:56:CYS:CB	1:A:85:LEU:HD12	0.71	2.13	1	16
1:A:67:THR:HG22	1:B:55:HIS:NE2	0.71	1.99	4	4
1:B:54:TRP:CZ3	1:B:72:HIS:HB3	0.71	2.19	13	6
1:A:13:MET:SD	1:A:74:ILE:N	0.71	2.63	16	1
1:A:40:ALA:HA	1:B:65:TYR:CD2	0.71	2.20	2	19
1:B:73:PHE:HA	1:B:85:LEU:O	0.71	1.86	13	11
1:A:53:THR:O	1:A:87:LYS:HG2	0.71	1.85	2	4
1:B:21:SER:HB2	1:B:85:LEU:HD22	0.71	1.61	18	6
1:B:27:GLN:O	1:B:31:LYS:HG2	0.71	1.86	17	11
1:A:78:LEU:HB2	1:A:81:VAL:HB	0.71	1.61	6	4
1:A:43:LYS:HE2	1:A:54:TRP:H	0.71	1.45	6	1
1:A:65:TYR:CD1	1:B:40:ALA:HA	0.71	2.21	8	9
1:A:65:TYR:CE2	1:B:40:ALA:HA	0.71	2.21	13	16
1:B:62:PHE:HE2	1:B:64:SER:HB3	0.71	1.46	20	13
1:A:7:VAL:O	1:A:9:LYS:HD2	0.71	1.86	2	1
1:B:15:GLU:O	1:B:18:GLN:HG2	0.71	1.86	13	12
1:A:16:GLU:HG2	1:A:19:GLN:OE1	0.71	1.85	15	1
1:A:13:MET:SD	1:A:17:MET:HE2	0.71	2.25	1	3
1:B:70:THR:HG22	1:B:71:LYS:N	0.71	2.00	16	4
1:B:68:HIS:HB3	1:B:73:PHE:CD2	0.71	2.21	20	1
1:A:62:PHE:HE2	1:A:64:SER:HB3	0.71	1.46	1	6
1:A:73:PHE:HA	1:A:85:LEU:O	0.71	1.86	1	9
1:B:57:ILE:HB	1:B:84:LEU:HB3	0.71	1.63	14	8
1:B:56:CYS:HA	1:B:84:LEU:O	0.71	1.86	9	15
1:A:81:VAL:HG12	1:A:82:ALA:H	0.71	1.46	9	9
1:A:84:LEU:CD2	1:B:57:ILE:HD11	0.71	2.16	19	6
1:B:13:MET:SD	1:B:74:ILE:HB	0.71	2.26	13	1
1:A:10:ASN:HB3	1:A:75:TYR:HB3	0.71	1.61	18	2
1:A:35:GLU:CA	1:A:38:ILE:HD12	0.71	2.16	20	2
1:A:14:SER:O	1:A:17:MET:HB2	0.70	1.86	1	12
1:A:14:SER:O	1:A:18:GLN:HG2	0.70	1.86	15	19
1:A:47:ASP:O	1:A:52:PRO:HD3	0.70	1.85	20	19
1:B:22:VAL:HG13	1:B:76:PHE:CD2	0.70	2.21	3	5
1:B:68:HIS:NE2	1:B:87:LYS:HG3	0.70	2.00	4	1
1:B:13:MET:HG2	1:B:17:MET:HB3	0.70	1.63	10	4
1:A:54:TRP:CZ3	1:A:72:HIS:HB3	0.70	2.21	10	9
1:A:5:LYS:O	1:A:78:LEU:HD13	0.70	1.86	3	6
1:B:57:ILE:HD12	1:B:84:LEU:CD2	0.70	2.16	18	2
1:A:8:ILE:HA	1:A:76:PHE:HB3	0.70	1.63	4	18
1:A:72:HIS:O	1:A:73:PHE:HB3	0.70	1.85	17	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:49:LYS:O	1:B:49:LYS:HD3	0.70	1.86	12	1
1:A:40:ALA:HA	1:B:65:TYR:CE2	0.70	2.21	20	19
1:B:29:LEU:HD21	1:B:81:VAL:CG1	0.70	2.12	1	4
1:A:65:TYR:CE2	1:B:43:LYS:HB3	0.70	2.22	3	6
1:B:13:MET:H	1:B:18:GLN:HE22	0.70	1.30	8	5
1:B:45:GLU:O	1:B:49:LYS:HB2	0.70	1.86	19	18
1:B:75:TYR:CE1	1:B:84:LEU:HB2	0.70	2.21	3	5
1:A:67:THR:HG21	1:B:53:THR:OG1	0.70	1.86	2	2
1:B:55:HIS:CE1	1:B:88:SER:HB2	0.70	2.21	3	10
1:A:13:MET:HB2	1:A:72:HIS:HA	0.70	1.61	10	4
1:B:50:TYR:O	1:B:51:ASN:HB2	0.70	1.86	7	14
1:B:45:GLU:O	1:B:48:LYS:HG3	0.70	1.87	7	1
1:A:50:TYR:O	1:A:51:ASN:HB3	0.70	1.85	10	4
1:A:67:THR:HG23	1:A:68:HIS:N	0.70	2.01	18	4
1:B:12:ASP:O	1:B:71:LYS:HA	0.70	1.87	5	2
1:A:54:TRP:CD2	1:A:87:LYS:HD2	0.70	2.21	16	6
1:B:66:VAL:HB	1:B:86:PHE:CZ	0.70	2.22	4	3
1:B:13:MET:HG3	1:B:71:LYS:HG2	0.70	1.63	4	1
1:A:73:PHE:CD1	1:A:86:PHE:HB3	0.70	2.22	20	8
1:A:15:GLU:O	1:A:18:GLN:HG2	0.70	1.86	10	10
1:B:11:ALA:CB	1:B:74:ILE:HG13	0.70	2.17	12	12
1:A:27:GLN:O	1:A:31:LYS:HD2	0.70	1.87	20	5
1:A:73:PHE:HD1	1:A:86:PHE:HB3	0.70	1.47	18	8
1:A:11:ALA:CB	1:A:74:ILE:HG13	0.70	2.17	3	14
1:A:22:VAL:HG22	1:A:76:PHE:CE2	0.70	2.20	5	10
1:A:26:THR:CA	1:A:29:LEU:HD12	0.70	2.16	10	4
1:A:65:TYR:CG	1:B:40:ALA:HA	0.69	2.22	20	10
1:A:9:LYS:HE3	1:A:76:PHE:C	0.69	2.08	2	1
1:A:65:TYR:CE2	1:B:43:LYS:HD3	0.69	2.22	3	2
1:A:12:ASP:HB3	1:A:72:HIS:ND1	0.69	2.02	19	4
1:A:61:ASN:ND2	1:B:60:ARG:NH1	0.69	2.41	4	1
1:B:32:TYR:HB2	1:B:34:ILE:HD13	0.69	1.64	7	1
1:A:67:THR:HG22	1:B:55:HIS:HE1	0.69	1.46	16	2
1:A:65:TYR:HD2	1:B:43:LYS:HG2	0.69	1.47	19	1
1:A:73:PHE:HB2	1:A:85:LEU:O	0.69	1.86	4	9
1:A:13:MET:HG3	1:A:72:HIS:HA	0.69	1.64	13	2
1:A:36:LYS:N	1:B:63:GLY:HA3	0.69	2.01	17	9
1:A:39:ALA:CB	1:B:65:TYR:HB2	0.69	2.18	1	11
1:B:8:ILE:HD12	1:B:76:PHE:HB3	0.69	1.64	1	8
1:B:8:ILE:HA	1:B:76:PHE:HB3	0.69	1.63	17	16
1:B:84:LEU:HG	1:B:84:LEU:O	0.69	1.87	5	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:TYR:CD2	1:B:43:LYS:HG2	0.69	2.22	19	1
1:A:81:VAL:HG12	1:A:82:ALA:N	0.69	2.03	6	20
1:B:14:SER:O	1:B:18:GLN:HG2	0.69	1.86	12	17
1:A:76:PHE:CZ	1:A:83:ILE:HB	0.69	2.22	19	13
1:B:68:HIS:HB2	1:B:72:HIS:O	0.69	1.87	18	5
1:A:13:MET:HA	1:A:71:LYS:O	0.69	1.86	10	7
1:A:25:ALA:C	1:A:29:LEU:HD12	0.69	2.08	17	19
1:A:55:HIS:HB3	1:B:66:VAL:CB	0.69	2.17	8	16
1:B:56:CYS:HB3	1:B:85:LEU:CD1	0.69	2.17	19	7
1:A:20:ASP:HB3	1:A:50:TYR:OH	0.69	1.87	6	3
1:B:24:CYS:SG	1:B:45:GLU:HB3	0.69	2.27	16	3
1:A:53:THR:HG23	1:A:55:HIS:NE2	0.69	2.03	16	3
1:A:58:VAL:HA	1:A:82:ALA:O	0.69	1.88	13	16
1:A:73:PHE:HB2	1:A:86:PHE:HB2	0.69	1.64	18	7
1:B:13:MET:HB3	1:B:18:GLN:HE21	0.69	1.48	1	1
1:B:68:HIS:ND1	1:B:68:HIS:N	0.69	2.41	15	4
1:A:40:ALA:HA	1:B:65:TYR:CG	0.69	2.21	6	18
1:A:40:ALA:HA	1:B:65:TYR:CD1	0.69	2.22	8	13
1:A:57:ILE:HG13	1:B:57:ILE:CD1	0.69	2.18	2	4
1:A:65:TYR:HB2	1:B:39:ALA:CB	0.69	2.18	7	8
1:B:73:PHE:HA	1:B:86:PHE:HA	0.69	1.62	5	3
1:A:44:LYS:HD2	1:A:45:GLU:N	0.69	2.03	7	1
1:A:70:THR:C	1:A:71:LYS:HG2	0.69	2.08	13	2
1:B:7:VAL:O	1:B:9:LYS:HD2	0.69	1.88	14	1
1:A:25:ALA:HA	1:A:42:ILE:CD1	0.69	2.18	4	18
1:A:66:VAL:CG1	1:B:55:HIS:HB3	0.69	2.18	3	16
1:A:75:TYR:CE1	1:A:84:LEU:HB2	0.69	2.23	17	8
1:B:8:ILE:HA	1:B:75:TYR:O	0.69	1.88	20	9
1:B:25:ALA:HA	1:B:42:ILE:CD1	0.69	2.17	14	19
1:A:50:TYR:O	1:A:51:ASN:HB2	0.69	1.87	5	8
1:A:8:ILE:C	1:A:9:LYS:HG2	0.69	2.08	18	7
1:A:47:ASP:OD2	1:A:52:PRO:HG3	0.69	1.87	19	2
1:A:35:GLU:N	1:A:38:ILE:HD12	0.69	2.03	18	5
1:A:16:GLU:O	1:A:19:GLN:HG2	0.69	1.88	14	3
1:A:12:ASP:O	1:A:71:LYS:HA	0.69	1.86	2	3
1:B:20:ASP:HB3	1:B:50:TYR:OH	0.69	1.88	11	10
1:A:66:VAL:HG13	1:B:57:ILE:CD1	0.68	2.11	15	8
1:A:45:GLU:O	1:A:49:LYS:HB2	0.68	1.89	15	13
1:B:47:ASP:OD2	1:B:52:PRO:HB3	0.68	1.87	14	4
1:A:51:ASN:O	1:A:87:LYS:HE3	0.68	1.89	8	6
1:A:43:LYS:HE2	1:A:47:ASP:HB2	0.68	1.66	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:TYR:HB3	1:B:39:ALA:HB1	0.68	1.66	1	5
1:B:25:ALA:C	1:B:29:LEU:HD12	0.68	2.08	20	16
1:B:62:PHE:CE2	1:B:64:SER:HB3	0.68	2.24	2	14
1:A:62:PHE:HE1	1:A:64:SER:HB3	0.68	1.49	10	5
1:B:28:ALA:HB2	1:B:41:HIS:CG	0.68	2.23	16	11
1:A:43:LYS:HE3	1:B:65:TYR:HE2	0.68	1.46	10	1
1:A:46:PHE:HA	1:A:50:TYR:CD1	0.68	2.24	19	4
1:B:8:ILE:HA	1:B:76:PHE:CB	0.68	2.19	17	17
1:B:19:GLN:O	1:B:23:GLU:HG3	0.68	1.89	11	11
1:B:76:PHE:CZ	1:B:83:ILE:HB	0.68	2.23	7	16
1:A:62:PHE:CE2	1:A:64:SER:HB3	0.68	2.23	17	7
1:B:35:GLU:O	1:B:58:VAL:HG13	0.68	1.88	9	18
1:B:58:VAL:HG23	1:B:82:ALA:O	0.68	1.89	9	10
1:B:60:ARG:O	1:B:61:ASN:HB2	0.68	1.88	12	4
1:A:27:GLN:O	1:A:31:LYS:HB2	0.68	1.89	5	5
1:A:68:HIS:HB2	1:A:72:HIS:CA	0.68	2.19	6	5
1:B:13:MET:H	1:B:18:GLN:NE2	0.68	1.86	8	2
1:A:72:HIS:CB	1:A:87:LYS:HB2	0.68	2.18	18	2
1:B:56:CYS:SG	1:B:85:LEU:HG	0.68	2.29	19	4
1:A:19:GLN:HG3	1:A:20:ASP:N	0.68	2.03	3	3
1:B:29:LEU:HD11	1:B:83:ILE:HD11	0.68	1.65	1	3
1:A:57:ILE:O	1:A:83:ILE:HA	0.68	1.88	13	5
1:A:66:VAL:HB	1:B:55:HIS:ND1	0.68	2.04	4	4
1:B:39:ALA:HB2	1:B:58:VAL:CG1	0.68	2.15	5	5
1:A:8:ILE:HA	1:A:75:TYR:O	0.68	1.88	8	1
1:A:62:PHE:HA	1:B:59:GLY:CA	0.68	2.18	3	15
1:A:64:SER:CA	1:B:57:ILE:HG23	0.68	2.18	2	13
1:B:68:HIS:HB2	1:B:72:HIS:HA	0.68	1.64	7	4
1:A:73:PHE:HD2	1:A:86:PHE:HB3	0.68	1.49	2	2
1:B:39:ALA:CB	1:B:58:VAL:HG12	0.68	2.15	17	16
1:A:55:HIS:CE1	1:B:67:THR:HB	0.68	2.23	13	5
1:B:27:GLN:O	1:B:31:LYS:HD3	0.68	1.88	8	1
1:B:71:LYS:HE2	1:B:72:HIS:CE1	0.68	2.24	8	1
1:B:8:ILE:C	1:B:9:LYS:HG2	0.68	2.09	2	9
1:A:12:ASP:HB3	1:A:72:HIS:CG	0.68	2.24	4	3
1:A:70:THR:O	1:A:71:LYS:HG3	0.68	1.88	14	2
1:B:57:ILE:HG13	1:B:84:LEU:CD2	0.68	2.17	20	2
1:B:15:GLU:HA	1:B:18:GLN:OE1	0.67	1.89	20	5
1:B:72:HIS:CB	1:B:87:LYS:HB2	0.67	2.19	5	3
1:A:31:LYS:HB3	1:A:32:TYR:CE1	0.67	2.24	5	9
1:B:53:THR:HG23	1:B:55:HIS:CE1	0.67	2.24	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ASP:OD2	1:A:52:PRO:HB3	0.67	1.89	10	5
1:A:43:LYS:HD2	1:A:43:LYS:C	0.67	2.09	10	4
1:A:27:GLN:HB3	1:A:41:HIS:CE1	0.67	2.24	12	3
1:A:33:ASN:CA	1:A:38:ILE:HD11	0.67	2.19	13	4
1:B:24:CYS:HB3	1:B:42:ILE:HG23	0.67	1.67	16	1
1:A:43:LYS:HE2	1:A:47:ASP:CB	0.67	2.19	1	2
1:B:58:VAL:HG23	1:B:81:VAL:CG1	0.67	2.18	7	5
1:A:57:ILE:HG12	1:B:65:TYR:H	0.67	1.49	4	1
1:B:47:ASP:HB2	1:B:52:PRO:CD	0.67	2.20	17	5
1:A:47:ASP:OD1	1:A:48:LYS:HG2	0.67	1.88	19	1
1:A:47:ASP:HB3	1:A:52:PRO:HB3	0.67	1.65	20	1
1:A:55:HIS:CE1	1:A:88:SER:HB2	0.67	2.24	16	8
1:B:55:HIS:HB2	1:B:86:PHE:O	0.67	1.89	4	10
1:A:56:CYS:HB3	1:A:85:LEU:CD1	0.67	2.19	3	8
1:A:77:TYR:OH	1:A:80:GLN:HA	0.67	1.88	18	8
1:B:16:GLU:O	1:B:20:ASP:HB2	0.67	1.89	11	5
1:A:66:VAL:HA	1:B:55:HIS:HB3	0.67	1.66	14	2
1:A:11:ALA:HB1	1:A:18:GLN:HE21	0.67	1.49	19	3
1:A:62:PHE:HA	1:B:59:GLY:HA3	0.67	1.65	7	11
1:A:67:THR:HB	1:B:55:HIS:CE1	0.67	2.25	19	4
1:A:55:HIS:HB3	1:B:66:VAL:CG1	0.67	2.19	19	8
1:B:72:HIS:CG	1:B:87:LYS:HD3	0.67	2.25	10	3
1:A:72:HIS:O	1:A:86:PHE:HA	0.67	1.89	16	7
1:A:55:HIS:HB2	1:A:86:PHE:CZ	0.67	2.24	2	3
1:B:12:ASP:O	1:B:72:HIS:HB2	0.67	1.90	11	7
1:A:5:LYS:HG3	1:A:5:LYS:O	0.67	1.89	1	2
1:A:35:GLU:HB3	1:B:63:GLY:CA	0.67	2.19	20	12
1:B:13:MET:HB2	1:B:73:PHE:N	0.67	2.04	17	4
1:A:55:HIS:CD2	1:A:87:LYS:HA	0.67	2.25	8	8
1:A:62:PHE:CB	1:B:59:GLY:HA3	0.67	2.19	6	11
1:B:38:ILE:O	1:B:42:ILE:HG13	0.67	1.90	11	11
1:A:66:VAL:HB	1:B:55:HIS:CG	0.67	2.24	4	3
1:B:47:ASP:HB3	1:B:52:PRO:HG3	0.67	1.67	5	1
1:A:55:HIS:C	1:B:66:VAL:HG12	0.67	2.10	20	3
1:A:9:LYS:HB2	1:A:75:TYR:CD2	0.67	2.24	11	1
1:A:64:SER:HA	1:B:57:ILE:CD1	0.67	2.20	7	13
1:B:58:VAL:HA	1:B:82:ALA:O	0.67	1.90	14	17
1:A:55:HIS:HD2	1:A:87:LYS:HA	0.67	1.49	8	10
1:A:35:GLU:HG3	1:A:59:GLY:HA2	0.67	1.67	12	4
1:A:34:ILE:HB	1:A:37:ASP:CB	0.67	2.20	15	15
1:B:8:ILE:CG1	1:B:76:PHE:HB3	0.67	2.20	5	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:81:VAL:HG12	1:B:82:ALA:N	0.67	2.04	1	20
1:A:60:ARG:HG3	1:A:60:ARG:NH1	0.67	2.05	14	3
1:A:57:ILE:CB	1:A:84:LEU:HB3	0.67	2.20	7	4
1:B:4:ARG:HG2	1:B:4:ARG:HH11	0.67	1.49	12	3
1:A:8:ILE:HA	1:A:76:PHE:CB	0.67	2.20	20	19
1:B:6:ALA:HB2	1:B:78:LEU:HD22	0.67	1.67	20	12
1:B:8:ILE:HA	1:B:76:PHE:CA	0.67	2.20	7	20
1:B:27:GLN:HB3	1:B:41:HIS:CE1	0.67	2.25	16	3
1:A:65:TYR:CD2	1:B:43:LYS:HD3	0.67	2.25	7	4
1:A:8:ILE:HD12	1:A:76:PHE:HB3	0.66	1.66	11	8
1:A:72:HIS:HB2	1:A:87:LYS:CG	0.66	2.21	1	2
1:A:76:PHE:CE2	1:A:83:ILE:HG13	0.66	2.25	5	16
1:A:29:LEU:CD1	1:A:78:LEU:HG	0.66	2.19	16	14
1:A:72:HIS:CB	1:A:87:LYS:HD3	0.66	2.19	16	2
1:B:22:VAL:HG22	1:B:76:PHE:CE2	0.66	2.24	12	10
1:B:26:THR:CA	1:B:29:LEU:HD12	0.66	2.21	18	6
1:B:59:GLY:O	1:B:60:ARG:HB3	0.66	1.91	4	4
1:B:4:ARG:O	1:B:4:ARG:HG3	0.66	1.88	17	1
1:A:9:LYS:HE2	1:A:77:TYR:CB	0.66	2.20	2	1
1:B:4:ARG:HG2	1:B:19:GLN:CD	0.66	2.10	2	1
1:A:43:LYS:CE	1:A:56:CYS:HB3	0.66	2.19	5	1
1:A:56:CYS:HB2	1:A:85:LEU:CD1	0.66	2.19	13	7
1:A:65:TYR:CE2	1:B:43:LYS:HD2	0.66	2.26	13	2
1:B:14:SER:HB3	1:B:17:MET:HG3	0.66	1.67	19	2
1:A:8:ILE:CG1	1:A:76:PHE:HB3	0.66	2.21	13	17
1:A:7:VAL:O	1:A:9:LYS:HE2	0.66	1.89	3	1
1:B:7:VAL:O	1:B:9:LYS:HE3	0.66	1.90	17	4
1:B:37:ASP:HB3	1:B:41:HIS:CE1	0.66	2.25	8	3
1:A:38:ILE:O	1:A:42:ILE:HG13	0.66	1.90	10	11
1:A:57:ILE:HD13	1:B:65:TYR:H	0.66	1.48	3	15
1:A:66:VAL:CB	1:B:55:HIS:HB3	0.66	2.20	1	11
1:B:66:VAL:HG21	1:B:86:PHE:CD1	0.66	2.25	13	7
1:B:11:ALA:CB	1:B:74:ILE:HA	0.66	2.20	14	5
1:B:27:GLN:O	1:B:31:LYS:HD2	0.66	1.90	20	1
1:A:43:LYS:HB3	1:B:65:TYR:CD2	0.66	2.25	17	10
1:A:72:HIS:CG	1:A:87:LYS:HD3	0.66	2.25	16	3
1:A:62:PHE:CB	1:B:62:PHE:HB3	0.66	2.21	11	9
1:B:47:ASP:HB2	1:B:52:PRO:CB	0.66	2.20	16	7
1:A:53:THR:HG21	1:B:67:THR:CG2	0.66	2.20	12	3
1:B:35:GLU:HA	1:B:35:GLU:OE1	0.66	1.90	20	2
1:A:63:GLY:CA	1:B:35:GLU:HB3	0.66	2.20	9	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:58:VAL:HG23	1:B:83:ILE:HD13	0.66	1.65	10	15
1:A:13:MET:H	1:A:18:GLN:HE22	0.66	1.31	18	6
1:A:34:ILE:HG22	1:A:34:ILE:O	0.66	1.90	13	6
1:A:57:ILE:HB	1:A:84:LEU:HD23	0.66	1.68	8	4
1:A:46:PHE:CD2	1:A:85:LEU:HD21	0.66	2.26	13	3
1:A:8:ILE:O	1:A:9:LYS:HD3	0.66	1.90	19	2
1:A:8:ILE:HA	1:A:76:PHE:CA	0.66	2.21	6	20
1:A:75:TYR:CD1	1:A:84:LEU:HB2	0.66	2.26	3	5
1:B:31:LYS:HD3	1:B:41:HIS:CE1	0.66	2.26	16	3
1:B:13:MET:SD	1:B:18:GLN:N	0.66	2.68	3	4
1:A:60:ARG:O	1:A:61:ASN:HB2	0.66	1.91	12	11
1:B:29:LEU:HG	1:B:38:ILE:HG21	0.66	1.68	15	4
1:B:69:GLU:O	1:B:70:THR:HG22	0.66	1.91	5	1
1:A:63:GLY:HA3	1:B:35:GLU:C	0.66	2.11	7	18
1:B:56:CYS:HB2	1:B:85:LEU:CD1	0.66	2.19	13	4
1:A:11:ALA:CA	1:A:74:ILE:HA	0.66	2.20	16	2
1:A:84:LEU:HD22	1:B:57:ILE:HD11	0.66	1.68	19	2
1:A:10:ASN:CB	1:A:75:TYR:HB3	0.66	2.21	18	1
1:B:87:LYS:CE	1:B:89:GLY:HA2	0.66	2.21	18	1
1:A:25:ALA:HA	1:A:42:ILE:CG1	0.65	2.21	19	10
1:B:35:GLU:HB3	1:B:58:VAL:O	0.65	1.90	19	14
1:B:54:TRP:CZ2	1:B:87:LYS:HD2	0.65	2.26	11	9
1:A:59:GLY:O	1:A:60:ARG:HB3	0.65	1.89	5	1
1:B:11:ALA:CA	1:B:74:ILE:HA	0.65	2.21	8	6
1:A:40:ALA:HB2	1:B:65:TYR:CE1	0.65	2.26	14	7
1:A:64:SER:CA	1:B:57:ILE:HG12	0.65	2.21	13	3
1:A:13:MET:HB2	1:A:71:LYS:O	0.65	1.91	6	6
1:A:54:TRP:HA	1:A:87:LYS:HB3	0.65	1.66	17	5
1:A:43:LYS:HE2	1:A:47:ASP:HB3	0.65	1.67	8	2
1:A:17:MET:HA	1:A:20:ASP:OD2	0.65	1.91	15	1
1:B:55:HIS:ND1	1:B:55:HIS:N	0.65	2.44	18	3
1:A:60:ARG:HG3	1:A:60:ARG:HH11	0.65	1.50	4	3
1:A:13:MET:CB	1:A:17:MET:HG3	0.65	2.21	16	1
1:A:55:HIS:N	1:A:55:HIS:CD2	0.65	2.65	16	10
1:B:73:PHE:HD1	1:B:86:PHE:HB3	0.65	1.50	13	4
1:B:35:GLU:CG	1:B:59:GLY:HA2	0.65	2.22	6	4
1:A:16:GLU:HA	1:A:19:GLN:NE2	0.65	2.07	14	2
1:B:41:HIS:O	1:B:45:GLU:HG2	0.65	1.90	17	1
1:B:43:LYS:HE2	1:B:47:ASP:HB3	0.65	1.67	17	1
1:A:57:ILE:CD1	1:B:66:VAL:HG13	0.65	2.21	2	14
1:A:66:VAL:HG11	1:A:86:PHE:CZ	0.65	2.25	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LYS:HE3	1:B:65:TYR:CE2	0.65	2.27	10	3
1:A:8:ILE:CD1	1:A:76:PHE:HB3	0.65	2.21	8	10
1:A:67:THR:HG23	1:A:67:THR:O	0.65	1.92	1	2
1:B:74:ILE:HG23	1:B:76:PHE:CE1	0.65	2.26	15	9
1:A:65:TYR:CD1	1:B:40:ALA:HB2	0.65	2.27	19	3
1:B:51:ASN:O	1:B:87:LYS:HE3	0.65	1.91	14	3
1:B:7:VAL:HG12	1:B:9:LYS:HE3	0.65	1.68	10	1
1:A:39:ALA:N	1:A:58:VAL:HG11	0.65	2.07	1	13
1:A:63:GLY:HA3	1:B:35:GLU:HB3	0.65	1.67	6	10
1:A:66:VAL:HG12	1:B:55:HIS:C	0.65	2.12	8	5
1:A:64:SER:HA	1:B:57:ILE:CG2	0.65	2.20	2	3
1:A:74:ILE:O	1:A:74:ILE:HG23	0.65	1.92	3	6
1:B:4:ARG:HG2	1:B:19:GLN:NE2	0.65	2.07	2	1
1:B:7:VAL:HG23	1:B:77:TYR:O	0.65	1.90	10	9
1:A:6:ALA:HB1	1:A:76:PHE:HB2	0.65	1.68	8	1
1:B:43:LYS:HB3	1:B:56:CYS:SG	0.65	2.32	19	1
1:B:13:MET:HA	1:B:71:LYS:O	0.65	1.92	13	6
1:B:38:ILE:HG22	1:B:42:ILE:HD11	0.65	1.68	18	10
1:A:47:ASP:HA	1:A:54:TRP:CD1	0.65	2.26	5	10
1:A:7:VAL:HG23	1:A:77:TYR:O	0.65	1.92	16	3
1:B:13:MET:HB2	1:B:72:HIS:CA	0.65	2.21	13	4
1:A:43:LYS:HD2	1:A:55:HIS:CA	0.65	2.21	5	1
1:B:43:LYS:HD3	1:B:43:LYS:C	0.65	2.12	19	2
1:A:26:THR:HA	1:A:29:LEU:CD1	0.65	2.21	10	5
1:B:25:ALA:HB2	1:B:83:ILE:HG21	0.65	1.68	16	13
1:A:24:CYS:SG	1:A:42:ILE:HA	0.65	2.32	12	4
1:A:64:SER:HA	1:B:57:ILE:CG1	0.65	2.22	13	5
1:A:57:ILE:HA	1:B:63:GLY:O	0.65	1.92	14	2
1:A:47:ASP:OD1	1:A:54:TRP:HB2	0.64	1.92	7	3
1:B:7:VAL:HG12	1:B:9:LYS:CE	0.64	2.22	3	2
1:A:47:ASP:OD1	1:A:53:THR:HA	0.64	1.91	15	2
1:A:57:ILE:HG21	1:A:62:PHE:CE2	0.64	2.27	15	3
1:A:13:MET:HG2	1:A:17:MET:CG	0.64	2.22	16	1
1:A:69:GLU:CB	1:A:88:SER:HA	0.64	2.21	4	3
1:A:43:LYS:HB3	1:B:65:TYR:CE2	0.64	2.28	12	7
1:A:57:ILE:CG1	1:B:64:SER:HA	0.64	2.20	4	1
1:A:29:LEU:HD11	1:A:83:ILE:HD11	0.64	1.68	17	2
1:A:84:LEU:O	1:A:84:LEU:HG	0.64	1.93	8	12
1:A:57:ILE:HG23	1:B:64:SER:CA	0.64	2.21	11	12
1:B:25:ALA:HA	1:B:42:ILE:CG1	0.64	2.22	15	9
1:B:42:ILE:HG21	1:B:85:LEU:CD1	0.64	2.20	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:GLU:HA	1:A:18:GLN:OE1	0.64	1.92	6	4
1:A:43:LYS:HD2	1:B:65:TYR:HE2	0.64	1.52	18	2
1:B:46:PHE:CE2	1:B:85:LEU:HD21	0.64	2.27	14	3
1:B:26:THR:HA	1:B:29:LEU:CD1	0.64	2.23	18	6
1:A:43:LYS:HD3	1:A:54:TRP:O	0.64	1.91	16	2
1:A:67:THR:HG22	1:B:53:THR:HG21	0.64	1.68	13	1
1:B:6:ALA:HB2	1:B:78:LEU:CD2	0.64	2.22	6	13
1:B:18:GLN:HB3	1:B:74:ILE:CD1	0.64	2.21	1	5
1:B:54:TRP:HA	1:B:87:LYS:CB	0.64	2.22	18	2
1:A:65:TYR:CE1	1:B:40:ALA:HA	0.64	2.28	8	6
1:B:17:MET:HA	1:B:20:ASP:OD2	0.64	1.91	3	1
1:B:50:TYR:O	1:B:51:ASN:HB3	0.64	1.92	16	2
1:B:74:ILE:HG22	1:B:85:LEU:HB2	0.64	1.67	14	3
1:A:55:HIS:CA	1:B:66:VAL:HG12	0.64	2.23	20	3
1:A:25:ALA:CB	1:A:83:ILE:HG13	0.64	2.21	9	4
1:A:59:GLY:HA3	1:A:62:PHE:CD1	0.64	2.26	9	1
1:A:7:VAL:CG1	1:A:9:LYS:HE2	0.64	2.23	18	3
1:B:15:GLU:HA	1:B:18:GLN:CG	0.64	2.23	2	9
1:A:70:THR:HG22	1:A:71:LYS:N	0.64	2.08	3	1
1:A:71:LYS:HG2	1:A:87:LYS:HZ3	0.64	1.52	11	2
1:A:11:ALA:CB	1:A:74:ILE:HA	0.64	2.22	16	4
1:A:65:TYR:CE2	1:B:40:ALA:HB2	0.64	2.28	6	2
1:A:55:HIS:CD2	1:B:67:THR:HB	0.64	2.28	9	1
1:B:72:HIS:HB2	1:B:87:LYS:HD3	0.64	1.69	10	1
1:B:48:LYS:HE3	1:B:48:LYS:CA	0.64	2.23	1	2
1:A:43:LYS:HD2	1:A:54:TRP:O	0.64	1.93	20	3
1:B:22:VAL:HG22	1:B:76:PHE:CG	0.64	2.28	18	9
1:A:53:THR:O	1:A:87:LYS:HB2	0.64	1.92	9	5
1:A:77:TYR:HA	1:A:82:ALA:HA	0.64	1.70	4	15
1:B:54:TRP:CD2	1:B:87:LYS:HD2	0.64	2.28	15	13
1:A:65:TYR:CD2	1:B:43:LYS:HB3	0.64	2.28	10	10
1:A:69:GLU:CG	1:A:88:SER:HA	0.64	2.23	3	6
1:B:55:HIS:HE2	1:B:88:SER:HB2	0.64	1.53	19	3
1:B:47:ASP:OD2	1:B:52:PRO:HG3	0.64	1.93	19	2
1:B:84:LEU:O	1:B:85:LEU:HD12	0.64	1.93	13	1
1:B:13:MET:HG2	1:B:17:MET:CB	0.64	2.23	10	12
1:B:29:LEU:CD1	1:B:78:LEU:HG	0.64	2.23	11	11
1:B:53:THR:O	1:B:87:LYS:HG2	0.64	1.92	2	3
1:A:46:PHE:HB3	1:A:54:TRP:CG	0.64	2.28	18	5
1:B:14:SER:O	1:B:17:MET:HB2	0.63	1.92	19	10
1:A:18:GLN:O	1:A:74:ILE:HD12	0.63	1.94	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:CYS:HB2	1:A:85:LEU:HG	0.63	1.69	5	3
1:B:48:LYS:C	1:B:48:LYS:HE2	0.63	2.14	11	1
1:A:43:LYS:HD3	1:B:65:TYR:CD2	0.63	2.27	19	1
1:A:67:THR:HB	1:B:55:HIS:ND1	0.63	2.07	19	1
1:A:13:MET:HG2	1:A:17:MET:CB	0.63	2.24	2	9
1:A:57:ILE:CD1	1:B:64:SER:HA	0.63	2.22	7	18
1:A:61:ASN:O	1:B:60:ARG:HG2	0.63	1.93	1	1
1:B:55:HIS:HB2	1:B:86:PHE:CD1	0.63	2.28	4	3
1:B:55:HIS:N	1:B:55:HIS:CD2	0.63	2.65	2	7
1:A:13:MET:SD	1:A:18:GLN:N	0.63	2.72	6	5
1:A:54:TRP:CZ2	1:A:87:LYS:HD2	0.63	2.29	8	7
1:B:47:ASP:OD1	1:B:52:PRO:HG3	0.63	1.94	18	2
1:A:11:ALA:HB2	1:A:74:ILE:HG13	0.63	1.68	13	10
1:B:53:THR:HG23	1:B:55:HIS:NE2	0.63	2.07	2	2
1:A:57:ILE:HG21	1:A:62:PHE:HE2	0.63	1.53	15	2
1:A:66:VAL:HG21	1:A:86:PHE:CZ	0.63	2.28	1	5
1:B:32:TYR:CD1	1:B:32:TYR:N	0.63	2.66	20	8
1:B:34:ILE:HB	1:B:37:ASP:CB	0.63	2.24	15	11
1:A:32:TYR:N	1:A:32:TYR:CD1	0.63	2.67	7	9
1:A:39:ALA:HB1	1:B:65:TYR:HB3	0.63	1.68	20	4
1:A:78:LEU:HD23	1:A:83:ILE:CG1	0.63	2.24	9	4
1:A:27:GLN:HB2	1:A:41:HIS:NE2	0.63	2.09	19	2
1:B:21:SER:CB	1:B:74:ILE:HG21	0.63	2.24	17	3
1:A:62:PHE:HB2	1:B:59:GLY:HA3	0.63	1.69	6	8
1:A:51:ASN:O	1:A:87:LYS:HE2	0.63	1.93	2	2
1:A:33:ASN:C	1:A:34:ILE:HD12	0.63	2.14	5	1
1:B:47:ASP:OD2	1:B:53:THR:HA	0.63	1.93	12	1
1:A:66:VAL:HB	1:B:55:HIS:CB	0.63	2.23	1	5
1:B:6:ALA:CB	1:B:78:LEU:HD13	0.63	2.22	18	4
1:A:68:HIS:CD2	1:A:69:GLU:N	0.63	2.67	2	2
1:A:70:THR:HG21	1:A:87:LYS:NZ	0.63	2.09	3	1
1:A:74:ILE:HG22	1:A:85:LEU:CB	0.63	2.24	7	5
1:B:19:GLN:HG3	1:B:20:ASP:N	0.63	2.09	5	2
1:B:13:MET:HG2	1:B:17:MET:HB2	0.63	1.69	8	9
1:B:78:LEU:HD23	1:B:83:ILE:HD11	0.63	1.70	14	2
1:A:55:HIS:HB2	1:A:86:PHE:O	0.63	1.94	12	6
1:A:13:MET:H	1:A:18:GLN:NE2	0.63	1.90	18	2
1:B:8:ILE:CD1	1:B:76:PHE:HB3	0.63	2.23	13	13
1:A:6:ALA:CB	1:A:78:LEU:HD13	0.63	2.22	4	5
1:A:53:THR:HG22	1:B:67:THR:HG21	0.63	1.70	17	1
1:A:6:ALA:HB2	1:A:78:LEU:CD2	0.63	2.24	17	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:VAL:HG12	1:B:56:CYS:N	0.63	2.09	8	3
1:A:16:GLU:O	1:A:20:ASP:HB2	0.63	1.93	17	3
1:B:15:GLU:HA	1:B:18:GLN:NE2	0.63	2.09	11	1
1:A:13:MET:CG	1:A:17:MET:HG3	0.63	2.24	16	1
1:A:46:PHE:HA	1:A:50:TYR:HD1	0.63	1.54	19	2
1:A:39:ALA:HB1	1:B:65:TYR:CB	0.62	2.24	1	15
1:B:76:PHE:CD1	1:B:76:PHE:N	0.62	2.67	12	16
1:A:6:ALA:HB1	1:A:76:PHE:HD2	0.62	1.52	16	7
1:B:72:HIS:CB	1:B:87:LYS:HD3	0.62	2.23	10	1
1:A:68:HIS:CB	1:A:86:PHE:HB2	0.62	2.24	12	1
1:A:40:ALA:HA	1:B:65:TYR:CE1	0.62	2.28	7	8
1:A:11:ALA:O	1:A:12:ASP:HB2	0.62	1.93	7	3
1:B:35:GLU:OE1	1:B:58:VAL:HG22	0.62	1.94	20	2
1:B:62:PHE:CD1	1:B:63:GLY:N	0.62	2.67	19	1
1:A:55:HIS:HB3	1:B:66:VAL:CA	0.62	2.25	8	7
1:A:68:HIS:ND1	1:A:68:HIS:N	0.62	2.48	3	5
1:A:45:GLU:OE1	1:A:45:GLU:HA	0.62	1.94	10	2
1:A:13:MET:HG3	1:A:14:SER:N	0.62	2.09	5	9
1:B:72:HIS:O	1:B:86:PHE:HA	0.62	1.95	8	7
1:A:47:ASP:OD1	1:A:52:PRO:HA	0.62	1.94	15	2
1:A:13:MET:HB2	1:A:72:HIS:CA	0.62	2.24	18	5
1:A:18:GLN:CB	1:A:74:ILE:HD12	0.62	2.25	1	7
1:B:73:PHE:HE1	1:B:84:LEU:HD12	0.62	1.54	17	2
1:A:32:TYR:CE1	1:A:41:HIS:ND1	0.62	2.68	13	13
1:B:39:ALA:N	1:B:58:VAL:HG11	0.62	2.10	14	12
1:B:74:ILE:N	1:B:85:LEU:O	0.62	2.33	5	6
1:B:71:LYS:O	1:B:72:HIS:HB2	0.62	1.94	16	5
1:A:74:ILE:HG23	1:A:76:PHE:CE1	0.62	2.29	5	8
1:B:54:TRP:CD1	1:B:87:LYS:HD2	0.62	2.29	12	2
1:B:70:THR:C	1:B:71:LYS:HG2	0.62	2.14	5	2
1:A:34:ILE:O	1:A:36:LYS:N	0.62	2.32	18	6
1:A:35:GLU:CG	1:A:59:GLY:HA2	0.62	2.25	17	4
1:B:51:ASN:HD22	1:B:52:PRO:HD2	0.62	1.53	17	2
1:B:9:LYS:HD2	1:B:76:PHE:HA	0.62	1.70	14	1
1:A:19:GLN:O	1:A:23:GLU:HG3	0.62	1.93	18	10
1:A:65:TYR:H	1:B:57:ILE:HG12	0.62	1.53	19	4
1:A:56:CYS:HB2	1:A:85:LEU:CG	0.62	2.25	5	3
1:A:66:VAL:HG21	1:A:86:PHE:CG	0.62	2.29	19	2
1:B:46:PHE:CZ	1:B:85:LEU:HD23	0.62	2.29	11	1
1:B:8:ILE:CA	1:B:76:PHE:HA	0.62	2.23	9	9
1:B:16:GLU:O	1:B:19:GLN:HG2	0.62	1.94	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:32:TYR:CE1	1:B:41:HIS:ND1	0.62	2.68	5	10
1:A:55:HIS:ND1	1:A:55:HIS:N	0.62	2.48	19	4
1:B:47:ASP:HB2	1:B:52:PRO:HD3	0.62	1.71	17	2
1:A:13:MET:HG3	1:A:14:SER:H	0.62	1.54	5	9
1:B:25:ALA:HA	1:B:42:ILE:HD11	0.62	1.72	6	12
1:A:23:GLU:O	1:A:27:GLN:HG3	0.62	1.94	19	2
1:A:68:HIS:N	1:A:68:HIS:ND1	0.62	2.47	4	1
1:B:43:LYS:HG3	1:B:54:TRP:O	0.62	1.94	15	8
1:A:66:VAL:HB	1:A:86:PHE:CZ	0.62	2.30	14	2
1:A:78:LEU:N	1:A:81:VAL:O	0.62	2.33	9	20
1:A:18:GLN:HB3	1:A:74:ILE:CD1	0.62	2.25	18	3
1:A:39:ALA:HB2	1:A:58:VAL:CG1	0.62	2.17	16	5
1:B:77:TYR:HA	1:B:81:VAL:O	0.62	1.95	3	5
1:A:7:VAL:HG12	1:A:7:VAL:O	0.62	1.94	6	6
1:B:60:ARG:HG3	1:B:61:ASN:HD22	0.62	1.54	10	1
1:B:17:MET:SD	1:B:72:HIS:ND1	0.62	2.73	13	1
1:B:5:LYS:O	1:B:78:LEU:HD13	0.61	1.94	2	7
1:A:33:ASN:C	1:A:34:ILE:HD13	0.61	2.14	6	3
1:A:68:HIS:HB2	1:A:72:HIS:O	0.61	1.94	8	4
1:B:13:MET:HG3	1:B:17:MET:HG2	0.61	1.72	13	1
1:B:64:SER:CB	1:B:84:LEU:HD13	0.61	2.25	19	1
1:B:68:HIS:HE1	1:B:70:THR:HB	0.61	1.55	9	1
1:A:27:GLN:O	1:A:31:LYS:HD3	0.61	1.95	11	1
1:B:17:MET:SD	1:B:54:TRP:HH2	0.61	2.18	13	2
1:B:68:HIS:HB3	1:B:72:HIS:O	0.61	1.95	15	2
1:A:76:PHE:CD1	1:A:76:PHE:N	0.61	2.69	19	20
1:B:13:MET:SD	1:B:17:MET:C	0.61	2.78	3	4
1:B:55:HIS:N	1:B:86:PHE:O	0.61	2.34	11	5
1:A:55:HIS:NE2	1:B:67:THR:HG22	0.61	2.11	16	2
1:A:65:TYR:HB3	1:B:56:CYS:O	0.61	1.95	16	1
1:A:28:ALA:HB3	1:A:38:ILE:CG2	0.61	2.25	17	13
1:A:73:PHE:CD1	1:A:74:ILE:N	0.61	2.69	2	1
1:A:13:MET:SD	1:A:17:MET:C	0.61	2.79	17	5
1:A:35:GLU:HB3	1:B:63:GLY:HA3	0.61	1.73	20	6
1:B:4:ARG:HG2	1:B:19:GLN:OE1	0.61	1.95	4	1
1:B:13:MET:HG2	1:B:18:GLN:OE1	0.61	1.95	8	2
1:B:9:LYS:HE3	1:B:76:PHE:C	0.61	2.16	14	1
1:A:67:THR:HG22	1:A:67:THR:O	0.61	1.96	15	2
1:B:78:LEU:N	1:B:81:VAL:O	0.61	2.33	2	20
1:A:54:TRP:CH2	1:A:87:LYS:HD3	0.61	2.30	3	2
1:A:43:LYS:HB3	1:B:65:TYR:HE2	0.61	1.55	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:HIS:HB2	1:A:86:PHE:CD1	0.61	2.30	14	4
1:B:46:PHE:HA	1:B:50:TYR:CD1	0.61	2.31	17	2
1:B:54:TRP:HA	1:B:87:LYS:HG2	0.61	1.71	19	6
1:A:49:LYS:HB3	1:A:50:TYR:CE1	0.61	2.31	4	3
1:A:35:GLU:HG2	1:B:62:PHE:HA	0.61	1.72	10	4
1:B:57:ILE:CD1	1:B:84:LEU:HD23	0.61	2.25	18	2
1:A:58:VAL:O	1:B:63:GLY:N	0.61	2.34	1	19
1:A:12:ASP:N	1:A:73:PHE:O	0.61	2.33	13	8
1:A:43:LYS:HD2	1:A:56:CYS:N	0.61	2.10	5	1
1:A:73:PHE:HB3	1:A:86:PHE:CB	0.61	2.25	8	1
1:B:9:LYS:HE2	1:B:9:LYS:CA	0.61	2.23	18	2
1:A:12:ASP:HB3	1:A:72:HIS:HD1	0.61	1.56	19	1
1:A:66:VAL:HG12	1:B:55:HIS:CA	0.61	2.26	17	5
1:A:6:ALA:HB1	1:A:78:LEU:HD22	0.61	1.73	4	12
1:A:34:ILE:HG22	1:A:36:LYS:CD	0.61	2.26	2	1
1:B:24:CYS:SG	1:B:46:PHE:CE1	0.61	2.94	7	1
1:B:4:ARG:NH1	1:B:19:GLN:HG3	0.61	2.10	12	1
1:A:49:LYS:HD2	1:A:50:TYR:CE1	0.61	2.30	13	1
1:A:24:CYS:SG	1:A:46:PHE:CE1	0.61	2.94	16	2
1:A:59:GLY:HA3	1:B:62:PHE:CB	0.61	2.25	20	6
1:B:13:MET:HG3	1:B:14:SER:N	0.61	2.11	2	11
1:A:55:HIS:HB3	1:B:66:VAL:HG12	0.61	1.73	17	6
1:A:58:VAL:HG23	1:A:83:ILE:HD12	0.61	1.70	13	2
1:A:58:VAL:HG13	1:A:58:VAL:O	0.61	1.95	13	1
1:A:63:GLY:N	1:B:58:VAL:O	0.60	2.34	4	20
1:B:47:ASP:HB2	1:B:52:PRO:HG3	0.60	1.71	7	2
1:B:73:PHE:CD1	1:B:86:PHE:HB3	0.60	2.30	17	4
1:A:12:ASP:HB3	1:A:72:HIS:CB	0.60	2.26	4	2
1:B:46:PHE:O	1:B:50:TYR:HB2	0.60	1.96	18	5
1:A:61:ASN:O	1:B:35:GLU:HG2	0.60	1.95	14	3
1:B:71:LYS:O	1:B:71:LYS:HG2	0.60	1.95	11	1
1:B:12:ASP:N	1:B:73:PHE:O	0.60	2.34	1	7
1:B:55:HIS:HB2	1:B:86:PHE:CE1	0.60	2.32	20	5
1:A:56:CYS:SG	1:A:85:LEU:HG	0.60	2.37	3	1
1:A:73:PHE:HB2	1:A:86:PHE:CB	0.60	2.26	17	7
1:A:13:MET:HB3	1:A:18:GLN:NE2	0.60	2.11	4	2
1:B:68:HIS:HE2	1:B:87:LYS:HG3	0.60	1.55	4	1
1:A:24:CYS:O	1:A:27:GLN:HG2	0.60	1.95	16	2
1:B:24:CYS:HA	1:B:27:GLN:HG3	0.60	1.73	11	1
1:A:34:ILE:CG2	1:A:36:LYS:HD2	0.60	2.25	16	1
1:B:7:VAL:N	1:B:77:TYR:O	0.60	2.34	20	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:54:TRP:CH2	1:B:72:HIS:HB3	0.60	2.32	10	2
1:B:38:ILE:O	1:B:42:ILE:HD12	0.60	1.96	2	2
1:B:13:MET:HA	1:B:71:LYS:HG3	0.60	1.73	4	1
1:B:13:MET:N	1:B:18:GLN:HE22	0.60	1.94	8	1
1:B:87:LYS:NZ	1:B:87:LYS:HB3	0.60	2.11	8	1
1:A:17:MET:SD	1:A:54:TRP:HH2	0.60	2.18	10	1
1:A:12:ASP:HB2	1:A:73:PHE:HD2	0.60	1.55	13	5
1:A:45:GLU:O	1:A:49:LYS:N	0.60	2.34	3	17
1:A:62:PHE:HB3	1:B:62:PHE:CB	0.60	2.25	14	6
1:A:54:TRP:CD2	1:A:87:LYS:HG3	0.60	2.30	2	3
1:B:13:MET:HG3	1:B:14:SER:H	0.60	1.55	7	11
1:B:12:ASP:HB3	1:B:72:HIS:CG	0.60	2.32	4	2
1:B:14:SER:C	1:B:18:GLN:NE2	0.60	2.55	11	1
1:A:64:SER:OG	1:A:84:LEU:HD13	0.60	1.96	12	2
1:B:13:MET:SD	1:B:18:GLN:HA	0.60	2.36	13	1
1:A:74:ILE:HG22	1:A:85:LEU:HB3	0.60	1.74	7	2
1:A:62:PHE:HA	1:B:59:GLY:HA2	0.60	1.74	15	11
1:B:29:LEU:HD13	1:B:78:LEU:HG	0.60	1.72	20	5
1:A:41:HIS:H	1:A:41:HIS:CD2	0.60	2.15	10	5
1:B:43:LYS:HD2	1:B:54:TRP:O	0.60	1.96	4	5
1:A:65:TYR:CD2	1:B:40:ALA:HB2	0.60	2.32	6	2
1:A:10:ASN:O	1:A:75:TYR:N	0.60	2.35	13	8
1:A:13:MET:HB3	1:A:17:MET:HG3	0.60	1.71	16	1
1:B:78:LEU:O	1:B:80:GLN:N	0.60	2.34	3	12
1:A:5:LYS:O	1:A:6:ALA:HB2	0.60	1.97	3	3
1:B:44:LYS:HA	1:B:47:ASP:OD2	0.60	1.96	17	5
1:A:7:VAL:HG12	1:A:9:LYS:HE2	0.60	1.73	12	3
1:B:53:THR:HG22	1:B:55:HIS:CD2	0.60	2.32	13	2
1:A:13:MET:O	1:A:18:GLN:NE2	0.60	2.35	10	10
1:B:58:VAL:HG23	1:B:83:ILE:CD1	0.60	2.26	4	11
1:A:78:LEU:O	1:A:80:GLN:N	0.60	2.35	17	7
1:A:34:ILE:CB	1:A:37:ASP:HB2	0.60	2.27	15	3
1:A:44:LYS:HE2	1:A:44:LYS:HA	0.60	1.71	5	1
1:B:46:PHE:CE2	1:B:85:LEU:HD23	0.60	2.32	9	4
1:A:14:SER:OG	1:A:17:MET:HG3	0.60	1.97	12	2
1:A:55:HIS:ND1	1:B:67:THR:HB	0.60	2.12	15	1
1:A:25:ALA:HB2	1:A:83:ILE:HG21	0.60	1.74	17	10
1:B:21:SER:HB2	1:B:46:PHE:CZ	0.60	2.32	5	10
1:B:14:SER:O	1:B:17:MET:N	0.60	2.35	11	5
1:B:47:ASP:OD2	1:B:52:PRO:HA	0.60	1.97	12	1
1:B:69:GLU:O	1:B:70:THR:HG23	0.60	1.97	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:PHE:CD2	1:A:78:LEU:HD21	0.60	2.32	19	4
1:A:73:PHE:CG	1:A:74:ILE:N	0.59	2.70	2	2
1:B:13:MET:CG	1:B:17:MET:HB3	0.59	2.26	10	7
1:B:7:VAL:O	1:B:9:LYS:HE2	0.59	1.97	5	3
1:A:24:CYS:HA	1:A:27:GLN:HG3	0.59	1.73	13	1
1:A:80:GLN:O	1:A:80:GLN:HG3	0.59	1.97	1	1
1:B:81:VAL:CG1	1:B:82:ALA:N	0.59	2.65	7	20
1:B:47:ASP:HB2	1:B:52:PRO:CG	0.59	2.27	17	3
1:A:68:HIS:HB3	1:A:73:PHE:CD2	0.59	2.32	8	2
1:A:34:ILE:O	1:A:37:ASP:HB3	0.59	1.97	11	3
1:A:54:TRP:CH2	1:A:72:HIS:HB3	0.59	2.32	16	5
1:B:6:ALA:HB2	1:B:22:VAL:HG13	0.59	1.73	9	11
1:A:43:LYS:HB3	1:B:65:TYR:HD2	0.59	1.56	7	4
1:B:13:MET:HB2	1:B:71:LYS:O	0.59	1.97	6	4
1:B:39:ALA:HA	1:B:56:CYS:SG	0.59	2.37	7	2
1:A:65:TYR:HD2	1:B:43:LYS:HD3	0.59	1.56	7	1
1:A:64:SER:HB3	1:B:57:ILE:HD13	0.59	1.75	11	2
1:A:6:ALA:CA	1:A:78:LEU:HA	0.59	2.21	14	11
1:B:6:ALA:HB3	1:B:22:VAL:HG11	0.59	1.74	4	9
1:B:74:ILE:HG23	1:B:74:ILE:O	0.59	1.97	4	13
1:B:5:LYS:O	1:B:6:ALA:HB2	0.59	1.97	13	6
1:B:13:MET:O	1:B:18:GLN:NE2	0.59	2.36	13	16
1:B:13:MET:CG	1:B:14:SER:N	0.59	2.66	7	13
1:A:70:THR:HG21	1:A:87:LYS:HZ3	0.59	1.58	3	1
1:B:11:ALA:HA	1:B:73:PHE:O	0.59	1.97	8	2
1:A:84:LEU:HD21	1:A:86:PHE:CE2	0.59	2.31	4	1
1:A:29:LEU:CD2	1:A:81:VAL:HG11	0.59	2.20	13	1
1:B:8:ILE:HD12	1:B:76:PHE:CB	0.59	2.27	8	5
1:B:25:ALA:HB1	1:B:83:ILE:HD12	0.59	1.73	1	1
1:A:46:PHE:O	1:A:54:TRP:NE1	0.59	2.36	20	3
1:B:34:ILE:O	1:B:37:ASP:N	0.59	2.36	16	5
1:A:57:ILE:HG22	1:A:58:VAL:N	0.59	2.13	11	6
1:B:33:ASN:C	1:B:34:ILE:HD13	0.59	2.18	4	4
1:B:68:HIS:HB2	1:B:72:HIS:CA	0.59	2.27	7	3
1:B:58:VAL:CG2	1:B:81:VAL:HG11	0.59	2.26	7	3
1:A:10:ASN:O	1:A:11:ALA:HB2	0.59	1.96	2	3
1:B:51:ASN:N	1:B:51:ASN:HD22	0.59	1.94	4	1
1:B:73:PHE:HB2	1:B:86:PHE:HB3	0.59	1.72	7	2
1:A:75:TYR:CZ	1:A:84:LEU:HD13	0.59	2.33	8	1
1:A:62:PHE:HB2	1:B:62:PHE:CD2	0.59	2.32	13	1
1:A:41:HIS:N	1:A:41:HIS:CD2	0.59	2.70	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:GLU:O	1:A:17:MET:N	0.59	2.36	16	3
1:A:74:ILE:N	1:A:85:LEU:O	0.59	2.35	18	9
1:A:81:VAL:CG1	1:A:82:ALA:N	0.59	2.66	17	20
1:A:58:VAL:N	1:B:63:GLY:O	0.59	2.35	14	4
1:A:13:MET:SD	1:A:18:GLN:CA	0.59	2.91	10	2
1:B:6:ALA:N	1:B:78:LEU:HD13	0.59	2.13	6	1
1:B:34:ILE:O	1:B:38:ILE:HD12	0.59	1.98	7	1
1:A:13:MET:SD	1:A:18:GLN:HA	0.59	2.37	10	1
1:A:69:GLU:OE2	1:A:88:SER:HA	0.59	1.98	13	2
1:B:7:VAL:CG1	1:B:9:LYS:HE2	0.59	2.28	19	3
1:A:73:PHE:HB2	1:A:86:PHE:HB3	0.59	1.75	4	5
1:B:6:ALA:HB1	1:B:78:LEU:HD22	0.59	1.73	18	6
1:A:39:ALA:O	1:A:56:CYS:SG	0.59	2.61	8	3
1:B:41:HIS:NE2	1:B:45:GLU:OE2	0.59	2.36	19	1
1:A:62:PHE:CD2	1:A:63:GLY:N	0.59	2.71	1	1
1:B:41:HIS:CD2	1:B:41:HIS:H	0.59	2.14	18	9
1:A:9:LYS:CD	1:A:76:PHE:HA	0.59	2.28	2	1
1:A:41:HIS:CD2	1:A:41:HIS:H	0.59	2.16	17	5
1:B:28:ALA:HB3	1:B:38:ILE:CG2	0.59	2.28	16	17
1:A:62:PHE:CD1	1:A:63:GLY:N	0.59	2.71	12	3
1:B:49:LYS:HE3	1:B:50:TYR:OH	0.59	1.97	16	1
1:A:62:PHE:HE1	1:A:82:ALA:HB3	0.59	1.58	19	1
1:B:10:ASN:O	1:B:75:TYR:N	0.59	2.35	3	9
1:B:7:VAL:O	1:B:9:LYS:HG2	0.59	1.96	2	9
1:B:11:ALA:HB2	1:B:74:ILE:HG12	0.59	1.74	16	5
1:B:6:ALA:CA	1:B:78:LEU:HD13	0.58	2.28	18	4
1:B:55:HIS:HB2	1:B:86:PHE:CE2	0.58	2.33	8	5
1:A:25:ALA:HA	1:A:42:ILE:HD11	0.58	1.75	11	9
1:A:46:PHE:CE2	1:A:85:LEU:HD21	0.58	2.32	15	3
1:A:9:LYS:HE3	1:A:77:TYR:HB3	0.58	1.74	16	2
1:B:9:LYS:HB2	1:B:75:TYR:HD2	0.58	1.58	16	3
1:B:55:HIS:HB2	1:B:86:PHE:CZ	0.58	2.33	2	1
1:A:13:MET:SD	1:A:17:MET:CB	0.58	2.90	17	6
1:A:47:ASP:HA	1:A:54:TRP:HD1	0.58	1.58	15	6
1:A:58:VAL:HG23	1:A:82:ALA:O	0.58	1.98	4	1
1:A:34:ILE:CD1	1:A:34:ILE:N	0.58	2.66	5	1
1:B:70:THR:CG2	1:B:71:LYS:N	0.58	2.66	5	3
1:A:34:ILE:O	1:A:37:ASP:N	0.58	2.36	16	10
1:B:76:PHE:CE2	1:B:78:LEU:HD21	0.58	2.33	13	3
1:A:49:LYS:HD3	1:A:50:TYR:CE1	0.58	2.34	4	1
1:A:56:CYS:SG	1:A:57:ILE:N	0.58	2.76	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:THR:OG1	1:A:71:LYS:N	0.58	2.36	6	2
1:A:46:PHE:HA	1:A:50:TYR:CD2	0.58	2.33	7	3
1:B:6:ALA:HA	1:B:78:LEU:CA	0.58	2.21	7	2
1:A:69:GLU:O	1:A:70:THR:HG23	0.58	1.98	16	2
1:A:47:ASP:HB2	1:A:52:PRO:HB3	0.58	1.73	18	1
1:A:43:LYS:O	1:A:46:PHE:N	0.58	2.36	20	1
1:A:69:GLU:OE1	1:A:69:GLU:HA	0.58	1.97	3	1
1:B:13:MET:SD	1:B:18:GLN:CA	0.58	2.91	13	2
1:A:55:HIS:NE2	1:A:88:SER:CB	0.58	2.66	4	4
1:A:45:GLU:HG3	1:A:49:LYS:HG3	0.58	1.73	12	1
1:B:70:THR:OG1	1:B:71:LYS:N	0.58	2.36	15	3
1:A:38:ILE:HG21	1:A:58:VAL:HG21	0.58	1.74	19	2
1:A:54:TRP:CH2	1:A:72:HIS:ND1	0.58	2.72	18	1
1:A:61:ASN:O	1:B:60:ARG:NE	0.58	2.37	19	1
1:A:47:ASP:OD1	1:A:52:PRO:HG3	0.58	1.97	9	3
1:B:43:LYS:HG2	1:B:54:TRP:O	0.58	1.99	1	1
1:A:21:SER:HB2	1:A:46:PHE:CZ	0.58	2.34	7	6
1:A:86:PHE:CZ	1:B:55:HIS:ND1	0.58	2.72	9	1
1:B:14:SER:HB2	1:B:17:MET:CG	0.58	2.28	11	1
1:B:35:GLU:CA	1:B:38:ILE:HD12	0.58	2.28	17	1
1:A:39:ALA:HB1	1:A:56:CYS:SG	0.58	2.39	20	1
1:A:55:HIS:N	1:A:86:PHE:O	0.58	2.36	3	9
1:B:7:VAL:HG12	1:B:7:VAL:O	0.58	1.98	3	3
1:A:15:GLU:O	1:A:18:GLN:N	0.58	2.37	16	6
1:B:48:LYS:HG3	1:B:49:LYS:N	0.58	2.14	11	2
1:A:35:GLU:N	1:A:35:GLU:CD	0.58	2.56	18	1
1:B:17:MET:O	1:B:21:SER:HB3	0.58	1.98	18	4
1:A:54:TRP:HA	1:A:87:LYS:HG2	0.58	1.74	16	1
1:B:47:ASP:OD1	1:B:48:LYS:N	0.58	2.37	15	3
1:A:55:HIS:HB3	1:B:66:VAL:HA	0.58	1.76	8	4
1:B:75:TYR:CD1	1:B:84:LEU:HB2	0.58	2.34	13	3
1:B:34:ILE:O	1:B:38:ILE:HG13	0.58	1.98	6	5
1:A:58:VAL:O	1:A:58:VAL:HG13	0.58	1.98	11	5
1:B:52:PRO:C	1:B:87:LYS:HZ1	0.58	2.01	17	1
1:A:13:MET:CG	1:A:14:SER:N	0.58	2.67	11	16
1:A:84:LEU:HD22	1:B:57:ILE:CD1	0.58	2.28	19	4
1:A:12:ASP:HB2	1:A:72:HIS:HB3	0.58	1.75	6	3
1:A:74:ILE:HG23	1:A:74:ILE:O	0.58	1.96	8	5
1:B:15:GLU:CA	1:B:18:GLN:NE2	0.58	2.66	11	1
1:A:43:LYS:HG3	1:A:54:TRP:O	0.58	1.99	14	4
1:B:55:HIS:CD2	1:B:87:LYS:HA	0.58	2.34	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:TYR:CE1	1:B:43:LYS:HB3	0.58	2.33	1	1
1:A:11:ALA:HB1	1:A:74:ILE:HG13	0.58	1.76	19	8
1:B:75:TYR:HD1	1:B:76:PHE:N	0.58	1.96	8	2
1:A:35:GLU:OE2	1:A:60:ARG:HD3	0.58	1.98	11	2
1:A:13:MET:HG2	1:A:17:MET:HB2	0.57	1.75	2	5
1:A:37:ASP:O	1:A:41:HIS:NE2	0.57	2.37	16	7
1:B:6:ALA:CA	1:B:78:LEU:HA	0.57	2.23	7	5
1:B:10:ASN:O	1:B:11:ALA:HB3	0.57	1.98	8	4
1:B:72:HIS:CD2	1:B:87:LYS:HD3	0.57	2.34	8	1
1:A:7:VAL:N	1:A:77:TYR:O	0.57	2.36	20	8
1:A:28:ALA:HB1	1:A:38:ILE:CA	0.57	2.26	19	5
1:A:70:THR:CG2	1:A:87:LYS:HZ3	0.57	2.12	3	1
1:B:57:ILE:O	1:B:84:LEU:N	0.57	2.37	3	3
1:B:68:HIS:ND1	1:B:69:GLU:N	0.57	2.52	9	2
1:B:77:TYR:OH	1:B:80:GLN:HA	0.57	1.99	14	4
1:A:55:HIS:CB	1:B:66:VAL:HB	0.57	2.28	20	2
1:A:34:ILE:O	1:A:36:LYS:HG3	0.57	1.98	18	2
1:B:18:GLN:CB	1:B:74:ILE:HD12	0.57	2.28	1	5
1:B:55:HIS:CE1	1:B:88:SER:H	0.57	2.18	1	1
1:B:74:ILE:HD13	1:B:76:PHE:CD1	0.57	2.33	17	13
1:B:13:MET:SD	1:B:17:MET:CB	0.57	2.91	4	4
1:B:71:LYS:O	1:B:73:PHE:N	0.57	2.37	19	3
1:B:30:GLU:OE1	1:B:31:LYS:HD2	0.57	1.99	10	1
1:A:14:SER:O	1:A:16:GLU:N	0.57	2.37	16	1
1:A:43:LYS:HD3	1:A:54:TRP:HB2	0.57	1.75	16	1
1:A:5:LYS:O	1:A:6:ALA:HB3	0.57	1.99	17	1
1:A:55:HIS:CD2	1:A:55:HIS:N	0.57	2.72	8	2
1:B:27:GLN:O	1:B:30:GLU:HG3	0.57	1.99	17	2
1:B:8:ILE:CA	1:B:76:PHE:HB3	0.57	2.30	12	9
1:A:77:TYR:HE1	1:A:80:GLN:HA	0.57	1.59	12	1
1:B:4:ARG:NH1	1:B:4:ARG:HG2	0.57	2.14	15	1
1:A:46:PHE:O	1:A:50:TYR:HB2	0.57	1.99	16	3
1:A:35:GLU:HG2	1:A:59:GLY:HA2	0.57	1.76	16	3
1:B:12:ASP:HB2	1:B:72:HIS:CB	0.57	2.27	11	3
1:B:4:ARG:HD2	1:B:19:GLN:OE1	0.57	1.99	18	1
1:A:73:PHE:HB3	1:A:86:PHE:HB2	0.57	1.75	8	2
1:B:6:ALA:HB2	1:B:22:VAL:CG1	0.57	2.29	12	7
1:A:21:SER:HB2	1:A:85:LEU:CD2	0.57	2.25	4	2
1:A:49:LYS:HD3	1:A:50:TYR:CZ	0.57	2.34	4	1
1:B:74:ILE:HG22	1:B:85:LEU:CB	0.57	2.30	14	5
1:B:34:ILE:N	1:B:34:ILE:CD1	0.57	2.68	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:MET:SD	1:A:17:MET:O	0.57	2.62	16	1
1:B:46:PHE:CD2	1:B:85:LEU:HD21	0.57	2.34	19	5
1:A:13:MET:HA	1:A:71:LYS:C	0.57	2.20	2	1
1:B:25:ALA:CB	1:B:83:ILE:HG21	0.57	2.29	16	10
1:B:23:GLU:O	1:B:27:GLN:HG3	0.57	2.00	11	3
1:A:39:ALA:HA	1:A:42:ILE:HD12	0.57	1.76	13	2
1:A:8:ILE:CA	1:A:76:PHE:HB3	0.57	2.30	6	8
1:A:57:ILE:HG12	1:A:84:LEU:CD2	0.57	2.28	9	2
1:B:70:THR:HG23	1:B:71:LYS:H	0.57	1.59	2	3
1:A:65:TYR:OH	1:B:44:LYS:HE2	0.57	2.00	4	1
1:A:14:SER:HB2	1:A:17:MET:CG	0.56	2.30	11	3
1:A:59:GLY:O	1:A:82:ALA:N	0.56	2.37	1	4
1:A:15:GLU:HA	1:A:18:GLN:CG	0.56	2.30	10	9
1:B:20:ASP:O	1:B:24:CYS:SG	0.56	2.62	5	1
1:A:18:GLN:CB	1:A:74:ILE:HG13	0.56	2.30	10	2
1:A:34:ILE:O	1:A:38:ILE:HG13	0.56	2.00	6	1
1:A:14:SER:HB3	1:A:17:MET:HB3	0.56	1.76	10	1
1:A:65:TYR:N	1:B:56:CYS:O	0.56	2.38	16	3
1:B:53:THR:HG22	1:B:55:HIS:CE1	0.56	2.35	15	1
1:A:55:HIS:HD1	1:B:66:VAL:HB	0.56	1.59	17	1
1:B:8:ILE:HG13	1:B:75:TYR:O	0.56	2.00	6	6
1:A:73:PHE:CD2	1:A:86:PHE:HB3	0.56	2.36	5	2
1:B:11:ALA:CB	1:B:18:GLN:NE2	0.56	2.68	5	3
1:B:75:TYR:HE1	1:B:84:LEU:HB2	0.56	1.59	7	4
1:B:39:ALA:N	1:B:58:VAL:CG1	0.56	2.69	9	12
1:A:43:LYS:CE	1:A:43:LYS:HA	0.56	2.30	5	1
1:A:43:LYS:HD2	1:B:65:TYR:CE2	0.56	2.35	7	2
1:A:86:PHE:CE1	1:B:55:HIS:ND1	0.56	2.73	9	1
1:B:68:HIS:C	1:B:69:GLU:HG2	0.56	2.19	4	10
1:A:11:ALA:HA	1:A:73:PHE:CD1	0.56	2.35	2	1
1:A:62:PHE:CE1	1:A:64:SER:HB3	0.56	2.35	12	4
1:A:64:SER:HB2	1:A:84:LEU:HD13	0.56	1.77	11	4
1:A:66:VAL:HG22	1:A:84:LEU:HD11	0.56	1.78	4	1
1:A:12:ASP:H	1:A:73:PHE:HD1	0.56	1.43	5	1
1:A:69:GLU:HG3	1:A:88:SER:OG	0.56	1.99	9	2
1:A:47:ASP:HB3	1:A:52:PRO:CB	0.56	2.30	20	1
1:A:13:MET:HG2	1:A:18:GLN:OE1	0.56	2.01	18	1
1:B:32:TYR:CD1	1:B:41:HIS:CE1	0.56	2.94	5	9
1:A:13:MET:HG3	1:A:71:LYS:O	0.56	2.01	2	1
1:B:10:ASN:HB3	1:B:75:TYR:CB	0.56	2.27	2	1
1:A:67:THR:CB	1:B:53:THR:HG21	0.56	2.30	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:51:ASN:O	1:B:87:LYS:HE2	0.56	2.01	17	2
1:A:6:ALA:HA	1:A:78:LEU:CA	0.56	2.23	17	4
1:B:14:SER:CB	1:B:17:MET:HB3	0.56	2.31	13	1
1:B:80:GLN:HE21	1:B:80:GLN:HA	0.56	1.60	20	1
1:B:17:MET:HE1	1:B:50:TYR:CE2	0.56	2.36	19	3
1:A:8:ILE:C	1:A:9:LYS:HD2	0.56	2.21	2	1
1:B:11:ALA:HB1	1:B:74:ILE:HG13	0.56	1.78	12	11
1:A:77:TYR:HA	1:A:81:VAL:O	0.56	2.01	2	9
1:A:78:LEU:N	1:A:78:LEU:CD2	0.56	2.69	13	9
1:A:51:ASN:O	1:A:54:TRP:NE1	0.56	2.39	17	8
1:B:58:VAL:HB	1:B:83:ILE:HG23	0.56	1.77	3	8
1:A:79:GLY:O	1:A:80:GLN:HB2	0.56	2.00	20	4
1:A:68:HIS:HB2	1:A:72:HIS:C	0.56	2.20	6	2
1:A:38:ILE:O	1:A:42:ILE:HD12	0.56	2.01	15	3
1:A:54:TRP:CH2	1:A:87:LYS:HD2	0.56	2.36	10	1
1:A:70:THR:HG23	1:A:71:LYS:H	0.56	1.60	14	2
1:B:41:HIS:CD2	1:B:41:HIS:N	0.56	2.73	11	9
1:B:57:ILE:HG22	1:B:58:VAL:N	0.56	2.16	19	4
1:A:14:SER:OG	1:A:71:LYS:NZ	0.56	2.35	7	1
1:A:57:ILE:CG1	1:A:84:LEU:HB3	0.56	2.29	18	3
1:A:54:TRP:CE2	1:A:87:LYS:HE3	0.56	2.36	10	1
1:B:47:ASP:HB3	1:B:52:PRO:HB3	0.56	1.77	20	1
1:B:62:PHE:CD2	1:B:63:GLY:N	0.56	2.73	20	1
1:A:40:ALA:HA	1:B:65:TYR:CZ	0.56	2.35	2	13
1:A:41:HIS:CD2	1:A:41:HIS:C	0.56	2.79	20	8
1:A:54:TRP:CZ2	1:A:87:LYS:HD3	0.56	2.36	15	2
1:A:14:SER:CB	1:A:17:MET:HG3	0.56	2.30	9	1
1:A:11:ALA:CB	1:A:18:GLN:NE2	0.56	2.68	15	5
1:A:68:HIS:HB3	1:A:86:PHE:CD2	0.56	2.36	12	1
1:A:29:LEU:HD21	1:A:81:VAL:CG1	0.56	2.20	13	1
1:A:10:ASN:HB3	1:A:75:TYR:CB	0.56	2.31	18	1
1:A:35:GLU:HB3	1:B:62:PHE:C	0.56	2.20	14	4
1:A:62:PHE:C	1:B:35:GLU:HB3	0.56	2.22	13	8
1:B:32:TYR:CG	1:B:41:HIS:CE1	0.56	2.94	11	9
1:B:84:LEU:O	1:B:84:LEU:HG	0.56	1.99	8	4
1:A:5:LYS:O	1:A:5:LYS:HG3	0.56	2.00	2	1
1:A:32:TYR:CD1	1:A:41:HIS:CE1	0.56	2.94	16	12
1:A:35:GLU:C	1:B:63:GLY:HA3	0.56	2.21	2	5
1:A:41:HIS:CD2	1:A:41:HIS:N	0.56	2.74	4	10
1:A:65:TYR:CE2	1:B:43:LYS:HE3	0.56	2.36	2	4
1:B:12:ASP:HB3	1:B:72:HIS:ND1	0.56	2.16	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:55:HIS:HE1	1:B:88:SER:HB2	0.56	1.60	12	1
1:A:46:PHE:CD2	1:A:54:TRP:CZ3	0.55	2.95	4	14
1:A:63:GLY:O	1:B:39:ALA:HB2	0.55	2.01	14	8
1:B:18:GLN:O	1:B:74:ILE:HD12	0.55	2.02	17	8
1:B:77:TYR:CD2	1:B:82:ALA:HB2	0.55	2.37	18	3
1:A:62:PHE:HD1	1:A:63:GLY:N	0.55	1.98	12	1
1:A:66:VAL:CA	1:B:55:HIS:HB3	0.55	2.31	14	3
1:A:18:GLN:HB3	1:A:74:ILE:HD12	0.55	1.78	14	1
1:B:56:CYS:HB3	1:B:85:LEU:CG	0.55	2.31	14	1
1:B:71:LYS:HD2	1:B:72:HIS:NE2	0.55	2.16	2	1
1:A:8:ILE:O	1:A:9:LYS:HG2	0.55	2.01	5	1
1:A:39:ALA:H	1:A:58:VAL:HG11	0.55	1.62	18	2
1:A:43:LYS:CA	1:A:56:CYS:SG	0.55	2.94	14	2
1:B:53:THR:HG22	1:B:55:HIS:NE2	0.55	2.16	14	1
1:A:13:MET:HG2	1:A:17:MET:HB3	0.55	1.77	1	6
1:A:8:ILE:HD11	1:A:22:VAL:CG2	0.55	2.31	4	2
1:B:14:SER:HB2	1:B:17:MET:HG3	0.55	1.78	18	2
1:B:15:GLU:CA	1:B:18:GLN:HG3	0.55	2.29	15	1
1:B:12:ASP:HB2	1:B:73:PHE:CE1	0.55	2.37	16	1
1:A:16:GLU:CA	1:A:19:GLN:HG2	0.55	2.31	15	2
1:A:14:SER:O	1:A:17:MET:N	0.55	2.39	3	6
1:B:72:HIS:HB2	1:B:87:LYS:HG3	0.55	1.77	13	2
1:B:66:VAL:HG11	1:B:86:PHE:CZ	0.55	2.37	17	1
1:A:25:ALA:CB	1:A:83:ILE:HG21	0.55	2.31	2	11
1:A:35:GLU:O	1:A:58:VAL:HG13	0.55	2.01	19	4
1:B:69:GLU:HG3	1:B:88:SER:HA	0.55	1.77	20	6
1:A:34:ILE:C	1:A:38:ILE:HD12	0.55	2.22	3	1
1:A:78:LEU:HD23	1:A:83:ILE:HG12	0.55	1.78	19	5
1:A:57:ILE:HG12	1:B:64:SER:CA	0.55	2.30	4	1
1:A:76:PHE:CE2	1:A:83:ILE:HB	0.55	2.36	9	3
1:B:68:HIS:CE1	1:B:70:THR:HB	0.55	2.36	4	1
1:B:68:HIS:ND1	1:B:87:LYS:O	0.55	2.40	4	1
1:A:62:PHE:CD2	1:B:62:PHE:HB2	0.55	2.36	14	2
1:B:13:MET:SD	1:B:71:LYS:CG	0.55	2.94	11	1
1:B:9:LYS:CD	1:B:76:PHE:HA	0.55	2.32	14	1
1:A:65:TYR:CZ	1:B:40:ALA:HA	0.55	2.37	14	9
1:B:80:GLN:O	1:B:81:VAL:HG23	0.55	2.01	7	5
1:B:43:LYS:HD3	1:B:47:ASP:OD2	0.55	2.02	20	2
1:A:13:MET:SD	1:A:72:HIS:CA	0.55	2.95	15	4
1:B:72:HIS:ND1	1:B:87:LYS:HD3	0.55	2.17	3	1
1:A:43:LYS:HA	1:A:56:CYS:SG	0.55	2.42	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ASP:HB2	1:A:72:HIS:CB	0.55	2.31	6	1
1:A:43:LYS:NZ	1:A:47:ASP:HB2	0.55	2.17	6	1
1:B:68:HIS:HB2	1:B:72:HIS:C	0.55	2.22	16	3
1:A:48:LYS:HG3	1:A:48:LYS:O	0.55	2.02	13	2
1:B:12:ASP:HB2	1:B:73:PHE:HD2	0.55	1.62	13	1
1:A:29:LEU:HD22	1:A:81:VAL:HG21	0.55	1.79	17	1
1:A:49:LYS:HE2	1:A:50:TYR:CZ	0.55	2.37	20	1
1:A:34:ILE:O	1:A:35:GLU:C	0.55	2.44	5	18
1:B:76:PHE:CD2	1:B:78:LEU:HD21	0.55	2.36	3	2
1:B:9:LYS:HE3	1:B:77:TYR:HB3	0.55	1.79	4	2
1:A:18:GLN:HA	1:A:21:SER:OG	0.55	2.01	5	1
1:B:4:ARG:HH22	1:B:8:ILE:HD13	0.55	1.61	5	1
1:A:7:VAL:O	1:A:9:LYS:HG2	0.55	2.02	18	4
1:A:6:ALA:HB1	1:A:76:PHE:CD2	0.55	2.37	16	2
1:A:43:LYS:HD2	1:A:43:LYS:O	0.55	2.02	16	1
1:B:46:PHE:CD2	1:B:54:TRP:CE3	0.55	2.95	4	13
1:A:12:ASP:O	1:A:72:HIS:HB2	0.55	2.02	11	6
1:A:38:ILE:CG2	1:A:42:ILE:HD11	0.55	2.30	5	3
1:A:57:ILE:HG22	1:A:58:VAL:H	0.55	1.60	7	4
1:B:13:MET:SD	1:B:71:LYS:HB3	0.55	2.42	19	3
1:A:6:ALA:CB	1:A:22:VAL:HG13	0.55	2.32	9	6
1:B:13:MET:SD	1:B:72:HIS:CA	0.55	2.94	1	1
1:B:46:PHE:CD1	1:B:50:TYR:CE1	0.55	2.95	1	5
1:A:57:ILE:CD1	1:B:64:SER:HB2	0.55	2.22	12	3
1:A:57:ILE:HG12	1:B:65:TYR:N	0.55	2.17	4	1
1:A:55:HIS:HB2	1:A:86:PHE:CD2	0.55	2.37	7	1
1:A:25:ALA:HB1	1:A:83:ILE:HG13	0.55	1.78	9	1
1:B:8:ILE:O	1:B:9:LYS:HE3	0.55	2.02	16	1
1:A:46:PHE:CD2	1:A:54:TRP:CE3	0.54	2.95	20	12
1:A:55:HIS:CB	1:B:66:VAL:HG12	0.54	2.31	9	4
1:B:18:GLN:HB3	1:B:74:ILE:HD12	0.54	1.79	1	1
1:B:46:PHE:CD2	1:B:50:TYR:CE2	0.54	2.95	9	5
1:B:46:PHE:CD2	1:B:54:TRP:CZ3	0.54	2.95	11	9
1:B:73:PHE:HB3	1:B:86:PHE:CB	0.54	2.32	11	3
1:A:65:TYR:N	1:B:57:ILE:HD13	0.54	2.13	7	2
1:B:43:LYS:CB	1:B:56:CYS:SG	0.54	2.95	14	5
1:B:34:ILE:HG22	1:B:36:LYS:HG3	0.54	1.79	12	3
1:B:70:THR:HG22	1:B:71:LYS:H	0.54	1.60	16	3
1:B:78:LEU:N	1:B:78:LEU:CD2	0.54	2.70	4	8
1:B:78:LEU:O	1:B:79:GLY:C	0.54	2.45	6	20
1:A:8:ILE:CG2	1:A:9:LYS:N	0.54	2.70	15	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:TYR:CG	1:A:41:HIS:CE1	0.54	2.95	10	9
1:A:50:TYR:O	1:A:51:ASN:ND2	0.54	2.40	17	1
1:A:13:MET:N	1:A:18:GLN:HE22	0.54	1.99	18	1
1:A:42:ILE:HG21	1:A:85:LEU:CD1	0.54	2.31	19	2
1:A:59:GLY:O	1:A:82:ALA:HB3	0.54	2.02	8	3
1:B:68:HIS:HE2	1:B:87:LYS:H	0.54	1.45	9	1
1:B:73:PHE:CD1	1:B:75:TYR:CE1	0.54	2.96	20	1
1:A:39:ALA:N	1:A:58:VAL:CG1	0.54	2.70	19	8
1:A:42:ILE:HG22	1:A:85:LEU:HD11	0.54	1.80	4	3
1:A:57:ILE:CG2	1:A:58:VAL:N	0.54	2.71	4	2
1:A:67:THR:CG2	1:A:68:HIS:N	0.54	2.70	18	3
1:B:5:LYS:HA	1:B:5:LYS:CE	0.54	2.33	4	1
1:A:35:GLU:HG2	1:B:61:ASN:O	0.54	2.02	7	3
1:B:28:ALA:CB	1:B:38:ILE:HA	0.54	2.23	7	1
1:A:13:MET:HB3	1:A:17:MET:CG	0.54	2.32	16	1
1:B:47:ASP:CB	1:B:52:PRO:HB3	0.54	2.32	17	2
1:B:35:GLU:OE2	1:B:59:GLY:HA2	0.54	2.02	2	1
1:B:38:ILE:CG2	1:B:42:ILE:HD11	0.54	2.32	7	1
1:A:26:THR:N	1:A:29:LEU:HD12	0.54	2.17	10	1
1:A:48:LYS:HA	1:A:48:LYS:CE	0.54	2.32	11	1
1:B:11:ALA:HB1	1:B:18:GLN:HG2	0.54	1.80	11	1
1:A:46:PHE:CE2	1:A:54:TRP:CZ3	0.54	2.96	12	7
1:A:86:PHE:CZ	1:B:86:PHE:CZ	0.54	2.95	17	10
1:A:28:ALA:HA	1:A:32:TYR:CD1	0.54	2.37	17	4
1:B:54:TRP:CG	1:B:87:LYS:HD2	0.54	2.37	12	2
1:A:54:TRP:HA	1:A:87:LYS:HG3	0.54	1.78	18	2
1:B:38:ILE:HG22	1:B:42:ILE:CD1	0.54	2.33	7	3
1:B:4:ARG:O	1:B:5:LYS:HB3	0.54	2.03	8	1
1:B:46:PHE:CE2	1:B:50:TYR:CE2	0.54	2.96	9	2
1:B:43:LYS:CA	1:B:56:CYS:SG	0.54	2.95	14	3
1:B:78:LEU:HB2	1:B:81:VAL:HB	0.54	1.79	13	1
1:A:23:GLU:O	1:A:27:GLN:HG2	0.54	2.03	20	2
1:A:68:HIS:CG	1:A:73:PHE:CD2	0.54	2.96	1	4
1:B:41:HIS:CD2	1:B:41:HIS:C	0.54	2.81	2	11
1:A:6:ALA:HB2	1:A:22:VAL:HG13	0.54	1.80	6	7
1:A:57:ILE:CB	1:A:84:LEU:HD23	0.54	2.32	9	7
1:B:52:PRO:CB	1:B:53:THR:HA	0.54	2.32	13	4
1:B:18:GLN:CG	1:B:74:ILE:HG13	0.54	2.32	11	1
1:B:68:HIS:CD2	1:B:73:PHE:CD2	0.54	2.96	17	1
1:B:61:ASN:OD1	1:B:61:ASN:N	0.54	2.40	19	1
1:B:11:ALA:HB2	1:B:74:ILE:HG13	0.54	1.79	1	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:39:ALA:CA	1:B:58:VAL:HG12	0.54	2.33	15	4
1:A:75:TYR:N	1:A:75:TYR:CD1	0.54	2.76	8	1
1:A:46:PHE:CD2	1:A:50:TYR:CE2	0.54	2.96	12	1
1:B:73:PHE:CD1	1:B:73:PHE:C	0.54	2.81	20	2
1:A:46:PHE:CD1	1:A:50:TYR:CD2	0.54	2.96	15	1
1:A:39:ALA:HB2	1:B:63:GLY:O	0.54	2.03	12	5
1:B:46:PHE:CE1	1:B:50:TYR:CZ	0.54	2.96	19	2
1:B:46:PHE:CD1	1:B:54:TRP:CZ3	0.54	2.96	14	2
1:A:43:LYS:CE	1:A:54:TRP:HB3	0.54	2.32	5	1
1:B:6:ALA:CB	1:B:22:VAL:HG13	0.54	2.33	6	5
1:A:35:GLU:HB3	1:B:62:PHE:O	0.54	2.03	14	1
1:A:17:MET:HE1	1:A:54:TRP:CH2	0.54	2.38	1	1
1:B:46:PHE:CD1	1:B:50:TYR:CD1	0.54	2.96	5	4
1:B:68:HIS:O	1:B:69:GLU:HG2	0.54	2.03	1	2
1:A:28:ALA:O	1:A:32:TYR:HD1	0.54	1.86	18	16
1:B:32:TYR:CD1	1:B:41:HIS:ND1	0.54	2.76	5	4
1:A:46:PHE:CD1	1:A:54:TRP:CZ3	0.54	2.95	15	2
1:A:57:ILE:HG13	1:A:84:LEU:CD2	0.54	2.31	18	2
1:B:35:GLU:HG3	1:B:58:VAL:O	0.54	2.03	6	1
1:B:54:TRP:CD1	1:B:87:LYS:HE2	0.54	2.38	8	1
1:B:4:ARG:HH11	1:B:19:GLN:HG3	0.54	1.63	12	1
1:A:28:ALA:O	1:A:38:ILE:HG12	0.54	2.03	16	2
1:A:58:VAL:HG23	1:A:81:VAL:CG1	0.54	2.33	14	1
1:A:13:MET:CG	1:A:17:MET:HB3	0.53	2.33	1	7
1:A:36:LYS:HB2	1:A:36:LYS:HZ2	0.53	1.61	2	1
1:B:47:ASP:HB3	1:B:52:PRO:CB	0.53	2.33	20	2
1:B:46:PHE:CE2	1:B:54:TRP:CZ3	0.53	2.96	8	6
1:A:34:ILE:CG2	1:A:37:ASP:HB2	0.53	2.33	15	3
1:A:35:GLU:HG2	1:B:62:PHE:C	0.53	2.23	11	1
1:B:87:LYS:HE2	1:B:89:GLY:O	0.53	2.04	12	1
1:A:37:ASP:OD1	1:A:38:ILE:N	0.53	2.40	17	1
1:B:17:MET:HE1	1:B:50:TYR:CE1	0.53	2.38	18	1
1:B:54:TRP:CE2	1:B:87:LYS:CD	0.53	2.92	12	16
1:A:35:GLU:CD	1:A:35:GLU:H	0.53	2.06	6	3
1:B:73:PHE:HB3	1:B:86:PHE:HB2	0.53	1.79	4	5
1:A:12:ASP:HB2	1:A:73:PHE:CD1	0.53	2.38	5	1
1:B:56:CYS:HB3	1:B:85:LEU:HG	0.53	1.78	14	1
1:B:69:GLU:O	1:B:71:LYS:N	0.53	2.41	17	1
1:B:56:CYS:SG	1:B:85:LEU:CD1	0.53	2.96	1	5
1:A:67:THR:HB	1:B:53:THR:CG2	0.53	2.32	8	2
1:A:78:LEU:CD2	1:A:78:LEU:H	0.53	2.17	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:4:ARG:NH2	1:B:8:ILE:HD13	0.53	2.18	5	2
1:B:70:THR:HG23	1:B:71:LYS:CG	0.53	2.21	5	1
1:A:55:HIS:HE1	1:A:88:SER:HB2	0.53	1.64	9	1
1:B:27:GLN:HG3	1:B:28:ALA:H	0.53	1.63	18	1
1:B:17:MET:HE1	1:B:50:TYR:CD2	0.53	2.38	14	2
1:B:12:ASP:HB3	1:B:72:HIS:CB	0.53	2.32	20	2
1:A:73:PHE:HA	1:A:86:PHE:CA	0.53	2.28	18	2
1:B:67:THR:HG22	1:B:67:THR:O	0.53	2.03	11	2
1:A:55:HIS:HE2	1:A:88:SER:CB	0.53	2.17	14	3
1:A:43:LYS:NZ	1:A:47:ASP:CB	0.53	2.71	6	1
1:B:73:PHE:CG	1:B:74:ILE:N	0.53	2.75	6	1
1:A:35:GLU:HG3	1:A:58:VAL:O	0.53	2.03	11	1
1:A:11:ALA:HB1	1:A:18:GLN:CD	0.53	2.24	14	1
1:A:56:CYS:HB3	1:A:85:LEU:HG	0.53	1.81	16	2
1:A:62:PHE:HA	1:B:35:GLU:HG2	0.53	1.79	1	2
1:B:32:TYR:HE1	1:B:41:HIS:ND1	0.53	2.02	2	3
1:B:68:HIS:HB3	1:B:73:PHE:CG	0.53	2.39	5	3
1:A:32:TYR:CD1	1:A:32:TYR:N	0.53	2.77	5	4
1:A:43:LYS:NZ	1:A:54:TRP:HB3	0.53	2.19	5	1
1:A:29:LEU:HD13	1:A:78:LEU:CD1	0.53	2.34	6	1
1:B:13:MET:CB	1:B:72:HIS:HA	0.53	2.30	13	2
1:B:20:ASP:HA	1:B:23:GLU:OE1	0.53	2.04	11	1
1:A:17:MET:SD	1:A:46:PHE:CE2	0.53	3.01	16	1
1:A:43:LYS:C	1:A:43:LYS:HD3	0.53	2.23	1	2
1:A:57:ILE:N	1:A:84:LEU:O	0.53	2.41	15	5
1:A:87:LYS:HB3	1:A:87:LYS:NZ	0.53	2.19	5	1
1:A:75:TYR:CE1	1:A:84:LEU:HD13	0.53	2.39	8	1
1:B:4:ARG:HG2	1:B:4:ARG:NH1	0.53	2.19	12	1
1:B:37:ASP:C	1:B:41:HIS:CE1	0.53	2.82	8	8
1:A:76:PHE:HE2	1:A:78:LEU:HD21	0.53	1.61	16	2
1:A:54:TRP:HA	1:A:87:LYS:CB	0.53	2.33	17	3
1:A:43:LYS:HB2	1:B:65:TYR:HD2	0.53	1.63	12	1
1:B:9:LYS:HE2	1:B:77:TYR:CB	0.53	2.34	14	1
1:A:7:VAL:O	1:A:7:VAL:HG12	0.53	2.03	2	1
1:A:46:PHE:HD2	1:A:54:TRP:CE3	0.53	2.22	2	5
1:A:68:HIS:CE1	1:A:88:SER:HA	0.53	2.38	2	1
1:B:24:CYS:SG	1:B:42:ILE:HG23	0.53	2.44	11	2
1:B:51:ASN:ND2	1:B:51:ASN:O	0.53	2.42	4	1
1:A:29:LEU:O	1:A:33:ASN:ND2	0.53	2.42	12	1
1:B:73:PHE:HD2	1:B:86:PHE:HB3	0.53	1.62	14	1
1:B:68:HIS:HB3	1:B:73:PHE:HD2	0.53	1.59	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:35:GLU:HG2	1:B:59:GLY:HA2	0.53	1.81	9	4
1:A:56:CYS:SG	1:A:85:LEU:CD1	0.53	2.97	6	4
1:A:68:HIS:HB3	1:A:86:PHE:CB	0.53	2.34	12	1
1:B:17:MET:HE3	1:B:50:TYR:CE1	0.53	2.39	13	1
1:B:75:TYR:HD1	1:B:84:LEU:HD12	0.53	1.64	14	1
1:A:8:ILE:CG1	1:A:74:ILE:HD11	0.53	2.34	16	1
1:A:37:ASP:CG	1:A:41:HIS:CE1	0.53	2.83	17	1
1:A:65:TYR:CB	1:B:39:ALA:HB1	0.52	2.34	7	6
1:A:43:LYS:CD	1:A:54:TRP:HB2	0.52	2.35	6	1
1:A:38:ILE:CB	1:A:58:VAL:HG11	0.52	2.34	19	2
1:A:72:HIS:CD2	1:A:87:LYS:NZ	0.52	2.78	16	1
1:A:32:TYR:CE1	1:A:41:HIS:HB2	0.52	2.39	9	4
1:A:17:MET:HE1	1:A:50:TYR:CD1	0.52	2.39	2	1
1:B:8:ILE:O	1:B:9:LYS:HG2	0.52	2.03	10	3
1:A:17:MET:SD	1:A:54:TRP:CH2	0.52	3.01	10	1
1:A:72:HIS:HB2	1:A:87:LYS:CD	0.52	2.34	16	1
1:B:55:HIS:O	1:B:86:PHE:CD1	0.52	2.63	18	5
1:B:77:TYR:CD1	1:B:81:VAL:O	0.52	2.63	17	4
1:A:32:TYR:CE2	1:A:41:HIS:CE1	0.52	2.97	17	2
1:B:68:HIS:ND1	1:B:70:THR:N	0.52	2.57	9	1
1:B:75:TYR:N	1:B:75:TYR:CD1	0.52	2.77	20	1
1:A:63:GLY:HA3	1:B:35:GLU:CB	0.52	2.34	17	12
1:B:57:ILE:O	1:B:83:ILE:HA	0.52	2.04	14	5
1:A:62:PHE:CD2	1:B:62:PHE:CD2	0.52	2.98	15	1
1:B:68:HIS:CD2	1:B:72:HIS:ND1	0.52	2.77	16	1
1:A:55:HIS:CD2	1:A:55:HIS:H	0.52	2.22	20	1
1:A:77:TYR:CD1	1:A:78:LEU:O	0.52	2.63	4	7
1:A:37:ASP:O	1:A:41:HIS:CD2	0.52	2.63	13	11
1:A:37:ASP:C	1:A:41:HIS:CE1	0.52	2.83	10	10
1:B:77:TYR:CD1	1:B:78:LEU:O	0.52	2.63	16	5
1:A:63:GLY:N	1:B:35:GLU:CB	0.52	2.72	10	3
1:A:65:TYR:HE2	1:B:43:LYS:HB3	0.52	1.64	16	3
1:A:77:TYR:O	1:A:77:TYR:CD1	0.52	2.63	15	4
1:A:8:ILE:HG13	1:A:75:TYR:O	0.52	2.05	8	2
1:B:9:LYS:HE2	1:B:77:TYR:HB3	0.52	1.81	14	1
1:A:72:HIS:HB2	1:A:87:LYS:CB	0.52	2.33	18	1
1:A:12:ASP:HB2	1:A:73:PHE:CD2	0.52	2.38	13	4
1:A:65:TYR:HB3	1:B:39:ALA:CB	0.52	2.33	1	2
1:A:55:HIS:O	1:A:86:PHE:CD2	0.52	2.63	11	3
1:B:71:LYS:NZ	1:B:71:LYS:HB3	0.52	2.18	3	1
1:A:43:LYS:HA	1:A:43:LYS:HE2	0.52	1.82	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:ASN:O	1:A:11:ALA:HB3	0.52	2.05	7	2
1:A:46:PHE:HD2	1:A:54:TRP:CZ3	0.52	2.22	7	2
1:B:46:PHE:HD2	1:B:54:TRP:CE3	0.52	2.22	9	6
1:A:46:PHE:CD2	1:A:50:TYR:CE1	0.52	2.97	10	1
1:A:43:LYS:C	1:A:43:LYS:HE2	0.52	2.25	11	1
1:B:57:ILE:HB	1:B:84:LEU:CD2	0.52	2.35	13	4
1:A:71:LYS:O	1:A:73:PHE:N	0.52	2.43	13	5
1:B:55:HIS:NE2	1:B:88:SER:CB	0.52	2.71	15	2
1:B:5:LYS:O	1:B:5:LYS:HG3	0.52	2.05	15	4
1:B:31:LYS:O	1:B:32:TYR:CD1	0.52	2.63	15	2
1:A:55:HIS:O	1:A:86:PHE:CD1	0.52	2.63	10	8
1:B:55:HIS:CE1	1:B:88:SER:N	0.52	2.77	1	1
1:A:26:THR:HA	1:A:29:LEU:HB2	0.52	1.81	17	4
1:A:86:PHE:CE1	1:B:86:PHE:HZ	0.52	2.23	2	1
1:B:28:ALA:O	1:B:32:TYR:CD1	0.52	2.63	17	8
1:B:39:ALA:HB1	1:B:56:CYS:O	0.52	2.05	4	2
1:A:8:ILE:CA	1:A:76:PHE:HA	0.52	2.32	8	4
1:B:49:LYS:CB	1:B:49:LYS:NZ	0.52	2.70	15	1
1:A:17:MET:SD	1:A:46:PHE:HE2	0.52	2.27	16	1
1:B:62:PHE:HD1	1:B:63:GLY:N	0.52	2.02	19	1
1:A:27:GLN:OE1	1:A:27:GLN:HA	0.52	2.05	1	1
1:A:78:LEU:O	1:A:79:GLY:C	0.52	2.48	9	14
1:A:86:PHE:CZ	1:B:86:PHE:HZ	0.52	2.23	16	12
1:B:54:TRP:CE3	1:B:85:LEU:HD23	0.52	2.40	1	2
1:B:47:ASP:OD1	1:B:54:TRP:CD1	0.52	2.63	3	4
1:A:43:LYS:HB2	1:A:56:CYS:SG	0.52	2.44	4	5
1:A:79:GLY:C	1:A:80:GLN:NE2	0.52	2.64	4	1
1:B:68:HIS:CD2	1:B:72:HIS:O	0.52	2.63	4	1
1:A:34:ILE:HD12	1:A:34:ILE:N	0.52	2.20	5	1
1:B:7:VAL:O	1:B:7:VAL:HG12	0.52	2.04	5	3
1:B:22:VAL:HA	1:B:76:PHE:HE2	0.52	1.62	14	1
1:B:18:GLN:CB	1:B:74:ILE:HG13	0.52	2.29	17	2
1:A:67:THR:HG21	1:B:53:THR:HG23	0.52	1.82	1	1
1:A:86:PHE:HZ	1:B:86:PHE:CZ	0.52	2.23	17	12
1:B:18:GLN:HB3	1:B:74:ILE:CG1	0.52	2.32	16	4
1:A:42:ILE:O	1:A:46:PHE:HB2	0.52	2.04	2	2
1:A:65:TYR:HE2	1:B:43:LYS:HE3	0.52	1.65	2	1
1:B:21:SER:OG	1:B:74:ILE:HD12	0.52	2.05	12	2
1:A:55:HIS:CE1	1:B:67:THR:O	0.52	2.63	4	3
1:B:64:SER:OG	1:B:75:TYR:CE2	0.52	2.63	19	6
1:A:77:TYR:CD2	1:A:77:TYR:O	0.52	2.63	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:68:HIS:CG	1:B:72:HIS:O	0.52	2.63	9	1
1:B:17:MET:SD	1:B:54:TRP:CH2	0.52	3.02	13	1
1:B:31:LYS:HB2	1:B:32:TYR:CD1	0.51	2.40	3	3
1:B:22:VAL:HG22	1:B:76:PHE:CE1	0.51	2.40	5	1
1:B:18:GLN:C	1:B:74:ILE:HD12	0.51	2.26	11	2
1:A:54:TRP:CE3	1:A:87:LYS:HG2	0.51	2.40	3	1
1:A:7:VAL:HG12	1:A:9:LYS:CE	0.51	2.33	5	1
1:A:13:MET:HB2	1:A:73:PHE:H	0.51	1.63	13	3
1:B:31:LYS:C	1:B:32:TYR:CG	0.51	2.83	13	7
1:B:73:PHE:CB	1:B:86:PHE:HB3	0.51	2.36	7	2
1:A:54:TRP:CE2	1:A:87:LYS:CD	0.51	2.93	2	12
1:A:57:ILE:CG2	1:B:62:PHE:CD2	0.51	2.94	2	10
1:B:11:ALA:HB1	1:B:18:GLN:CD	0.51	2.25	1	2
1:B:26:THR:HA	1:B:29:LEU:HB2	0.51	1.82	3	4
1:A:9:LYS:HD2	1:A:76:PHE:HA	0.51	1.82	2	1
1:B:46:PHE:CE1	1:B:85:LEU:HD21	0.51	2.40	16	3
1:B:77:TYR:CG	1:B:81:VAL:O	0.51	2.63	18	4
1:A:32:TYR:CD2	1:A:41:HIS:HE1	0.51	2.23	17	2
1:A:73:PHE:CD1	1:A:75:TYR:CE1	0.51	2.98	8	1
1:A:74:ILE:O	1:A:76:PHE:CE1	0.51	2.64	8	1
1:B:62:PHE:HE1	1:B:64:SER:HG	0.51	1.48	13	1
1:A:63:GLY:HA3	1:B:36:LYS:N	0.51	2.20	9	8
1:B:54:TRP:NE1	1:B:87:LYS:HD2	0.51	2.21	5	4
1:B:47:ASP:HB3	1:B:52:PRO:HD3	0.51	1.82	3	1
1:A:8:ILE:CD1	1:A:74:ILE:HD11	0.51	2.35	16	3
1:A:10:ASN:O	1:A:73:PHE:CE1	0.51	2.63	8	1
1:B:31:LYS:HB3	1:B:32:TYR:CE1	0.51	2.39	8	4
1:B:21:SER:OG	1:B:76:PHE:CZ	0.51	2.64	9	2
1:B:69:GLU:C	1:B:70:THR:HG22	0.51	2.26	13	1
1:A:57:ILE:HD11	1:B:84:LEU:CD2	0.51	2.35	14	1
1:B:28:ALA:O	1:B:32:TYR:HD1	0.51	1.88	3	11
1:B:69:GLU:O	1:B:70:THR:HB	0.51	2.05	10	3
1:A:12:ASP:O	1:A:72:HIS:CG	0.51	2.64	9	3
1:B:72:HIS:O	1:B:73:PHE:CB	0.51	2.59	4	4
1:B:13:MET:HB2	1:B:72:HIS:N	0.51	2.21	5	1
1:B:25:ALA:CB	1:B:83:ILE:HG13	0.51	2.35	11	3
1:A:41:HIS:CD2	1:A:42:ILE:N	0.51	2.78	9	5
1:A:13:MET:SD	1:A:74:ILE:CB	0.51	2.95	16	1
1:A:17:MET:HE1	1:A:46:PHE:CE2	0.51	2.40	16	1
1:B:87:LYS:HE2	1:B:89:GLY:HA2	0.51	1.83	18	1
1:B:4:ARG:HG3	1:B:4:ARG:NH1	0.51	2.19	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ASP:OD2	1:A:68:HIS:NE2	0.51	2.44	20	3
1:A:68:HIS:C	1:A:69:GLU:HG2	0.51	2.26	1	2
1:B:12:ASP:CG	1:B:68:HIS:CD2	0.51	2.84	2	2
1:B:21:SER:CA	1:B:46:PHE:CZ	0.51	2.94	14	20
1:A:65:TYR:CE2	1:B:40:ALA:CB	0.51	2.94	4	3
1:A:73:PHE:CD1	1:A:73:PHE:C	0.51	2.84	5	2
1:B:77:TYR:CE1	1:B:78:LEU:O	0.51	2.64	10	8
1:A:43:LYS:HB2	1:B:65:TYR:CD2	0.51	2.41	12	1
1:A:28:ALA:O	1:A:32:TYR:CD1	0.51	2.63	14	5
1:A:56:CYS:C	1:A:57:ILE:HD13	0.51	2.25	19	7
1:B:5:LYS:C	1:B:78:LEU:HD13	0.51	2.25	1	4
1:B:68:HIS:HA	1:B:86:PHE:HD2	0.51	1.64	1	1
1:A:6:ALA:HB3	1:A:22:VAL:HG11	0.51	1.81	4	8
1:A:21:SER:CB	1:A:85:LEU:HD22	0.51	2.35	17	2
1:B:77:TYR:O	1:B:77:TYR:CD1	0.51	2.64	15	3
1:A:13:MET:HG2	1:A:17:MET:HG3	0.51	1.80	16	1
1:A:54:TRP:C	1:A:55:HIS:CD2	0.51	2.84	2	4
1:B:12:ASP:OD2	1:B:68:HIS:CD2	0.51	2.64	2	1
1:A:32:TYR:CZ	1:A:41:HIS:CE1	0.51	2.99	17	2
1:B:55:HIS:CD2	1:B:86:PHE:O	0.51	2.63	5	2
1:A:43:LYS:CD	1:A:44:LYS:N	0.51	2.74	7	1
1:A:67:THR:O	1:B:55:HIS:NE2	0.51	2.44	7	1
1:B:43:LYS:HZ3	1:B:53:THR:HG23	0.51	1.63	7	1
1:B:47:ASP:C	1:B:47:ASP:OD1	0.51	2.49	14	3
1:A:73:PHE:CA	1:A:86:PHE:HA	0.51	2.29	18	1
1:A:65:TYR:HE1	1:B:43:LYS:HB3	0.51	1.66	1	1
1:A:17:MET:SD	1:A:50:TYR:CE1	0.51	3.04	2	1
1:A:32:TYR:CG	1:A:41:HIS:HE1	0.51	2.24	4	3
1:B:73:PHE:O	1:B:73:PHE:CG	0.51	2.63	13	3
1:B:32:TYR:CG	1:B:41:HIS:HE1	0.51	2.22	11	1
1:A:65:TYR:HE2	1:B:43:LYS:HD2	0.51	1.64	18	1
1:A:29:LEU:HG	1:A:38:ILE:CG2	0.51	2.32	11	2
1:B:4:ARG:HD2	1:B:19:GLN:HA	0.51	1.82	1	1
1:B:8:ILE:HD11	1:B:22:VAL:HG21	0.51	1.82	5	2
1:B:68:HIS:CE1	1:B:87:LYS:O	0.51	2.64	4	2
1:B:37:ASP:O	1:B:41:HIS:CD2	0.51	2.63	18	6
1:A:54:TRP:CE2	1:A:87:LYS:CE	0.51	2.94	10	1
1:A:35:GLU:CB	1:B:63:GLY:HA3	0.50	2.36	17	2
1:A:37:ASP:O	1:A:41:HIS:CE1	0.50	2.64	13	5
1:A:66:VAL:HG11	1:A:86:PHE:CE2	0.50	2.41	2	1
1:A:73:PHE:O	1:A:74:ILE:HB	0.50	2.06	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LYS:CB	1:A:32:TYR:CE1	0.50	2.94	6	11
1:A:64:SER:HB3	1:A:84:LEU:HD22	0.50	1.84	3	2
1:B:73:PHE:O	1:B:73:PHE:CD1	0.50	2.64	3	1
1:A:77:TYR:CD1	1:A:81:VAL:O	0.50	2.64	13	6
1:B:87:LYS:HB3	1:B:87:LYS:HZ3	0.50	1.66	8	1
1:A:64:SER:CB	1:A:84:LEU:HD13	0.50	2.36	11	2
1:B:57:ILE:CB	1:B:84:LEU:HB3	0.50	2.35	14	1
1:A:55:HIS:ND1	1:B:66:VAL:HB	0.50	2.21	17	1
1:B:32:TYR:CE1	1:B:41:HIS:HB2	0.50	2.41	2	5
1:B:50:TYR:O	1:B:51:ASN:CB	0.50	2.59	4	17
1:A:62:PHE:CA	1:B:59:GLY:HA3	0.50	2.35	16	9
1:A:73:PHE:CB	1:A:86:PHE:HB2	0.50	2.36	17	3
1:A:13:MET:SD	1:A:17:MET:SD	0.50	3.09	8	2
1:A:73:PHE:CB	1:A:86:PHE:HB3	0.50	2.36	12	3
1:B:70:THR:C	1:B:72:HIS:H	0.50	2.10	15	6
1:A:62:PHE:CD1	1:A:62:PHE:C	0.50	2.84	12	3
1:A:62:PHE:CD2	1:B:57:ILE:CG2	0.50	2.94	1	10
1:A:77:TYR:CG	1:A:81:VAL:O	0.50	2.64	4	5
1:A:55:HIS:HA	1:B:66:VAL:HA	0.50	1.83	7	3
1:B:71:LYS:HE3	1:B:87:LYS:H	0.50	1.67	11	1
1:A:15:GLU:CA	1:A:18:GLN:HG3	0.50	2.36	20	1
1:A:17:MET:HE1	1:A:50:TYR:CD2	0.50	2.41	1	2
1:B:69:GLU:O	1:B:70:THR:O	0.50	2.30	19	5
1:B:55:HIS:CG	1:B:86:PHE:CE1	0.50	3.00	11	1
1:A:60:ARG:HH11	1:A:60:ARG:CG	0.50	2.20	14	1
1:B:12:ASP:CG	1:B:72:HIS:CD2	0.50	2.84	15	1
1:B:34:ILE:O	1:B:35:GLU:C	0.50	2.49	8	19
1:A:46:PHE:CD2	1:A:50:TYR:CD2	0.50	2.99	9	4
1:B:54:TRP:CE2	1:B:87:LYS:HE3	0.50	2.41	3	3
1:B:50:TYR:CD1	1:B:50:TYR:N	0.50	2.80	4	2
1:A:12:ASP:CB	1:A:68:HIS:NE2	0.50	2.75	5	1
1:A:62:PHE:CD1	1:B:57:ILE:CG2	0.50	2.95	6	3
1:A:52:PRO:CB	1:A:53:THR:HA	0.50	2.36	10	5
1:A:86:PHE:HZ	1:B:86:PHE:HZ	0.50	1.48	14	2
1:B:73:PHE:CD2	1:B:73:PHE:O	0.50	2.65	10	1
1:B:48:LYS:HE2	1:B:48:LYS:O	0.50	2.07	11	1
1:B:46:PHE:HA	1:B:50:TYR:HD1	0.50	1.66	14	2
1:B:57:ILE:CG2	1:B:58:VAL:N	0.50	2.75	19	3
1:A:32:TYR:CD2	1:A:41:HIS:CE1	0.50	3.00	4	4
1:B:46:PHE:HD2	1:B:54:TRP:CD2	0.50	2.24	17	9
1:B:33:ASN:C	1:B:34:ILE:HD12	0.50	2.26	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ASP:CG	1:A:52:PRO:HB3	0.50	2.27	12	1
1:A:48:LYS:O	1:A:48:LYS:NZ	0.50	2.38	13	1
1:A:66:VAL:CG2	1:A:84:LEU:HD21	0.50	2.37	18	1
1:A:81:VAL:CG1	1:A:82:ALA:H	0.50	2.19	9	11
1:B:76:PHE:CE2	1:B:83:ILE:CG1	0.50	2.95	8	12
1:B:46:PHE:CD2	1:B:50:TYR:CD2	0.50	2.99	20	6
1:B:68:HIS:NE2	1:B:87:LYS:CG	0.50	2.75	4	1
1:B:77:TYR:CD2	1:B:81:VAL:O	0.50	2.65	8	4
1:A:48:LYS:HE3	1:A:48:LYS:CA	0.50	2.37	10	2
1:B:30:GLU:OE2	1:B:31:LYS:HE3	0.50	2.06	17	1
1:B:11:ALA:HB2	1:B:74:ILE:CG1	0.50	2.37	5	11
1:A:67:THR:O	1:B:55:HIS:CE1	0.50	2.64	2	3
1:B:34:ILE:HG22	1:B:36:LYS:HD3	0.50	1.84	3	1
1:B:55:HIS:HB2	1:B:86:PHE:CD2	0.50	2.41	6	5
1:A:65:TYR:CD1	1:B:43:LYS:HD3	0.50	2.42	6	2
1:B:47:ASP:CA	1:B:52:PRO:HD3	0.50	2.37	13	4
1:B:28:ALA:HB1	1:B:38:ILE:CA	0.50	2.31	17	2
1:B:68:HIS:CD2	1:B:87:LYS:N	0.50	2.79	9	1
1:A:12:ASP:OD2	1:A:68:HIS:CD2	0.50	2.64	14	3
1:B:4:ARG:O	1:B:5:LYS:HB2	0.50	2.06	19	1
1:A:21:SER:CA	1:A:46:PHE:CZ	0.50	2.95	12	20
1:A:11:ALA:HB2	1:A:74:ILE:CG1	0.50	2.37	3	9
1:B:47:ASP:CB	1:B:52:PRO:HD3	0.50	2.36	17	3
1:B:73:PHE:CD1	1:B:86:PHE:HB2	0.50	2.42	5	1
1:B:56:CYS:C	1:B:57:ILE:HD13	0.50	2.26	9	2
1:A:32:TYR:CE1	1:A:41:HIS:CE1	0.50	3.00	16	3
1:A:62:PHE:HD2	1:B:57:ILE:CG2	0.50	2.20	16	2
1:B:12:ASP:HB2	1:B:68:HIS:CD2	0.50	2.42	17	1
1:B:21:SER:HB2	1:B:85:LEU:CD2	0.50	2.36	18	1
1:B:70:THR:CG2	1:B:87:LYS:HB2	0.50	2.37	19	1
1:A:35:GLU:HB3	1:A:58:VAL:O	0.49	2.07	17	4
1:A:65:TYR:CE1	1:B:40:ALA:CB	0.49	2.95	14	12
1:B:46:PHE:CE2	1:B:85:LEU:CD2	0.49	2.95	19	4
1:A:62:PHE:HD1	1:A:62:PHE:H	0.49	1.48	16	5
1:B:13:MET:CA	1:B:71:LYS:HG3	0.49	2.37	4	1
1:A:69:GLU:O	1:A:70:THR:O	0.49	2.30	17	3
1:B:49:LYS:HD3	1:B:50:TYR:CE1	0.49	2.42	16	3
1:A:65:TYR:CZ	1:B:40:ALA:CB	0.49	2.94	19	4
1:B:53:THR:HG22	1:B:55:HIS:HD2	0.49	1.65	13	2
1:A:13:MET:HG3	1:A:17:MET:HG2	0.49	1.80	10	1
1:A:40:ALA:HB2	1:B:65:TYR:CZ	0.49	2.42	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:VAL:CB	1:A:86:PHE:CZ	0.49	2.95	14	2
1:B:49:LYS:HZ2	1:B:49:LYS:HB3	0.49	1.65	15	1
1:A:28:ALA:CB	1:A:41:HIS:CG	0.49	2.95	1	7
1:B:31:LYS:CB	1:B:32:TYR:CE1	0.49	2.95	8	6
1:B:77:TYR:HA	1:B:82:ALA:HA	0.49	1.83	6	6
1:A:55:HIS:CD2	1:A:86:PHE:O	0.49	2.64	7	2
1:A:78:LEU:CD2	1:A:78:LEU:N	0.49	2.75	5	3
1:A:29:LEU:HD13	1:A:78:LEU:HD12	0.49	1.84	6	1
1:A:62:PHE:CD2	1:B:62:PHE:CB	0.49	2.95	8	4
1:A:32:TYR:HE1	1:A:41:HIS:ND1	0.49	2.05	14	2
1:A:47:ASP:CG	1:A:52:PRO:HG3	0.49	2.27	19	4
1:A:73:PHE:CD1	1:A:86:PHE:CB	0.49	2.96	13	5
1:B:13:MET:O	1:B:18:GLN:CD	0.49	2.51	11	13
1:B:66:VAL:CB	1:B:86:PHE:CZ	0.49	2.94	4	3
1:A:76:PHE:CD2	1:A:78:LEU:CD2	0.49	2.95	20	6
1:B:55:HIS:CB	1:B:86:PHE:CZ	0.49	2.95	11	2
1:B:77:TYR:HD2	1:B:82:ALA:HB2	0.49	1.67	13	4
1:B:47:ASP:HB3	1:B:52:PRO:CD	0.49	2.38	3	2
1:B:19:GLN:OE1	1:B:19:GLN:HA	0.49	2.06	4	1
1:B:46:PHE:CD2	1:B:54:TRP:CD2	0.49	3.00	16	4
1:A:61:ASN:N	1:A:61:ASN:ND2	0.49	2.59	7	1
1:A:65:TYR:HB2	1:B:39:ALA:HB3	0.49	1.83	7	2
1:A:65:TYR:CE2	1:B:43:LYS:CD	0.49	2.95	9	2
1:A:62:PHE:CB	1:B:62:PHE:CD2	0.49	2.96	13	1
1:B:34:ILE:CG2	1:B:36:LYS:HE3	0.49	2.33	14	1
1:A:54:TRP:HA	1:A:87:LYS:CG	0.49	2.37	16	1
1:A:27:GLN:NE2	1:A:45:GLU:OE1	0.49	2.45	17	1
1:A:70:THR:OG1	1:A:87:LYS:HE2	0.49	2.07	17	1
1:A:13:MET:HB3	1:A:18:GLN:OE1	0.49	2.06	18	1
1:A:44:LYS:HA	1:A:47:ASP:OD2	0.49	2.06	18	1
1:A:40:ALA:CB	1:B:65:TYR:CE1	0.49	2.96	1	10
1:A:5:LYS:O	1:A:6:ALA:CB	0.49	2.61	3	4
1:A:46:PHE:CZ	1:A:85:LEU:CD2	0.49	2.95	8	4
1:B:12:ASP:O	1:B:72:HIS:CG	0.49	2.65	18	2
1:A:77:TYR:HD1	1:A:77:TYR:O	0.49	1.90	9	1
1:B:68:HIS:CB	1:B:73:PHE:CD2	0.49	2.95	10	1
1:B:17:MET:CE	1:B:50:TYR:CE1	0.49	2.95	13	2
1:B:73:PHE:CD2	1:B:86:PHE:HB3	0.49	2.42	14	1
1:A:22:VAL:HG22	1:A:76:PHE:CG	0.49	2.42	15	2
1:B:18:GLN:HA	1:B:74:ILE:CD1	0.49	2.35	16	2
1:B:76:PHE:O	1:B:82:ALA:HA	0.49	2.06	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:21:SER:CB	1:B:85:LEU:HD22	0.49	2.37	11	2
1:A:65:TYR:HD2	1:B:43:LYS:HB3	0.49	1.67	12	3
1:A:43:LYS:HE3	1:B:65:TYR:CD2	0.49	2.43	14	1
1:A:55:HIS:CE1	1:B:67:THR:CG2	0.49	2.96	19	2
1:A:76:PHE:CE2	1:A:83:ILE:CG1	0.49	2.95	15	14
1:B:29:LEU:CD2	1:B:81:VAL:HG11	0.49	2.22	1	1
1:A:86:PHE:HZ	1:B:86:PHE:CE2	0.49	2.26	6	4
1:B:44:LYS:O	1:B:47:ASP:OD1	0.49	2.31	2	1
1:A:69:GLU:O	1:A:72:HIS:N	0.49	2.46	12	3
1:B:56:CYS:SG	1:B:85:LEU:HD12	0.49	2.48	4	2
1:A:43:LYS:HG3	1:B:65:TYR:O	0.49	2.08	5	1
1:A:43:LYS:CB	1:B:65:TYR:CD2	0.49	2.96	12	6
1:B:46:PHE:CZ	1:B:85:LEU:CD2	0.49	2.96	11	6
1:B:70:THR:HG22	1:B:72:HIS:CD2	0.49	2.43	10	1
1:A:55:HIS:CB	1:A:86:PHE:CE1	0.49	2.95	19	2
1:A:66:VAL:CG2	1:A:86:PHE:CZ	0.49	2.96	14	1
1:B:15:GLU:O	1:B:18:GLN:CG	0.49	2.60	13	13
1:B:67:THR:O	1:B:68:HIS:O	0.49	2.31	9	4
1:A:40:ALA:CB	1:B:65:TYR:CZ	0.49	2.95	14	1
1:A:50:TYR:O	1:A:51:ASN:CB	0.49	2.61	19	18
1:A:14:SER:O	1:A:15:GLU:C	0.49	2.51	20	7
1:A:46:PHE:CE2	1:A:85:LEU:CD2	0.49	2.95	19	4
1:A:53:THR:C	1:A:87:LYS:HG2	0.49	2.28	2	1
1:B:13:MET:CG	1:B:71:LYS:HG2	0.49	2.36	4	1
1:A:45:GLU:O	1:A:48:LYS:N	0.49	2.46	9	3
1:B:28:ALA:C	1:B:38:ILE:HG23	0.49	2.27	20	4
1:B:53:THR:CG2	1:B:55:HIS:CE1	0.49	2.96	5	2
1:B:68:HIS:CB	1:B:73:PHE:CG	0.49	2.96	10	1
1:A:35:GLU:CD	1:B:61:ASN:O	0.49	2.51	13	2
1:B:71:LYS:CD	1:B:87:LYS:HD3	0.49	2.37	11	1
1:B:71:LYS:O	1:B:72:HIS:C	0.49	2.51	19	1
1:A:46:PHE:HD2	1:A:54:TRP:CD2	0.49	2.25	20	5
1:B:43:LYS:O	1:B:47:ASP:OD1	0.49	2.31	3	2
1:B:28:ALA:CB	1:B:41:HIS:CG	0.49	2.96	14	8
1:B:32:TYR:CE1	1:B:41:HIS:CB	0.49	2.96	4	1
1:A:43:LYS:CB	1:B:65:TYR:HD2	0.49	2.21	10	5
1:B:47:ASP:C	1:B:52:PRO:HD3	0.49	2.28	16	4
1:A:11:ALA:C	1:A:73:PHE:O	0.49	2.52	16	2
1:B:68:HIS:O	1:B:69:GLU:CB	0.49	2.61	9	1
1:A:29:LEU:HD11	1:A:83:ILE:CD1	0.49	2.37	17	1
1:A:47:ASP:OD1	1:A:48:LYS:N	0.49	2.46	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:86:PHE:O	1:B:86:PHE:CG	0.48	2.66	18	9
1:B:5:LYS:O	1:B:6:ALA:CB	0.48	2.61	19	6
1:B:10:ASN:CB	1:B:75:TYR:HB3	0.48	2.34	2	1
1:A:55:HIS:CD2	1:A:87:LYS:CA	0.48	2.96	8	2
1:B:12:ASP:H	1:B:73:PHE:HD1	0.48	1.50	3	2
1:A:17:MET:O	1:A:21:SER:HB3	0.48	2.08	4	2
1:A:43:LYS:HD2	1:A:44:LYS:N	0.48	2.23	4	2
1:B:64:SER:OG	1:B:75:TYR:HE2	0.48	1.91	19	2
1:B:75:TYR:CD1	1:B:76:PHE:N	0.48	2.80	8	1
1:B:87:LYS:NZ	1:B:87:LYS:CB	0.48	2.76	8	1
1:A:35:GLU:H	1:A:38:ILE:HD12	0.48	1.68	13	1
1:B:70:THR:O	1:B:71:LYS:HG2	0.48	2.07	13	1
1:A:62:PHE:HD2	1:B:62:PHE:HB2	0.48	1.66	14	1
1:A:66:VAL:HG11	1:B:55:HIS:HB3	0.48	1.84	17	1
1:B:17:MET:CE	1:B:54:TRP:HH2	0.48	2.21	19	2
1:A:9:LYS:CE	1:A:77:TYR:HB2	0.48	2.38	2	2
1:B:86:PHE:O	1:B:86:PHE:CD1	0.48	2.66	2	3
1:A:42:ILE:HD13	1:A:83:ILE:HG21	0.48	1.84	4	2
1:B:4:ARG:N	1:B:4:ARG:CD	0.48	2.69	4	1
1:A:18:GLN:HB3	1:A:74:ILE:CG1	0.48	2.38	5	3
1:B:22:VAL:HG22	1:B:76:PHE:CZ	0.48	2.44	5	1
1:B:55:HIS:CE1	1:B:88:SER:CB	0.48	2.96	6	1
1:A:49:LYS:O	1:A:50:TYR:CG	0.48	2.66	7	2
1:B:29:LEU:HD21	1:B:81:VAL:HG21	0.48	1.84	8	2
1:A:5:LYS:O	1:A:6:ALA:O	0.48	2.31	10	1
1:B:35:GLU:CD	1:B:59:GLY:HA2	0.48	2.28	17	1
1:B:51:ASN:HD22	1:B:52:PRO:CD	0.48	2.19	17	1
1:A:17:MET:CE	1:A:50:TYR:CE2	0.48	2.96	10	2
1:A:50:TYR:CB	1:A:54:TRP:CZ2	0.48	2.96	1	1
1:B:7:VAL:O	1:B:8:ILE:C	0.48	2.52	11	11
1:A:74:ILE:O	1:A:74:ILE:CG2	0.48	2.62	7	9
1:B:55:HIS:CB	1:B:86:PHE:CE1	0.48	2.96	16	2
1:B:12:ASP:CB	1:B:68:HIS:CD2	0.48	2.96	14	3
1:B:78:LEU:HD23	1:B:83:ILE:CG1	0.48	2.38	6	2
1:A:54:TRP:CZ3	1:A:87:LYS:HD2	0.48	2.42	10	1
1:B:4:ARG:O	1:B:5:LYS:C	0.48	2.51	17	2
1:B:12:ASP:OD2	1:B:73:PHE:CE1	0.48	2.66	11	1
1:B:14:SER:O	1:B:18:GLN:NE2	0.48	2.46	11	1
1:B:6:ALA:HB1	1:B:76:PHE:HD2	0.48	1.67	13	2
1:B:46:PHE:CD1	1:B:50:TYR:HE2	0.48	2.26	15	1
1:B:66:VAL:CG2	1:B:86:PHE:CE2	0.48	2.96	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ASP:O	1:A:72:HIS:ND1	0.48	2.46	19	1
1:A:62:PHE:CB	1:B:62:PHE:CD1	0.48	2.96	20	1
1:A:13:MET:O	1:A:18:GLN:CD	0.48	2.51	12	12
1:A:61:ASN:OD1	1:B:60:ARG:HG3	0.48	2.09	1	1
1:B:7:VAL:O	1:B:8:ILE:O	0.48	2.31	6	3
1:A:9:LYS:CD	1:A:9:LYS:N	0.48	2.76	2	1
1:B:54:TRP:CA	1:B:87:LYS:HG3	0.48	2.35	2	3
1:B:68:HIS:CB	1:B:72:HIS:O	0.48	2.61	4	5
1:A:13:MET:HB3	1:A:18:GLN:HE21	0.48	1.69	5	1
1:B:46:PHE:O	1:B:50:TYR:HD1	0.48	1.91	17	3
1:B:15:GLU:N	1:B:18:GLN:HE22	0.48	2.07	11	1
1:B:46:PHE:CE1	1:B:85:LEU:CD2	0.48	2.96	16	2
1:B:44:LYS:O	1:B:48:LYS:HB3	0.48	2.09	20	1
1:A:43:LYS:HG2	1:A:54:TRP:O	0.48	2.07	9	3
1:A:54:TRP:C	1:A:55:HIS:CG	0.48	2.86	3	2
1:B:21:SER:CB	1:B:46:PHE:CZ	0.48	2.96	14	6
1:B:84:LEU:O	1:B:84:LEU:CG	0.48	2.62	2	2
1:A:69:GLU:HB2	1:A:88:SER:HA	0.48	1.85	4	3
1:A:77:TYR:O	1:A:78:LEU:O	0.48	2.32	3	3
1:A:44:LYS:O	1:A:47:ASP:OD1	0.48	2.31	4	2
1:A:57:ILE:HG23	1:B:63:GLY:O	0.48	2.08	4	1
1:B:8:ILE:HD11	1:B:22:VAL:CG2	0.48	2.39	5	3
1:B:10:ASN:HB3	1:B:73:PHE:CZ	0.48	2.44	6	1
1:B:66:VAL:HG11	1:B:86:PHE:CE1	0.48	2.44	9	2
1:A:46:PHE:CG	1:A:50:TYR:CE1	0.48	3.01	10	1
1:B:43:LYS:HA	1:B:56:CYS:SG	0.48	2.49	14	2
1:B:14:SER:HB3	1:B:17:MET:HB3	0.48	1.85	13	1
1:B:49:LYS:HB3	1:B:50:TYR:CD1	0.48	2.43	16	1
1:A:37:ASP:OD1	1:A:41:HIS:CE1	0.48	2.66	17	1
1:B:4:ARG:CD	1:B:19:GLN:HA	0.48	2.37	1	1
1:B:55:HIS:CB	1:B:86:PHE:O	0.48	2.62	11	10
1:B:73:PHE:HB2	1:B:86:PHE:HB2	0.48	1.86	3	3
1:B:81:VAL:HG12	1:B:82:ALA:H	0.48	1.66	2	5
1:A:87:LYS:NZ	1:A:87:LYS:HB3	0.48	2.22	2	2
1:B:13:MET:O	1:B:18:GLN:OE1	0.48	2.31	7	7
1:B:12:ASP:O	1:B:72:HIS:CD2	0.48	2.67	15	1
1:B:32:TYR:CE2	1:B:41:HIS:HB2	0.48	2.43	16	2
1:A:10:ASN:O	1:A:75:TYR:HB3	0.48	2.09	18	1
1:B:10:ASN:HD22	1:B:10:ASN:C	0.48	2.12	18	1
1:B:21:SER:HA	1:B:46:PHE:HZ	0.48	1.65	1	1
1:B:25:ALA:HB1	1:B:83:ILE:CD1	0.48	2.39	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:28:ALA:O	1:B:38:ILE:HG12	0.48	2.09	5	2
1:B:79:GLY:O	1:B:80:GLN:HG3	0.48	2.09	4	1
1:A:15:GLU:O	1:A:16:GLU:C	0.48	2.52	16	2
1:A:84:LEU:O	1:A:84:LEU:CG	0.48	2.61	8	1
1:A:8:ILE:O	1:A:9:LYS:HE2	0.48	2.09	9	1
1:B:68:HIS:O	1:B:69:GLU:HB3	0.48	2.09	9	1
1:A:11:ALA:HA	1:A:74:ILE:CA	0.48	2.36	16	2
1:A:27:GLN:CB	1:A:41:HIS:CE1	0.48	2.96	11	1
1:B:43:LYS:HZ2	1:B:55:HIS:HA	0.48	1.68	12	1
1:B:76:PHE:CE1	1:B:83:ILE:HB	0.48	2.43	14	2
1:A:69:GLU:O	1:A:70:THR:HB	0.48	2.08	14	1
1:B:53:THR:C	1:B:87:LYS:NZ	0.48	2.66	17	1
1:A:17:MET:SD	1:A:71:LYS:HD3	0.48	2.48	19	1
1:A:13:MET:O	1:A:18:GLN:OE1	0.48	2.32	16	3
1:A:62:PHE:C	1:B:35:GLU:CB	0.48	2.82	10	7
1:B:12:ASP:CG	1:B:68:HIS:HD2	0.48	2.12	1	1
1:B:44:LYS:O	1:B:47:ASP:OD2	0.48	2.32	9	6
1:B:74:ILE:O	1:B:74:ILE:CG2	0.48	2.61	18	4
1:A:65:TYR:H	1:B:57:ILE:CD1	0.48	2.21	4	6
1:A:54:TRP:CE3	1:A:87:LYS:HG3	0.48	2.42	4	1
1:B:34:ILE:HD13	1:B:34:ILE:N	0.48	2.24	20	2
1:B:55:HIS:CE1	1:B:88:SER:OG	0.48	2.67	4	2
1:B:54:TRP:CD2	1:B:87:LYS:CD	0.48	2.96	19	6
1:A:6:ALA:HB2	1:A:22:VAL:CG1	0.48	2.38	6	2
1:A:7:VAL:HB	1:A:77:TYR:HB3	0.48	1.84	6	1
1:B:32:TYR:C	1:B:34:ILE:CD1	0.48	2.82	7	1
1:B:53:THR:O	1:B:87:LYS:CB	0.48	2.62	7	5
1:B:72:HIS:CB	1:B:87:LYS:HG3	0.48	2.39	8	1
1:A:35:GLU:OE2	1:B:61:ASN:O	0.48	2.32	11	2
1:B:15:GLU:N	1:B:18:GLN:NE2	0.48	2.62	11	1
1:A:74:ILE:O	1:A:85:LEU:N	0.48	2.47	13	1
1:A:46:PHE:HB3	1:A:54:TRP:CD1	0.48	2.44	19	2
1:A:43:LYS:O	1:A:44:LYS:C	0.48	2.51	5	7
1:B:22:VAL:HG22	1:B:76:PHE:CD1	0.48	2.43	5	2
1:B:60:ARG:O	1:B:61:ASN:OD1	0.48	2.32	17	2
1:B:68:HIS:CG	1:B:73:PHE:CD2	0.48	3.02	5	1
1:A:74:ILE:CG2	1:A:76:PHE:HE1	0.48	2.22	14	2
1:A:46:PHE:CE1	1:A:85:LEU:CD2	0.48	2.97	8	2
1:B:54:TRP:CD2	1:B:87:LYS:CG	0.48	2.97	11	1
1:A:66:VAL:HG22	1:A:84:LEU:HD21	0.48	1.85	13	1
1:A:77:TYR:CD2	1:A:81:VAL:O	0.48	2.67	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:69:GLU:O	1:B:70:THR:OG1	0.48	2.32	1	1
1:B:8:ILE:CD1	1:B:74:ILE:HD11	0.48	2.37	2	1
1:A:7:VAL:O	1:A:8:ILE:C	0.48	2.51	11	8
1:A:7:VAL:O	1:A:8:ILE:O	0.48	2.31	9	4
1:B:10:ASN:O	1:B:75:TYR:CB	0.48	2.62	5	2
1:B:68:HIS:CG	1:B:69:GLU:H	0.48	2.25	4	1
1:B:47:ASP:HB3	1:B:52:PRO:CG	0.48	2.39	5	1
1:B:73:PHE:HB2	1:B:86:PHE:CB	0.48	2.39	6	1
1:B:6:ALA:HB1	1:B:76:PHE:HB2	0.48	1.86	20	2
1:B:55:HIS:HD2	1:B:87:LYS:HA	0.48	1.69	9	1
1:B:71:LYS:HZ3	1:B:72:HIS:N	0.48	2.07	11	1
1:A:46:PHE:CD1	1:A:54:TRP:CH2	0.48	3.02	15	2
1:A:46:PHE:CD1	1:A:50:TYR:CE2	0.48	3.02	15	1
1:A:62:PHE:CD2	1:B:62:PHE:CG	0.48	3.02	15	1
1:A:13:MET:HG2	1:A:72:HIS:HA	0.48	1.85	16	1
1:A:11:ALA:HA	1:A:73:PHE:O	0.48	2.09	18	1
1:A:66:VAL:HG11	1:A:86:PHE:CE1	0.48	2.43	19	1
1:A:51:ASN:OD1	1:A:51:ASN:O	0.47	2.31	1	1
1:A:50:TYR:O	1:A:51:ASN:CG	0.47	2.52	2	1
1:B:14:SER:O	1:B:18:GLN:CG	0.47	2.62	13	5
1:B:17:MET:CE	1:B:50:TYR:CE2	0.47	2.96	14	4
1:A:69:GLU:O	1:A:70:THR:C	0.47	2.52	6	5
1:B:46:PHE:HD2	1:B:54:TRP:CE2	0.47	2.27	4	4
1:A:43:LYS:HD2	1:A:54:TRP:HB2	0.47	1.85	6	1
1:A:57:ILE:CG2	1:B:62:PHE:HD2	0.47	2.22	12	3
1:B:43:LYS:HE2	1:B:54:TRP:O	0.47	2.09	9	1
1:B:61:ASN:OD1	1:B:61:ASN:O	0.47	2.32	9	1
1:A:67:THR:O	1:A:68:HIS:O	0.47	2.32	12	1
1:A:13:MET:HB2	1:A:72:HIS:C	0.47	2.29	13	1
1:B:51:ASN:O	1:B:54:TRP:NE1	0.47	2.47	20	3
1:A:17:MET:CE	1:A:54:TRP:HH2	0.47	2.23	1	1
1:A:47:ASP:OD1	1:A:47:ASP:C	0.47	2.52	13	3
1:A:68:HIS:CB	1:A:73:PHE:CG	0.47	2.96	1	1
1:B:25:ALA:O	1:B:29:LEU:CD1	0.47	2.62	20	12
1:A:25:ALA:O	1:A:29:LEU:CD1	0.47	2.63	17	15
1:A:62:PHE:HB3	1:B:62:PHE:CG	0.47	2.44	20	2
1:B:59:GLY:O	1:B:82:ALA:N	0.47	2.47	2	1
1:B:47:ASP:OD1	1:B:54:TRP:HD1	0.47	1.92	5	1
1:B:44:LYS:O	1:B:47:ASP:CG	0.47	2.52	7	1
1:A:14:SER:CB	1:A:17:MET:HB3	0.47	2.37	10	1
1:A:43:LYS:CE	1:B:65:TYR:CE2	0.47	2.96	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:ALA:O	1:A:44:LYS:HB2	0.47	2.09	19	2
1:A:50:TYR:O	1:A:51:ASN:OD1	0.47	2.32	14	1
1:A:64:SER:HB2	1:B:57:ILE:CD1	0.47	2.22	17	3
1:A:69:GLU:OE2	1:A:88:SER:O	0.47	2.32	14	1
1:A:24:CYS:SG	1:A:46:PHE:HE1	0.47	2.32	16	1
1:B:55:HIS:O	1:B:86:PHE:O	0.47	2.32	19	1
1:A:66:VAL:HA	1:B:55:HIS:HA	0.47	1.85	20	1
1:A:67:THR:CG2	1:B:55:HIS:NE2	0.47	2.78	1	1
1:B:29:LEU:HD22	1:B:81:VAL:HG21	0.47	1.86	1	1
1:A:21:SER:CA	1:A:46:PHE:HZ	0.47	2.23	18	10
1:B:88:SER:O	1:B:89:GLY:C	0.47	2.53	4	2
1:A:67:THR:HB	1:B:43:LYS:HE3	0.47	1.85	9	1
1:B:43:LYS:NZ	1:B:55:HIS:HA	0.47	2.24	12	1
1:A:65:TYR:HE2	1:B:43:LYS:CD	0.47	2.22	13	1
1:A:66:VAL:CG1	1:B:86:PHE:CE2	0.47	2.97	14	1
1:A:46:PHE:HB3	1:A:54:TRP:CD2	0.47	2.44	15	2
1:A:20:ASP:OD1	1:A:50:TYR:OH	0.47	2.33	17	1
1:B:54:TRP:CD1	1:B:87:LYS:NZ	0.47	2.79	17	1
1:A:86:PHE:CG	1:A:86:PHE:O	0.47	2.67	19	2
1:B:17:MET:HE1	1:B:54:TRP:CH2	0.47	2.44	19	1
1:A:62:PHE:HB3	1:B:62:PHE:CD1	0.47	2.44	20	1
1:A:15:GLU:O	1:A:18:GLN:CG	0.47	2.63	9	14
1:A:86:PHE:CE1	1:B:86:PHE:CZ	0.47	3.03	2	1
1:B:73:PHE:CG	1:B:73:PHE:O	0.47	2.66	5	1
1:A:61:ASN:N	1:A:61:ASN:HD22	0.47	2.06	7	1
1:A:75:TYR:N	1:A:75:TYR:HD1	0.47	2.07	8	1
1:A:77:TYR:CD1	1:A:77:TYR:O	0.47	2.67	9	1
1:B:49:LYS:NZ	1:B:49:LYS:HB3	0.47	2.24	15	1
1:A:14:SER:O	1:A:14:SER:OG	0.47	2.31	16	1
1:A:86:PHE:O	1:A:86:PHE:CG	0.47	2.67	11	4
1:A:35:GLU:O	1:A:58:VAL:CG1	0.47	2.63	13	14
1:A:70:THR:C	1:A:72:HIS:H	0.47	2.12	11	5
1:B:12:ASP:O	1:B:72:HIS:CB	0.47	2.62	16	4
1:B:87:LYS:NZ	1:B:89:GLY:OXT	0.47	2.47	6	1
1:B:32:TYR:O	1:B:33:ASN:CB	0.47	2.62	7	1
1:A:16:GLU:O	1:A:20:ASP:OD2	0.47	2.32	15	2
1:B:55:HIS:CD2	1:B:55:HIS:N	0.47	2.80	8	1
1:B:76:PHE:O	1:B:83:ILE:HG12	0.47	2.10	9	1
1:A:35:GLU:HG2	1:B:63:GLY:N	0.47	2.24	11	1
1:A:86:PHE:O	1:A:86:PHE:CD1	0.47	2.67	11	2
1:A:56:CYS:O	1:B:65:TYR:N	0.47	2.48	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LYS:CB	1:A:56:CYS:SG	0.47	3.03	14	1
1:A:62:PHE:HD2	1:B:62:PHE:CD2	0.47	2.27	15	1
1:A:65:TYR:CB	1:B:56:CYS:O	0.47	2.63	16	1
1:B:75:TYR:N	1:B:75:TYR:HD1	0.47	2.07	20	1
1:B:45:GLU:O	1:B:49:LYS:CB	0.47	2.62	2	12
1:B:62:PHE:HD1	1:B:62:PHE:H	0.47	1.53	12	3
1:A:65:TYR:HD2	1:B:43:LYS:CB	0.47	2.23	14	2
1:B:11:ALA:C	1:B:13:MET:H	0.47	2.12	13	1
1:A:29:LEU:O	1:A:33:ASN:OD1	0.47	2.32	15	1
1:A:36:LYS:CD	1:A:36:LYS:H	0.47	2.20	19	1
1:A:51:ASN:O	1:A:51:ASN:CG	0.47	2.52	1	1
1:B:35:GLU:O	1:B:58:VAL:CG1	0.47	2.62	15	17
1:A:77:TYR:CA	1:A:81:VAL:O	0.47	2.63	15	7
1:A:70:THR:HB	1:A:87:LYS:HE2	0.47	1.86	3	1
1:A:53:THR:HG22	1:A:55:HIS:NE2	0.47	2.23	5	2
1:A:79:GLY:O	1:A:80:GLN:CB	0.47	2.62	6	5
1:B:12:ASP:HB3	1:B:72:HIS:CD2	0.47	2.44	11	2
1:B:18:GLN:O	1:B:74:ILE:CD1	0.47	2.63	17	7
1:A:10:ASN:O	1:A:75:TYR:CB	0.47	2.63	5	3
1:A:32:TYR:O	1:A:33:ASN:CB	0.47	2.62	18	2
1:B:6:ALA:HB3	1:B:22:VAL:CG1	0.47	2.40	6	2
1:B:33:ASN:OD1	1:B:33:ASN:N	0.47	2.47	6	1
1:A:21:SER:HG	1:A:74:ILE:HG21	0.47	1.67	7	1
1:A:24:CYS:O	1:A:27:GLN:CG	0.47	2.63	16	2
1:A:37:ASP:OD2	1:A:41:HIS:CE1	0.47	2.67	7	2
1:A:43:LYS:HD3	1:A:44:LYS:N	0.47	2.24	8	2
1:A:53:THR:OG1	1:B:67:THR:HG21	0.47	2.09	7	1
1:B:28:ALA:CB	1:B:41:HIS:HB3	0.47	2.40	7	1
1:B:37:ASP:HB3	1:B:41:HIS:NE2	0.47	2.24	8	1
1:A:65:TYR:CD2	1:B:43:LYS:CB	0.47	2.98	20	3
1:B:8:ILE:CA	1:B:75:TYR:O	0.47	2.62	9	2
1:B:31:LYS:O	1:B:32:TYR:CD2	0.47	2.67	13	2
1:A:51:ASN:O	1:A:51:ASN:OD1	0.47	2.33	10	1
1:A:55:HIS:CB	1:A:86:PHE:O	0.47	2.63	12	7
1:A:32:TYR:HE1	1:A:41:HIS:HB2	0.47	1.69	12	1
1:A:61:ASN:O	1:B:35:GLU:CG	0.47	2.63	14	1
1:B:60:ARG:O	1:B:61:ASN:CG	0.47	2.53	15	1
1:A:56:CYS:HB3	1:A:85:LEU:CG	0.47	2.39	16	1
1:B:39:ALA:H	1:B:58:VAL:CG1	0.47	2.22	19	1
1:B:21:SER:CA	1:B:46:PHE:HZ	0.47	2.23	10	15
1:B:78:LEU:HD22	1:B:78:LEU:N	0.47	2.25	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:TRP:CG	1:A:87:LYS:HG3	0.47	2.44	2	1
1:B:5:LYS:O	1:B:78:LEU:CD1	0.47	2.62	13	6
1:A:53:THR:O	1:A:87:LYS:CB	0.47	2.63	9	9
1:B:20:ASP:OD1	1:B:21:SER:N	0.47	2.47	3	1
1:B:39:ALA:O	1:B:56:CYS:SG	0.47	2.70	20	2
1:B:88:SER:O	1:B:89:GLY:O	0.47	2.33	4	1
1:A:28:ALA:O	1:A:32:TYR:O	0.47	2.33	13	4
1:B:43:LYS:NZ	1:B:53:THR:CG2	0.47	2.75	7	1
1:B:46:PHE:O	1:B:50:TYR:N	0.47	2.48	7	2
1:B:70:THR:O	1:B:71:LYS:HB2	0.47	2.09	10	1
1:A:43:LYS:CB	1:B:65:TYR:CE2	0.47	2.97	12	1
1:A:65:TYR:CD2	1:B:43:LYS:CD	0.47	2.98	12	1
1:A:68:HIS:CE1	1:A:73:PHE:CE2	0.47	3.02	15	1
1:B:32:TYR:HE2	1:B:41:HIS:HB2	0.47	1.68	16	1
1:A:43:LYS:CG	1:A:54:TRP:O	0.47	2.63	12	3
1:B:67:THR:O	1:B:68:HIS:C	0.47	2.53	1	1
1:B:5:LYS:O	1:B:22:VAL:CG1	0.47	2.63	9	6
1:A:34:ILE:HD13	1:A:34:ILE:N	0.47	2.25	6	1
1:A:72:HIS:O	1:A:73:PHE:CB	0.47	2.63	8	3
1:B:70:THR:O	1:B:71:LYS:CB	0.47	2.63	17	3
1:A:13:MET:HG2	1:A:17:MET:HG2	0.47	1.85	16	2
1:B:4:ARG:HH11	1:B:4:ARG:CG	0.47	2.22	12	2
1:B:17:MET:CE	1:B:54:TRP:CH2	0.47	2.98	19	3
1:A:80:GLN:O	1:A:81:VAL:HG23	0.47	2.09	14	1
1:A:46:PHE:O	1:A:54:TRP:CD1	0.47	2.68	15	1
1:A:68:HIS:CD2	1:A:73:PHE:CD2	0.47	3.03	15	1
1:A:17:MET:HE2	1:A:50:TYR:CE1	0.47	2.45	16	1
1:B:80:GLN:CA	1:B:80:GLN:NE2	0.47	2.78	20	1
1:A:5:LYS:O	1:A:78:LEU:CD1	0.47	2.63	15	5
1:B:56:CYS:CA	1:B:84:LEU:O	0.47	2.63	2	2
1:A:65:TYR:CE2	1:B:43:LYS:CB	0.47	2.98	16	2
1:B:62:PHE:CE2	1:B:64:SER:CB	0.47	2.98	16	2
1:A:46:PHE:CE1	1:A:85:LEU:HD21	0.47	2.45	8	2
1:B:24:CYS:O	1:B:27:GLN:CG	0.47	2.63	18	1
1:B:40:ALA:O	1:B:43:LYS:HG3	0.47	2.09	19	1
1:A:57:ILE:CD1	1:B:65:TYR:H	0.46	2.22	12	6
1:A:73:PHE:CG	1:A:73:PHE:O	0.46	2.68	1	1
1:A:10:ASN:O	1:A:11:ALA:CB	0.46	2.62	2	2
1:A:12:ASP:O	1:A:72:HIS:CD2	0.46	2.69	4	1
1:B:55:HIS:ND1	1:B:86:PHE:CZ	0.46	2.83	6	1
1:B:34:ILE:O	1:B:38:ILE:CG1	0.46	2.63	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:GLU:OE2	1:A:49:LYS:HG3	0.46	2.09	9	1
1:B:58:VAL:O	1:B:58:VAL:HG13	0.46	2.10	14	1
1:B:79:GLY:O	1:B:80:GLN:HG2	0.46	2.10	14	1
1:A:17:MET:O	1:A:20:ASP:OD1	0.46	2.33	15	1
1:B:46:PHE:HB3	1:B:54:TRP:CG	0.46	2.45	16	3
1:B:35:GLU:OE1	1:B:35:GLU:CA	0.46	2.63	20	1
1:A:67:THR:CG2	1:B:53:THR:OG1	0.46	2.63	1	2
1:A:12:ASP:HB2	1:A:69:GLU:HB3	0.46	1.85	2	1
1:A:25:ALA:O	1:A:29:LEU:CG	0.46	2.63	13	5
1:B:40:ALA:O	1:B:41:HIS:C	0.46	2.54	6	6
1:A:32:TYR:O	1:A:34:ILE:CD1	0.46	2.63	5	1
1:B:69:GLU:O	1:B:70:THR:CG2	0.46	2.62	5	1
1:B:55:HIS:CB	1:B:86:PHE:CE2	0.46	2.98	8	3
1:A:46:PHE:HA	1:A:50:TYR:HD2	0.46	1.69	7	3
1:B:54:TRP:CA	1:B:87:LYS:HB3	0.46	2.28	18	2
1:A:69:GLU:O	1:A:71:LYS:N	0.46	2.49	10	1
1:A:69:GLU:C	1:A:70:THR:CG2	0.46	2.84	10	1
1:A:20:ASP:OD1	1:A:21:SER:N	0.46	2.47	15	1
1:A:61:ASN:CG	1:B:60:ARG:HD3	0.46	2.31	15	1
1:A:69:GLU:C	1:A:70:THR:OG1	0.46	2.53	15	2
1:A:55:HIS:NE2	1:B:67:THR:CG2	0.46	2.78	16	1
1:A:69:GLU:HG3	1:A:88:SER:CA	0.46	2.33	17	1
1:A:61:ASN:CG	1:B:60:ARG:NH2	0.46	2.68	19	1
1:B:35:GLU:OE1	1:B:58:VAL:O	0.46	2.33	20	1
1:A:73:PHE:HD1	1:A:86:PHE:CB	0.46	2.23	7	2
1:B:67:THR:O	1:B:69:GLU:HG2	0.46	2.10	1	1
1:A:13:MET:C	1:A:18:GLN:NE2	0.46	2.68	5	2
1:B:70:THR:C	1:B:71:LYS:CG	0.46	2.83	5	1
1:A:68:HIS:CD2	1:A:72:HIS:HA	0.46	2.45	8	1
1:A:78:LEU:HD23	1:A:83:ILE:HD11	0.46	1.85	10	2
1:B:43:LYS:CE	1:B:54:TRP:O	0.46	2.64	9	2
1:A:12:ASP:O	1:A:72:HIS:CB	0.46	2.63	11	3
1:B:14:SER:O	1:B:15:GLU:C	0.46	2.54	15	3
1:B:43:LYS:HZ2	1:B:54:TRP:C	0.46	2.13	12	1
1:A:12:ASP:OD1	1:A:12:ASP:O	0.46	2.33	14	2
1:B:17:MET:HE3	1:B:50:TYR:CE2	0.46	2.44	14	1
1:A:32:TYR:O	1:A:38:ILE:CG1	0.46	2.64	16	1
1:B:9:LYS:HB2	1:B:75:TYR:CD2	0.46	2.43	16	1
1:B:4:ARG:HG3	1:B:4:ARG:HH11	0.46	1.70	19	1
1:A:57:ILE:CG2	1:B:62:PHE:CE2	0.46	2.98	20	1
1:A:26:THR:OG1	1:A:78:LEU:HD11	0.46	2.09	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:69:GLU:OE2	1:B:88:SER:OG	0.46	2.32	18	2
1:B:53:THR:O	1:B:87:LYS:CG	0.46	2.64	12	3
1:A:55:HIS:CD2	1:A:87:LYS:C	0.46	2.89	4	3
1:A:70:THR:HG22	1:A:71:LYS:HG2	0.46	1.86	3	1
1:B:28:ALA:HB3	1:B:38:ILE:HG22	0.46	1.87	4	1
1:B:43:LYS:CD	1:B:54:TRP:O	0.46	2.64	14	2
1:A:43:LYS:HZ3	1:A:54:TRP:HB3	0.46	1.71	5	1
1:A:67:THR:CG2	1:A:67:THR:O	0.46	2.63	6	3
1:A:27:GLN:CB	1:A:41:HIS:NE2	0.46	2.78	11	1
1:A:66:VAL:HG11	1:B:86:PHE:HE2	0.46	1.70	14	1
1:A:55:HIS:ND1	1:B:86:PHE:CE2	0.46	2.84	17	1
1:B:43:LYS:CG	1:B:54:TRP:O	0.46	2.64	8	7
1:A:44:LYS:HD2	1:A:44:LYS:C	0.46	2.30	2	1
1:B:32:TYR:HE1	1:B:41:HIS:CB	0.46	2.24	4	3
1:B:68:HIS:HE2	1:B:87:LYS:CG	0.46	2.22	4	1
1:A:11:ALA:C	1:A:13:MET:H	0.46	2.14	17	4
1:A:59:GLY:O	1:A:81:VAL:CG1	0.46	2.63	15	2
1:A:46:PHE:CE2	1:A:85:LEU:HD23	0.46	2.44	8	2
1:B:19:GLN:O	1:B:23:GLU:CG	0.46	2.63	8	1
1:A:70:THR:O	1:A:71:LYS:HG2	0.46	2.11	13	3
1:A:58:VAL:O	1:A:58:VAL:CG1	0.46	2.63	13	2
1:A:76:PHE:CE2	1:A:78:LEU:CD2	0.46	2.97	16	1
1:B:13:MET:HB3	1:B:18:GLN:OE1	0.46	2.10	16	1
1:A:38:ILE:CG2	1:A:58:VAL:HG21	0.46	2.39	19	2
1:A:18:GLN:O	1:A:74:ILE:CD1	0.46	2.64	5	6
1:A:56:CYS:CB	1:A:85:LEU:CD1	0.46	2.93	13	11
1:B:69:GLU:O	1:B:70:THR:CB	0.46	2.64	13	3
1:A:21:SER:CB	1:A:74:ILE:HG21	0.46	2.40	17	3
1:A:41:HIS:HD2	1:A:42:ILE:N	0.46	2.09	9	3
1:A:86:PHE:CE1	1:B:55:HIS:CE1	0.46	3.04	9	1
1:B:28:ALA:O	1:B:32:TYR:CD2	0.46	2.69	14	2
1:A:53:THR:O	1:A:87:LYS:CG	0.46	2.63	18	1
1:A:54:TRP:CD2	1:A:87:LYS:CG	0.46	2.99	4	3
1:B:26:THR:N	1:B:29:LEU:HD12	0.46	2.25	5	4
1:A:28:ALA:C	1:A:38:ILE:HG23	0.46	2.31	6	3
1:A:68:HIS:HB3	1:A:73:PHE:HD2	0.46	1.68	8	1
1:B:78:LEU:CD2	1:B:78:LEU:N	0.46	2.78	15	2
1:A:43:LYS:HE2	1:A:43:LYS:O	0.46	2.11	11	1
1:B:49:LYS:CE	1:B:50:TYR:CZ	0.46	2.99	16	1
1:B:70:THR:O	1:B:71:LYS:HB3	0.46	2.11	17	1
1:B:55:HIS:O	1:B:86:PHE:N	0.46	2.48	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:11:ALA:CB	1:B:74:ILE:CG1	0.46	2.94	11	9
1:B:15:GLU:O	1:B:18:GLN:N	0.46	2.48	8	3
1:B:81:VAL:CG1	1:B:82:ALA:H	0.46	2.23	1	12
1:A:28:ALA:HA	1:A:32:TYR:CE1	0.46	2.45	2	10
1:A:87:LYS:HB3	1:A:87:LYS:HZ2	0.46	1.71	2	1
1:B:43:LYS:CD	1:B:43:LYS:C	0.46	2.84	2	1
1:B:56:CYS:CB	1:B:85:LEU:CD1	0.46	2.94	14	6
1:A:8:ILE:CD1	1:A:22:VAL:HG21	0.46	2.40	4	1
1:B:51:ASN:N	1:B:51:ASN:ND2	0.46	2.64	4	1
1:A:62:PHE:CD2	1:B:62:PHE:HB3	0.46	2.46	8	1
1:A:35:GLU:CG	1:A:58:VAL:O	0.46	2.64	11	1
1:A:46:PHE:CE2	1:A:50:TYR:CE2	0.46	3.03	12	1
1:B:57:ILE:N	1:B:84:LEU:O	0.46	2.49	14	2
1:A:9:LYS:HE3	1:A:77:TYR:CB	0.46	2.40	15	1
1:B:62:PHE:CZ	1:B:75:TYR:HE1	0.46	2.28	16	1
1:A:55:HIS:CB	1:A:86:PHE:CE2	0.46	2.97	7	1
1:B:78:LEU:HD23	1:B:83:ILE:HG12	0.46	1.88	7	1
1:B:10:ASN:O	1:B:11:ALA:CB	0.46	2.64	8	3
1:B:75:TYR:CD1	1:B:84:LEU:CD1	0.46	2.99	12	1
1:A:17:MET:SD	1:A:17:MET:C	0.46	2.94	16	1
1:A:11:ALA:O	1:A:12:ASP:OD1	0.46	2.33	18	1
1:A:41:HIS:O	1:A:45:GLU:OE1	0.46	2.34	1	1
1:B:11:ALA:HB1	1:B:18:GLN:HE22	0.46	1.69	1	2
1:B:58:VAL:CA	1:B:82:ALA:O	0.46	2.63	19	7
1:B:76:PHE:CD2	1:B:78:LEU:CD2	0.46	2.99	5	2
1:B:42:ILE:HD12	1:B:56:CYS:SG	0.46	2.51	4	1
1:A:27:GLN:O	1:A:31:LYS:CD	0.46	2.64	8	2
1:A:6:ALA:CB	1:A:76:PHE:HD2	0.46	2.24	10	4
1:B:5:LYS:HD2	1:B:5:LYS:O	0.46	2.12	10	1
1:B:47:ASP:OD2	1:B:52:PRO:CA	0.46	2.64	12	1
1:A:29:LEU:O	1:A:32:TYR:O	0.46	2.34	14	1
1:A:74:ILE:CG2	1:A:76:PHE:CE1	0.46	2.99	14	1
1:B:4:ARG:O	1:B:78:LEU:CD1	0.46	2.64	15	2
1:B:71:LYS:O	1:B:72:HIS:CB	0.46	2.64	16	2
1:B:17:MET:SD	1:B:71:LYS:HE2	0.46	2.51	16	1
1:A:74:ILE:CG2	1:A:85:LEU:HB2	0.46	2.41	17	1
1:B:46:PHE:O	1:B:50:TYR:CD1	0.46	2.69	19	2
1:B:38:ILE:O	1:B:42:ILE:CD1	0.46	2.64	18	1
1:B:45:GLU:OE1	1:B:49:LYS:HG3	0.46	2.10	20	1
1:B:75:TYR:C	1:B:76:PHE:CD1	0.46	2.89	20	1
1:A:17:MET:CE	1:A:54:TRP:CH2	0.45	2.99	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:GLU:O	1:A:49:LYS:CB	0.45	2.64	13	5
1:A:60:ARG:HB3	1:A:81:VAL:HA	0.45	1.87	1	1
1:A:86:PHE:HE2	1:B:55:HIS:HD2	0.45	1.54	1	1
1:A:9:LYS:HE2	1:A:77:TYR:HB3	0.45	1.87	2	1
1:A:62:PHE:CD1	1:B:62:PHE:HB3	0.45	2.47	3	1
1:B:77:TYR:CD1	1:B:77:TYR:C	0.45	2.90	15	2
1:A:32:TYR:CB	1:A:37:ASP:OD2	0.45	2.64	9	1
1:B:31:LYS:C	1:B:32:TYR:CD1	0.45	2.89	15	2
1:A:55:HIS:HE1	1:B:69:GLU:OE2	0.45	1.95	13	1
1:A:8:ILE:C	1:A:9:LYS:CG	0.45	2.84	15	2
1:A:69:GLU:O	1:A:70:THR:OG1	0.45	2.34	15	1
1:B:31:LYS:HB3	1:B:32:TYR:CZ	0.45	2.46	16	1
1:B:21:SER:OG	1:B:74:ILE:CG2	0.45	2.63	17	1
1:B:41:HIS:CE1	1:B:45:GLU:OE2	0.45	2.69	17	1
1:B:4:ARG:HD3	1:B:19:GLN:HG2	0.45	1.87	19	1
1:A:55:HIS:CB	1:B:66:VAL:CG1	0.45	2.94	20	1
1:B:25:ALA:O	1:B:29:LEU:CG	0.45	2.64	11	4
1:A:54:TRP:NE1	1:A:87:LYS:HD2	0.45	2.25	18	3
1:A:60:ARG:O	1:A:61:ASN:CB	0.45	2.63	6	2
1:A:46:PHE:CD1	1:A:50:TYR:CD1	0.45	3.04	19	2
1:B:70:THR:OG1	1:B:89:GLY:C	0.45	2.54	6	1
1:B:80:GLN:HG2	1:B:80:GLN:O	0.45	2.11	10	1
1:A:71:LYS:O	1:A:72:HIS:C	0.45	2.53	13	1
1:B:24:CYS:O	1:B:27:GLN:HG3	0.45	2.10	18	1
1:B:56:CYS:O	1:B:57:ILE:CG1	0.45	2.64	18	1
1:A:18:GLN:CB	1:A:74:ILE:CD1	0.45	2.94	15	7
1:A:67:THR:CG2	1:B:55:HIS:CE1	0.45	2.99	1	1
1:A:77:TYR:CD2	1:A:82:ALA:HB2	0.45	2.45	1	2
1:A:65:TYR:CE2	1:B:43:LYS:CE	0.45	2.99	2	1
1:B:70:THR:HG23	1:B:71:LYS:N	0.45	2.25	2	1
1:B:8:ILE:CG2	1:B:9:LYS:N	0.45	2.79	15	4
1:A:57:ILE:O	1:A:83:ILE:CG2	0.45	2.64	7	3
1:B:68:HIS:NE2	1:B:87:LYS:O	0.45	2.49	9	1
1:B:70:THR:CG2	1:B:72:HIS:CD2	0.45	2.99	10	1
1:B:13:MET:SD	1:B:18:GLN:HB3	0.45	2.52	13	1
1:A:67:THR:H	1:B:55:HIS:CG	0.45	2.29	15	1
1:A:60:ARG:O	1:A:77:TYR:CE2	0.45	2.69	19	1
1:A:6:ALA:CB	1:A:22:VAL:CG1	0.45	2.95	1	15
1:B:6:ALA:CB	1:B:22:VAL:CG1	0.45	2.95	11	19
1:A:62:PHE:HE2	1:A:64:SER:CB	0.45	2.25	3	2
1:B:73:PHE:CB	1:B:85:LEU:O	0.45	2.63	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ASP:CB	1:A:72:HIS:CG	0.45	2.99	6	1
1:B:21:SER:OG	1:B:76:PHE:CE1	0.45	2.69	10	2
1:A:31:LYS:C	1:A:32:TYR:CG	0.45	2.89	15	2
1:B:46:PHE:HA	1:B:50:TYR:HD2	0.45	1.72	18	2
1:A:56:CYS:O	1:B:65:TYR:CB	0.45	2.64	14	1
1:B:47:ASP:OD1	1:B:47:ASP:C	0.45	2.54	15	1
1:A:62:PHE:O	1:B:35:GLU:CB	0.45	2.64	16	1
1:A:88:SER:OG	1:B:88:SER:OG	0.45	2.31	10	3
1:B:38:ILE:O	1:B:42:ILE:CG1	0.45	2.65	18	4
1:B:47:ASP:CG	1:B:48:LYS:N	0.45	2.68	1	2
1:A:13:MET:CB	1:A:73:PHE:O	0.45	2.65	19	2
1:B:60:ARG:O	1:B:61:ASN:CB	0.45	2.63	11	3
1:A:22:VAL:O	1:A:26:THR:OG1	0.45	2.33	4	5
1:B:70:THR:C	1:B:72:HIS:N	0.45	2.68	15	2
1:A:39:ALA:HB3	1:B:65:TYR:HB2	0.45	1.89	13	2
1:A:43:LYS:CE	1:A:47:ASP:HB2	0.45	2.42	11	1
1:A:62:PHE:CG	1:B:62:PHE:HB3	0.45	2.47	16	2
1:A:74:ILE:HG22	1:A:85:LEU:HB2	0.45	1.88	16	2
1:B:55:HIS:CD2	1:B:88:SER:N	0.45	2.84	19	1
1:B:80:GLN:HA	1:B:80:GLN:NE2	0.45	2.26	20	1
1:A:17:MET:CE	1:A:50:TYR:CE1	0.45	2.99	16	2
1:A:57:ILE:CG1	1:A:84:LEU:CD2	0.45	2.95	8	3
1:B:77:TYR:CA	1:B:81:VAL:O	0.45	2.65	3	3
1:A:32:TYR:C	1:A:34:ILE:HD13	0.45	2.32	5	1
1:B:34:ILE:O	1:B:38:ILE:CD1	0.45	2.64	7	1
1:A:8:ILE:CA	1:A:75:TYR:O	0.45	2.62	8	1
1:A:78:LEU:C	1:A:80:GLN:N	0.45	2.70	17	2
1:A:12:ASP:CB	1:A:68:HIS:CD2	0.45	3.00	10	1
1:B:18:GLN:CB	1:B:74:ILE:CD1	0.45	2.95	13	3
1:B:4:ARG:NH1	1:B:4:ARG:CG	0.45	2.79	12	1
1:A:35:GLU:CB	1:B:62:PHE:O	0.45	2.64	14	1
1:A:62:PHE:HB2	1:B:62:PHE:CD1	0.45	2.47	15	1
1:A:13:MET:HG3	1:A:72:HIS:CA	0.45	2.41	16	1
1:A:88:SER:CB	1:B:88:SER:OG	0.45	2.64	17	1
1:A:5:LYS:C	1:A:78:LEU:HD13	0.45	2.32	18	2
1:B:43:LYS:HD3	1:B:44:LYS:N	0.45	2.27	19	1
1:A:39:ALA:CB	1:B:65:TYR:CB	0.45	2.95	20	1
1:A:6:ALA:HB3	1:A:22:VAL:CG1	0.45	2.41	14	5
1:A:86:PHE:CE2	1:B:55:HIS:HD2	0.45	2.30	1	1
1:B:29:LEU:O	1:B:32:TYR:O	0.45	2.34	4	4
1:B:33:ASN:C	1:B:33:ASN:OD1	0.45	2.55	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:GLY:O	1:B:39:ALA:CB	0.45	2.65	19	3
1:A:18:GLN:C	1:A:74:ILE:HD12	0.45	2.32	5	1
1:B:73:PHE:HA	1:B:86:PHE:CA	0.45	2.40	5	1
1:B:74:ILE:CG2	1:B:76:PHE:HE1	0.45	2.25	5	2
1:B:62:PHE:HE2	1:B:64:SER:CB	0.45	2.24	10	2
1:A:35:GLU:HG2	1:B:62:PHE:CA	0.45	2.41	7	3
1:B:57:ILE:O	1:B:83:ILE:CG2	0.45	2.65	7	1
1:A:10:ASN:O	1:A:73:PHE:HE1	0.45	1.93	8	1
1:A:39:ALA:HA	1:A:56:CYS:SG	0.45	2.52	9	1
1:B:54:TRP:CG	1:B:87:LYS:HG2	0.45	2.46	11	1
1:A:77:TYR:HD1	1:A:78:LEU:O	0.45	1.95	12	1
1:A:69:GLU:OE2	1:A:88:SER:CA	0.45	2.65	20	2
1:B:46:PHE:HB3	1:B:54:TRP:CD2	0.45	2.47	14	1
1:A:13:MET:CE	1:A:17:MET:SD	0.45	3.04	16	1
1:B:62:PHE:HE1	1:B:64:SER:CB	0.45	2.24	19	1
1:A:15:GLU:C	1:A:17:MET:N	0.45	2.70	1	4
1:A:7:VAL:O	1:A:9:LYS:CD	0.45	2.63	2	1
1:A:9:LYS:CE	1:A:76:PHE:C	0.45	2.84	2	1
1:A:64:SER:N	1:B:57:ILE:HG23	0.45	2.26	2	1
1:B:13:MET:CG	1:B:17:MET:CB	0.45	2.95	2	9
1:B:28:ALA:CB	1:B:38:ILE:CG2	0.45	2.95	12	8
1:A:24:CYS:SG	1:A:42:ILE:CG2	0.45	2.98	8	1
1:A:40:ALA:CB	1:B:65:TYR:CE2	0.45	3.00	8	1
1:B:11:ALA:CA	1:B:73:PHE:O	0.45	2.65	8	1
1:B:13:MET:CG	1:B:18:GLN:OE1	0.45	2.63	8	2
1:A:77:TYR:C	1:A:81:VAL:O	0.45	2.54	17	3
1:B:22:VAL:O	1:B:26:THR:OG1	0.45	2.32	10	1
1:A:32:TYR:O	1:A:38:ILE:HG12	0.45	2.11	13	1
1:A:72:HIS:CB	1:A:87:LYS:CD	0.45	2.94	16	1
1:B:43:LYS:HE3	1:B:53:THR:HA	0.45	1.88	17	1
1:A:77:TYR:O	1:A:77:TYR:HD1	0.45	1.95	18	1
1:A:54:TRP:CD2	1:A:87:LYS:CD	0.45	2.99	1	3
1:B:13:MET:CB	1:B:71:LYS:O	0.45	2.64	2	1
1:B:70:THR:CG2	1:B:71:LYS:H	0.45	2.24	2	1
1:B:20:ASP:OD1	1:B:20:ASP:C	0.45	2.55	3	1
1:B:47:ASP:O	1:B:52:PRO:CD	0.45	2.63	3	5
1:A:6:ALA:CA	1:A:78:LEU:HD13	0.45	2.41	4	1
1:A:16:GLU:O	1:A:19:GLN:CG	0.45	2.65	15	1
1:A:72:HIS:CB	1:A:87:LYS:HG3	0.45	2.30	15	1
1:A:32:TYR:O	1:A:38:ILE:HD11	0.45	2.11	16	1
1:A:51:ASN:O	1:A:87:LYS:CE	0.45	2.64	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:46:PHE:HA	1:B:50:TYR:CD2	0.45	2.46	18	1
1:A:13:MET:CG	1:A:17:MET:CB	0.45	2.95	18	7
1:A:65:TYR:HE2	1:B:43:LYS:CE	0.45	2.25	19	2
1:A:84:LEU:CD2	1:B:57:ILE:CD1	0.45	2.95	16	2
1:A:64:SER:OG	1:A:75:TYR:CE1	0.45	2.70	4	4
1:A:55:HIS:HD2	1:A:87:LYS:CA	0.45	2.22	8	3
1:B:68:HIS:C	1:B:69:GLU:CG	0.45	2.84	5	2
1:A:43:LYS:CD	1:A:54:TRP:C	0.45	2.85	5	1
1:B:73:PHE:CB	1:B:86:PHE:CB	0.45	2.95	7	4
1:B:74:ILE:HG22	1:B:85:LEU:HB3	0.45	1.88	12	2
1:A:59:GLY:HA2	1:B:62:PHE:HA	0.45	1.89	14	1
1:A:46:PHE:C	1:A:54:TRP:CD1	0.45	2.91	15	1
1:A:7:VAL:HB	1:A:9:LYS:HE2	0.45	1.87	16	1
1:A:44:LYS:O	1:A:47:ASP:OD2	0.45	2.35	16	1
1:A:28:ALA:CB	1:A:38:ILE:HA	0.45	2.36	17	1
1:B:21:SER:HA	1:B:46:PHE:HE2	0.45	1.69	19	1
1:B:73:PHE:C	1:B:73:PHE:HD1	0.45	2.16	20	1
1:A:13:MET:CB	1:A:72:HIS:HA	0.44	2.41	1	3
1:A:37:ASP:OD2	1:A:41:HIS:NE2	0.44	2.50	3	1
1:A:73:PHE:CB	1:A:86:PHE:CB	0.44	2.95	8	6
1:B:4:ARG:HB3	1:B:22:VAL:HG11	0.44	1.89	4	1
1:A:74:ILE:O	1:A:76:PHE:HE1	0.44	1.95	8	1
1:A:17:MET:CE	1:A:50:TYR:CD2	0.44	3.00	17	2
1:A:54:TRP:CE3	1:A:87:LYS:HD2	0.44	2.46	16	2
1:A:62:PHE:O	1:B:35:GLU:OE1	0.44	2.35	11	1
1:A:67:THR:O	1:A:68:HIS:C	0.44	2.55	12	1
1:B:41:HIS:O	1:B:44:LYS:HB2	0.44	2.12	12	1
1:B:7:VAL:CB	1:B:77:TYR:O	0.44	2.65	18	2
1:A:62:PHE:CE2	1:B:57:ILE:HG21	0.44	2.47	15	1
1:A:65:TYR:CZ	1:B:40:ALA:HB2	0.44	2.46	15	2
1:B:12:ASP:OD1	1:B:72:HIS:CD2	0.44	2.70	15	1
1:B:21:SER:HB3	1:B:46:PHE:CZ	0.44	2.46	15	1
1:A:65:TYR:O	1:B:56:CYS:O	0.44	2.35	19	1
1:B:11:ALA:CB	1:B:18:GLN:OE1	0.44	2.65	1	1
1:A:68:HIS:CD2	1:A:87:LYS:O	0.44	2.70	2	1
1:B:49:LYS:HB3	1:B:50:TYR:CE1	0.44	2.48	16	3
1:B:70:THR:HG21	1:B:87:LYS:HZ3	0.44	1.67	4	1
1:B:64:SER:OG	1:B:75:TYR:CE1	0.44	2.69	6	1
1:A:61:ASN:HD22	1:A:61:ASN:H	0.44	1.55	7	1
1:B:27:GLN:O	1:B:31:LYS:HB2	0.44	2.12	8	1
1:B:54:TRP:CE2	1:B:87:LYS:CE	0.44	3.00	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ILE:HB	1:A:84:LEU:CD2	0.44	2.42	9	1
1:A:80:GLN:O	1:A:80:GLN:OE1	0.44	2.35	10	1
1:B:4:ARG:HH11	1:B:19:GLN:CB	0.44	2.25	10	1
1:A:35:GLU:OE2	1:A:60:ARG:CD	0.44	2.65	11	1
1:B:74:ILE:CG2	1:B:85:LEU:HB2	0.44	2.38	14	2
1:A:69:GLU:O	1:A:70:THR:CB	0.44	2.65	14	3
1:A:43:LYS:HE3	1:A:54:TRP:H	0.44	1.72	16	1
1:A:55:HIS:CD2	1:B:67:THR:HG22	0.44	2.46	16	1
1:A:63:GLY:CA	1:B:35:GLU:CB	0.44	2.95	3	8
1:A:28:ALA:CB	1:A:38:ILE:CG2	0.44	2.95	6	5
1:A:63:GLY:CA	1:B:35:GLU:HB2	0.44	2.42	12	2
1:B:12:ASP:OD2	1:B:68:HIS:NE2	0.44	2.50	5	1
1:B:38:ILE:CB	1:B:58:VAL:HG11	0.44	2.39	11	2
1:A:16:GLU:HA	1:A:19:GLN:HE21	0.44	1.72	8	1
1:B:46:PHE:O	1:B:50:TYR:HD2	0.44	1.95	18	2
1:B:33:ASN:HD22	1:B:34:ILE:HD13	0.44	1.72	11	1
1:A:28:ALA:CB	1:A:41:HIS:HB3	0.44	2.43	12	1
1:B:42:ILE:O	1:B:43:LYS:C	0.44	2.55	16	7
1:A:21:SER:HB3	1:A:46:PHE:CZ	0.44	2.47	5	2
1:B:43:LYS:C	1:B:43:LYS:HD2	0.44	2.33	2	1
1:B:73:PHE:HD2	1:B:86:PHE:CB	0.44	2.26	3	2
1:B:10:ASN:HB3	1:B:75:TYR:HB2	0.44	1.89	4	1
1:B:72:HIS:C	1:B:73:PHE:HD1	0.44	2.16	11	2
1:A:59:GLY:HA3	1:B:62:PHE:HA	0.44	1.90	18	3
1:B:4:ARG:O	1:B:6:ALA:N	0.44	2.50	5	1
1:A:62:PHE:CB	1:B:62:PHE:CG	0.44	3.00	7	1
1:A:67:THR:HG22	1:B:55:HIS:CD2	0.44	2.46	7	1
1:A:14:SER:O	1:A:18:GLN:CG	0.44	2.62	10	2
1:A:72:HIS:CD2	1:A:87:LYS:HD3	0.44	2.47	10	1
1:A:21:SER:HA	1:A:46:PHE:HE1	0.44	1.67	12	2
1:B:32:TYR:CB	1:B:37:ASP:OD2	0.44	2.65	17	1
1:B:49:LYS:HE3	1:B:50:TYR:CZ	0.44	2.47	17	1
1:B:53:THR:O	1:B:87:LYS:HB2	0.44	2.13	18	1
1:B:4:ARG:CD	1:B:19:GLN:HG2	0.44	2.43	19	1
1:A:43:LYS:C	1:A:43:LYS:CD	0.44	2.86	1	4
1:A:17:MET:HE1	1:A:50:TYR:CE1	0.44	2.48	2	1
1:B:73:PHE:CD1	1:B:86:PHE:CB	0.44	3.00	2	2
1:A:78:LEU:HD22	1:A:78:LEU:N	0.44	2.27	13	5
1:A:13:MET:SD	1:A:18:GLN:HB3	0.44	2.53	10	1
1:A:14:SER:HB2	1:A:17:MET:HB2	0.44	1.89	11	1
1:B:76:PHE:HE2	1:B:78:LEU:HD21	0.44	1.71	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:75:TYR:CD1	1:B:84:LEU:HD12	0.44	2.46	14	1
1:A:25:ALA:CA	1:A:42:ILE:HG12	0.44	2.42	19	1
1:A:24:CYS:HB2	1:A:46:PHE:HE1	0.44	1.73	1	1
1:A:35:GLU:CB	1:B:62:PHE:C	0.44	2.86	10	3
1:B:68:HIS:HB3	1:B:73:PHE:CB	0.44	2.43	2	2
1:B:46:PHE:CE1	1:B:54:TRP:CZ3	0.44	3.06	3	1
1:A:47:ASP:O	1:A:52:PRO:CD	0.44	2.65	16	2
1:B:6:ALA:HA	1:B:77:TYR:O	0.44	2.13	7	1
1:A:32:TYR:CE1	1:A:41:HIS:CB	0.44	3.01	9	1
1:A:31:LYS:HB3	1:A:32:TYR:CZ	0.44	2.47	11	1
1:A:57:ILE:HD13	1:B:64:SER:HB2	0.44	1.88	14	1
1:A:68:HIS:HB2	1:A:73:PHE:CG	0.44	2.47	1	1
1:B:47:ASP:CG	1:B:52:PRO:HG3	0.44	2.33	1	1
1:A:6:ALA:CB	1:A:78:LEU:CD2	0.44	2.96	4	1
1:A:44:LYS:HE2	1:A:44:LYS:CA	0.44	2.42	5	1
1:A:62:PHE:HE1	1:A:64:SER:CB	0.44	2.25	12	2
1:B:47:ASP:OD2	1:B:52:PRO:CG	0.44	2.64	6	1
1:B:57:ILE:CG1	1:B:84:LEU:CD2	0.44	2.94	8	2
1:A:14:SER:O	1:A:17:MET:CB	0.44	2.64	11	1
1:B:56:CYS:HB2	1:B:84:LEU:O	0.44	2.13	13	1
1:B:12:ASP:HB3	1:B:72:HIS:HB3	0.44	1.89	18	2
1:B:42:ILE:O	1:B:44:LYS:N	0.44	2.51	17	1
1:A:69:GLU:HB2	1:A:87:LYS:O	0.44	2.12	19	1
1:B:5:LYS:O	1:B:6:ALA:HB3	0.44	2.12	20	1
1:B:15:GLU:CA	1:B:18:GLN:OE1	0.44	2.65	20	1
1:A:8:ILE:HD12	1:A:76:PHE:CB	0.44	2.41	1	2
1:B:73:PHE:HD1	1:B:86:PHE:CB	0.44	2.26	2	1
1:B:68:HIS:CE1	1:B:70:THR:H	0.44	2.31	9	1
1:A:7:VAL:O	1:A:9:LYS:HE3	0.44	2.13	11	1
1:A:38:ILE:O	1:A:42:ILE:CD1	0.44	2.65	15	2
1:B:54:TRP:CE3	1:B:87:LYS:HD2	0.44	2.48	19	1
1:A:31:LYS:HD3	1:A:41:HIS:CE1	0.44	2.47	1	2
1:A:65:TYR:CB	1:B:39:ALA:CB	0.44	2.96	9	2
1:A:35:GLU:CB	1:B:63:GLY:CA	0.44	2.95	2	1
1:A:69:GLU:HG2	1:A:73:PHE:CD2	0.44	2.48	2	1
1:B:32:TYR:HE1	1:B:41:HIS:CG	0.44	2.30	2	1
1:B:45:GLU:O	1:B:49:LYS:N	0.44	2.51	16	4
1:B:33:ASN:OD1	1:B:34:ILE:HD13	0.44	2.13	3	1
1:B:80:GLN:O	1:B:81:VAL:CG2	0.44	2.66	3	5
1:B:9:LYS:CE	1:B:77:TYR:HB3	0.44	2.42	4	1
1:A:86:PHE:HE2	1:B:55:HIS:HD1	0.44	1.55	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:49:LYS:HD3	1:B:50:TYR:CZ	0.44	2.47	13	2
1:B:68:HIS:HD1	1:B:68:HIS:C	0.44	2.16	6	1
1:B:73:PHE:HE1	1:B:84:LEU:CD1	0.44	2.26	12	1
1:A:43:LYS:CD	1:B:65:TYR:HD2	0.44	2.25	14	1
1:B:11:ALA:HA	1:B:73:PHE:CD1	0.44	2.47	14	1
1:B:12:ASP:HB2	1:B:73:PHE:HE1	0.44	1.73	16	1
1:B:58:VAL:CG2	1:B:81:VAL:CG1	0.44	2.96	19	2
1:A:78:LEU:CD2	1:A:83:ILE:HG12	0.44	2.42	19	1
1:A:46:PHE:CD2	1:A:54:TRP:CD2	0.44	3.06	20	1
1:A:55:HIS:ND1	1:B:67:THR:O	0.43	2.50	4	2
1:A:11:ALA:CB	1:A:74:ILE:CG1	0.43	2.96	11	4
1:B:75:TYR:CD1	1:B:83:ILE:O	0.43	2.71	3	1
1:B:32:TYR:C	1:B:34:ILE:HD12	0.43	2.34	7	1
1:A:17:MET:HE3	1:A:50:TYR:CE2	0.43	2.48	10	1
1:B:7:VAL:CG1	1:B:9:LYS:HE3	0.43	2.42	10	1
1:A:21:SER:HB2	1:A:46:PHE:HZ	0.43	1.71	12	1
1:A:43:LYS:HE2	1:B:65:TYR:O	0.43	2.12	14	1
1:B:4:ARG:CD	1:B:19:GLN:CD	0.43	2.86	16	1
1:A:8:ILE:HD11	1:A:22:VAL:HG21	0.43	1.89	2	1
1:A:34:ILE:O	1:A:37:ASP:CB	0.43	2.65	9	2
1:A:32:TYR:CD1	1:A:41:HIS:ND1	0.43	2.86	10	1
1:A:77:TYR:CE1	1:A:81:VAL:N	0.43	2.86	12	1
1:B:21:SER:OG	1:B:74:ILE:CD1	0.43	2.65	12	1
1:A:57:ILE:CA	1:B:63:GLY:O	0.43	2.63	14	1
1:A:67:THR:CB	1:B:53:THR:CG2	0.43	2.96	15	1
1:B:13:MET:CB	1:B:18:GLN:OE1	0.43	2.65	16	1
1:B:9:LYS:O	1:B:10:ASN:HB2	0.43	2.12	20	1
1:A:32:TYR:HE1	1:A:41:HIS:CB	0.43	2.26	9	4
1:B:72:HIS:HB2	1:B:87:LYS:CB	0.43	2.36	2	1
1:A:56:CYS:CA	1:A:84:LEU:O	0.43	2.63	8	3
1:A:43:LYS:HD2	1:A:55:HIS:N	0.43	2.28	5	1
1:B:78:LEU:HD23	1:B:83:ILE:CD1	0.43	2.42	6	1
1:A:64:SER:CA	1:B:57:ILE:CD1	0.43	2.94	14	4
1:A:66:VAL:CG1	1:B:86:PHE:HE2	0.43	2.25	14	1
1:A:17:MET:CE	1:A:46:PHE:HE1	0.43	2.25	15	1
1:B:42:ILE:O	1:B:45:GLU:N	0.43	2.52	16	1
1:B:53:THR:HG23	1:B:55:HIS:HE1	0.43	1.66	18	1
1:A:10:ASN:O	1:A:73:PHE:CE2	0.43	2.71	19	1
1:A:70:THR:C	1:A:71:LYS:CG	0.43	2.85	20	1
1:A:16:GLU:C	1:A:19:GLN:HG2	0.43	2.34	1	1
1:A:39:ALA:CB	1:B:63:GLY:O	0.43	2.66	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LEU:HD23	1:A:38:ILE:HD13	0.43	1.90	5	1
1:B:21:SER:HB2	1:B:46:PHE:HZ	0.43	1.70	5	3
1:B:68:HIS:NE2	1:B:87:LYS:N	0.43	2.66	9	1
1:B:15:GLU:CA	1:B:18:GLN:HE22	0.43	2.27	11	1
1:B:4:ARG:NH1	1:B:19:GLN:CG	0.43	2.81	12	1
1:B:49:LYS:HD2	1:B:50:TYR:CE2	0.43	2.47	12	1
1:A:39:ALA:H	1:A:58:VAL:CG1	0.43	2.26	18	1
1:A:17:MET:SD	1:A:50:TYR:CD1	0.43	3.11	2	1
1:B:12:ASP:HB3	1:B:68:HIS:HD2	0.43	1.74	2	1
1:A:68:HIS:CE1	1:A:72:HIS:ND1	0.43	2.87	6	1
1:A:11:ALA:O	1:A:12:ASP:CB	0.43	2.65	7	1
1:B:4:ARG:NH1	1:B:19:GLN:HE22	0.43	2.12	7	1
1:B:68:HIS:HD2	1:B:86:PHE:CB	0.43	2.27	9	1
1:A:12:ASP:HB3	1:A:72:HIS:HB3	0.43	1.89	17	2
1:B:24:CYS:SG	1:B:42:ILE:HA	0.43	2.53	11	1
1:B:33:ASN:CG	1:B:33:ASN:O	0.43	2.57	12	1
1:A:57:ILE:CG2	1:A:62:PHE:CE2	0.43	3.00	15	1
1:B:32:TYR:HE2	1:B:41:HIS:CB	0.43	2.26	15	2
1:A:13:MET:SD	1:A:73:PHE:N	0.43	2.91	16	1
1:B:27:GLN:CG	1:B:28:ALA:N	0.43	2.78	18	1
1:A:19:GLN:CG	1:A:20:ASP:N	0.43	2.81	1	2
1:A:9:LYS:CE	1:A:77:TYR:CB	0.43	2.95	2	2
1:B:12:ASP:CB	1:B:68:HIS:HD2	0.43	2.27	3	4
1:B:6:ALA:CB	1:B:22:VAL:HG11	0.43	2.43	3	3
1:A:69:GLU:OE1	1:A:88:SER:O	0.43	2.37	7	1
1:B:5:LYS:HG2	1:B:6:ALA:H	0.43	1.73	7	1
1:B:46:PHE:HD2	1:B:54:TRP:CZ3	0.43	2.30	9	1
1:B:14:SER:HB2	1:B:17:MET:HB2	0.43	1.89	11	1
1:A:33:ASN:HA	1:A:38:ILE:CD1	0.43	2.36	19	1
1:B:66:VAL:CG2	1:B:86:PHE:CZ	0.43	3.00	19	1
1:A:62:PHE:CE2	1:B:57:ILE:CG2	0.43	3.02	1	1
1:A:66:VAL:CG1	1:B:55:HIS:CB	0.43	2.96	1	2
1:A:36:LYS:NZ	1:A:36:LYS:CB	0.43	2.76	2	1
1:B:70:THR:HG21	1:B:87:LYS:HZ1	0.43	1.68	4	1
1:A:43:LYS:HD3	1:A:54:TRP:C	0.43	2.33	6	2
1:A:63:GLY:O	1:B:57:ILE:HA	0.43	2.14	7	1
1:B:23:GLU:O	1:B:27:GLN:CG	0.43	2.66	11	1
1:A:55:HIS:CE1	1:A:88:SER:CB	0.43	3.02	13	1
1:B:40:ALA:O	1:B:43:LYS:N	0.43	2.52	15	1
1:A:68:HIS:HD2	1:A:72:HIS:ND1	0.43	2.11	17	1
1:B:54:TRP:CH2	1:B:87:LYS:HD2	0.43	2.48	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:12:ASP:OD2	1:B:68:HIS:HD2	0.43	1.95	1	1
1:A:77:TYR:CD1	1:A:77:TYR:C	0.43	2.92	9	3
1:B:13:MET:CB	1:B:71:LYS:HG3	0.43	2.43	4	1
1:A:66:VAL:CG1	1:B:55:HIS:CA	0.43	2.96	8	2
1:B:70:THR:O	1:B:72:HIS:N	0.43	2.51	15	2
1:A:18:GLN:CB	1:A:74:ILE:CG1	0.43	2.96	10	1
1:B:34:ILE:CG2	1:B:36:LYS:CE	0.43	2.96	14	1
1:B:79:GLY:C	1:B:80:GLN:HG2	0.43	2.34	18	1
1:A:13:MET:SD	1:A:54:TRP:CZ3	0.43	3.12	7	1
1:B:11:ALA:C	1:B:73:PHE:O	0.43	2.57	8	1
1:B:27:GLN:O	1:B:31:LYS:CD	0.43	2.63	8	1
1:B:57:ILE:HG12	1:B:84:LEU:CD2	0.43	2.32	9	2
1:A:61:ASN:O	1:B:35:GLU:OE2	0.43	2.37	11	1
1:B:71:LYS:HE3	1:B:87:LYS:HG3	0.43	1.90	11	1
1:A:16:GLU:OE1	1:A:16:GLU:HA	0.43	2.14	12	1
1:A:72:HIS:CD2	1:A:72:HIS:N	0.43	2.87	13	1
1:A:55:HIS:CG	1:A:86:PHE:O	0.43	2.71	14	1
1:B:9:LYS:CE	1:B:77:TYR:CB	0.43	2.96	14	1
1:B:15:GLU:O	1:B:18:GLN:HG3	0.43	2.13	15	1
1:A:13:MET:CG	1:A:18:GLN:OE1	0.43	2.66	18	1
1:B:70:THR:HG21	1:B:89:GLY:CA	0.43	2.43	18	1
1:A:21:SER:HA	1:A:46:PHE:HE2	0.43	1.68	19	1
1:A:61:ASN:CB	1:B:60:ARG:NH2	0.43	2.81	19	1
1:A:55:HIS:CA	1:B:66:VAL:CG1	0.43	2.97	20	1
1:B:73:PHE:CG	1:B:75:TYR:HE1	0.43	2.31	20	1
1:A:67:THR:O	1:A:67:THR:CG2	0.43	2.63	1	1
1:B:17:MET:O	1:B:21:SER:HB2	0.43	2.13	1	1
1:B:15:GLU:CA	1:B:18:GLN:CG	0.43	2.95	2	1
1:B:62:PHE:CE1	1:B:82:ALA:O	0.43	2.72	3	1
1:B:76:PHE:CE2	1:B:83:ILE:HB	0.43	2.49	9	2
1:A:86:PHE:HZ	1:B:86:PHE:HE2	0.43	1.56	5	1
1:A:18:GLN:HB2	1:A:74:ILE:CD1	0.43	2.44	10	1
1:B:46:PHE:CG	1:B:50:TYR:CE2	0.43	3.06	10	2
1:B:12:ASP:HB2	1:B:73:PHE:CD2	0.43	2.46	13	1
1:B:56:CYS:HB3	1:B:85:LEU:HA	0.43	1.91	14	1
1:A:27:GLN:HE21	1:A:41:HIS:CE1	0.43	2.32	15	1
1:A:7:VAL:CB	1:A:9:LYS:HE2	0.43	2.44	16	1
1:A:13:MET:HE3	1:A:17:MET:SD	0.43	2.54	16	1
1:A:68:HIS:ND1	1:A:68:HIS:C	0.43	2.72	16	1
1:B:11:ALA:HB3	1:B:18:GLN:OE1	0.42	2.14	1	1
1:A:12:ASP:O	1:A:71:LYS:CA	0.42	2.63	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:LYS:HD2	1:B:44:LYS:N	0.42	2.29	2	1
1:A:55:HIS:NE2	1:A:87:LYS:C	0.42	2.73	3	1
1:A:57:ILE:CD1	1:B:64:SER:CA	0.42	2.96	12	3
1:A:64:SER:HB2	1:A:84:LEU:CD2	0.42	2.30	5	2
1:A:16:GLU:CD	1:A:16:GLU:H	0.42	2.17	6	1
1:A:62:PHE:CA	1:B:59:GLY:CA	0.42	2.96	19	2
1:A:73:PHE:CB	1:A:85:LEU:O	0.42	2.66	12	2
1:A:28:ALA:CB	1:A:38:ILE:O	0.42	2.67	19	2
1:B:43:LYS:N	1:B:56:CYS:SG	0.42	2.92	16	2
1:A:32:TYR:CD2	1:A:37:ASP:OD2	0.42	2.72	17	1
1:A:70:THR:OG1	1:A:87:LYS:CE	0.42	2.67	17	1
1:B:68:HIS:O	1:B:69:GLU:CG	0.42	2.67	1	1
1:A:7:VAL:HB	1:A:77:TYR:O	0.42	2.14	6	1
1:B:10:ASN:HB3	1:B:73:PHE:HZ	0.42	1.74	6	1
1:B:46:PHE:HB3	1:B:54:TRP:CD1	0.42	2.49	16	2
1:B:18:GLN:CA	1:B:74:ILE:CD1	0.42	2.95	9	3
1:B:68:HIS:HB2	1:B:73:PHE:CB	0.42	2.45	10	1
1:B:56:CYS:SG	1:B:85:LEU:HD11	0.42	2.55	11	1
1:B:7:VAL:HB	1:B:77:TYR:HB3	0.42	1.91	12	1
1:B:39:ALA:HB1	1:B:56:CYS:SG	0.42	2.55	13	1
1:A:57:ILE:HD12	1:A:84:LEU:HD23	0.42	1.91	14	1
1:A:5:LYS:O	1:A:78:LEU:HA	0.42	2.14	19	2
1:A:51:ASN:N	1:A:51:ASN:HD22	0.42	2.12	20	1
1:A:50:TYR:HB3	1:A:54:TRP:HZ2	0.42	1.73	1	2
1:A:55:HIS:HD1	1:B:67:THR:H	0.42	1.56	2	1
1:A:9:LYS:O	1:A:10:ASN:OD1	0.42	2.38	4	1
1:A:77:TYR:CE1	1:A:78:LEU:O	0.42	2.72	18	3
1:B:12:ASP:CB	1:B:72:HIS:CB	0.42	2.97	9	2
1:B:38:ILE:CG2	1:B:58:VAL:HG11	0.42	2.44	7	1
1:B:51:ASN:O	1:B:52:PRO:O	0.42	2.37	9	1
1:B:13:MET:O	1:B:14:SER:C	0.42	2.58	10	2
1:A:73:PHE:CA	1:A:85:LEU:O	0.42	2.67	12	1
1:A:43:LYS:CE	1:B:65:TYR:HD2	0.42	2.27	14	1
1:A:56:CYS:O	1:B:65:TYR:HB2	0.42	2.14	14	1
1:A:57:ILE:CD1	1:B:84:LEU:HD22	0.42	2.44	14	1
1:B:24:CYS:HB2	1:B:46:PHE:HE1	0.42	1.73	17	1
1:A:65:TYR:CD2	1:B:43:LYS:CG	0.42	3.00	19	1
1:B:75:TYR:CE1	1:B:84:LEU:HD13	0.42	2.48	20	1
1:A:57:ILE:O	1:A:84:LEU:N	0.42	2.52	1	1
1:B:43:LYS:O	1:B:47:ASP:CG	0.42	2.57	3	1
1:A:57:ILE:HD12	1:A:84:LEU:CD2	0.42	2.45	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ALA:O	1:A:29:LEU:HG	0.42	2.13	5	1
1:A:38:ILE:O	1:A:42:ILE:CG1	0.42	2.66	8	2
1:A:51:ASN:HD22	1:A:52:PRO:HD2	0.42	1.73	8	1
1:B:62:PHE:HE1	1:B:82:ALA:O	0.42	1.97	11	1
1:B:27:GLN:HE21	1:B:41:HIS:CE1	0.42	2.32	13	1
1:A:59:GLY:CA	1:B:62:PHE:HA	0.42	2.45	14	1
1:B:11:ALA:CB	1:B:74:ILE:HG12	0.42	2.44	16	1
1:B:28:ALA:CB	1:B:38:ILE:O	0.42	2.67	17	1
1:B:6:ALA:C	1:B:7:VAL:CG2	0.42	2.88	18	1
1:B:46:PHE:O	1:B:50:TYR:CD2	0.42	2.73	18	1
1:A:61:ASN:HB3	1:B:60:ARG:NH2	0.42	2.28	19	1
1:A:62:PHE:CD1	1:A:62:PHE:N	0.42	2.88	19	1
1:A:5:LYS:O	1:A:5:LYS:CG	0.42	2.62	1	1
1:B:55:HIS:ND1	1:B:87:LYS:HA	0.42	2.30	1	1
1:B:87:LYS:NZ	1:B:89:GLY:HA2	0.42	2.29	2	1
1:A:13:MET:CB	1:A:18:GLN:NE2	0.42	2.81	4	1
1:A:31:LYS:C	1:A:32:TYR:CD1	0.42	2.92	17	2
1:B:42:ILE:HG22	1:B:56:CYS:SG	0.42	2.55	11	1
1:B:13:MET:CG	1:B:17:MET:CG	0.42	2.93	13	1
1:B:21:SER:CB	1:B:46:PHE:HZ	0.42	2.27	13	2
1:A:43:LYS:CE	1:A:54:TRP:H	0.42	2.27	16	1
1:B:10:ASN:CG	1:B:73:PHE:HZ	0.42	2.17	19	1
1:A:38:ILE:C	1:A:42:ILE:HD12	0.42	2.34	20	1
1:A:35:GLU:O	1:A:36:LYS:C	0.42	2.57	1	2
1:A:80:GLN:O	1:A:80:GLN:CG	0.42	2.67	1	1
1:B:64:SER:HB2	1:B:84:LEU:CD2	0.42	2.43	2	3
1:A:65:TYR:N	1:B:57:ILE:CD1	0.42	2.83	5	2
1:B:4:ARG:O	1:B:5:LYS:CB	0.42	2.67	7	3
1:B:43:LYS:HZ1	1:B:53:THR:HG23	0.42	1.72	7	1
1:A:40:ALA:HB2	1:B:65:TYR:CD2	0.42	2.50	8	1
1:A:63:GLY:O	1:B:58:VAL:N	0.42	2.51	10	2
1:B:28:ALA:HA	1:B:32:TYR:CE1	0.42	2.50	10	2
1:B:62:PHE:CG	1:B:63:GLY:N	0.42	2.87	14	1
1:B:17:MET:SD	1:B:71:LYS:CD	0.42	3.04	16	1
1:B:13:MET:N	1:B:73:PHE:O	0.42	2.53	17	1
1:A:39:ALA:CB	1:A:56:CYS:SG	0.42	3.08	20	1
1:A:55:HIS:HE1	1:A:88:SER:CB	0.42	2.28	1	1
1:A:68:HIS:CB	1:A:73:PHE:CD2	0.42	3.02	1	2
1:A:75:TYR:HD1	1:A:84:LEU:HA	0.42	1.74	1	2
1:B:55:HIS:O	1:B:86:PHE:HD1	0.42	1.96	1	1
1:A:71:LYS:HG3	1:A:72:HIS:NE2	0.42	2.29	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:73:PHE:CA	1:B:85:LEU:O	0.42	2.63	5	4
1:B:42:ILE:CD1	1:B:56:CYS:SG	0.42	3.08	4	1
1:B:13:MET:N	1:B:18:GLN:NE2	0.42	2.59	8	1
1:A:54:TRP:NE1	1:A:87:LYS:HE3	0.42	2.29	10	1
1:B:8:ILE:CA	1:B:76:PHE:CB	0.42	2.96	10	3
1:B:43:LYS:HZ2	1:B:55:HIS:CA	0.42	2.28	12	1
1:A:67:THR:HG22	1:B:53:THR:CG2	0.42	2.43	13	1
1:A:77:TYR:CZ	1:A:80:GLN:HA	0.42	2.49	15	1
1:A:13:MET:SD	1:A:73:PHE:C	0.42	2.97	16	1
1:A:72:HIS:CD2	1:A:87:LYS:HZ2	0.42	2.32	16	1
1:B:48:LYS:HA	1:B:48:LYS:HE2	0.42	1.91	16	1
1:B:67:THR:O	1:B:67:THR:HG23	0.42	2.14	16	1
1:A:32:TYR:O	1:A:33:ASN:CG	0.42	2.58	18	1
1:A:18:GLN:HE21	1:A:18:GLN:HB3	0.42	1.50	1	2
1:A:60:ARG:HD2	1:A:80:GLN:O	0.42	2.14	1	1
1:B:55:HIS:N	1:B:55:HIS:HD2	0.42	2.10	2	1
1:B:71:LYS:HE3	1:B:71:LYS:HA	0.42	1.92	4	1
1:A:43:LYS:CD	1:A:56:CYS:N	0.42	2.83	5	1
1:B:4:ARG:C	1:B:6:ALA:N	0.42	2.73	5	1
1:B:30:GLU:OE1	1:B:31:LYS:CD	0.42	2.68	10	1
1:A:56:CYS:HG	1:A:57:ILE:N	0.42	2.12	11	1
1:A:61:ASN:O	1:A:61:ASN:OD1	0.42	2.37	12	1
1:B:37:ASP:O	1:B:41:HIS:NE2	0.42	2.53	12	1
1:B:18:GLN:HG2	1:B:18:GLN:H	0.42	1.38	17	3
1:B:35:GLU:CD	1:B:35:GLU:H	0.42	2.18	13	1
1:A:13:MET:O	1:A:15:GLU:N	0.42	2.53	16	1
1:B:41:HIS:CD2	1:B:42:ILE:N	0.42	2.88	16	1
1:A:17:MET:SD	1:A:50:TYR:CE2	0.42	3.12	17	1
1:B:43:LYS:CD	1:B:54:TRP:H	0.42	2.28	17	1
1:B:46:PHE:HA	1:B:50:TYR:CE1	0.42	2.49	17	1
1:B:37:ASP:C	1:B:41:HIS:NE2	0.42	2.72	18	1
1:A:79:GLY:O	1:A:80:GLN:HB3	0.42	2.15	19	1
1:A:75:TYR:CD1	1:A:84:LEU:CB	0.42	3.02	3	1
1:B:7:VAL:O	1:B:7:VAL:CG1	0.42	2.68	3	1
1:A:67:THR:O	1:A:67:THR:HG23	0.42	2.15	7	1
1:B:43:LYS:O	1:B:47:ASP:OD2	0.42	2.38	7	2
1:A:66:VAL:HB	1:B:55:HIS:HD1	0.42	1.73	10	2
1:B:70:THR:HB	1:B:71:LYS:H	0.42	1.51	11	1
1:A:46:PHE:HA	1:A:50:TYR:CE1	0.42	2.50	14	1
1:A:58:VAL:CG2	1:A:81:VAL:HG11	0.42	2.44	14	1
1:A:53:THR:HG23	1:A:55:HIS:CD2	0.42	2.50	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:GLU:O	1:A:70:THR:CG2	0.42	2.67	16	1
1:A:65:TYR:N	1:B:57:ILE:HG12	0.42	2.27	19	1
1:A:47:ASP:CB	1:A:52:PRO:HB3	0.42	2.41	20	1
1:B:78:LEU:C	1:B:80:GLN:N	0.42	2.74	7	2
1:A:49:LYS:HB3	1:A:50:TYR:CD1	0.42	2.50	13	2
1:A:73:PHE:HD2	1:A:86:PHE:CB	0.42	2.27	5	1
1:B:72:HIS:HB3	1:B:87:LYS:HB2	0.42	1.91	5	1
1:B:51:ASN:O	1:B:87:LYS:CE	0.42	2.67	17	2
1:A:53:THR:CG2	1:B:67:THR:CG2	0.42	2.97	12	1
1:B:27:GLN:O	1:B:31:LYS:CG	0.42	2.65	13	2
1:B:62:PHE:HE1	1:B:64:SER:OG	0.42	1.97	13	1
1:A:61:ASN:O	1:B:35:GLU:CD	0.42	2.59	14	1
1:A:70:THR:HG23	1:A:71:LYS:N	0.42	2.28	14	1
1:A:35:GLU:CB	1:B:63:GLY:N	0.41	2.83	2	1
1:A:16:GLU:HG2	1:A:17:MET:N	0.41	2.30	10	1
1:A:75:TYR:C	1:A:76:PHE:CD1	0.41	2.94	12	1
1:B:13:MET:HB2	1:B:73:PHE:H	0.41	1.74	17	2
1:A:7:VAL:O	1:A:9:LYS:CE	0.41	2.68	14	1
1:B:5:LYS:HE3	1:B:6:ALA:H	0.41	1.74	14	1
1:B:10:ASN:O	1:B:75:TYR:HB3	0.41	2.15	2	1
1:A:62:PHE:CG	1:B:62:PHE:CB	0.41	3.03	9	2
1:A:65:TYR:CE1	1:B:43:LYS:HD2	0.41	2.51	8	1
1:B:17:MET:CE	1:B:46:PHE:CE2	0.41	3.03	9	1
1:A:15:GLU:H	1:A:15:GLU:HG2	0.41	1.45	11	1
1:A:88:SER:CB	1:B:69:GLU:OE2	0.41	2.67	12	1
1:A:9:LYS:N	1:A:75:TYR:O	0.41	2.52	14	1
1:A:66:VAL:HA	1:B:55:HIS:CB	0.41	2.43	14	1
1:B:46:PHE:CD1	1:B:54:TRP:CH2	0.41	3.08	14	1
1:A:63:GLY:CA	1:B:58:VAL:O	0.41	2.68	17	1
1:B:14:SER:OG	1:B:17:MET:HG3	0.41	2.14	17	1
1:A:43:LYS:CD	1:B:65:TYR:HE2	0.41	2.26	18	1
1:A:66:VAL:HG21	1:A:84:LEU:HD21	0.41	1.91	18	1
1:B:56:CYS:O	1:B:57:ILE:HG13	0.41	2.15	18	1
1:B:4:ARG:HB3	1:B:22:VAL:CG1	0.41	2.45	4	1
1:B:54:TRP:HA	1:B:87:LYS:HA	0.41	1.92	4	1
1:A:40:ALA:CA	1:B:65:TYR:CD1	0.41	3.03	9	1
1:A:86:PHE:CZ	1:B:86:PHE:CE2	0.41	3.08	12	1
1:A:7:VAL:O	1:A:9:LYS:HD3	0.41	2.14	13	1
1:A:74:ILE:HG12	1:A:75:TYR:N	0.41	2.30	13	1
1:B:72:HIS:HB2	1:B:87:LYS:CG	0.41	2.44	13	1
1:A:43:LYS:CD	1:A:43:LYS:C	0.41	2.89	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LYS:HD2	1:A:55:HIS:C	0.41	2.35	5	1
1:B:35:GLU:OE2	1:B:60:ARG:NH2	0.41	2.53	10	1
1:A:50:TYR:C	1:A:51:ASN:OD1	0.41	2.58	14	1
1:A:8:ILE:CA	1:A:76:PHE:CB	0.41	2.97	16	1
1:B:11:ALA:HB2	1:B:74:ILE:HA	0.41	1.90	18	1
1:A:39:ALA:CA	1:A:56:CYS:SG	0.41	3.08	20	1
1:A:88:SER:OG	1:B:88:SER:HB3	0.41	2.15	1	1
1:B:72:HIS:C	1:B:73:PHE:CD1	0.41	2.94	4	2
1:B:53:THR:O	1:B:53:THR:CG2	0.41	2.68	16	2
1:A:35:GLU:CG	1:B:61:ASN:O	0.41	2.69	7	1
1:B:14:SER:CB	1:B:17:MET:HG3	0.41	2.45	7	2
1:B:28:ALA:HB2	1:B:41:HIS:HB3	0.41	1.92	7	1
1:A:13:MET:HG3	1:A:71:LYS:HG3	0.41	1.91	9	1
1:A:65:TYR:HE2	1:B:43:LYS:HD3	0.41	1.76	9	1
1:B:84:LEU:HD21	1:B:86:PHE:CE2	0.41	2.50	11	1
1:A:43:LYS:HD2	1:B:65:TYR:CD2	0.41	2.49	14	1
1:A:70:THR:O	1:A:71:LYS:HB3	0.41	2.16	18	1
1:A:9:LYS:HE2	1:A:77:TYR:HB2	0.41	1.85	2	1
1:A:17:MET:CE	1:A:46:PHE:HE2	0.41	2.28	3	1
1:A:62:PHE:CD1	1:B:62:PHE:CB	0.41	3.03	3	2
1:A:86:PHE:CE2	1:B:86:PHE:HZ	0.41	2.33	7	1
1:A:43:LYS:CD	1:A:54:TRP:O	0.41	2.68	11	2
1:B:84:LEU:HD21	1:B:86:PHE:HE2	0.41	1.75	11	1
1:A:17:MET:SD	1:A:72:HIS:CE1	0.41	3.14	14	1
1:A:88:SER:OG	1:B:88:SER:CB	0.41	2.68	1	1
1:A:11:ALA:HA	1:A:73:PHE:HD1	0.41	1.74	2	1
1:A:13:MET:HB2	1:A:72:HIS:N	0.41	2.30	7	1
1:A:55:HIS:CA	1:B:66:VAL:HA	0.41	2.45	7	1
1:B:44:LYS:CA	1:B:47:ASP:OD2	0.41	2.68	7	1
1:B:70:THR:OG1	1:B:89:GLY:CA	0.41	2.69	11	1
1:A:68:HIS:CG	1:A:73:PHE:CG	0.41	3.08	15	1
1:A:8:ILE:HG13	1:A:76:PHE:CB	0.41	2.39	18	1
1:A:13:MET:CB	1:A:18:GLN:OE1	0.41	2.68	18	1
1:B:86:PHE:O	1:B:86:PHE:CD2	0.41	2.74	18	1
1:B:62:PHE:CZ	1:B:75:TYR:CE2	0.41	3.08	19	1
1:A:57:ILE:HG23	1:B:63:GLY:C	0.41	2.36	4	1
1:B:5:LYS:HA	1:B:5:LYS:HE3	0.41	1.92	4	1
1:A:7:VAL:CB	1:A:77:TYR:O	0.41	2.69	6	1
1:B:45:GLU:O	1:B:48:LYS:CG	0.41	2.67	7	1
1:A:61:ASN:OD1	1:B:60:ARG:NE	0.41	2.53	8	1
1:A:59:GLY:CA	1:A:62:PHE:CE1	0.41	3.04	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:54:TRP:HA	1:B:87:LYS:CA	0.41	2.45	9	1
1:A:46:PHE:HD1	1:A:54:TRP:CZ2	0.41	2.34	15	1
1:B:21:SER:HB3	1:B:74:ILE:HG21	0.41	1.92	1	1
1:B:29:LEU:CD2	1:B:81:VAL:CG2	0.41	2.98	1	1
1:A:8:ILE:C	1:A:9:LYS:CD	0.41	2.88	2	1
1:B:86:PHE:CD1	1:B:86:PHE:C	0.41	2.93	6	2
1:B:28:ALA:O	1:B:32:TYR:O	0.41	2.38	3	1
1:A:64:SER:HG	1:A:75:TYR:HE1	0.41	1.58	5	2
1:A:87:LYS:HB3	1:A:87:LYS:HZ3	0.41	1.75	5	1
1:A:43:LYS:HE2	1:A:54:TRP:N	0.41	2.24	6	1
1:A:57:ILE:CD1	1:B:65:TYR:N	0.41	2.84	6	1
1:A:71:LYS:C	1:A:72:HIS:CG	0.41	2.94	7	1
1:A:17:MET:HE2	1:A:46:PHE:CE2	0.41	2.51	8	1
1:A:71:LYS:O	1:A:72:HIS:HB2	0.41	2.15	8	1
1:A:84:LEU:HD11	1:A:86:PHE:CD1	0.41	2.51	8	1
1:B:7:VAL:CG2	1:B:77:TYR:O	0.41	2.67	9	1
1:B:26:THR:O	1:B:29:LEU:HB2	0.41	2.16	9	2
1:A:13:MET:CG	1:A:17:MET:CG	0.41	2.95	10	1
1:A:70:THR:CG2	1:A:87:LYS:HE2	0.41	2.45	11	1
1:B:71:LYS:HE3	1:B:87:LYS:N	0.41	2.30	11	1
1:A:21:SER:CB	1:A:46:PHE:HZ	0.41	2.29	12	1
1:A:43:LYS:CE	1:B:65:TYR:CD2	0.41	3.04	14	1
1:B:33:ASN:O	1:B:34:ILE:HD13	0.41	2.16	15	1
1:B:67:THR:CG2	1:B:67:THR:O	0.41	2.68	16	1
1:A:66:VAL:HG12	1:B:55:HIS:HA	0.41	1.90	17	1
1:B:42:ILE:C	1:B:44:LYS:N	0.41	2.74	17	1
1:B:62:PHE:CD1	1:B:62:PHE:C	0.41	2.94	19	1
1:B:53:THR:O	1:B:53:THR:HG23	0.41	2.15	20	1
1:B:9:LYS:HE3	1:B:77:TYR:CB	0.41	2.45	4	1
1:A:20:ASP:CB	1:A:50:TYR:OH	0.41	2.66	6	1
1:A:45:GLU:O	1:A:46:PHE:C	0.41	2.60	9	1
1:A:54:TRP:CZ2	1:A:87:LYS:CD	0.41	3.03	11	1
1:A:42:ILE:O	1:A:43:LYS:C	0.41	2.59	12	1
1:A:50:TYR:CD1	1:A:50:TYR:N	0.41	2.89	13	1
1:B:64:SER:HG	1:B:75:TYR:HE2	0.41	1.59	19	1
1:B:8:ILE:CD1	1:B:22:VAL:HG21	0.40	2.45	5	1
1:A:65:TYR:HD1	1:B:43:LYS:HD3	0.40	1.75	6	1
1:B:54:TRP:CG	1:B:87:LYS:HG3	0.40	2.50	6	1
1:A:47:ASP:CA	1:A:54:TRP:CD1	0.40	3.01	8	1
1:B:68:HIS:CD2	1:B:87:LYS:O	0.40	2.74	9	1
1:B:6:ALA:CB	1:B:78:LEU:CD2	0.40	2.97	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:VAL:HG23	1:A:81:VAL:HG11	0.40	1.91	14	1
1:A:46:PHE:CE1	1:A:50:TYR:CE2	0.40	3.08	15	1
1:A:15:GLU:H	1:A:15:GLU:HG3	0.40	1.57	2	1
1:B:71:LYS:HD2	1:B:72:HIS:CD2	0.40	2.52	2	1
1:B:62:PHE:H	1:B:62:PHE:HD1	0.40	1.56	3	1
1:B:73:PHE:HD2	1:B:86:PHE:HB2	0.40	1.77	3	1
1:A:8:ILE:CD1	1:A:22:VAL:CG2	0.40	2.99	4	1
1:A:24:CYS:SG	1:A:42:ILE:CA	0.40	3.07	8	1
1:B:11:ALA:HA	1:B:74:ILE:CA	0.40	2.39	8	1
1:A:13:MET:SD	1:A:18:GLN:CB	0.40	3.10	10	1
1:B:24:CYS:CA	1:B:27:GLN:HG3	0.40	2.45	11	1
1:A:75:TYR:C	1:A:76:PHE:HD1	0.40	2.19	12	1
1:A:68:HIS:CG	1:A:69:GLU:N	0.40	2.88	13	1
1:B:54:TRP:CZ2	1:B:87:LYS:HD3	0.40	2.51	13	1
1:A:37:ASP:C	1:A:41:HIS:NE2	0.40	2.74	16	1
1:A:9:LYS:HE3	1:A:77:TYR:HB2	0.40	1.92	17	1
1:B:44:LYS:O	1:B:44:LYS:HE2	0.40	2.15	18	1
1:B:53:THR:CG2	1:B:55:HIS:HE1	0.40	2.28	18	1
1:A:8:ILE:O	1:A:9:LYS:CD	0.40	2.67	19	1
1:B:62:PHE:CZ	1:B:75:TYR:CZ	0.40	3.09	19	1
1:B:54:TRP:CD1	1:B:87:LYS:HE3	0.40	2.51	1	1
1:A:75:TYR:HD1	1:A:84:LEU:CB	0.40	2.29	3	1
1:A:70:THR:HG21	1:A:87:LYS:HE2	0.40	1.92	4	1
1:A:86:PHE:CZ	1:B:66:VAL:CG1	0.40	3.04	4	1
1:B:36:LYS:H	1:B:36:LYS:HG2	0.40	1.38	5	1
1:A:68:HIS:CB	1:A:72:HIS:O	0.40	2.69	6	1
1:B:54:TRP:C	1:B:55:HIS:CD2	0.40	2.94	9	1
1:B:5:LYS:O	1:B:5:LYS:CG	0.40	2.69	11	1
1:B:13:MET:SD	1:B:17:MET:HG3	0.40	2.55	13	1
1:B:72:HIS:HB3	1:B:87:LYS:HG3	0.40	1.93	14	1
1:B:82:ALA:C	1:B:83:ILE:CD1	0.40	2.87	14	1
1:A:46:PHE:CD1	1:A:54:TRP:CE3	0.40	3.09	15	1
1:B:4:ARG:HD3	1:B:19:GLN:NE2	0.40	2.32	17	1
1:A:14:SER:OG	1:A:17:MET:HB2	0.40	2.15	20	1
1:A:62:PHE:CA	1:B:35:GLU:HG2	0.40	2.46	1	1
1:A:64:SER:CB	1:B:57:ILE:HD13	0.40	2.45	2	1
1:B:56:CYS:HB2	1:B:85:LEU:HA	0.40	1.94	2	1
1:A:70:THR:HB	1:A:71:LYS:H	0.40	1.54	5	1
1:A:58:VAL:CG2	1:A:83:ILE:CD1	0.40	2.99	6	1
1:A:21:SER:CB	1:A:46:PHE:CZ	0.40	3.03	15	2
1:A:71:LYS:C	1:A:72:HIS:ND1	0.40	2.75	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:PHE:CD1	1:A:85:LEU:HD21	0.40	2.52	8	1
1:A:24:CYS:HB3	1:A:42:ILE:HG23	0.40	1.93	9	1
1:A:61:ASN:HB3	1:B:60:ARG:HE	0.40	1.76	10	1
1:B:32:TYR:CD2	1:B:41:HIS:CE1	0.40	3.09	11	1
1:A:68:HIS:O	1:A:69:GLU:CB	0.40	2.68	12	1
1:B:54:TRP:CH2	1:B:87:LYS:HD3	0.40	2.52	13	1
1:A:81:VAL:HG12	1:A:83:ILE:HD13	0.40	1.93	14	1
1:B:32:TYR:CG	1:B:37:ASP:OD2	0.40	2.74	17	1
1:B:46:PHE:CA	1:B:50:TYR:HD1	0.40	2.28	17	1
1:B:6:ALA:O	1:B:7:VAL:CG2	0.40	2.69	18	1
1:B:7:VAL:H	1:B:77:TYR:N	0.40	2.14	20	1
1:A:55:HIS:HD2	1:A:86:PHE:O	0.40	2.00	2	1
1:A:57:ILE:HD13	1:B:64:SER:HB3	0.40	1.92	4	1
1:A:16:GLU:CD	1:A:16:GLU:N	0.40	2.75	6	1
1:A:6:ALA:CB	1:A:22:VAL:HG11	0.40	2.46	15	1
1:A:85:LEU:O	1:A:86:PHE:HB3	0.40	2.16	15	1
1:B:18:GLN:HA	1:B:21:SER:OG	0.40	2.17	15	1
1:A:27:GLN:O	1:A:31:LYS:CG	0.40	2.70	18	1
1:B:18:GLN:HE21	1:B:18:GLN:HB3	0.40	1.50	20	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	84/89 (94%)	54±3 (64±3%)	20±3 (24±4%)	10±2 (12±3%)	1 6
1	B	85/89 (96%)	56±3 (65±4%)	20±2 (23±3%)	10±2 (12±2%)	1 7
All	All	3380/3560 (95%)	2183 (65%)	793 (23%)	404 (12%)	1 7

All 59 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	35	GLU	20
1	A	51	ASN	20

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Mol	Chain	Res	Type	Models (Total)
1	B	51	ASN	20
1	B	79	GLY	19
1	B	60	ARG	17
1	B	8	ILE	15
1	A	61	ASN	14
1	B	61	ASN	14
1	B	70	THR	14
1	A	79	GLY	14
1	A	71	LYS	12
1	B	7	VAL	12
1	A	70	THR	12
1	B	71	LYS	11
1	A	8	ILE	10
1	A	72	HIS	10
1	B	73	PHE	10
1	A	15	GLU	9
1	A	73	PHE	9
1	B	72	HIS	9
1	B	10	ASN	8
1	A	78	LEU	8
1	B	6	ALA	7
1	B	68	HIS	7
1	A	60	ARG	7
1	A	68	HIS	6
1	B	4	ARG	6
1	A	6	ALA	5
1	A	10	ASN	5
1	A	5	LYS	5
1	A	58	VAL	5
1	A	42	ILE	5
1	A	69	GLU	4
1	A	74	ILE	4
1	B	35	GLU	4
1	B	69	GLU	4
1	B	5	LYS	4
1	A	12	ASP	4
1	A	11	ALA	3
1	B	52	PRO	3
1	B	11	ALA	3
1	B	58	VAL	3
1	B	42	ILE	2
1	A	7	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	67	THR	2
1	A	33	ASN	2
1	A	16	GLU	2
1	B	14	SER	2
1	A	66	VAL	1
1	A	88	SER	1
1	B	12	ASP	1
1	B	33	ASN	1
1	A	86	PHE	1
1	A	9	LYS	1
1	A	52	PRO	1
1	A	65	TYR	1
1	B	43	LYS	1
1	B	74	ILE	1
1	A	55	HIS	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	74/78 (95%)	44±4 (59±6%)	30±4 (41±6%)	0 4
1	B	75/78 (96%)	45±4 (60±5%)	30±4 (40±5%)	0 5
All	All	2980/3120 (96%)	1770 (59%)	1210 (41%)	0 4

All 123 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	32	TYR	20
1	A	83	ILE	20
1	B	18	GLN	20
1	B	32	TYR	20
1	B	83	ILE	20
1	A	18	GLN	19
1	A	41	HIS	19
1	A	36	LYS	18
1	A	60	ARG	18

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Mol	Chain	Res	Type	Models (Total)
1	B	41	HIS	18
1	B	46	PHE	18
1	A	88	SER	17
1	B	36	LYS	17
1	A	8	ILE	16
1	A	48	LYS	16
1	A	85	LEU	16
1	B	10	ASN	16
1	A	49	LYS	15
1	A	55	HIS	15
1	B	4	ARG	15
1	B	17	MET	15
1	B	48	LYS	15
1	B	49	LYS	15
1	B	74	ILE	15
1	A	76	PHE	15
1	B	5	LYS	15
1	B	69	GLU	15
1	B	88	SER	15
1	A	10	ASN	14
1	A	17	MET	14
1	A	47	ASP	14
1	B	14	SER	14
1	B	21	SER	14
1	B	84	LEU	14
1	B	87	LYS	14
1	B	30	GLU	13
1	B	47	ASP	13
1	A	43	LYS	13
1	B	8	ILE	13
1	B	20	ASP	12
1	B	60	ARG	12
1	B	85	LEU	12
1	A	44	LYS	12
1	A	5	LYS	12
1	A	37	ASP	12
1	A	46	PHE	11
1	A	70	THR	11
1	A	87	LYS	11
1	A	20	ASP	11
1	B	71	LYS	11
1	A	68	HIS	11

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Mol	Chain	Res	Type	Models (Total)
1	A	80	GLN	11
1	A	16	GLU	10
1	A	30	GLU	10
1	A	69	GLU	10
1	B	43	LYS	10
1	B	68	HIS	10
1	A	14	SER	10
1	A	78	LEU	10
1	A	84	LEU	10
1	B	61	ASN	10
1	A	56	CYS	10
1	A	61	ASN	10
1	A	74	ILE	10
1	B	70	THR	10
1	A	15	GLU	9
1	B	44	LYS	9
1	B	56	CYS	9
1	A	21	SER	9
1	B	16	GLU	9
1	B	78	LEU	9
1	B	76	PHE	9
1	B	80	GLN	9
1	B	33	ASN	8
1	B	45	GLU	8
1	A	9	LYS	8
1	B	86	PHE	8
1	B	9	LYS	8
1	A	62	PHE	8
1	A	71	LYS	8
1	A	51	ASN	8
1	A	12	ASP	7
1	B	37	ASP	7
1	B	55	HIS	7
1	A	13	MET	7
1	A	24	CYS	7
1	A	31	LYS	7
1	B	12	ASP	7
1	B	75	TYR	7
1	A	27	GLN	7
1	B	73	PHE	7
1	A	19	GLN	6
1	A	33	ASN	6

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Mol	Chain	Res	Type	Models (Total)
1	A	73	PHE	6
1	B	27	GLN	6
1	A	45	GLU	5
1	B	13	MET	5
1	B	24	CYS	5
1	B	35	GLU	5
1	B	62	PHE	4
1	A	26	THR	4
1	A	35	GLU	4
1	B	15	GLU	4
1	B	51	ASN	4
1	B	31	LYS	4
1	B	53	THR	3
1	B	19	GLN	3
1	A	67	THR	3
1	A	86	PHE	3
1	A	53	THR	3
1	B	64	SER	2
1	A	72	HIS	2
1	A	75	TYR	2
1	B	72	HIS	2
1	A	64	SER	2
1	B	29	LEU	2
1	A	29	LEU	1
1	B	38	ILE	1
1	A	34	ILE	1
1	B	26	THR	1
1	B	65	TYR	1
1	B	77	TYR	1
1	B	67	THR	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided