



Full wwPDB NMR Structure Validation Report ⓘ

Feb 18, 2018 – 08:53 pm GMT

PDB ID : 1F3C
Title : REFINED SOLUTION STRUCTURE OF 8KDA DYNEIN LIGHT CHAIN (DLC8)
Authors : Fan, J.-S.; Zhang, Q.; Tochio, H.; Zhang, M.
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 ⓘ symbol.

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk30686
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30686

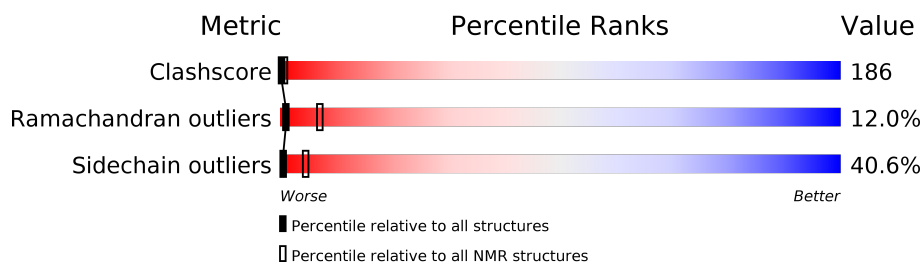
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

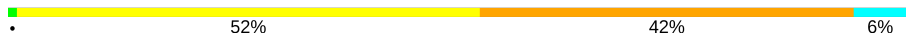

The overall completeness of chemical shifts assignment is 76%.

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	89	
1	B	89	

2 Ensemble composition and analysis

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.

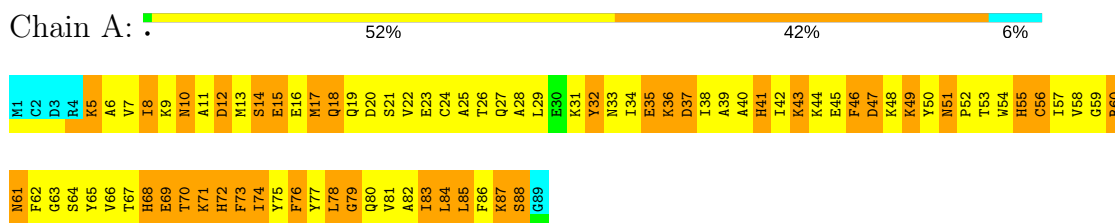
Mol	Chain	Residues	Atoms						Trace
1	A	89	Total	C	H	N	O	S	0
			1446	465	718	122	135	6	
1	B	89	Total	C	H	N	O	S	0
			1446	465	718	122	135	6	

4 Residue-property plots

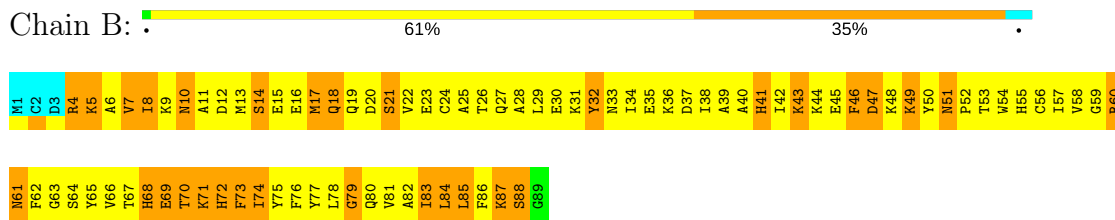
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: DYNEIN



- Molecule 1: DYNEIN

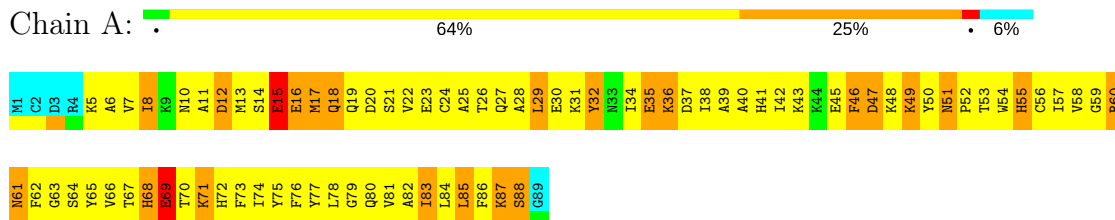


4.2 Scores per residue for each member of the ensemble

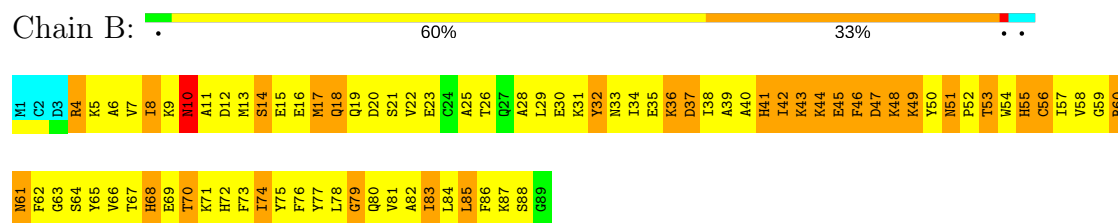
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: DYNEIN

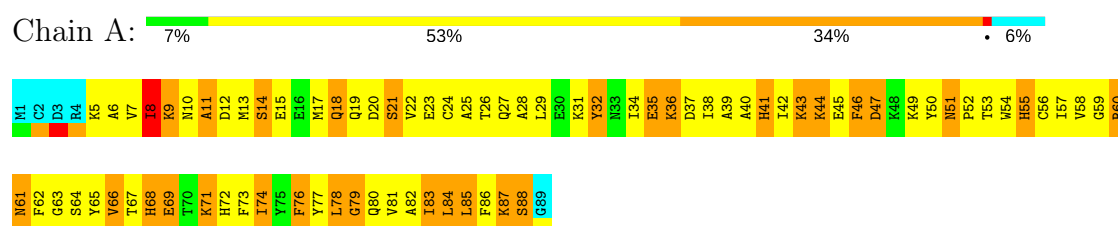


- Molecule 1: DYNEIN

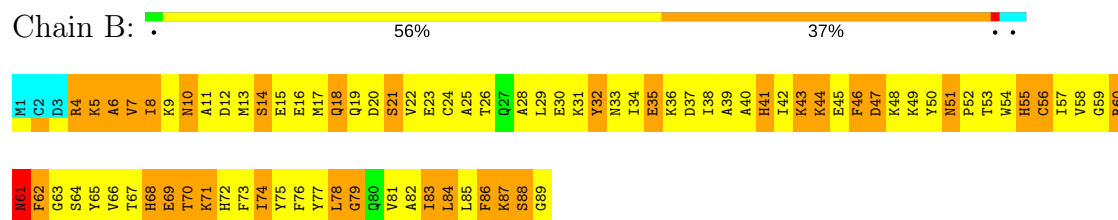


4.2.2 Score per residue for model 2

- Molecule 1: DYNEIN

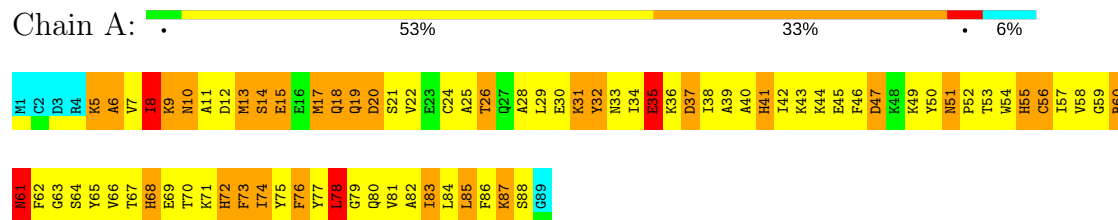


- Molecule 1: DYNEIN

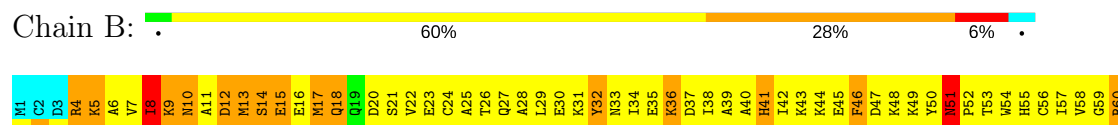


4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: DYNEIN



- Molecule 1: DYNEIN





4.2.4 Score per residue for model 4

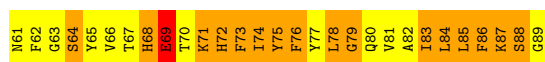
- Molecule 1: DYNEIN

Chain A: . 54% 34% 6%



- Molecule 1: DYNEIN

Chain B: . 49% 42% 6%



4.2.5 Score per residue for model 5

- Molecule 1: DYNEIN

Chain A: . 52% 33% 8% 6%



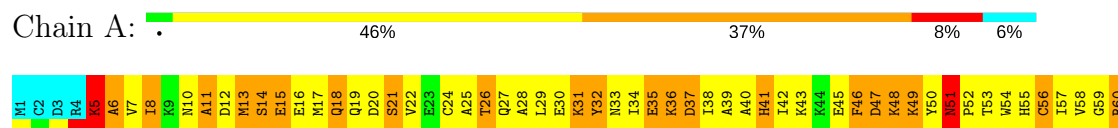
- Molecule 1: DYNEIN

Chain B: . 54% 33% 6%

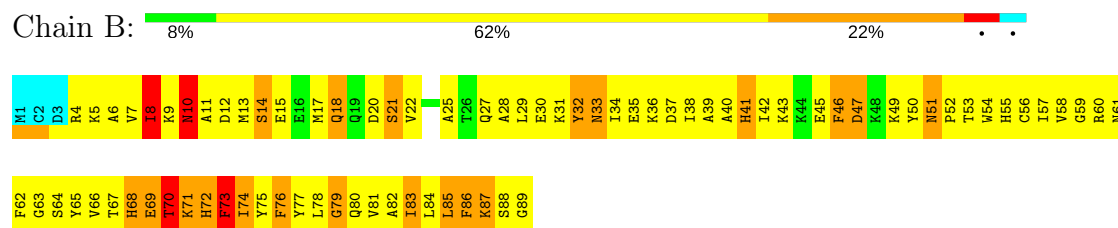


4.2.6 Score per residue for model 6

- Molecule 1: DYNEIN

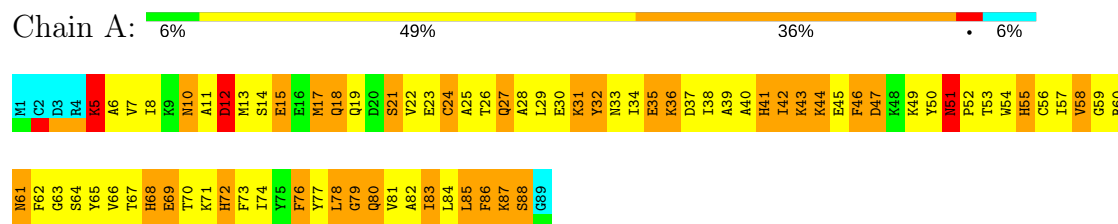


- Molecule 1: DYNEIN

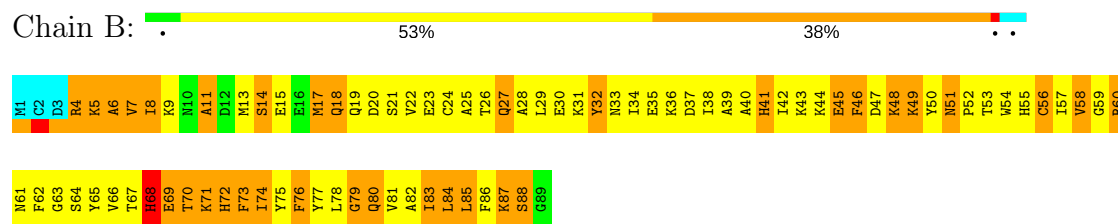


4.2.7 Score per residue for model 7

- Molecule 1: DYNEIN

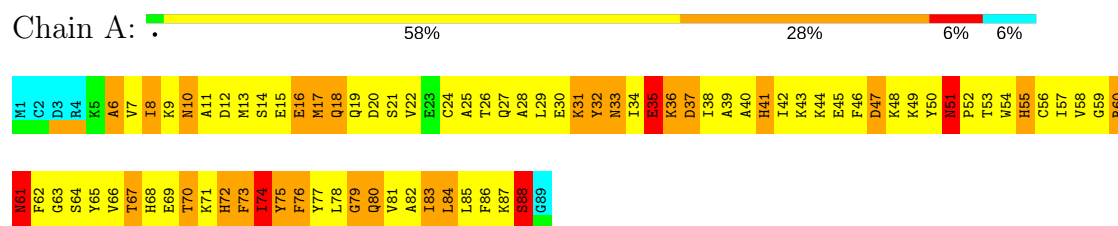


- Molecule 1: DYNEIN

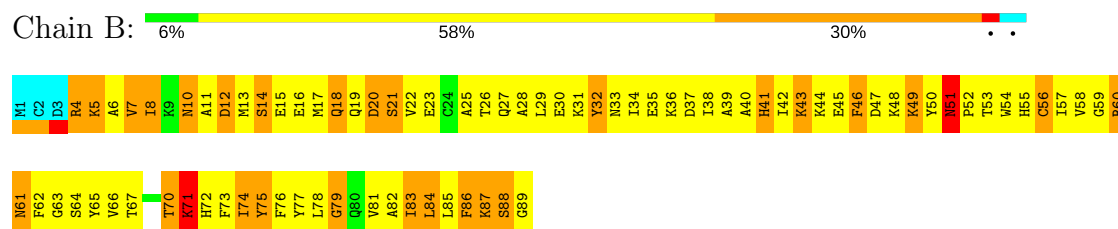


4.2.8 Score per residue for model 8

- Molecule 1: DYNEIN

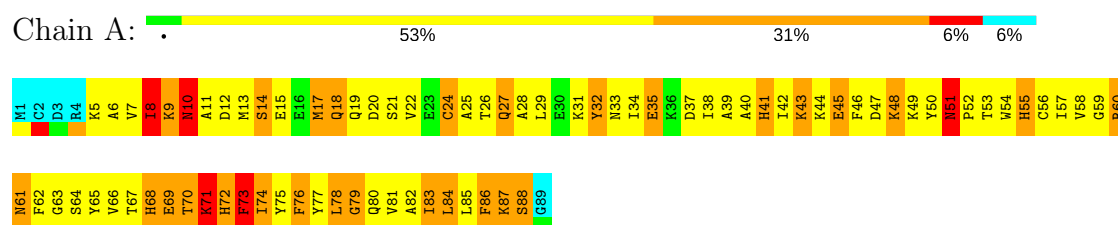


- Molecule 1: DYNEIN

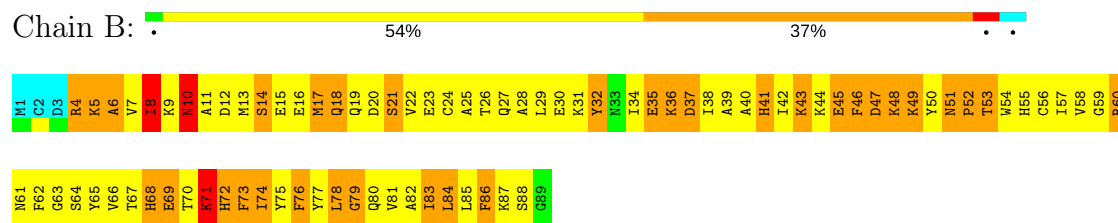


4.2.9 Score per residue for model 9

- Molecule 1: DYNEIN

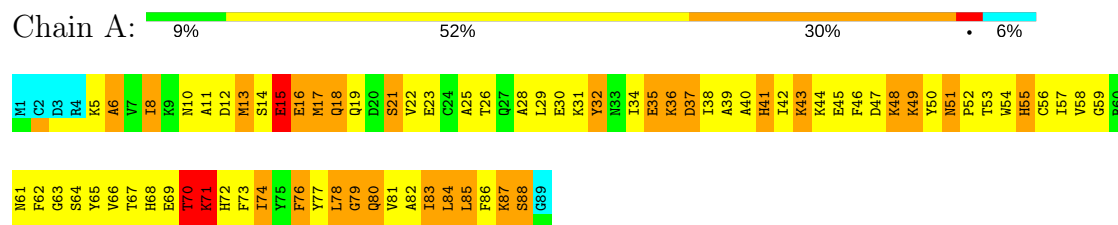


- Molecule 1: DYNEIN



4.2.10 Score per residue for model 10

- Molecule 1: DYNEIN



- Molecule 1: DYNEIN





4.2.11 Score per residue for model 11

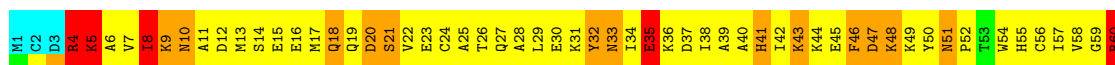
- Molecule 1: DYNEIN

Chain A: 9% 44% 35% 7% 6%



- Molecule 1: DYNEIN

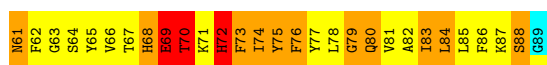
Chain B: 61% 26% 8% 5%



4.2.12 Score per residue for model 12

- Molecule 1: DYNEIN

Chain A: 53% 28% 10% 6%



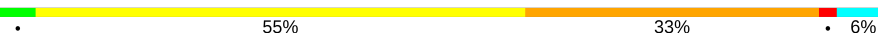
- Molecule 1: DYNEIN

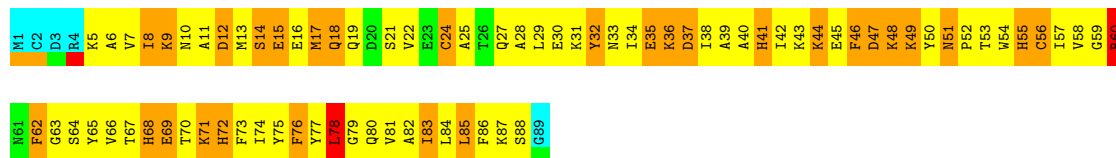
Chain B: 51% 39% 10% 5%



4.2.13 Score per residue for model 13

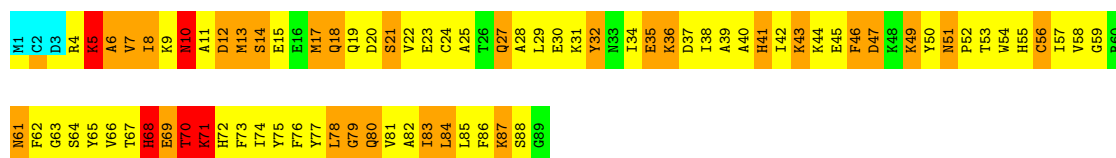
- Molecule 1: DYNEIN

Chain A: 




- Molecule 1: DYNEIN

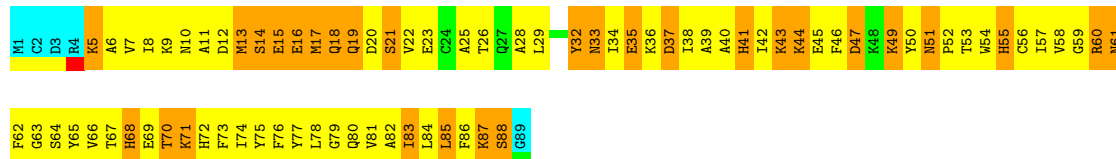
Chain B: 



4.2.14 Score per residue for model 14

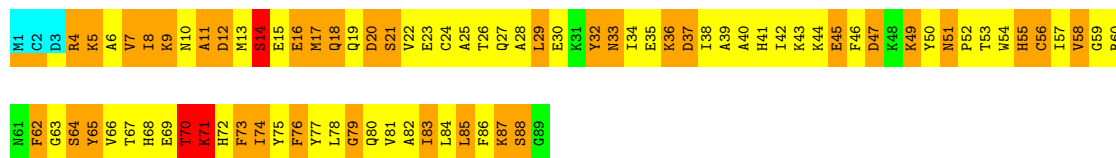
- Molecule 1: DYNEIN

Chain A: 



- Molecule 1: DYNEIN

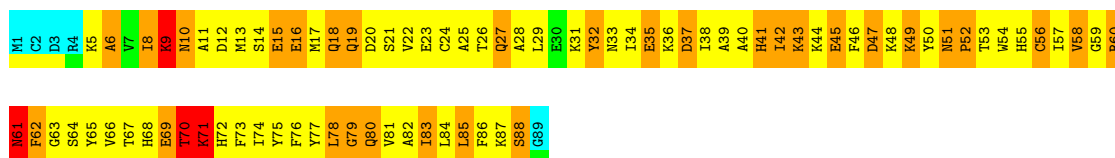
Chain B: 



4.2.15 Score per residue for model 15

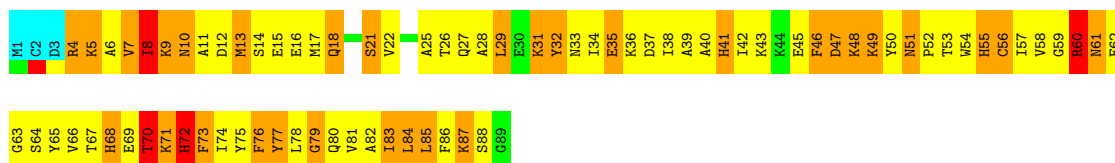
- Molecule 1: DYNEIN

Chain A: 



- Molecule 1: DYNEIN

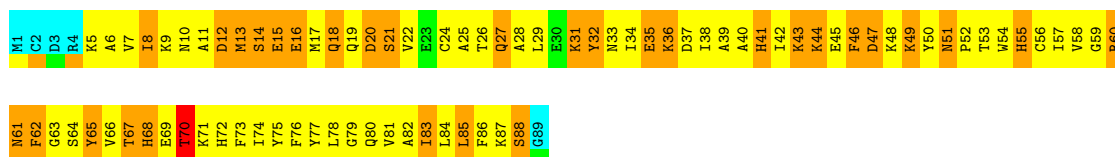
Chain B: 8% 49% 35%



4.2.16 Score per residue for model 16

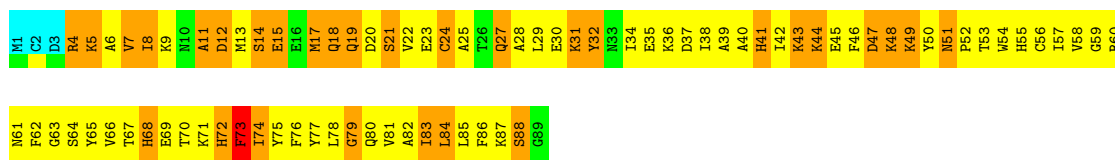
- Molecule 1: DYNEIN

Chain A: 56% 35% 6%



- Molecule 1: DYNEIN

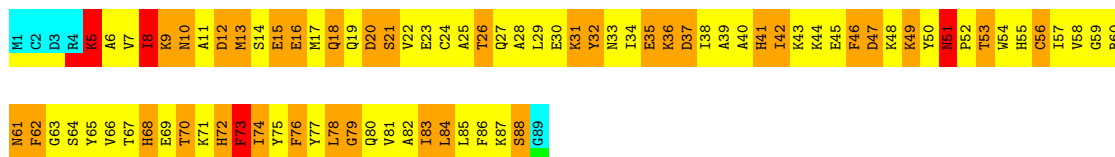
Chain B: 6% 56% 34%



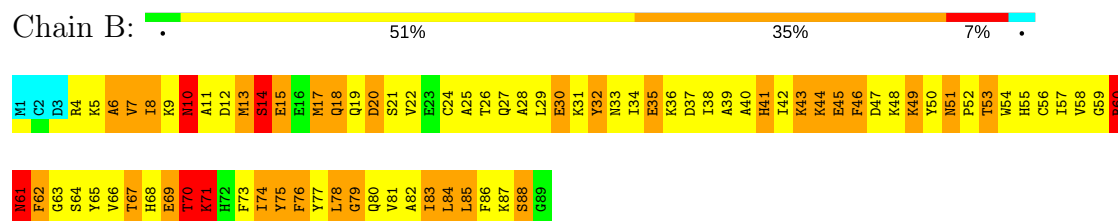
4.2.17 Score per residue for model 17

- Molecule 1: DYNEIN

Chain A: 52% 38% 6%

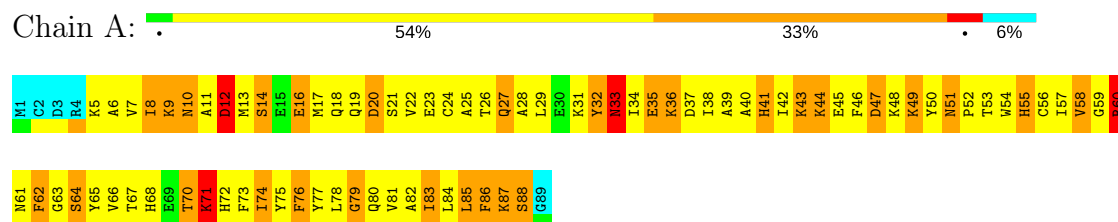


- Molecule 1: DYNEIN

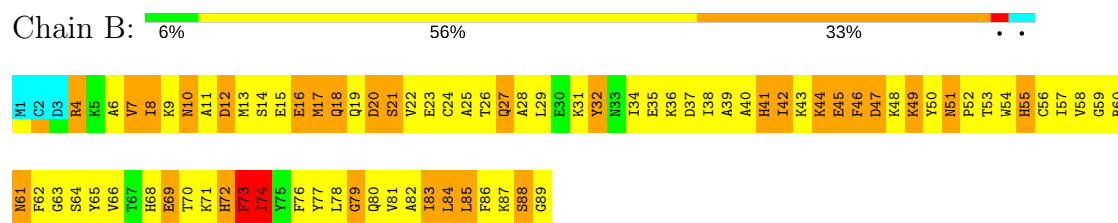


4.2.18 Score per residue for model 18

- Molecule 1: DYNEIN

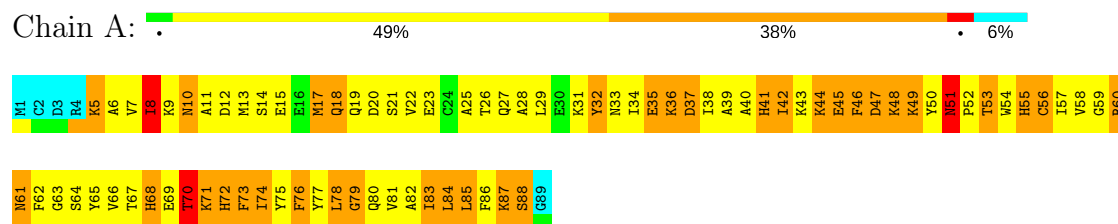


- Molecule 1: DYNEIN

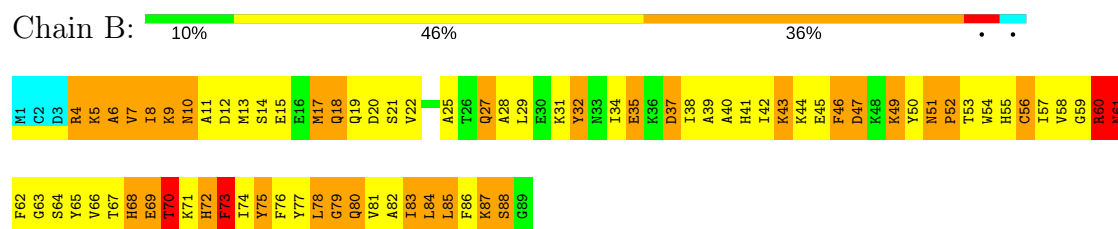


4.2.19 Score per residue for model 19

- Molecule 1: DYNEIN



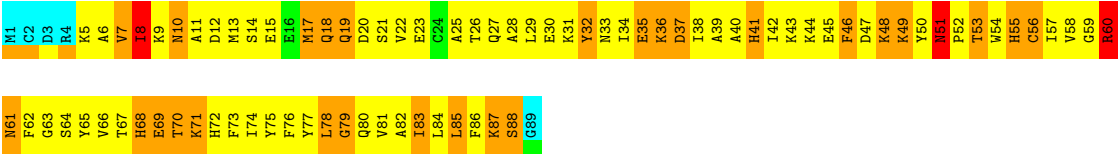
- Molecule 1: DYNEIN



4.2.20 Score per residue for model 20

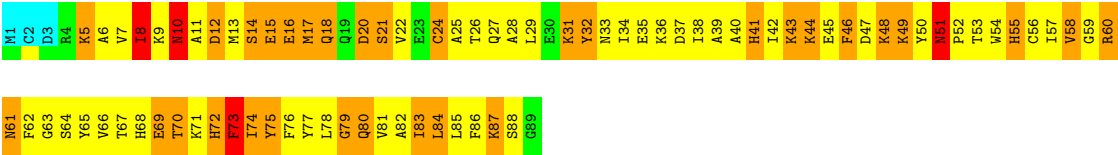
● Molecule 1: DYNEIN

Chain A: 58% 30% 6%



● Molecule 1: DYNEIN

Chain B: 6% 51% 36%



5 Refinement protocol and experimental data overview

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

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 4912
Number of chemical shift lists	1
Total number of shifts	1920
Number of shifts mapped to atoms	1920
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

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

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	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:68:HIS:HB2	1:A:72:HIS:HA	0.89	1.42	9	6
1:A:56:CYS:HB2	1:A:85:LEU:HD12	0.89	1.40	20	14
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:56:CYS:HB3	1:A:85:LEU:HD12	0.89	1.43	19	6
1:A:57:ILE:HD11	1:B:66:VAL:HG13	0.89	1.45	2	18
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:64:SER:CB	1:B:57:ILE:HD12	0.88	1.99	17	14
1:A:57:ILE:HD12	1:B:64:SER:CB	0.88	1.99	19	18
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:B:66:VAL:HG21	1:B:86:PHE:CZ	0.87	2.05	11	8
1:A:53:THR:HG21	1:B:67:THR:HG21	0.87	1.42	9	9

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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:B:66:VAL:HG21	1:B:86:PHE:CE2	0.86	2.06	8	7
1:A:18:GLN:O	1:A:22:VAL:HG23	0.86	1.71	18	18
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:74:ILE:HD13	1:A:76:PHE:CE1	0.85	2.05	8	13
1:A:6:ALA:HB2	1:A:78:LEU:HD13	0.85	1.49	4	12
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	1
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:B:18:GLN:CA	1:B:74:ILE:HD12	0.84	2.02	11	20
1:A:57:ILE:HG12	1:A:84:LEU:HD23	0.84	1.45	2	14
1:A:25:ALA:HA	1:A:42:ILE:HG12	0.84	1.48	20	13
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:64:SER:HA	1:B:57:ILE:HG23	0.83	1.50	2	16
1:A:22:VAL:HG13	1:A:76:PHE:CE2	0.83	2.08	2	5
1:B:13:MET:HB2	1:B:72:HIS:HA	0.83	1.48	13	5
1:A:42:ILE:HG21	1:A:85:LEU:HD11	0.83	1.48	15	16
1:A:28:ALA:HB2	1:A:41:HIS:CD2	0.83	2.09	20	8
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:B:8:ILE:HG13	1:B:76:PHE:HB3	0.82	1.48	19	15
1:A:57:ILE:HG23	1:B:64:SER:HA	0.82	1.47	11	18
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:55:HIS:NE2	1:A:88:SER:HB2	0.82	1.88	15	12
1:A:24:CYS:SG	1:A:42:ILE:HG23	0.82	2.13	8	3
1:A:57:ILE:HG12	1:B:64:SER:HA	0.81	1.52	4	2
1:B:13:MET:SD	1:B:17:MET:HE2	0.81	2.15	1	6
1:A:67:THR:HG21	1:B:53:THR:CG2	0.81	2.05	1	2
1:B:48:LYS:HA	1:B:48:LYS:HE3	0.81	1.50	15	1
1:A:77:TYR:HD1	1:A:82:ALA:HB2	0.81	1.34	17	2
1:A:69:GLU:HG3	1:A:88:SER:HA	0.81	1.52	17	7
1:A:73:PHE:HA	1:A:86:PHE:HA	0.81	1.50	18	2
1:B:21:SER:OG	1:B:85:LEU:HD22	0.81	1.75	1	1
1:B:13:MET:HG2	1:B:14:SER:N	0.81	1.90	15	5
1:B:28:ALA:HB2	1:B:41:HIS:CD2	0.81	2.10	4	11
1:A:57:ILE:HG13	1:B:57:ILE:HG13	0.81	1.49	9	3
1:A:5:LYS:O	1:A:22:VAL:HG11	0.81	1.73	17	1
1:B:48:LYS:HE3	1:B:48:LYS:HA	0.81	1.52	1	1
1:A:35:GLU:HB3	1:B:63:GLY:N	0.81	1.90	10	13
1:A:13:MET:SD	1:A:72:HIS:HA	0.81	2.15	7	7
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:HA	1:A:48:LYS:HE3	0.80	1.53	19	1
1:A:63:GLY:N	1:B:35:GLU:HB3	0.80	1.92	5	18
1:A:28:ALA:CB	1:A:38:ILE:HG23	0.80	2.05	16	17
1:A:64:SER:CB	1:A:84:LEU:HD22	0.80	2.06	17	13
1:A:6:ALA:HB2	1:A:78:LEU:CD1	0.80	2.06	4	12
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:42:ILE:CG2	1:B:85:LEU:HD11	0.79	2.07	19	7
1:B:26:THR:HA	1:B:29:LEU:HD12	0.79	1.51	18	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:66:VAL:HG21	1:B:86:PHE:CD2	0.79	2.13	8	5
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:66:VAL:CG1	1:B:57:ILE:HD11	0.78	2.08	4	8
1:A:55:HIS:HB3	1:B:66:VAL:HB	0.78	1.56	18	13
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:A:65:TYR:CE1	1:B:40:ALA:HB2	0.77	2.13	19	7
1:B:13:MET:SD	1:B:72:HIS:HA	0.77	2.18	1	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:55:HIS:HE2	1:A:88:SER:HB2	0.77	1.40	4	6
1:A:36:LYS:HB2	1:A:36:LYS:NZ	0.77	1.95	2	1
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:54:TRP:CE2	1:A:87:LYS:HD2	0.76	2.15	4	18
1:A:26:THR:HA	1:A:29:LEU:HD12	0.76	1.55	10	11
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:N	1:B:4:ARG:HD2	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:22:VAL:HG13	1:B:76:PHE:CE2	0.75	2.17	5	3
1:B:34:ILE:HG22	1:B:36:LYS:HE3	0.75	1.57	14	1
1:B:9:LYS:HA	1:B:9:LYS:HE2	0.75	1.59	16	2
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:57:ILE:HD11	1:B:66:VAL:CG1	0.75	2.11	13	13
1:A:66:VAL:HG21	1:A:86:PHE:CE2	0.75	2.17	15	3
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:A:67:THR:HB	1:B:53:THR:HG21	0.74	1.58	8	2
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: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:B:22:VAL:HA	1:B:76:PHE:CZ	0.74	2.18	5	9
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: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:A:38:ILE:HG22	1:A:42:ILE:CD1	0.74	2.12	5	11
1:B:64:SER:HB3	1:B:84:LEU:HD22	0.74	1.59	19	8
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:B:43:LYS:NZ	1:B:53:THR:HG23	0.74	1.97	7	1
1:A:55:HIS:CE1	1:B:67:THR:HG22	0.74	2.18	14	5
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:21:SER:HA	1:A:46:PHE:CE1	0.73	2.19	20	16
1:A:21:SER:HA	1:A:46:PHE:CZ	0.73	2.19	20	20
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:13:MET:CG	1:A:72:HIS:HA	0.73	2.14	16	5
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:B:22:VAL:HA	1:B:76:PHE:CE2	0.72	2.19	9	20
1:A:22:VAL:HA	1:A:76:PHE:CZ	0.72	2.20	13	10
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:72:HIS:O	1:B:73:PHE:HB3	0.72	1.85	18	10
1:B:21:SER:HG	1:B:85:LEU:HD22	0.72	1.43	1	1
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:76:PHE:CE2	1:B:83:ILE:HG13	0.72	2.19	6	18
1:B:56:CYS:CB	1:B:85:LEU:HD12	0.72	2.14	1	11
1:B:68:HIS:CE1	1:B:87:LYS:HG3	0.72	2.19	4	1
1:A:27:GLN:O	1:A:31:LYS:HG2	0.72	1.84	15	5
1:B:27:GLN:HG3	1:B:28:ALA:N	0.72	1.98	18	1
1:B:17:MET:SD	1:B:71:LYS:HD3	0.72	2.25	16	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:53:THR:O	1:B:87:LYS:HB3	0.71	1.84	13	6
1:B:34:ILE:N	1:B:34:ILE:HD12	0.71	2.00	7	1
1:B:11:ALA:HB1	1:B:18:GLN:HE21	0.71	1.44	20	2
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: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: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:A:43:LYS:HE2	1:A:54:TRP:H	0.71	1.45	6	1
1:A:65:TYR:CE2	1:B:40:ALA:HA	0.71	2.21	13	16
1:A:65:TYR:CD1	1:B:40:ALA:HA	0.71	2.21	8	9
1:B:15:GLU:O	1:B:18:GLN:HG2	0.71	1.86	13	12
1:B:62:PHE:HE2	1:B:64:SER:HB3	0.71	1.46	20	13
1:A:16:GLU:HG2	1:A:19:GLN:OE1	0.71	1.85	15	1
1:A:7:VAL:O	1:A:9:LYS:HD2	0.71	1.86	2	1
1:B:70:THR:HG22	1:B:71:LYS:N	0.71	2.00	16	4
1:A:13:MET:SD	1:A:17:MET:HE2	0.71	2.25	1	3
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:B:57:ILE:HB	1:B:84:LEU:HB3	0.71	1.63	14	8
1:A:73:PHE:HA	1:A:85:LEU:O	0.71	1.86	1	9
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:35:GLU:CA	1:A:38:ILE:HD12	0.71	2.16	20	2
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:B:22:VAL:HG13	1:B:76:PHE:CD2	0.70	2.21	3	5
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: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:5:LYS:O	1:A:78:LEU:HD13	0.70	1.86	3	6
1:A:54:TRP:CZ3	1:A:72:HIS:HB3	0.70	2.21	10	9
1:B:57:ILE:HD12	1:B:84:LEU:CD2	0.70	2.16	18	2

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

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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:ASN:O	1:A:87:LYS:HE3	0.68	1.89	8	6
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:65:TYR:HB3	1:B:39:ALA:HB1	0.68	1.66	1	5
1:B:28:ALA:HB2	1:B:41:HIS:CG	0.68	2.23	16	11
1:A:62:PHE:HE1	1:A:64:SER:HB3	0.68	1.49	10	5
1:A:43:LYS:HE3	1:B:65:TYR:HE2	0.68	1.46	10	1
1:A:43:LYS:HE2	1:A:47:ASP:HB2	0.68	1.66	1	1
1:B:8:ILE:HA	1:B:76:PHE:CB	0.68	2.19	17	17
1:A:46:PHE:HA	1:A:50:TYR:CD1	0.68	2.24	19	4
1:B:76:PHE:CZ	1:B:83:ILE:HB	0.68	2.23	7	16
1:B:19:GLN:O	1:B:23:GLU:HG3	0.68	1.89	11	11
1:B:35:GLU:O	1:B:58:VAL:HG13	0.68	1.88	9	18
1:A:62:PHE:CE2	1:A:64:SER:HB3	0.68	2.23	17	7
1:B:58:VAL:HG23	1:B:82:ALA:O	0.68	1.89	9	10
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:60:ARG:O	1:B:61:ASN:HB2	0.68	1.88	12	4
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:B:39:ALA:HB2	1:B:58:VAL:CG1	0.68	2.15	5	5
1:A:66:VAL:HB	1:B:55:HIS:ND1	0.68	2.04	4	4
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: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:A:73:PHE:HD2	1:A:86:PHE:HB3	0.68	1.49	2	2
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:A:12:ASP:HB3	1:A:72:HIS:CG	0.68	2.24	4	3
1:B:8:ILE:C	1:B:9:LYS:HG2	0.68	2.09	2	9
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:A:31:LYS:HB3	1:A:32:TYR:CE1	0.67	2.24	5	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LYS:C	1:A:43:LYS:HD2	0.67	2.09	10	2
1:A:47:ASP:OD2	1:A:52:PRO:HB3	0.67	1.89	10	5
1:A:27:GLN:HB3	1:A:41:HIS:CE1	0.67	2.24	12	3
1:B:72:HIS:CB	1:B:87:LYS:HB2	0.67	2.19	5	3
1:A:33:ASN:CA	1:A:38:ILE:HD11	0.67	2.19	13	4
1:B:53:THR:HG23	1:B:55:HIS:CE1	0.67	2.24	18	2
1:B:24:CYS:HB3	1:B:42:ILE:HG23	0.67	1.67	16	1
1:B:58:VAL:HG23	1:B:81:VAL:CG1	0.67	2.18	7	5
1:B:47:ASP:HB2	1:B:52:PRO:CD	0.67	2.20	17	5
1:A:57:ILE:HG12	1:B:65:TYR:H	0.67	1.49	4	1
1:A:43:LYS:HD2	1:A:43:LYS:C	0.67	2.08	15	2
1:A:43:LYS:HE2	1:A:47:ASP:CB	0.67	2.19	1	2
1:A:47:ASP:HB3	1:A:52:PRO:HB3	0.67	1.65	20	1
1:A:47:ASP:OD1	1:A:48:LYS:HG2	0.67	1.88	19	1
1:A:56:CYS:HB3	1:A:85:LEU:CD1	0.67	2.19	3	8
1:B:55:HIS:HB2	1:B:86:PHE:O	0.67	1.89	4	10
1:A:11:ALA:HB1	1:A:18:GLN:HE21	0.67	1.49	19	3
1:A:77:TYR:OH	1:A:80:GLN:HA	0.67	1.88	18	8
1:A:55:HIS:CE1	1:A:88:SER:HB2	0.67	2.24	16	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:62:PHE:HA	1:B:59:GLY:HA3	0.67	1.65	7	11
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:67:THR:HB	1:B:55:HIS:CE1	0.67	2.25	19	4
1:B:12:ASP:O	1:B:72:HIS:HB2	0.67	1.90	11	7
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:A:35:GLU:HB3	1:B:63:GLY:CA	0.67	2.19	20	12
1:A:55:HIS:CD2	1:A:87:LYS:HA	0.67	2.25	8	8
1:B:13:MET:HB2	1:B:73:PHE:N	0.67	2.04	17	4
1:A:5:LYS:O	1:A:5:LYS:HG3	0.67	1.89	1	2
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: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:B:47:ASP:HB3	1:B:52:PRO:HG3	0.67	1.67	5	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:35:GLU:HG3	1:A:59:GLY:HA2	0.67	1.67	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:HIS:HD2	1:A:87:LYS:HA	0.67	1.49	8	10
1:B:8:ILE:CG1	1:B:76:PHE:HB3	0.67	2.20	5	18
1:A:34:ILE:HB	1:A:37:ASP:CB	0.67	2.20	15	15
1:B:81:VAL:HG12	1:B:82:ALA:N	0.67	2.04	1	20
1:A:60:ARG:NH1	1:A:60:ARG:HG3	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:HH11	1:B:4:ARG:HG2	0.67	1.49	12	1
1:A:8:ILE:HA	1:A:76:PHE:CB	0.67	2.20	20	19
1:B:8:ILE:HA	1:B:76:PHE:CA	0.67	2.20	7	20
1:B:6:ALA:HB2	1:B:78:LEU:HD22	0.67	1.67	20	12
1:A:65:TYR:CD2	1:B:43:LYS:HD3	0.67	2.25	7	4
1:B:27:GLN:HB3	1:B:41:HIS:CE1	0.67	2.25	16	3
1:A:8:ILE:HD12	1:A:76:PHE:HB3	0.66	1.66	11	8
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:HB2	1:A:87:LYS:CG	0.66	2.21	1	2
1:A:72:HIS:CB	1:A:87:LYS:HD3	0.66	2.19	16	2
1:B:4:ARG:HG3	1:B:4:ARG:O	0.66	1.88	17	1
1:B:22:VAL:HG22	1:B:76:PHE:CE2	0.66	2.24	12	10
1:B:59:GLY:O	1:B:60:ARG:HB3	0.66	1.91	4	4
1:B:26:THR:CA	1:B:29:LEU:HD12	0.66	2.21	18	6
1:A:56:CYS:HB2	1:A:85:LEU:CD1	0.66	2.19	13	7
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:B:14:SER:HB3	1:B:17:MET:HG3	0.66	1.65	20	2
1:A:65:TYR:CE2	1:B:43:LYS:HD2	0.66	2.26	13	2
1:A:43:LYS:CE	1:A:56:CYS:HB3	0.66	2.19	5	1
1:A:7:VAL:O	1:A:9:LYS:HE2	0.66	1.89	3	1
1:A:8:ILE:CG1	1:A:76:PHE:HB3	0.66	2.21	13	17
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: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:A:38:ILE:O	1:A:42:ILE:HG13	0.66	1.90	10	11
1:B:11:ALA:CB	1:B:74:ILE:HA	0.66	2.20	14	5
1:B:66:VAL:HG21	1:B:86:PHE:CD1	0.66	2.25	13	7
1:B:27:GLN:O	1:B:31:LYS:HD2	0.66	1.90	20	1
1:A:62:PHE:CB	1:B:62:PHE:HB3	0.66	2.21	11	9
1:A:43:LYS:HB3	1:B:65:TYR:CD2	0.66	2.25	17	10
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:HIS:CG	1:A:87:LYS:HD3	0.66	2.25	16	3
1:B:35:GLU:HA	1:B:35:GLU:OE1	0.66	1.90	20	1
1:B:58:VAL:HG23	1:B:83:ILE:HD13	0.66	1.65	10	15
1:A:63:GLY:CA	1:B:35:GLU:HB3	0.66	2.20	9	15
1:A:34:ILE:O	1:A:34:ILE:HG22	0.66	1.90	13	4
1:A:13:MET:H	1:A:18:GLN:HE22	0.66	1.31	18	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:75:TYR:CD1	1:A:84:LEU:HB2	0.66	2.26	3	5
1:B:13:MET:SD	1:B:18:GLN:N	0.66	2.68	3	4
1:A:8:ILE:HA	1:A:76:PHE:CA	0.66	2.21	6	20
1:B:31:LYS:HD3	1:B:41:HIS:CE1	0.66	2.26	16	3
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:A:11:ALA:CA	1:A:74:ILE:HA	0.66	2.20	16	2
1:B:56:CYS:HB2	1:B:85:LEU:CD1	0.66	2.19	13	4
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: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:25:ALA:HA	1:A:42:ILE:CG1	0.65	2.21	19	10
1:B:11:ALA:CA	1:B:74:ILE:HA	0.65	2.21	8	6
1:A:59:GLY:O	1:A:60:ARG:HB3	0.65	1.89	5	1
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:40:ALA:HB2	1:B:65:TYR:CE1	0.65	2.26	14	7
1:A:17:MET:HA	1:A:20:ASP:OD2	0.65	1.91	15	1
1:A:64:SER:CA	1:B:57:ILE:HG12	0.65	2.21	13	3
1:A:43:LYS:HE2	1:A:47:ASP:HB3	0.65	1.67	8	2
1:A:60:ARG:HG3	1:A:60:ARG:HH11	0.65	1.50	4	2
1:B:55:HIS:ND1	1:B:55:HIS:N	0.65	2.44	18	2
1:A:13:MET:CB	1:A:17:MET:HG3	0.65	2.21	16	1
1:B:73:PHE:HD1	1:B:86:PHE:HB3	0.65	1.50	13	4
1:A:55:HIS:CD2	1:A:55:HIS:N	0.65	2.65	16	8
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:LYS:HE2	1:B:47:ASP:HB3	0.65	1.67	17	1
1:A:43:LYS:HE3	1:B:65:TYR:CE2	0.65	2.27	10	3
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
1:A:8:ILE:CD1	1:A:76:PHE:HB3	0.65	2.21	8	10
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:7:VAL:HG12	1:B:9:LYS:HE3	0.65	1.68	10	1
1:A:67:THR:HG23	1:A:67:THR:O	0.65	1.92	1	3
1:B:51:ASN:O	1:B:87:LYS:HE3	0.65	1.91	14	3
1:A:74:ILE:O	1:A:74:ILE:HG23	0.65	1.92	3	5
1:A:66:VAL:HG12	1:B:55:HIS:C	0.65	2.12	8	5
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:B:7:VAL:HG23	1:B:77:TYR:O	0.65	1.90	10	9
1:A:64:SER:HA	1:B:57:ILE:CG2	0.65	2.20	2	3
1:B:4:ARG:HG2	1:B:19:GLN:NE2	0.65	2.07	2	1
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:HB2	1:B:72:HIS:CA	0.65	2.21	13	4
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: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:B:43:LYS:HD3	1:B:43:LYS:C	0.65	2.12	19	1
1:A:43:LYS:HD2	1:A:55:HIS:CA	0.65	2.21	5	1
1:B:25:ALA:HB2	1:B:83:ILE:HG21	0.65	1.68	16	13
1:A:26:THR:HA	1:A:29:LEU:CD1	0.65	2.21	10	5
1:A:57:ILE:HA	1:B:63:GLY:O	0.65	1.92	14	2
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:B:7:VAL:HG12	1:B:9:LYS:CE	0.64	2.22	3	2
1:A:47:ASP:OD1	1:A:54:TRP:HB2	0.64	1.92	7	3
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:29:LEU:HD11	1:A:83:ILE:HD11	0.64	1.68	17	2
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:57:ILE:HG23	1:B:64:SER:CA	0.64	2.21	11	12

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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:18:GLN:O	1:A:74:ILE:HD12	0.63	1.94	10	5
1:B:14:SER:O	1:B:17:MET:HB2	0.63	1.92	19	10
1:A:34:ILE:HG22	1:A:34:ILE:O	0.63	1.93	14	2
1:B:48:LYS:HE2	1:B:48:LYS:C	0.63	2.14	11	1
1:A:56:CYS:HB2	1:A:85:LEU:HG	0.63	1.69	5	3
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:57:ILE:CD1	1:B:64:SER:HA	0.63	2.22	7	18
1:A:13:MET:SD	1:A:18:GLN:N	0.63	2.72	6	5
1:B:55:HIS:HB2	1:B:86:PHE:CD1	0.63	2.28	4	3
1:A:13:MET:HG2	1:A:17:MET:CB	0.63	2.24	2	9
1:A:54:TRP:CZ2	1:A:87:LYS:HD2	0.63	2.29	8	7
1:B:55:HIS:CD2	1:B:55:HIS:N	0.63	2.65	2	3
1:A:61:ASN:O	1:B:60:ARG:HG2	0.63	1.93	1	1
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:B:47:ASP:OD1	1:B:52:PRO:HG3	0.63	1.94	18	2
1:A:57:ILE:HG21	1:A:62:PHE:HE2	0.63	1.53	15	2
1:A:32:TYR:N	1:A:32:TYR:CD1	0.63	2.67	7	12
1:B:34:ILE:HB	1:B:37:ASP:CB	0.63	2.24	15	11
1:B:32:TYR:CD1	1:B:32:TYR:N	0.63	2.66	20	7
1:B:21:SER:CB	1:B:74:ILE:HG21	0.63	2.24	17	3
1:A:39:ALA:HB1	1:B:65:TYR:HB3	0.63	1.68	20	4
1:A:66:VAL:HG21	1:A:86:PHE:CZ	0.63	2.28	1	5
1:A:78:LEU:HD23	1:A:83:ILE:CG1	0.63	2.24	9	4
1:A:48:LYS:HE3	1:A:48:LYS:HA	0.63	1.68	10	2
1:A:27:GLN:HB2	1:A:41:HIS:NE2	0.63	2.09	19	2
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:B:47:ASP:OD2	1:B:53:THR:HA	0.63	1.93	12	1
1:A:33:ASN:C	1:A:34:ILE:HD12	0.63	2.14	5	1
1:A:70:THR:HG21	1:A:87:LYS:NZ	0.63	2.09	3	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:55:HIS:HB2	1:A:86:PHE:O	0.63	1.94	12	6
1:B:19:GLN:HG3	1:B:20:ASP:N	0.63	2.09	5	2
1:A:74:ILE:HG22	1:A:85:LEU:CB	0.63	2.24	7	5
1:B:13:MET:HG2	1:B:17:MET:HB2	0.63	1.69	8	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:HIS:CD2	1:A:69:GLU:N	0.63	2.67	2	2
1:B:78:LEU:HD23	1:B:83:ILE:HD11	0.63	1.70	14	2
1:A:13:MET:H	1:A:18:GLN:NE2	0.63	1.90	18	2
1:A:53:THR:HG22	1:B:67:THR:HG21	0.63	1.70	17	1
1:A:6:ALA:CB	1:A:78:LEU:HD13	0.63	2.22	4	5
1:B:8:ILE:CD1	1:B:76:PHE:HB3	0.63	2.23	13	13
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:A:6:ALA:HB2	1:A:78:LEU:CD2	0.63	2.24	17	13
1:A:46:PHE:HA	1:A:50:TYR:HD1	0.63	1.54	19	2
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:B:76:PHE:N	1:B:76:PHE:CD1	0.62	2.67	12	10
1:A:39:ALA:HB1	1:B:65:TYR:CB	0.62	2.24	1	15
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:B:35:GLU:OE1	1:B:58:VAL:HG22	0.62	1.94	20	2
1:A:11:ALA:O	1:A:12:ASP:HB2	0.62	1.93	7	3
1:B:62:PHE:CD1	1:B:63:GLY:N	0.62	2.67	19	1
1:A:68:HIS:N	1:A:68:HIS:ND1	0.62	2.48	3	3
1:A:55:HIS:HB3	1:B:66:VAL:CA	0.62	2.25	8	7
1:A:45:GLU:HA	1:A:45:GLU:OE1	0.62	1.94	10	1
1:A:13:MET:HG3	1:A:14:SER:N	0.62	2.09	5	9
1:A:13:MET:HB2	1:A:72:HIS:CA	0.62	2.24	18	5
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:68:HIS:ND1	1:A:68:HIS:N	0.62	2.47	11	3
1:A:32:TYR:CE1	1:A:41:HIS:ND1	0.62	2.68	13	13
1:B:74:ILE:N	1:B:85:LEU:O	0.62	2.33	5	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:73:PHE:HE1	1:B:84:LEU:HD12	0.62	1.54	17	2
1:B:39:ALA:N	1:B:58:VAL:HG11	0.62	2.10	14	12
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:A:34:ILE:O	1:A:36:LYS:N	0.62	2.32	18	6
1:B:54:TRP:CD1	1:B:87:LYS:HD2	0.62	2.29	12	2
1:A:18:GLN:CB	1:A:74:ILE:HD12	0.62	2.25	1	7
1:B:9:LYS:HD2	1:B:76:PHE:HA	0.62	1.70	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:70:THR:C	1:B:71:LYS:HG2	0.62	2.14	5	2
1:A:19:GLN:O	1:A:23:GLU:HG3	0.62	1.93	18	10
1:B:46:PHE:CZ	1:B:85:LEU:HD23	0.62	2.29	11	1
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:A:65:TYR:H	1:B:57:ILE:HG12	0.62	1.53	19	4
1:B:32:TYR:CE1	1:B:41:HIS:ND1	0.62	2.68	5	10
1:B:47:ASP:HB2	1:B:52:PRO:HD3	0.62	1.71	17	2
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
1:A:55:HIS:N	1:A:55:HIS:ND1	0.62	2.48	19	1
1:B:25:ALA:HA	1:B:42:ILE:HD11	0.62	1.72	7	12
1:B:43:LYS:HG3	1:B:54:TRP:O	0.62	1.94	15	8
1:A:23:GLU:O	1:A:27:GLN:HG3	0.62	1.94	19	2
1:A:13:MET:HG3	1:A:14:SER:H	0.62	1.54	5	9
1:A:55:HIS:ND1	1:A:55:HIS:N	0.62	2.47	10	3
1:A:66:VAL:HB	1:A:86:PHE:CZ	0.62	2.30	14	2
1:B:77:TYR:HA	1:B:81:VAL:O	0.62	1.95	3	5
1:A:78:LEU:N	1:A:81:VAL:O	0.62	2.33	9	20
1:A:39:ALA:HB2	1:A:58:VAL:CG1	0.62	2.17	16	5
1:B:60:ARG:HG3	1:B:61:ASN:HD22	0.62	1.54	10	1
1:A:7:VAL:HG12	1:A:7:VAL:O	0.62	1.94	6	4
1:A:18:GLN:HB3	1:A:74:ILE:CD1	0.62	2.25	18	3
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:68:HIS:HB2	1:A:72:HIS:O	0.61	1.94	8	4
1:A:33:ASN:C	1:A:34:ILE:HD13	0.61	2.14	6	3
1:B:64:SER:CB	1:B:84:LEU:HD13	0.61	2.25	19	1
1:B:13:MET:HG3	1:B:17:MET:HG2	0.61	1.72	13	1
1:B:17:MET:SD	1:B:54:TRP:HH2	0.61	2.18	13	2
1:A:27:GLN:O	1:A:31:LYS:HD3	0.61	1.95	11	1
1:B:68:HIS:HE1	1:B:70:THR:HB	0.61	1.55	9	1
1:B:68:HIS:HB3	1:B:72:HIS:O	0.61	1.95	15	2
1:B:13:MET:SD	1:B:17:MET:C	0.61	2.78	3	4
1:A:76:PHE:N	1:A:76:PHE:CD1	0.61	2.69	19	12
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: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:A:28:ALA:HB3	1:A:38:ILE:CG2	0.61	2.25	17	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:4:ARG:HG2	1:B:19:GLN:OE1	0.61	1.95	4	1
1:A:67:THR:O	1:A:67:THR:HG22	0.61	1.96	15	2
1:A:73:PHE:CD1	1:A:74:ILE:N	0.61	2.69	2	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:54:TRP:CH2	1:A:87:LYS:HD3	0.61	2.30	3	2
1:B:78:LEU:N	1:B:81:VAL:O	0.61	2.33	2	20
1:B:46:PHE:HA	1:B:50:TYR:CD1	0.61	2.31	17	2
1:A:55:HIS:HB2	1:A:86:PHE:CD1	0.61	2.30	14	4
1:A:43:LYS:HB3	1:B:65:TYR:HE2	0.61	1.55	12	1
1:B:54:TRP:HA	1:B:87:LYS:HG2	0.61	1.71	19	6
1:A:35:GLU:HG2	1:B:62:PHE:HA	0.61	1.72	10	4
1:A:49:LYS:HB3	1:A:50:TYR:CE1	0.61	2.31	4	3
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:73:PHE:HB3	1:A:86:PHE:CB	0.61	2.25	8	1
1:A:12:ASP:HB3	1:A:72:HIS:HD1	0.61	1.56	19	1
1:A:43:LYS:HD2	1:A:56:CYS:N	0.61	2.10	5	1
1:B:9:LYS:HE2	1:B:9:LYS:CA	0.61	2.23	18	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:24:CYS:SG	1:A:46:PHE:CE1	0.61	2.94	16	2
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:34:ILE:HG22	1:A:36:LYS:CD	0.61	2.26	2	1
1:A:49:LYS:HD2	1:A:50:TYR:CE1	0.61	2.30	13	1
1:A:55:HIS:HB3	1:B:66:VAL:HG12	0.61	1.73	17	6
1:A:59:GLY:HA3	1:B:62:PHE:CB	0.61	2.25	20	6
1:A:55:HIS:N	1:A:55:HIS:CD2	0.61	2.68	7	4
1:B:13:MET:HG3	1:B:14:SER:N	0.61	2.11	2	11
1:A:58:VAL:HG13	1:A:58:VAL:O	0.61	1.95	13	3
1:A:58:VAL:HG23	1:A:83:ILE:HD12	0.61	1.70	13	2
1:A:63:GLY:N	1:B:58:VAL:O	0.60	2.34	4	20
1:B:55:HIS:N	1:B:55:HIS:CD2	0.60	2.68	12	5
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:A:61:ASN:O	1:B:35:GLU:HG2	0.60	1.95	14	3
1:B:47:ASP:HB2	1:B:52:PRO:HG3	0.60	1.71	7	2
1:B:71:LYS:HG2	1:B:71:LYS:O	0.60	1.95	11	1
1:B:46:PHE:O	1:B:50:TYR:HB2	0.60	1.96	18	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:12:ASP:N	1:B:73:PHE:O	0.60	2.34	1	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:B:55:HIS:HB2	1:B:86:PHE:CE1	0.60	2.32	20	5
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
1:B:13:MET:HA	1:B:71:LYS:HG3	0.60	1.73	4	1
1:A:17:MET:SD	1:A:54:TRP:HH2	0.60	2.18	10	1
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:N	1:B:18:GLN:HE22	0.60	1.94	8	1
1:B:87:LYS:HB3	1:B:87:LYS:NZ	0.60	2.11	8	1
1:A:45:GLU:O	1:A:49:LYS:N	0.60	2.34	3	17
1:A:64:SER:OG	1:A:84:LEU:HD13	0.60	1.96	12	2
1:A:62:PHE:HB3	1:B:62:PHE:CB	0.60	2.25	14	6
1:B:12:ASP:HB3	1:B:72:HIS:CG	0.60	2.32	4	2
1:A:54:TRP:CD2	1:A:87:LYS:HG3	0.60	2.30	2	3
1:A:12:ASP:HB2	1:A:73:PHE:HD2	0.60	1.55	13	5
1:B:13:MET:HG3	1:B:14:SER:H	0.60	1.55	7	11
1:B:14:SER:C	1:B:18:GLN:NE2	0.60	2.55	11	1
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:B:43:LYS:HD2	1:B:54:TRP:O	0.60	1.96	4	5
1:A:41:HIS:CD2	1:A:41:HIS:H	0.60	2.15	10	5
1:A:10:ASN:O	1:A:75:TYR:N	0.60	2.35	13	8
1:A:65:TYR:CD2	1:B:40:ALA:HB2	0.60	2.32	6	2
1:A:13:MET:HB3	1:A:17:MET:HG3	0.60	1.71	16	1
1:A:5:LYS:O	1:A:6:ALA:HB2	0.60	1.97	3	3
1:B:78:LEU:O	1:B:80:GLN:N	0.60	2.34	3	12
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:34:ILE:CB	1:A:37:ASP:HB2	0.60	2.27	15	3
1:A:55:HIS:ND1	1:B:67:THR:HB	0.60	2.12	15	1
1:A:44:LYS:HA	1:A:44:LYS:HE2	0.60	1.71	5	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
1:A:76:PHE:CD2	1:A:78:LEU:HD21	0.60	2.32	19	4
1:A:41:HIS:H	1:A:41:HIS:CD2	0.59	2.14	4	5
1:B:7:VAL:O	1:B:9:LYS:HE2	0.59	1.97	5	3
1:B:13:MET:CG	1:B:17:MET:HB3	0.59	2.26	10	7
1:A:73:PHE:CG	1:A:74:ILE:N	0.59	2.70	2	2
1:A:45:GLU:OE1	1:A:45:GLU:HA	0.59	1.96	9	1
1:A:24:CYS:HA	1:A:27:GLN:HG3	0.59	1.73	13	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:34:ILE:O	1:A:37:ASP:HB3	0.59	1.97	11	3
1:A:80:GLN:HG3	1:A:80:GLN:O	0.59	1.97	1	1
1:A:68:HIS:HB3	1:A:73:PHE:CD2	0.59	2.32	8	2
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:A:65:TYR:HD2	1:B:43:LYS:HD3	0.59	1.56	7	1
1:B:39:ALA:HA	1:B:56:CYS:SG	0.59	2.37	7	2
1:A:54:TRP:CH2	1:A:72:HIS:HB3	0.59	2.32	16	5
1:B:13:MET:HB2	1:B:71:LYS:O	0.59	1.97	6	4
1:A:64:SER:HB3	1:B:57:ILE:HD13	0.59	1.75	11	2
1:A:70:THR:HG21	1:A:87:LYS:HZ3	0.59	1.58	3	1
1:B:6:ALA:HB3	1:B:22:VAL:HG11	0.59	1.74	4	9
1:A:6:ALA:CA	1:A:78:LEU:HA	0.59	2.21	14	11
1:B:13:MET:O	1:B:18:GLN:NE2	0.59	2.36	13	16
1:B:11:ALA:HA	1:B:73:PHE:O	0.59	1.97	8	2
1:B:5:LYS:O	1:B:6:ALA:HB2	0.59	1.97	13	6
1:B:74:ILE:O	1:B:74:ILE:HG23	0.59	1.97	4	7
1:A:84:LEU:HD21	1:A:86:PHE:CE2	0.59	2.31	4	1
1:B:13:MET:CG	1:B:14:SER:N	0.59	2.66	7	13
1:A:29:LEU:CD2	1:A:81:VAL:HG11	0.59	2.20	13	1
1:B:33:ASN:C	1:B:34:ILE:HD13	0.59	2.18	4	4
1:B:34:ILE:O	1:B:37:ASP:N	0.59	2.36	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ILE:HG22	1:A:58:VAL:N	0.59	2.13	11	6
1:B:58:VAL:CG2	1:B:81:VAL:HG11	0.59	2.26	7	3
1:B:68:HIS:HB2	1:B:72:HIS:CA	0.59	2.27	7	3
1:B:8:ILE:HD12	1:B:76:PHE:CB	0.59	2.27	8	5
1:A:46:PHE:O	1:A:54:TRP:NE1	0.59	2.36	20	3
1:B:25:ALA:HB1	1:B:83:ILE:HD12	0.59	1.73	1	1
1:A:41:HIS:CD2	1:A:41:HIS:N	0.59	2.70	17	8
1:B:51:ASN:N	1:B:51:ASN:HD22	0.59	1.94	4	1
1:A:10:ASN:O	1:A:11:ALA:HB2	0.59	1.96	2	3
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:81:VAL:CG1	1:A:82:ALA:N	0.59	2.66	17	20
1:A:13:MET:SD	1:A:18:GLN:CA	0.59	2.91	10	2
1:A:13:MET:SD	1:A:18:GLN:HA	0.59	2.37	10	1
1:A:74:ILE:N	1:A:85:LEU:O	0.59	2.35	18	9
1:B:34:ILE:O	1:B:38:ILE:HD12	0.59	1.98	7	1
1:A:58:VAL:N	1:B:63:GLY:O	0.59	2.35	14	4
1:A:15:GLU:O	1:A:17:MET:N	0.59	2.36	16	3
1:B:6:ALA:N	1:B:78:LEU:HD13	0.59	2.13	6	1
1:A:69:GLU:OE2	1:A:88:SER:HA	0.59	1.98	13	2
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:B:7:VAL:CG1	1:B:9:LYS:HE2	0.59	2.28	19	3
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: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:41:HIS:CD2	1:B:41:HIS:H	0.59	2.14	18	4
1:A:62:PHE:CD2	1:A:63:GLY:N	0.59	2.71	1	1
1:A:9:LYS:CD	1:A:76:PHE:HA	0.59	2.28	2	1
1:A:62:PHE:HE1	1:A:82:ALA:HB3	0.59	1.58	19	1
1:B:49:LYS:HE3	1:B:50:TYR:OH	0.59	1.97	16	1
1:B:10:ASN:O	1:B:75:TYR:N	0.59	2.35	3	9
1:B:11:ALA:HB2	1:B:74:ILE:HG12	0.59	1.74	16	5
1:B:7:VAL:O	1:B:9:LYS:HG2	0.59	1.96	2	9
1:A:25:ALA:HA	1:A:42:ILE:HD11	0.58	1.75	11	9
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:41:HIS:H	1:B:41:HIS:CD2	0.58	2.14	5	5
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: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: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:B:76:PHE:CE2	1:B:78:LEU:HD21	0.58	2.33	13	3
1:A:34:ILE:O	1:A:37:ASP:N	0.58	2.36	16	10
1:A:49:LYS:HD3	1:A:50:TYR:CE1	0.58	2.34	4	1
1:A:70:THR:OG1	1:A:71:LYS:N	0.58	2.36	6	2
1:A:69:GLU:O	1:A:70:THR:HG23	0.58	1.98	16	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:56:CYS:SG	1:A:57:ILE:N	0.58	2.76	15	3
1:A:43:LYS:O	1:A:46:PHE:N	0.58	2.36	20	1
1:A:47:ASP:HB2	1:A:52:PRO:HB3	0.58	1.73	18	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:B:70:THR:OG1	1:B:71:LYS:N	0.58	2.36	15	3
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:A:38:ILE:HG21	1:A:58:VAL:HG21	0.58	1.74	19	2
1:A:61:ASN:O	1:B:60:ARG:NE	0.58	2.37	19	1
1:A:54:TRP:CH2	1:A:72:HIS:ND1	0.58	2.72	18	1
1:B:35:GLU:CA	1:B:38:ILE:HD12	0.58	2.28	17	1
1:A:21:SER:HB2	1:A:46:PHE:CZ	0.58	2.34	7	6
1:B:14:SER:HB2	1:B:17:MET:CG	0.58	2.28	11	1
1:A:47:ASP:OD1	1:A:52:PRO:HG3	0.58	1.97	9	3
1:A:86:PHE:CZ	1:B:55:HIS:ND1	0.58	2.72	9	1
1:B:43:LYS:HG2	1:B:54:TRP:O	0.58	1.99	1	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:76:PHE:CD1	1:B:76:PHE:N	0.58	2.71	15	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:75:TYR:CD1	1:B:84:LEU:HB2	0.58	2.34	13	3
1:A:55:HIS:HB3	1:B:66:VAL:HA	0.58	1.76	8	4
1:B:52:PRO:C	1:B:87:LYS:HZ1	0.58	2.01	17	1
1:B:34:ILE:O	1:B:38:ILE:HG13	0.58	1.98	6	5
1:B:47:ASP:OD1	1:B:48:LYS:N	0.58	2.37	15	3
1:A:58:VAL:O	1:A:58:VAL:HG13	0.58	1.98	11	3
1:A:13:MET:CG	1:A:14:SER:N	0.58	2.67	11	16
1:A:74:ILE:HG23	1:A:74:ILE:O	0.58	1.96	8	6
1:A:43:LYS:HG3	1:A:54:TRP:O	0.58	1.99	14	4
1:B:15:GLU:CA	1:B:18:GLN:NE2	0.58	2.66	11	1
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:B:55:HIS:CD2	1:B:87:LYS:HA	0.58	2.34	19	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:65:TYR:CE1	1:B:43:LYS:HB3	0.58	2.33	1	1
1:A:37:ASP:O	1:A:41:HIS:NE2	0.57	2.37	16	7
1:B:10:ASN:O	1:B:11:ALA:HB3	0.57	1.98	8	4
1:A:13:MET:HG2	1:A:17:MET:HB2	0.57	1.75	2	5
1:B:6:ALA:CA	1:B:78:LEU:HA	0.57	2.23	7	5
1:B:72:HIS:CD2	1:B:87:LYS:HD3	0.57	2.34	8	1
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:A:28:ALA:HB1	1:A:38:ILE:CA	0.57	2.26	19	5
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:7:VAL:N	1:A:77:TYR:O	0.57	2.36	20	8
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:13:MET:SD	1:B:17:MET:CB	0.57	2.91	4	4
1:B:74:ILE:HD13	1:B:76:PHE:CD1	0.57	2.33	17	13
1:A:5:LYS:O	1:A:6:ALA:HB3	0.57	1.99	17	1
1:B:30:GLU:OE1	1:B:31:LYS:HD2	0.57	1.99	10	1
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:71:LYS:O	1:B:73:PHE:N	0.57	2.37	19	3
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	2
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:A:46:PHE:O	1:A:50:TYR:HB2	0.57	1.99	16	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:34:ILE:N	1:B:34:ILE:CD1	0.57	2.68	7	1
1:B:74:ILE:HG22	1:B:85:LEU:CB	0.57	2.30	14	5
1:A:17:MET:O	1:A:17:MET:SD	0.57	2.62	16	1
1:B:46:PHE:CD2	1:B:85:LEU:HD21	0.57	2.34	19	5
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:13:MET:HA	1:A:71:LYS:C	0.57	2.20	2	1
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:65:TYR:OH	1:B:44:LYS:HE2	0.57	2.00	4	1
1:A:57:ILE:HG12	1:A:84:LEU:CD2	0.57	2.28	9	2
1:B:74:ILE:HG23	1:B:74:ILE:O	0.57	1.99	19	6
1:B:70:THR:HG23	1:B:71:LYS:H	0.57	1.59	2	3
1:A:7:VAL:O	1:A:7:VAL:HG12	0.56	1.99	17	3
1:A:55:HIS:HD1	1:B:66:VAL:HB	0.56	1.59	17	1
1:A:15:GLU:HA	1:A:18:GLN:CG	0.56	2.30	10	9
1:A:59:GLY:O	1:A:82:ALA:N	0.56	2.37	1	4
1:A:14:SER:HB3	1:A:17:MET:HB3	0.56	1.76	10	1
1:A:18:GLN:CB	1:A:74:ILE:HG13	0.56	2.30	10	2
1:A:14:SER:HB2	1:A:17:MET:CG	0.56	2.30	11	3
1:B:53:THR:HG22	1:B:55:HIS:CE1	0.56	2.35	15	1
1:A:34:ILE:O	1:A:38:ILE:HG13	0.56	2.00	6	1
1:A:65:TYR:N	1:B:56:CYS:O	0.56	2.38	16	3
1:B:20:ASP:O	1:B:24:CYS:SG	0.56	2.62	5	1
1:B:75:TYR:HE1	1:B:84:LEU:HB2	0.56	1.59	7	4
1:B:11:ALA:CB	1:B:18:GLN:NE2	0.56	2.68	5	3
1:B:39:ALA:N	1:B:58:VAL:CG1	0.56	2.69	9	12
1:B:8:ILE:HG13	1:B:75:TYR:O	0.56	2.00	6	6
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:A:73:PHE:CD2	1:A:86:PHE:HB3	0.56	2.36	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LYS:HA	1:A:43:LYS:CE	0.56	2.30	5	1
1:B:68:HIS:C	1:B:69:GLU:HG2	0.56	2.19	4	10
1:A:66:VAL:HG22	1:A:84:LEU:HD11	0.56	1.78	4	1
1:A:64:SER:HB2	1:A:84:LEU:HD13	0.56	1.77	11	4
1:A:62:PHE:CE1	1:A:64:SER:HB3	0.56	2.35	12	4
1:A:69:GLU:HG3	1:A:88:SER:OG	0.56	1.99	9	2
1:A:11:ALA:HA	1:A:73:PHE:CD1	0.56	2.35	2	1
1:A:47:ASP:HB3	1:A:52:PRO:CB	0.56	2.30	20	1
1:A:12:ASP:H	1:A:73:PHE:HD1	0.56	1.43	5	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:76:PHE:CD1	1:A:76:PHE:N	0.56	2.73	8	8
1:A:6:ALA:HA	1:A:78:LEU:CA	0.56	2.23	17	4
1:B:51:ASN:O	1:B:87:LYS:HE2	0.56	2.01	17	2
1:A:67:THR:CB	1:B:53:THR:HG21	0.56	2.30	15	3
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:B:80:GLN:HE21	1:B:80:GLN:HA	0.56	1.60	20	1
1:B:14:SER:CB	1:B:17:MET:HB3	0.56	2.31	13	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:58:VAL:HB	1:B:83:ILE:HG23	0.56	1.77	3	8
1:A:51:ASN:O	1:A:54:TRP:NE1	0.56	2.39	17	8
1:A:78:LEU:CD2	1:A:78:LEU:N	0.56	2.69	13	8
1:A:77:TYR:HA	1:A:81:VAL:O	0.56	2.01	2	9
1:A:79:GLY:O	1:A:80:GLN:HB2	0.56	2.00	20	4
1:B:11:ALA:HB1	1:B:74:ILE:HG13	0.56	1.78	12	11
1:A:54:TRP:CH2	1:A:87:LYS:HD2	0.56	2.36	10	1
1:A:38:ILE:O	1:A:42:ILE:HD12	0.56	2.01	15	3
1:A:68:HIS:HB2	1:A:72:HIS:C	0.56	2.20	6	2
1:A:70:THR:HG23	1:A:71:LYS:H	0.56	1.60	14	2
1:B:41:HIS:N	1:B:41:HIS:CD2	0.56	2.73	11	7
1:A:54:TRP:CE2	1:A:87:LYS:HE3	0.56	2.36	10	1
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:B:57:ILE:HG22	1:B:58:VAL:N	0.56	2.16	19	4
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:54:TRP:CZ2	1:A:87:LYS:HD3	0.56	2.36	15	2
1:A:40:ALA:HA	1:B:65:TYR:CZ	0.56	2.35	2	13
1:A:11:ALA:CB	1:A:18:GLN:NE2	0.56	2.68	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:HIS:HB3	1:A:86:PHE:CD2	0.56	2.36	12	1
1:B:32:TYR:N	1:B:32:TYR:CD1	0.56	2.74	12	1
1:A:41:HIS:CD2	1:A:41:HIS:C	0.56	2.79	20	5
1:A:14:SER:CB	1:A:17:MET:HG3	0.56	2.30	9	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:32:TYR:CD1	1:A:41:HIS:CE1	0.56	2.94	16	12
1:B:32:TYR:CG	1:B:41:HIS:CE1	0.56	2.94	11	9
1:A:62:PHE:C	1:B:35:GLU:HB3	0.56	2.22	13	8
1:A:35:GLU:C	1:B:63:GLY:HA3	0.56	2.21	2	5
1:A:65:TYR:CE2	1:B:43:LYS:HE3	0.56	2.36	2	4
1:A:35:GLU:HB3	1:B:62:PHE:C	0.56	2.20	14	4
1:B:55:HIS:HE1	1:B:88:SER:HB2	0.56	1.60	12	1
1:B:12:ASP:HB3	1:B:72:HIS:ND1	0.56	2.16	9	1
1:A:5:LYS:HG3	1:A:5:LYS:O	0.56	2.00	2	1
1:B:18:GLN:O	1:B:74:ILE:HD12	0.55	2.02	17	8
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: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:B:77:TYR:CD2	1:B:82:ALA:HB2	0.55	2.37	18	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:A:43:LYS:CA	1:A:56:CYS:SG	0.55	2.94	14	2
1:B:71:LYS:HD2	1:B:72:HIS:NE2	0.55	2.16	2	1
1:A:39:ALA:H	1:A:58:VAL:HG11	0.55	1.62	18	2
1:B:53:THR:HG22	1:B:55:HIS:NE2	0.55	2.16	14	1
1:A:8:ILE:O	1:A:9:LYS:HG2	0.55	2.01	5	1
1:A:8:ILE:HD11	1:A:22:VAL:CG2	0.55	2.31	4	2
1:A:13:MET:HG2	1:A:17:MET:HB3	0.55	1.77	1	6
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:14:SER:O	1:A:17:MET:N	0.55	2.39	3	6
1:B:66:VAL:HG11	1:B:86:PHE:CZ	0.55	2.37	17	1
1:A:16:GLU:CA	1:A:19:GLN:HG2	0.55	2.31	15	2
1:B:72:HIS:HB2	1:B:87:LYS:HG3	0.55	1.77	13	2
1:A:34:ILE:C	1:A:38:ILE:HD12	0.55	2.22	3	1
1:A:25:ALA:CB	1:A:83:ILE:HG21	0.55	2.31	2	11
1:A:78:LEU:HD23	1:A:83:ILE:HG12	0.55	1.78	19	5
1:A:35:GLU:O	1:A:58:VAL:HG13	0.55	2.01	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ILE:HG12	1:B:64:SER:CA	0.55	2.30	4	1
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:76:PHE:CE2	1:A:83:ILE:HB	0.55	2.36	9	3
1:A:62:PHE:CD2	1:B:62:PHE:HB2	0.55	2.36	14	2
1:B:69:GLU:HG3	1:B:88:SER:HA	0.55	1.77	20	6
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:B:80:GLN:O	1:B:81:VAL:HG23	0.55	2.01	7	5
1:A:65:TYR:CZ	1:B:40:ALA:HA	0.55	2.37	14	9
1:B:43:LYS:HD3	1:B:47:ASP:OD2	0.55	2.02	20	2
1:B:72:HIS:ND1	1:B:87:LYS:HD3	0.55	2.17	3	1
1:A:29:LEU:HD22	1:A:81:VAL:HG21	0.55	1.79	17	1
1:A:43:LYS:HA	1:A:56:CYS:SG	0.55	2.42	14	3
1:B:68:HIS:HB2	1:B:72:HIS:C	0.55	2.22	16	3
1:A:13:MET:SD	1:A:72:HIS:CA	0.55	2.95	15	4
1:A:43:LYS:NZ	1:A:47:ASP:HB2	0.55	2.17	6	1
1:A:12:ASP:HB2	1:A:72:HIS:CB	0.55	2.31	6	1
1:A:49:LYS:HE2	1:A:50:TYR:CZ	0.55	2.37	20	1
1:A:48:LYS:HG3	1:A:48:LYS:O	0.55	2.02	13	1
1:B:12:ASP:HB2	1:B:73:PHE:HD2	0.55	1.62	13	1
1:B:76:PHE:CD2	1:B:78:LEU:HD21	0.55	2.36	3	2
1:A:34:ILE:O	1:A:35:GLU:C	0.55	2.44	5	18
1:B:9:LYS:HE3	1:B:77:TYR:HB3	0.55	1.79	4	2
1:A:6:ALA:HB1	1:A:76:PHE:CD2	0.55	2.37	16	2
1:A:7:VAL:O	1:A:9:LYS:HG2	0.55	2.02	18	4
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:43:LYS:O	1:A:43:LYS:HD2	0.55	2.02	16	1
1:A:12:ASP:O	1:A:72:HIS:HB2	0.55	2.02	11	6
1:B:46:PHE:CD2	1:B:54:TRP:CE3	0.55	2.95	4	13
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:38:ILE:CG2	1:A:42:ILE:HD11	0.55	2.30	5	3
1:B:46:PHE:CD1	1:B:50:TYR:CE1	0.55	2.95	1	5
1:A:6:ALA:CB	1:A:22:VAL:HG13	0.55	2.32	9	6
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:57:ILE:CD1	1:B:64:SER:HB2	0.55	2.22	12	3
1:A:25:ALA:HB1	1:A:83:ILE:HG13	0.55	1.78	9	1
1:B:13:MET:SD	1:B:72:HIS:CA	0.55	2.94	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:43:LYS:CB	1:B:56:CYS:SG	0.54	2.95	14	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:55:HIS:CB	1:B:66:VAL:HG12	0.54	2.31	9	4
1:B:46:PHE:CD2	1:B:50:TYR:CE2	0.54	2.95	9	5
1:A:65:TYR:N	1:B:57:ILE:HD13	0.54	2.13	7	2
1:B:18:GLN:HB3	1:B:74:ILE:HD12	0.54	1.79	1	1
1:A:32:TYR:CG	1:A:41:HIS:CE1	0.54	2.95	10	9
1:B:78:LEU:O	1:B:79:GLY:C	0.54	2.45	6	20
1:B:78:LEU:N	1:B:78:LEU:CD2	0.54	2.70	4	4
1:A:50:TYR:O	1:A:51:ASN:ND2	0.54	2.40	17	1
1:B:34:ILE:HG22	1:B:36:LYS:HG3	0.54	1.79	12	3
1:A:8:ILE:CG2	1:A:9:LYS:N	0.54	2.70	15	6
1:B:70:THR:HG22	1:B:71:LYS:H	0.54	1.60	16	3
1:A:13:MET:N	1:A:18:GLN:HE22	0.54	1.99	18	1
1:B:68:HIS:HE2	1:B:87:LYS:H	0.54	1.45	9	1
1:A:59:GLY:O	1:A:82:ALA:HB3	0.54	2.02	8	3
1:A:42:ILE:HG21	1:A:85:LEU:CD1	0.54	2.31	19	2
1:B:73:PHE:CD1	1:B:75:TYR:CE1	0.54	2.96	20	1
1:B:47:ASP:CB	1:B:52:PRO:HB3	0.54	2.32	17	2
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:B:5:LYS:HA	1:B:5:LYS:CE	0.54	2.33	4	1
1:A:67:THR:CG2	1:A:68:HIS:N	0.54	2.70	18	3
1:B:28:ALA:CB	1:B:38:ILE:HA	0.54	2.23	7	1
1:A:35:GLU:HG2	1:B:61:ASN:O	0.54	2.02	7	3
1:A:13:MET:HB3	1:A:17:MET:CG	0.54	2.32	16	1
1:A:26:THR:N	1:A:29:LEU:HD12	0.54	2.17	10	1
1:B:38:ILE:CG2	1:B:42:ILE:HD11	0.54	2.32	7	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:B:48:LYS:CA	1:B:48:LYS:HE3	0.54	2.28	15	1
1:B:35:GLU:OE2	1:B:59:GLY:HA2	0.54	2.02	2	1
1:A:28:ALA:HA	1:A:32:TYR:CD1	0.54	2.37	17	4
1:A:86:PHE:CZ	1:B:86:PHE:CZ	0.54	2.95	17	10
1:A:46:PHE:CE2	1:A:54:TRP:CZ3	0.54	2.96	12	7
1:B:38:ILE:HG22	1:B:42:ILE:CD1	0.54	2.33	7	3
1:A:54:TRP:HA	1:A:87:LYS:HG3	0.54	1.78	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:54:TRP:CG	1:B:87:LYS:HD2	0.54	2.37	12	2
1:B:43:LYS:CA	1:B:56:CYS:SG	0.54	2.95	14	3
1:B:46:PHE:CE2	1:B:50:TYR:CE2	0.54	2.96	9	2
1:B:4:ARG:O	1:B:5:LYS:HB3	0.54	2.03	8	1
1:B:78:LEU:HB2	1:B:81:VAL:HB	0.54	1.79	13	1
1:B:68:HIS:CD2	1:B:73:PHE:CD2	0.54	2.96	17	1
1:B:41:HIS:C	1:B:41:HIS:CD2	0.54	2.81	2	5
1:A:57:ILE:CB	1:A:84:LEU:HD23	0.54	2.32	9	7
1:A:6:ALA:HB2	1:A:22:VAL:HG13	0.54	1.80	6	7
1:B:52:PRO:CB	1:B:53:THR:HA	0.54	2.32	13	4
1:A:68:HIS:CG	1:A:73:PHE:CD2	0.54	2.96	1	4
1:B:18:GLN:CG	1:B:74:ILE:HG13	0.54	2.32	11	1
1:A:23:GLU:O	1:A:27:GLN:HG2	0.54	2.03	20	2
1:B:61:ASN:OD1	1:B:61:ASN:N	0.54	2.40	19	1
1:B:39:ALA:CA	1:B:58:VAL:HG12	0.54	2.33	15	4
1:A:46:PHE:CD2	1:A:50:TYR:CE2	0.54	2.96	12	1
1:B:11:ALA:HB2	1:B:74:ILE:HG13	0.54	1.79	1	6
1:A:46:PHE:CD1	1:A:50:TYR:CD2	0.54	2.96	15	1
1:A:75:TYR:CD1	1:A:75:TYR:N	0.54	2.76	8	1
1:B:73:PHE:CD1	1:B:73:PHE:C	0.54	2.81	20	2
1:B:46:PHE:CD1	1:B:54:TRP:CZ3	0.54	2.96	14	2
1:B:41:HIS:CD2	1:B:41:HIS:C	0.54	2.80	4	6
1:B:6:ALA:CB	1:B:22:VAL:HG13	0.54	2.33	6	5
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:A:35:GLU:HB3	1:B:62:PHE:O	0.54	2.03	14	1
1:A:43:LYS:CE	1:A:54:TRP:HB3	0.54	2.32	5	1
1:A:28:ALA:O	1:A:32:TYR:HD1	0.54	1.86	18	16
1:B:46:PHE:CD1	1:B:50:TYR:CD1	0.54	2.96	5	4
1:B:32:TYR:CD1	1:B:41:HIS:ND1	0.54	2.76	5	4
1:B:4:ARG:HH11	1:B:19:GLN:HG3	0.54	1.63	12	1
1:A:46:PHE:CD1	1:A:54:TRP:CZ3	0.54	2.95	15	2
1:A:17:MET:HE1	1:A:54:TRP:CH2	0.54	2.38	1	1
1:B:68:HIS:O	1:B:69:GLU:HG2	0.54	2.03	1	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: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:57:ILE:HG13	1:A:84:LEU:CD2	0.54	2.31	18	2
1:A:13:MET:CG	1:A:17:MET:HB3	0.53	2.33	1	7
1:B:47:ASP:HB3	1:B:52:PRO:CB	0.53	2.33	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ASP:OD1	1:A:38:ILE:N	0.53	2.40	17	1
1:B:46:PHE:CE2	1:B:54:TRP:CZ3	0.53	2.96	8	6
1:B:87:LYS:HE2	1:B:89:GLY:O	0.53	2.04	12	1
1:A:35:GLU:HG2	1:B:62:PHE:C	0.53	2.23	11	1
1:A:34:ILE:CG2	1:A:37:ASP:HB2	0.53	2.33	15	3
1:A:36:LYS:HB2	1:A:36:LYS:HZ2	0.53	1.61	2	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:69:GLU:O	1:B:71:LYS:N	0.53	2.41	17	1
1:B:73:PHE:HB3	1:B:86:PHE:HB2	0.53	1.79	4	5
1:B:56:CYS:HB3	1:B:85:LEU:HG	0.53	1.78	14	1
1:A:12:ASP:HB2	1:A:73:PHE:CD1	0.53	2.38	5	1
1:B:4:ARG:NH2	1:B:8:ILE:HD13	0.53	2.18	5	2
1:B:56:CYS:SG	1:B:85:LEU:CD1	0.53	2.96	9	5
1:A:67:THR:HB	1:B:53:THR:CG2	0.53	2.32	8	2
1:A:55:HIS:HE1	1:A:88:SER:HB2	0.53	1.64	9	1
1:A:78:LEU:CD2	1:A:78:LEU:H	0.53	2.17	13	2
1:B:70:THR:HG23	1:B:71:LYS:CG	0.53	2.21	5	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:35:GLU:HG3	1:A:58:VAL:O	0.53	2.03	11	1
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: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:B:32:TYR:HE1	1:B:41:HIS:ND1	0.53	2.02	2	3
1:B:13:MET:CB	1:B:72:HIS:HA	0.53	2.30	13	2
1:B:68:HIS:HB3	1:B:73:PHE:CG	0.53	2.39	5	3
1:B:20:ASP:HA	1:B:23:GLU:OE1	0.53	2.04	11	1
1:A:62:PHE:HA	1:B:35:GLU:HG2	0.53	1.79	1	2
1:A:29:LEU:HD13	1:A:78:LEU:CD1	0.53	2.34	6	1
1:A:32:TYR:CD1	1:A:32:TYR:N	0.53	2.77	5	1
1:A:43:LYS:NZ	1:A:54:TRP:HB3	0.53	2.19	5	1
1:A:17:MET:SD	1:A:46:PHE:CE2	0.53	3.01	16	1
1:A:57:ILE:N	1:A:84:LEU:O	0.53	2.41	15	5
1:A:43:LYS:C	1:A:43:LYS:HD3	0.53	2.23	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:TYR:CE1	1:A:84:LEU:HD13	0.53	2.39	8	1
1:A:87:LYS:HB3	1:A:87:LYS:NZ	0.53	2.19	5	1
1:B:37:ASP:C	1:B:41:HIS:CE1	0.53	2.82	8	8
1:A:54:TRP:HA	1:A:87:LYS:CB	0.53	2.33	17	3
1:B:4:ARG:HG2	1:B:4:ARG:HH11	0.53	1.63	15	2
1:A:43:LYS:HB2	1:B:65:TYR:HD2	0.53	1.63	12	1
1:A:76:PHE:HE2	1:A:78:LEU:HD21	0.53	1.61	16	2
1:B:9:LYS:HE2	1:B:77:TYR:CB	0.53	2.34	14	1
1:A:46:PHE:HD2	1:A:54:TRP:CE3	0.53	2.22	2	5
1:B:51:ASN:O	1:B:51:ASN:ND2	0.53	2.42	4	1
1:A:29:LEU:O	1:A:33:ASN:ND2	0.53	2.42	12	1
1:B:24:CYS:SG	1:B:42:ILE:HG23	0.53	2.44	11	2
1:A:68:HIS:CE1	1:A:88:SER:HA	0.53	2.38	2	1
1:B:68:HIS:HB3	1:B:73:PHE:HD2	0.53	1.59	20	1
1:B:73:PHE:HD2	1:B:86:PHE:HB3	0.53	1.62	14	1
1:A:37:ASP:CG	1:A:41:HIS:CE1	0.53	2.83	17	1
1:A:68:HIS:HB3	1:A:86:PHE:CB	0.53	2.34	12	1
1:A:56:CYS:SG	1:A:85:LEU:CD1	0.53	2.97	6	4
1:B:35:GLU:HG2	1:B:59:GLY:HA2	0.53	1.81	9	4
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: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:17:MET:SD	1:A:54:TRP:CH2	0.52	3.01	10	1
1:B:8:ILE:O	1:B:9:LYS:HG2	0.52	2.03	10	3
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:A:72:HIS:HB2	1:A:87:LYS:CD	0.52	2.34	16	1
1:A:32:TYR:CE2	1:A:41:HIS:CE1	0.52	2.97	17	2
1:B:77:TYR:CD1	1:B:81:VAL:O	0.52	2.63	17	4
1:B:55:HIS:O	1:B:86:PHE:CD1	0.52	2.63	18	5
1:A:41:HIS:C	1:A:41:HIS:CD2	0.52	2.82	14	3
1:B:68:HIS:ND1	1:B:70:THR:N	0.52	2.57	9	1
1:B:75:TYR:CD1	1:B:75:TYR:N	0.52	2.77	20	1
1:A:63:GLY:HA3	1:B:35:GLU:CB	0.52	2.34	17	12
1:A:62:PHE:CD2	1:B:62:PHE:CD2	0.52	2.98	15	1
1:B:57:ILE:O	1:B:83:ILE:HA	0.52	2.04	14	5
1:A:55:HIS:CD2	1:A:55:HIS:H	0.52	2.22	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:68:HIS:CD2	1:B:72:HIS:ND1	0.52	2.77	16	1
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:A:65:TYR:HE2	1:B:43:LYS:HB3	0.52	1.64	16	3
1:A:63:GLY:N	1:B:35:GLU:CB	0.52	2.72	10	3
1:A:77:TYR:CD1	1:A:78:LEU:O	0.52	2.63	4	7
1:B:77:TYR:CD1	1:B:78:LEU:O	0.52	2.63	16	5
1:A:8:ILE:HG13	1:A:75:TYR:O	0.52	2.05	8	2
1:A:77:TYR:O	1:A:77:TYR:CD1	0.52	2.63	15	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:B:71:LYS:HB3	1:B:71:LYS:NZ	0.52	2.18	3	1
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:12:ASP:HB2	1:A:73:PHE:CD2	0.52	2.38	13	4
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:A:43:LYS:C	1:A:43:LYS:HE2	0.52	2.25	11	1
1:A:55:HIS:O	1:A:86:PHE:CD2	0.52	2.63	11	3
1:A:65:TYR:HB3	1:B:39:ALA:CB	0.52	2.33	1	2
1:A:43:LYS:HE2	1:A:43:LYS:HA	0.52	1.82	5	1
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:HG3	1:B:5:LYS:O	0.52	2.05	15	4
1:B:31:LYS:O	1:B:32:TYR:CD1	0.52	2.63	15	2
1:B:57:ILE:HB	1:B:84:LEU:CD2	0.52	2.35	13	4
1:A:26:THR:HA	1:A:29:LEU:HB2	0.52	1.81	17	4
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:55:HIS:O	1:A:86:PHE:CD1	0.52	2.63	10	8
1:A:8:ILE:CA	1:A:76:PHE:HA	0.52	2.32	8	4
1:B:49:LYS:NZ	1:B:49:LYS:CB	0.52	2.70	15	1
1:B:55:HIS:CE1	1:B:88:SER:N	0.52	2.77	1	1
1:A:86:PHE:CE1	1:B:86:PHE:HZ	0.52	2.23	2	1
1:B:62:PHE:HD1	1:B:63:GLY:N	0.52	2.02	19	1
1:A:17:MET:SD	1:A:46:PHE:HE2	0.52	2.27	16	1
1:B:47:ASP:OD1	1:B:54:TRP:CD1	0.52	2.63	3	4
1:A:78:LEU:O	1:A:79:GLY:C	0.52	2.48	9	14
1:B:54:TRP:CE3	1:B:85:LEU:HD23	0.52	2.40	1	2
1:B:18:GLN:CB	1:B:74:ILE:HG13	0.52	2.29	17	2
1:A:86:PHE:CZ	1:B:86:PHE:HZ	0.52	2.23	16	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:27:GLN:OE1	1:A:27:GLN:HA	0.52	2.05	1	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:A:34:ILE:HD12	1:A:34:ILE:N	0.52	2.20	5	1
1:A:86:PHE:HZ	1:B:86:PHE:CZ	0.52	2.23	17	12
1:B:21:SER:OG	1:B:74:ILE:HD12	0.52	2.05	12	2
1:B:18:GLN:HB3	1:B:74:ILE:CG1	0.52	2.32	16	4
1:B:64:SER:OG	1:B:75:TYR:CE2	0.52	2.63	19	6
1:A:55:HIS:CE1	1:B:67:THR:O	0.52	2.63	4	3
1:B:68:HIS:CG	1:B:72:HIS:O	0.52	2.63	9	1
1:A:67:THR:HG21	1:B:53:THR:HG23	0.52	1.82	1	1
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:17:MET:SD	1:B:54:TRP:CH2	0.52	3.02	13	1
1:A:77:TYR:O	1:A:77:TYR:CD2	0.52	2.63	5	1
1:B:31:LYS:HB2	1:B:32:TYR:CD1	0.51	2.40	3	3
1:B:18:GLN:C	1:B:74:ILE:HD12	0.51	2.26	11	2
1:A:77:TYR:CD1	1:A:77:TYR:O	0.51	2.63	6	3
1:B:22:VAL:HG22	1:B:76:PHE:CE1	0.51	2.40	5	1
1:A:54:TRP:CE3	1:A:87:LYS:HG2	0.51	2.40	3	1
1:B:31:LYS:C	1:B:32:TYR:CG	0.51	2.83	13	7
1:A:13:MET:HB2	1:A:73:PHE:H	0.51	1.63	13	3
1:B:73:PHE:CB	1:B:86:PHE:HB3	0.51	2.36	7	2
1:A:7:VAL:HG12	1:A:9:LYS:CE	0.51	2.33	5	1
1:B:26:THR:HA	1:B:29:LEU:HB2	0.51	1.82	3	4
1:A:32:TYR:CD2	1:A:41:HIS:HE1	0.51	2.23	17	2
1:A:57:ILE:CG2	1:B:62:PHE:CD2	0.51	2.94	2	10
1:A:54:TRP:CE2	1:A:87:LYS:CD	0.51	2.93	2	12
1:B:11:ALA:HB1	1:B:18:GLN:CD	0.51	2.25	1	2
1:B:68:HIS:ND1	1:B:68:HIS:N	0.51	2.58	1	3
1:A:9:LYS:HD2	1:A:76:PHE:HA	0.51	1.82	2	1
1:B:77:TYR:CG	1:B:81:VAL:O	0.51	2.63	18	4
1:B:46:PHE:CE1	1:B:85:LEU:HD21	0.51	2.40	16	3
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:B:47:ASP:HB3	1:B:52:PRO:HD3	0.51	1.82	3	1
1:A:63:GLY:HA3	1:B:36:LYS:N	0.51	2.20	9	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:54:TRP:NE1	1:B:87:LYS:HD2	0.51	2.21	12	4
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: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: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: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:69:GLU:O	1:B:70:THR:HB	0.51	2.05	10	3
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:B:4:ARG:HG3	1:B:4:ARG:NH1	0.51	2.19	19	1
1:B:13:MET:HB2	1:B:72:HIS:N	0.51	2.21	5	1
1:B:87:LYS:HE2	1:B:89:GLY:HA2	0.51	1.83	18	1
1:A:17:MET:HE1	1:A:46:PHE:CE2	0.51	2.40	16	1
1:A:13:MET:SD	1:A:74:ILE:CB	0.51	2.95	16	1
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: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: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:A:12:ASP:OD2	1:A:68:HIS:NE2	0.51	2.44	20	3
1:A:73:PHE:C	1:A:73:PHE:CD1	0.51	2.84	5	1
1:B:5:LYS:C	1:B:78:LEU:HD13	0.51	2.25	1	4
1:A:21:SER:CB	1:A:85:LEU:HD22	0.51	2.35	17	2
1:A:6:ALA:HB3	1:A:22:VAL:HG11	0.51	1.81	4	8
1:A:56:CYS:C	1:A:57:ILE:HD13	0.51	2.25	19	7
1:A:28:ALA:O	1:A:32:TYR:CD1	0.51	2.63	14	5
1:B:77:TYR:CD1	1:B:77:TYR:O	0.51	2.64	15	2
1:B:68:HIS:HA	1:B:86:PHE:HD2	0.51	1.64	1	1
1:A:13:MET:HG2	1:A:17:MET:HG3	0.51	1.80	16	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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:47:ASP:C	1:B:47:ASP:OD1	0.51	2.49	14	2
1:A:73:PHE:CA	1:A:86:PHE:HA	0.51	2.29	18	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:A:78:LEU:N	1:A:78:LEU:CD2	0.51	2.74	11	4
1:B:32:TYR:CG	1:B:41:HIS:HE1	0.51	2.22	11	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:65:TYR:HE2	1:B:43:LYS:HD2	0.51	1.64	18	1
1:B:68:HIS:CE1	1:B:87:LYS:O	0.51	2.64	4	2
1:B:8:ILE:HD11	1:B:22:VAL:HG21	0.51	1.82	5	2
1:A:54:TRP:CE2	1:A:87:LYS:CE	0.51	2.94	10	1
1:B:37:ASP:O	1:B:41:HIS:CD2	0.51	2.63	18	6
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: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:31:LYS:CB	1:A:32:TYR:CE1	0.50	2.94	6	11
1:A:37:ASP:O	1:A:41:HIS:CE1	0.50	2.64	13	5
1:A:35:GLU:CB	1:B:63:GLY:HA3	0.50	2.36	17	2
1:A:55:HIS:ND1	1:B:66:VAL:HB	0.50	2.21	17	1
1:A:77:TYR:CD1	1:A:81:VAL:O	0.50	2.64	13	6
1:A:64:SER:CB	1:A:84:LEU:HD13	0.50	2.36	11	2
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
1:B:87:LYS:HZ3	1:B:87:LYS:HB3	0.50	1.66	8	1
1:B:57:ILE:CB	1:B:84:LEU:HB3	0.50	2.35	14	1
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:B:32:TYR:CE1	1:B:41:HIS:HB2	0.50	2.41	2	5
1:A:13:MET:SD	1:A:17:MET:SD	0.50	3.09	8	2
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:73:PHE:CB	1:A:86:PHE:HB3	0.50	2.36	12	3
1:A:62:PHE:CD2	1:B:57:ILE:CG2	0.50	2.95	9	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:B:69:GLU:O	1:B:70:THR:O	0.50	2.30	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:55:HIS:CG	1:B:86:PHE:CE1	0.50	3.00	11	1
1:B:12:ASP:CG	1:B:72:HIS:CD2	0.50	2.84	15	1
1:A:17:MET:HE1	1:A:50:TYR:CD2	0.50	2.41	1	2
1:A:60:ARG:CG	1:A:60:ARG:HH11	0.50	2.20	14	1
1:B:54:TRP:CE2	1:B:87:LYS:HE3	0.50	2.41	3	3
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:46:PHE:HA	1:B:50:TYR:HD1	0.50	1.66	14	2
1:B:50:TYR:N	1:B:50:TYR:CD1	0.50	2.80	4	1
1:A:52:PRO:CB	1:A:53:THR:HA	0.50	2.36	10	5
1:B:73:PHE:O	1:B:73:PHE:CD2	0.50	2.65	10	1
1:A:86:PHE:HZ	1:B:86:PHE:HZ	0.50	1.48	14	2
1:A:62:PHE:CD1	1:B:57:ILE:CG2	0.50	2.95	6	3
1:B:48:LYS:O	1:B:48:LYS:HE2	0.50	2.07	11	1
1:A:12:ASP:CB	1:A:68:HIS:NE2	0.50	2.75	5	1
1:B:46:PHE:HD2	1:B:54:TRP:CD2	0.50	2.24	17	9
1:A:32:TYR:CD2	1:A:41:HIS:CE1	0.50	3.00	4	4
1:B:33:ASN:C	1:B:34:ILE:HD12	0.50	2.26	7	1
1:A:47:ASP:CG	1:A:52:PRO:HB3	0.50	2.27	12	1
1:B:57:ILE:CG2	1:B:58:VAL:N	0.50	2.75	19	3
1:A:43:LYS:HD3	1:A:43:LYS:C	0.50	2.26	8	1
1:A:48:LYS:NZ	1:A:48:LYS:O	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:30:GLU:OE2	1:B:31:LYS:HE3	0.50	2.06	17	1
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	1
1:B:78:LEU:CD2	1:B:78:LEU:N	0.50	2.74	11	6
1:B:46:PHE:CD2	1:B:50:TYR:CD2	0.50	2.99	20	6
1:B:34:ILE:HG22	1:B:36:LYS:HD3	0.50	1.84	3	1
1:B:11:ALA:HB2	1:B:74:ILE:CG1	0.50	2.37	5	11
1:B:55:HIS:HB2	1:B:86:PHE:CD2	0.50	2.41	6	5
1:B:28:ALA:HB1	1:B:38:ILE:CA	0.50	2.31	17	2
1:B:47:ASP:CA	1:B:52:PRO:HD3	0.50	2.37	13	4
1:A:65:TYR:CD1	1:B:43:LYS:HD3	0.50	2.42	6	2
1:A:67:THR:O	1:B:55:HIS:CE1	0.50	2.64	2	3
1:B:68:HIS:CD2	1:B:87:LYS:N	0.50	2.79	9	1
1:B:4:ARG:O	1:B:5:LYS:HB2	0.50	2.06	19	1
1:A:12:ASP:OD2	1:A:68:HIS:CD2	0.50	2.64	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ALA:HB2	1:A:74:ILE:CG1	0.50	2.37	3	9
1:A:21:SER:CA	1:A:46:PHE:CZ	0.50	2.95	12	20
1:B:47:ASP:CB	1:B:52:PRO:HD3	0.50	2.36	17	3
1:B:12:ASP:HB2	1:B:68:HIS:CD2	0.50	2.42	17	1
1:A:62:PHE:HD2	1:B:57:ILE:CG2	0.50	2.20	16	2
1:A:32:TYR:CE1	1:A:41:HIS:CE1	0.50	3.00	16	3
1:B:56:CYS:C	1:B:57:ILE:HD13	0.50	2.26	9	2
1:B:70:THR:CG2	1:B:87:LYS:HB2	0.50	2.37	19	1
1:B:73:PHE:CD1	1:B:86:PHE:HB2	0.50	2.42	5	1
1:B:21:SER:HB2	1:B:85:LEU:CD2	0.50	2.36	18	1
1:B:46:PHE:CE2	1:B:85:LEU:CD2	0.49	2.95	19	4
1:A:65:TYR:CE1	1:B:40:ALA:CB	0.49	2.95	14	12
1:A:35:GLU:HB3	1:A:58:VAL:O	0.49	2.07	17	4
1:A:69:GLU:O	1:A:70:THR:O	0.49	2.30	17	3
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:13:MET:HG3	1:A:17:MET:HG2	0.49	1.80	10	1
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:49:LYS:HZ2	1:B:49:LYS:HB3	0.49	1.65	15	1
1:B:53:THR:HG22	1:B:55:HIS:HD2	0.49	1.65	13	2
1:A:66:VAL:CB	1:A:86:PHE:CZ	0.49	2.95	14	2
1:A:40:ALA:HB2	1:B:65:TYR:CZ	0.49	2.42	14	1
1:A:55:HIS:CD2	1:A:86:PHE:O	0.49	2.64	7	2
1:B:31:LYS:CB	1:B:32:TYR:CE1	0.49	2.95	8	6
1:A:62:PHE:CD2	1:B:62:PHE:CB	0.49	2.95	8	4
1:A:28:ALA:CB	1:A:41:HIS:CG	0.49	2.95	1	7
1:B:77:TYR:HA	1:B:82:ALA:HA	0.49	1.83	6	6
1:A:29:LEU:HD13	1:A:78:LEU:HD12	0.49	1.84	6	1
1:B:73:PHE:CG	1:B:73:PHE:O	0.49	2.66	8	1
1:A:32:TYR:HE1	1:A:41:HIS:ND1	0.49	2.05	14	2
1:B:47:ASP:HB3	1:B:52:PRO:CD	0.49	2.38	3	2
1:A:76:PHE:CD2	1:A:78:LEU:CD2	0.49	2.95	20	6
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:B:13:MET:O	1:B:18:GLN:CD	0.49	2.51	11	13
1:B:19:GLN:OE1	1:B:19:GLN:HA	0.49	2.06	4	1
1:B:66:VAL:CB	1:B:86:PHE:CZ	0.49	2.94	4	3
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:PHE:CD1	1:A:86:PHE:CB	0.49	2.96	13	5
1:B:55:HIS:CB	1:B:86:PHE:CZ	0.49	2.95	11	2
1:A:65:TYR:CE2	1:B:43:LYS:CD	0.49	2.95	9	2
1:A:47:ASP:CG	1:A:52:PRO:HG3	0.49	2.27	19	4
1:A:41:HIS:N	1:A:41:HIS:CD2	0.49	2.80	2	3
1:B:77:TYR:HD2	1:B:82:ALA:HB2	0.49	1.67	13	4
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: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:54:TRP:HA	1:A:87:LYS:CG	0.49	2.37	16	1
1:A:5:LYS:O	1:A:6:ALA:CB	0.49	2.61	3	4
1:A:40:ALA:CB	1:B:65:TYR:CE1	0.49	2.96	1	10
1:A:46:PHE:CZ	1:A:85:LEU:CD2	0.49	2.95	8	4
1:B:68:HIS:CB	1:B:73:PHE:CD2	0.49	2.95	10	1
1:A:77:TYR:HD1	1:A:77:TYR:O	0.49	1.90	9	1
1:A:22:VAL:HG22	1:A:76:PHE:CG	0.49	2.42	15	2
1:B:12:ASP:O	1:B:72:HIS:CG	0.49	2.65	18	2
1:B:18:GLN:HA	1:B:74:ILE:CD1	0.49	2.35	16	2
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:B:76:PHE:O	1:B:82:ALA:HA	0.49	2.06	3	1
1:A:65:TYR:HD2	1:B:43:LYS:HB3	0.49	1.67	12	3
1:B:21:SER:CB	1:B:85:LEU:HD22	0.49	2.37	11	2
1:A:55:HIS:CE1	1:B:67:THR:CG2	0.49	2.96	19	2
1:A:43:LYS:HE3	1:B:65:TYR:CD2	0.49	2.43	14	1
1:A:76:PHE:CE2	1:A:83:ILE:CG1	0.49	2.95	15	14
1:B:56:CYS:SG	1:B:85:LEU:HD12	0.49	2.48	4	2
1:A:69:GLU:O	1:A:72:HIS:N	0.49	2.46	12	3
1:B:70:THR:HG22	1:B:72:HIS:CD2	0.49	2.43	10	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:A:86:PHE:HZ	1:B:86:PHE:CE2	0.49	2.26	6	4
1:B:29:LEU:CD2	1:B:81:VAL:HG11	0.49	2.22	1	1
1:B:44:LYS:O	1:B:47:ASP:OD1	0.49	2.31	2	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:A:43:LYS:HG3	1:B:65:TYR:O	0.49	2.08	5	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:13:MET:CG	1:B:71:LYS:HG2	0.49	2.36	4	1
1:B:68:HIS:CB	1:B:73:PHE:CG	0.49	2.96	10	1
1:B:28:ALA:C	1:B:38:ILE:HG23	0.49	2.27	20	4
1:B:71:LYS:CD	1:B:87:LYS:HD3	0.49	2.37	11	1
1:A:35:GLU:CD	1:B:61:ASN:O	0.49	2.51	13	2
1:A:45:GLU:O	1:A:48:LYS:N	0.49	2.46	9	3
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:71:LYS:O	1:B:72:HIS:C	0.49	2.51	19	1
1:B:53:THR:CG2	1:B:55:HIS:CE1	0.49	2.96	5	2
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:46:PHE:HD2	1:A:54:TRP:CD2	0.49	2.25	20	5
1:B:47:ASP:C	1:B:52:PRO:HD3	0.49	2.28	16	4
1:A:29:LEU:HD11	1:A:83:ILE:CD1	0.49	2.37	17	1
1:A:43:LYS:CB	1:B:65:TYR:HD2	0.49	2.21	10	5
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:47:ASP:OD1	1:A:48:LYS:N	0.49	2.46	19	1
1:B:12:ASP:H	1:B:73:PHE:HD1	0.48	1.50	3	2
1:A:55:HIS:CD2	1:A:87:LYS:CA	0.48	2.96	8	2
1:A:66:VAL:HG11	1:B:55:HIS:HB3	0.48	1.84	17	1
1:B:5:LYS:O	1:B:6:ALA:CB	0.48	2.61	19	6
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:86:PHE:CG	1:B:86:PHE:O	0.48	2.66	18	4
1:B:10:ASN:CB	1:B:75:TYR:HB3	0.48	2.34	2	1
1:B:75:TYR:CD1	1:B:76:PHE:N	0.48	2.80	8	1
1:B:87:LYS:CB	1:B:87:LYS:NZ	0.48	2.76	8	1
1:B:64:SER:OG	1:B:75:TYR:HE2	0.48	1.91	19	2
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: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:9:LYS:CE	1:A:77:TYR:HB2	0.48	2.38	2	2
1:B:29:LEU:HD21	1:B:81:VAL:HG21	0.48	1.84	8	2
1:A:42:ILE:HD13	1:A:83:ILE:HG21	0.48	1.84	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:4:ARG:CD	1:B:4:ARG:N	0.48	2.69	4	1
1:B:86:PHE:O	1:B:86:PHE:CD1	0.48	2.66	2	3
1:A:5:LYS:O	1:A:6:ALA:O	0.48	2.31	10	1
1:A:18:GLN:HB3	1:A:74:ILE:CG1	0.48	2.38	5	3
1:A:49:LYS:O	1:A:50:TYR:CG	0.48	2.66	7	2
1:B:41:HIS:CD2	1:B:41:HIS:N	0.48	2.81	12	2
1:B:17:MET:CE	1:B:54:TRP:HH2	0.48	2.21	19	2
1:B:55:HIS:CE1	1:B:88:SER:CB	0.48	2.96	6	1
1:B:22:VAL:HG22	1:B:76:PHE:CZ	0.48	2.44	5	1
1:A:74:ILE:CG2	1:A:74:ILE:O	0.48	2.62	7	7
1:B:4:ARG:O	1:B:5:LYS:C	0.48	2.51	17	2
1:B:12:ASP:CB	1:B:68:HIS:CD2	0.48	2.96	14	3
1:B:55:HIS:CB	1:B:86:PHE:CE1	0.48	2.96	16	2
1:A:17:MET:CE	1:A:50:TYR:CE2	0.48	2.96	10	2
1:A:54:TRP:CZ3	1:A:87:LYS:HD2	0.48	2.42	10	1
1:B:7:VAL:O	1:B:8:ILE:C	0.48	2.52	11	11
1:B:78:LEU:HD23	1:B:83:ILE:CG1	0.48	2.38	6	2
1:B:6:ALA:HB1	1:B:76:PHE:HD2	0.48	1.67	13	2
1:B:14:SER:O	1:B:18:GLN:NE2	0.48	2.46	11	1
1:B:12:ASP:OD2	1:B:73:PHE:CE1	0.48	2.66	11	1
1:B:46:PHE:CD1	1:B:50:TYR:HE2	0.48	2.26	15	1
1:A:50:TYR:CB	1:A:54:TRP:CZ2	0.48	2.96	1	1
1:A:62:PHE:CB	1:B:62:PHE:CD1	0.48	2.96	20	1
1:A:12:ASP:O	1:A:72:HIS:ND1	0.48	2.46	19	1
1:B:66:VAL:CG2	1:B:86:PHE:CE2	0.48	2.96	19	2
1:A:13:MET:O	1:A:18:GLN:CD	0.48	2.51	12	12
1:B:46:PHE:O	1:B:50:TYR:HD1	0.48	1.91	17	3
1:B:68:HIS:CB	1:B:72:HIS:O	0.48	2.61	4	5
1:B:7:VAL:O	1:B:8:ILE:O	0.48	2.31	6	3
1:B:54:TRP:CA	1:B:87:LYS:HG3	0.48	2.35	2	3
1:B:15:GLU:N	1:B:18:GLN:HE22	0.48	2.07	11	1
1:A:61:ASN:OD1	1:B:60:ARG:HG3	0.48	2.09	1	1
1:A:9:LYS:CD	1:A:9:LYS:N	0.48	2.76	2	1
1:B:46:PHE:CE1	1:B:85:LEU:CD2	0.48	2.96	20	2
1:B:44:LYS:O	1:B:48:LYS:HB3	0.48	2.09	20	1
1:A:13:MET:HB3	1:A:18:GLN:HE21	0.48	1.69	5	1
1:A:54:TRP:C	1:A:55:HIS:CG	0.48	2.86	3	2
1:A:77:TYR:O	1:A:78:LEU:O	0.48	2.32	3	3
1:A:69:GLU:HB2	1:A:88:SER:HA	0.48	1.85	4	3
1:A:37:ASP:OD1	1:A:41:HIS:CE1	0.48	2.66	17	1
1:B:66:VAL:HG11	1:B:86:PHE:CE1	0.48	2.44	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:46:PHE:CG	1:A:50:TYR:CE1	0.48	3.01	10	1
1:A:43:LYS:HG2	1:A:54:TRP:O	0.48	2.07	9	3
1:B:86:PHE:O	1:B:86:PHE:CG	0.48	2.67	6	5
1:B:43:LYS:HA	1:B:56:CYS:SG	0.48	2.49	14	2
1:B:21:SER:CB	1:B:46:PHE:CZ	0.48	2.96	14	6
1:B:84:LEU:CG	1:B:84:LEU:O	0.48	2.62	2	2
1:B:10:ASN:HB3	1:B:73:PHE:CZ	0.48	2.44	6	1
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:B:73:PHE:HB2	1:B:86:PHE:HB2	0.48	1.86	3	3
1:B:55:HIS:CB	1:B:86:PHE:O	0.48	2.62	11	10
1:B:81:VAL:HG12	1:B:82:ALA:H	0.48	1.66	2	5
1:B:13:MET:O	1:B:18:GLN:OE1	0.48	2.31	7	7
1:A:87:LYS:NZ	1:A:87:LYS:HB3	0.48	2.22	2	2
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:B:4:ARG:CD	1:B:19:GLN:HA	0.48	2.37	1	1
1:A:10:ASN:O	1:A:75:TYR:HB3	0.48	2.09	18	1
1:B:10:ASN:C	1:B:10:ASN:HD22	0.48	2.12	18	1
1:B:28:ALA:O	1:B:38:ILE:HG12	0.48	2.09	5	2
1:B:53:THR:C	1:B:87:LYS:NZ	0.48	2.66	17	1
1:B:79:GLY:O	1:B:80:GLN:HG3	0.48	2.09	4	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:27:GLN:CB	1:A:41:HIS:CE1	0.48	2.96	11	1
1:A:11:ALA:HA	1:A:74:ILE:CA	0.48	2.36	16	2
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: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
1:A:84:LEU:CG	1:A:84:LEU:O	0.48	2.61	8	1
1:A:17:MET:SD	1:A:71:LYS:HD3	0.48	2.48	19	1
1:A:69:GLU:O	1:A:70:THR:HB	0.48	2.08	14	1
1:A:15:GLU:O	1:A:16:GLU:C	0.48	2.52	16	2
1:A:62:PHE:C	1:B:35:GLU:CB	0.48	2.82	10	7
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:55:HIS:CE1	1:B:88:SER:OG	0.48	2.67	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	2
1:B:34:ILE:N	1:B:34:ILE:HD13	0.48	2.24	20	2
1:A:35:GLU:OE2	1:B:61:ASN:O	0.48	2.32	11	2
1:A:13:MET:O	1:A:18:GLN:OE1	0.48	2.32	16	3
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:54:TRP:CD2	1:B:87:LYS:CD	0.48	2.96	19	6
1:B:15:GLU:N	1:B:18:GLN:NE2	0.48	2.62	11	1
1:A:6:ALA:HB2	1:A:22:VAL:CG1	0.48	2.38	6	2
1:B:12:ASP:CG	1:B:68:HIS:HD2	0.48	2.12	1	1
1:A:7:VAL:HB	1:A:77:TYR:HB3	0.48	1.84	6	1
1:B:72:HIS:CB	1:B:87:LYS:HG3	0.48	2.39	8	1
1:A:46:PHE:HB3	1:A:54:TRP:CD1	0.48	2.44	19	2
1:A:74:ILE:O	1:A:85:LEU:N	0.48	2.47	13	1
1:B:60:ARG:O	1:B:61:ASN:OD1	0.48	2.32	17	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: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:77:TYR:CD2	1:A:81:VAL:O	0.48	2.67	20	2
1:A:66:VAL:HG22	1:A:84:LEU:HD21	0.48	1.85	13	1
1:B:68:HIS:CG	1:B:73:PHE:CD2	0.48	3.02	5	1
1:A:7:VAL:O	1:A:8:ILE:C	0.48	2.51	11	8
1:B:10:ASN:O	1:B:75:TYR:CB	0.48	2.62	5	2
1:A:7:VAL:O	1:A:8:ILE:O	0.48	2.31	9	4
1:B:68:HIS:CG	1:B:69:GLU:H	0.48	2.25	4	1
1:B:71:LYS:HZ3	1:B:72:HIS:N	0.48	2.07	11	1
1:B:55:HIS:HD2	1:B:87:LYS:HA	0.48	1.69	9	1
1:B:6:ALA:HB1	1:B:76:PHE:HB2	0.48	1.86	20	2
1:A:46:PHE:CD1	1:A:50:TYR:CE2	0.48	3.02	15	1
1:A:46:PHE:CD1	1:A:54:TRP:CH2	0.48	3.02	15	2
1:A:62:PHE:CD2	1:B:62:PHE:CG	0.48	3.02	15	1
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:B:73:PHE:HB2	1:B:86:PHE:CB	0.48	2.39	6	1
1:A:66:VAL:HG11	1:A:86:PHE:CE1	0.48	2.43	19	1
1:B:47:ASP:HB3	1:B:52:PRO:CG	0.48	2.39	5	1
1:A:11:ALA:HA	1:A:73:PHE:O	0.48	2.09	18	1
1:A:13:MET:HG2	1:A:72:HIS:HA	0.48	1.85	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:17:MET:CE	1:B:50:TYR:CE2	0.47	2.96	14	4
1:B:14:SER:O	1:B:18:GLN:CG	0.47	2.62	13	5
1:A:57:ILE:CG2	1:B:62:PHE:HD2	0.47	2.22	12	3
1:B:51:ASN:O	1:B:54:TRP:NE1	0.47	2.47	20	3
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:51:ASN:O	1:A:51:ASN:OD1	0.47	2.31	1	2
1:A:67:THR:O	1:A:68:HIS:O	0.47	2.32	12	1
1:B:43:LYS:HE2	1:B:54:TRP:O	0.47	2.09	9	1
1:B:61:ASN:O	1:B:61:ASN:OD1	0.47	2.32	9	1
1:A:50:TYR:O	1:A:51:ASN:CG	0.47	2.52	2	1
1:A:43:LYS:HD2	1:A:54:TRP:HB2	0.47	1.85	6	1
1:A:13:MET:HB2	1:A:72:HIS:C	0.47	2.29	13	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:64:SER:HB2	1:B:57:ILE:CD1	0.47	2.22	17	3
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
1:B:44:LYS:O	1:B:47:ASP:CG	0.47	2.52	7	1
1:A:17:MET:CE	1:A:54:TRP:HH2	0.47	2.23	1	1
1:A:68:HIS:CB	1:A:73:PHE:CG	0.47	2.96	1	1
1:B:59:GLY:O	1:B:82:ALA:N	0.47	2.47	2	1
1:A:62:PHE:HB3	1:B:62:PHE:CG	0.47	2.44	20	2
1:A:66:VAL:HA	1:B:55:HIS:HA	0.47	1.85	20	1
1:A:40:ALA:O	1:A:44:LYS:HB2	0.47	2.09	19	2
1:B:55:HIS:O	1:B:86:PHE:O	0.47	2.32	19	1
1:A:47:ASP:C	1:A:47:ASP:OD1	0.47	2.52	13	1
1:A:50:TYR:O	1:A:51:ASN:OD1	0.47	2.32	14	1
1:A:69:GLU:OE2	1:A:88:SER:O	0.47	2.32	14	1
1:B:47:ASP:OD1	1:B:54:TRP:HD1	0.47	1.92	5	1
1:A:24:CYS:SG	1:A:46:PHE:HE1	0.47	2.32	16	1
1:A:21:SER:CA	1:A:46:PHE:HZ	0.47	2.23	18	10
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:B:88:SER:O	1:B:89:GLY:C	0.47	2.53	4	2
1:B:43:LYS:NZ	1:B:55:HIS:HA	0.47	2.24	12	1
1:A:67:THR:HB	1:B:43:LYS:HE3	0.47	1.85	9	1
1:A:46:PHE:HB3	1:A:54:TRP:CD2	0.47	2.44	15	2
1:B:29:LEU:HD22	1:B:81:VAL:HG21	0.47	1.86	1	1
1:A:67:THR:CG2	1:B:55:HIS:NE2	0.47	2.78	1	1
1:A:86:PHE:O	1:A:86:PHE:CG	0.47	2.67	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LYS:O	1:A:48:LYS:HG3	0.47	2.07	20	1
1:A:62:PHE:HB3	1:B:62:PHE:CD1	0.47	2.44	20	1
1:B:17:MET:HE1	1:B:54:TRP:CH2	0.47	2.44	19	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:15:GLU:O	1:A:18:GLN:CG	0.47	2.63	9	14
1:A:61:ASN:N	1:A:61:ASN:HD22	0.47	2.06	7	1
1:B:49:LYS:NZ	1:B:49:LYS:HB3	0.47	2.24	15	1
1:A:86:PHE:CE1	1:B:86:PHE:CZ	0.47	3.03	2	1
1:B:74:ILE:CG2	1:B:74:ILE:O	0.47	2.62	19	2
1:A:75:TYR:HD1	1:A:75:TYR:N	0.47	2.07	8	1
1:A:14:SER:O	1:A:14:SER:OG	0.47	2.31	16	1
1:A:35:GLU:O	1:A:58:VAL:CG1	0.47	2.63	13	14
1:A:86:PHE:CG	1:A:86:PHE:O	0.47	2.67	11	3
1:A:70:THR:C	1:A:72:HIS:H	0.47	2.12	11	5
1:B:32:TYR:O	1:B:33:ASN:CB	0.47	2.62	7	1
1:A:86:PHE:CD1	1:A:86:PHE:O	0.47	2.67	11	2
1:A:35:GLU:HG2	1:B:63:GLY:N	0.47	2.24	11	1
1:B:76:PHE:O	1:B:83:ILE:HG12	0.47	2.10	9	1
1:A:16:GLU:O	1:A:20:ASP:OD2	0.47	2.32	15	2
1:A:62:PHE:HD2	1:B:62:PHE:CD2	0.47	2.27	15	1
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:75:TYR:HD1	1:B:75:TYR:N	0.47	2.07	20	1
1:A:56:CYS:O	1:B:65:TYR:N	0.47	2.48	14	3
1:A:43:LYS:CB	1:A:56:CYS:SG	0.47	3.03	14	1
1:A:65:TYR:CB	1:B:56:CYS:O	0.47	2.63	16	1
1:B:45:GLU:O	1:B:49:LYS:CB	0.47	2.62	2	12
1:B:62:PHE:H	1:B:62:PHE:HD1	0.47	1.53	12	2
1:A:65:TYR:HD2	1:B:43:LYS:CB	0.47	2.23	14	2
1:A:29:LEU:O	1:A:33:ASN:OD1	0.47	2.32	15	1
1:A:36:LYS:H	1:A:36:LYS:CD	0.47	2.20	19	1
1:B:11:ALA:C	1:B:13:MET:H	0.47	2.12	13	1
1:A:70:THR:HB	1:A:87:LYS:HE2	0.47	1.86	3	1
1:B:35:GLU:O	1:B:58:VAL:CG1	0.47	2.62	15	17
1:B:18:GLN:O	1:B:74:ILE:CD1	0.47	2.63	17	7
1:A:55:HIS:CB	1:A:86:PHE:O	0.47	2.63	12	7
1:A:77:TYR:CA	1:A:81:VAL:O	0.47	2.63	15	7
1:A:37:ASP:OD2	1:A:41:HIS:CE1	0.47	2.67	7	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:12:ASP:HB3	1:B:72:HIS:CD2	0.47	2.44	11	2
1:A:65:TYR:CD2	1:B:43:LYS:CB	0.47	2.98	20	3
1:B:28:ALA:CB	1:B:41:HIS:HB3	0.47	2.40	7	1
1:A:21:SER:HG	1:A:74:ILE:HG21	0.47	1.67	7	1
1:A:53:THR:OG1	1:B:67:THR:HG21	0.47	2.09	7	1
1:A:24:CYS:O	1:A:27:GLN:CG	0.47	2.63	16	2
1:A:43:LYS:HD3	1:A:44:LYS:N	0.47	2.24	8	2
1:A:32:TYR:HE1	1:A:41:HIS:HB2	0.47	1.69	12	1
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:B:60:ARG:O	1:B:61:ASN:CG	0.47	2.53	15	1
1:A:10:ASN:O	1:A:75:TYR:CB	0.47	2.63	5	3
1:B:6:ALA:HB3	1:B:22:VAL:CG1	0.47	2.40	6	2
1:A:51:ASN:CG	1:A:51:ASN:O	0.47	2.52	1	1
1:B:33:ASN:OD1	1:B:33:ASN:N	0.47	2.47	6	1
1:B:37:ASP:HB3	1:B:41:HIS:NE2	0.47	2.24	8	1
1:B:39:ALA:H	1:B:58:VAL:CG1	0.47	2.22	19	1
1:A:61:ASN:O	1:B:35:GLU:CG	0.47	2.63	14	1
1:A:32:TYR:O	1:A:33:ASN:CB	0.47	2.62	18	2
1:A:56:CYS:HB3	1:A:85:LEU:CG	0.47	2.39	16	1
1:B:9:LYS:CA	1:B:9:LYS:HE2	0.47	2.34	16	1
1:B:20:ASP:OD1	1:B:21:SER:N	0.47	2.47	3	1
1:B:21:SER:CA	1:B:46:PHE:HZ	0.47	2.23	10	15
1:B:78:LEU:N	1:B:78:LEU:HD22	0.47	2.25	4	2
1:A:53:THR:O	1:A:87:LYS:CB	0.47	2.63	9	9
1:B:39:ALA:O	1:B:56:CYS:SG	0.47	2.70	20	2
1:B:5:LYS:O	1:B:78:LEU:CD1	0.47	2.62	13	6
1:B:88:SER:O	1:B:89:GLY:O	0.47	2.33	4	1
1:B:70:THR:O	1:B:71:LYS:HB2	0.47	2.09	10	1
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:A:28:ALA:O	1:A:32:TYR:O	0.47	2.33	13	4
1:A:65:TYR:CD2	1:B:43:LYS:CD	0.47	2.98	12	1
1:A:43:LYS:CB	1:B:65:TYR:CE2	0.47	2.97	12	1
1:A:68:HIS:CE1	1:A:73:PHE:CE2	0.47	3.02	15	1
1:A:54:TRP:CG	1:A:87:LYS:HG3	0.47	2.44	2	1
1:B:32:TYR:HE2	1:B:41:HIS:HB2	0.47	1.68	16	1
1:B:70:THR:O	1:B:71:LYS:CB	0.47	2.63	17	3
1:B:5:LYS:O	1:B:22:VAL:CG1	0.47	2.63	9	6
1:A:72:HIS:O	1:A:73:PHE:CB	0.47	2.63	8	3
1:A:13:MET:HG2	1:A:17:MET:HG2	0.47	1.85	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LYS:CG	1:A:54:TRP:O	0.47	2.63	12	3
1:B:4:ARG:HH11	1:B:4:ARG:CG	0.47	2.22	12	1
1:B:17:MET:CE	1:B:54:TRP:CH2	0.47	2.98	19	3
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:B:67:THR:O	1:B:68:HIS:C	0.47	2.53	1	1
1:A:34:ILE:HD13	1:A:34:ILE:N	0.47	2.25	6	1
1:B:80:GLN:NE2	1:B:80:GLN:CA	0.47	2.78	20	1
1:A:80:GLN:O	1:A:81:VAL:HG23	0.47	2.09	14	1
1:A:17:MET:HE2	1:A:50:TYR:CE1	0.47	2.45	16	1
1:A:5:LYS:O	1:A:78:LEU:CD1	0.47	2.63	15	5
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:55:HIS:N	1:B:55:HIS:ND1	0.47	2.61	1	1
1:B:56:CYS:CA	1:B:84:LEU:O	0.47	2.63	2	2
1:B:40:ALA:O	1:B:43:LYS:HG3	0.47	2.09	19	1
1:B:24:CYS:O	1:B:27:GLN:CG	0.47	2.63	18	1
1:A:12:ASP:O	1:A:72:HIS:CD2	0.46	2.69	4	1
1:A:10:ASN:O	1:A:11:ALA:CB	0.46	2.62	2	2
1:B:34:ILE:O	1:B:38:ILE:CG1	0.46	2.63	7	1
1:A:57:ILE:CD1	1:B:65:TYR:H	0.46	2.22	12	6
1:A:45:GLU:OE2	1:A:49:LYS:HG3	0.46	2.09	9	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:A:73:PHE:CG	1:A:73:PHE:O	0.46	2.68	1	1
1:B:62:PHE:HD1	1:B:62:PHE:H	0.46	1.52	2	2
1:B:55:HIS:ND1	1:B:86:PHE:CZ	0.46	2.83	6	1
1:B:35:GLU:CA	1:B:35:GLU:OE1	0.46	2.63	20	1
1:B:58:VAL:HG13	1:B:58:VAL:O	0.46	2.10	14	1
1:B:79:GLY:O	1:B:80:GLN:HG2	0.46	2.10	14	1
1:A:69:GLU:HG3	1:A:88:SER:CA	0.46	2.33	17	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: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:46:PHE:HA	1:A:50:TYR:HD2	0.46	1.69	7	3
1:B:55:HIS:CB	1:B:86:PHE:CE2	0.46	2.98	8	3
1:B:54:TRP:CA	1:B:87:LYS:HB3	0.46	2.28	18	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:GLU:C	1:A:70:THR:OG1	0.46	2.53	15	2
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:B:35:GLU:OE1	1:B:58:VAL:O	0.46	2.33	20	1
1:A:61:ASN:CG	1:B:60:ARG:NH2	0.46	2.68	19	1
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:43:LYS:C	1:B:43:LYS:HD3	0.46	2.31	18	1
1:A:55:HIS:NE2	1:B:67:THR:CG2	0.46	2.78	16	1
1:A:12:ASP:O	1:A:72:HIS:CB	0.46	2.63	11	3
1:A:13:MET:C	1:A:18:GLN:NE2	0.46	2.68	5	2
1:A:78:LEU:HD23	1:A:83:ILE:HD11	0.46	1.85	10	2
1:A:73:PHE:HD1	1:A:86:PHE:CB	0.46	2.23	7	2
1:B:43:LYS:HZ2	1:B:54:TRP:C	0.46	2.13	12	1
1:B:43:LYS:CE	1:B:54:TRP:O	0.46	2.64	9	2
1:B:14:SER:O	1:B:15:GLU:C	0.46	2.54	15	3
1:B:67:THR:O	1:B:69:GLU:HG2	0.46	2.10	1	1
1:A:68:HIS:CD2	1:A:72:HIS:HA	0.46	2.45	8	1
1:A:57:ILE:CG2	1:B:62:PHE:CE2	0.46	2.98	20	1
1:B:4:ARG:HG3	1:B:4:ARG:HH11	0.46	1.70	19	1
1:A:12:ASP:OD1	1:A:12:ASP:O	0.46	2.33	14	1
1:B:17:MET:HE3	1:B:50:TYR:CE2	0.46	2.44	14	1
1:B:70:THR:C	1:B:71:LYS:CG	0.46	2.83	5	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:A:70:THR:HG22	1:A:71:LYS:HG2	0.46	1.86	3	1
1:A:55:HIS:CD2	1:A:87:LYS:C	0.46	2.89	4	3
1:A:55:HIS:ND1	1:B:86:PHE:CE2	0.46	2.84	17	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:67:THR:O	1:A:67:THR:CG2	0.46	2.63	6	3
1:A:26:THR:OG1	1:A:78:LEU:HD11	0.46	2.09	1	2
1:B:53:THR:O	1:B:87:LYS:CG	0.46	2.64	12	3
1:A:27:GLN:CB	1:A:41:HIS:NE2	0.46	2.78	11	1
1:B:69:GLU:OE2	1:B:88:SER:OG	0.46	2.32	18	2
1:A:66:VAL:HG11	1:B:86:PHE:HE2	0.46	1.70	14	1
1:A:43:LYS:HZ3	1:A:54:TRP:HB3	0.46	1.71	5	1
1:A:11:ALA:C	1:A:13:MET:H	0.46	2.14	17	4
1:A:47:ASP:OD1	1:A:47:ASP:C	0.46	2.54	17	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:LYS:CG	1:B:54:TRP:O	0.46	2.64	8	7
1:A:70:THR:O	1:A:71:LYS:HG2	0.46	2.11	13	3
1:A:58:VAL:CG1	1:A:58:VAL:O	0.46	2.63	13	2
1:A:59:GLY:O	1:A:81:VAL:CG1	0.46	2.63	15	2
1:A:44:LYS:HD2	1:A:44:LYS:C	0.46	2.30	2	1
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:38:ILE:CG2	1:A:58:VAL:HG21	0.46	2.39	19	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: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:A:21:SER:CB	1:A:74:ILE:HG21	0.46	2.40	17	3
1:B:69:GLU:O	1:B:70:THR:CB	0.46	2.64	13	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:28:ALA:C	1:A:38:ILE:HG23	0.46	2.31	17	3
1:B:70:THR:O	1:B:71:LYS:HB3	0.46	2.11	17	1
1:A:54:TRP:CD2	1:A:87:LYS:CG	0.46	2.99	4	3
1:A:74:ILE:O	1:A:74:ILE:CG2	0.46	2.63	2	2
1:B:26:THR:N	1:B:29:LEU:HD12	0.46	2.25	5	4
1:A:43:LYS:O	1:A:43:LYS:HE2	0.46	2.11	11	1
1:A:68:HIS:HB3	1:A:73:PHE:HD2	0.46	1.68	8	1
1:B:55:HIS:O	1:B:86:PHE:N	0.46	2.48	19	1
1:B:49:LYS:CE	1:B:50:TYR:CZ	0.46	2.99	16	1
1:A:28:ALA:HA	1:A:32:TYR:CE1	0.46	2.45	2	10
1:B:11:ALA:CB	1:B:74:ILE:CG1	0.46	2.94	11	9
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:B:81:VAL:CG1	1:B:82:ALA:H	0.46	2.23	1	12
1:A:46:PHE:CE2	1:A:50:TYR:CE2	0.46	3.03	12	1
1:A:35:GLU:CG	1:A:58:VAL:O	0.46	2.64	11	1
1:A:9:LYS:HE3	1:A:77:TYR:CB	0.46	2.40	15	1
1:B:15:GLU:O	1:B:18:GLN:N	0.46	2.48	8	3
1:A:87:LYS:HZ2	1:A:87:LYS:HB3	0.46	1.71	2	1
1:B:43:LYS:C	1:B:43:LYS:CD	0.46	2.84	2	1
1:A:62:PHE:CD2	1:B:62:PHE:HB3	0.46	2.46	8	1
1:B:57:ILE:N	1:B:84:LEU:O	0.46	2.49	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:62:PHE:CZ	1:B:75:TYR:HE1	0.46	2.28	16	1
1:B:10:ASN:O	1:B:11:ALA:CB	0.46	2.64	8	3
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:75:TYR:CD1	1:B:84:LEU:CD1	0.46	2.99	12	1
1:A:11:ALA:O	1:A:12:ASP:OD1	0.46	2.33	18	1
1:A:17:MET:C	1:A:17:MET:SD	0.46	2.94	16	1
1:B:76:PHE:CD2	1:B:78:LEU:CD2	0.46	2.99	5	2
1:A:74:ILE:CG2	1:A:85:LEU:HB2	0.46	2.41	17	1
1:B:58:VAL:CA	1:B:82:ALA:O	0.46	2.63	19	7
1:B:46:PHE:O	1:B:50:TYR:CD1	0.46	2.69	19	2
1:B:42:ILE:HD12	1:B:56:CYS:SG	0.46	2.51	4	1
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:11:ALA:HB1	1:B:18:GLN:HE22	0.46	1.69	1	2
1:B:77:TYR:O	1:B:77:TYR:CD1	0.46	2.69	7	1
1:B:47:ASP:OD2	1:B:52:PRO:CA	0.46	2.64	12	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:A:41:HIS:O	1:A:45:GLU:OE1	0.46	2.34	1	1
1:A:27:GLN:O	1:A:31:LYS:CD	0.46	2.64	8	2
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:48:LYS:CA	1:A:48:LYS:HE3	0.46	2.34	19	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:38:ILE:O	1:B:42:ILE:CD1	0.46	2.64	18	1
1:B:17:MET:SD	1:B:71:LYS:HE2	0.46	2.51	16	1
1:A:62:PHE:CD1	1:B:62:PHE:HB3	0.45	2.47	3	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:A:45:GLU:O	1:A:49:LYS:CB	0.45	2.64	13	5
1:B:31:LYS:C	1:B:32:TYR:CD1	0.45	2.89	15	2
1:A:32:TYR:CB	1:A:37:ASP:OD2	0.45	2.64	9	1
1:A:69:GLU:O	1:A:70:THR:OG1	0.45	2.34	15	1
1:A:8:ILE:C	1:A:9:LYS:CG	0.45	2.84	15	2
1:B:77:TYR:CD1	1:B:77:TYR:C	0.45	2.90	15	1
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:17:MET:CE	1:A:54:TRP:CH2	0.45	2.99	14	2
1:A:9:LYS:HE2	1:A:77:TYR:HB3	0.45	1.87	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:HIS:CB	1:B:66:VAL:CG1	0.45	2.94	20	1
1:B:4:ARG:HD3	1:B:19:GLN:HG2	0.45	1.87	19	1
1:A:55:HIS:HE1	1:B:69:GLU:OE2	0.45	1.95	13	1
1:B:31:LYS:HB3	1:B:32:TYR:CZ	0.45	2.46	16	1
1:B:80:GLN:O	1:B:80:GLN:HG2	0.45	2.11	10	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:B:70:THR:OG1	1:B:89:GLY:C	0.45	2.54	6	1
1:A:46:PHE:CD1	1:A:50:TYR:CD1	0.45	3.04	19	2
1:B:50:TYR:CD1	1:B:50:TYR:N	0.45	2.83	19	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:B:8:ILE:CG2	1:B:9:LYS:N	0.45	2.79	15	4
1:B:70:THR:CG2	1:B:72:HIS:CD2	0.45	2.99	10	1
1:A:18:GLN:CB	1:A:74:ILE:CD1	0.45	2.94	15	7
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:A:67:THR:H	1:B:55:HIS:CG	0.45	2.29	15	1
1:A:77:TYR:CD2	1:A:82:ALA:HB2	0.45	2.45	1	2
1:A:67:THR:CG2	1:B:55:HIS:CE1	0.45	2.99	1	1
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:A:60:ARG:O	1:A:77:TYR:CE2	0.45	2.69	19	1
1:B:13:MET:SD	1:B:18:GLN:HB3	0.45	2.52	13	1
1:A:62:PHE:HE2	1:A:64:SER:CB	0.45	2.25	3	2
1:B:6:ALA:CB	1:B:22:VAL:CG1	0.45	2.95	11	19
1:A:6:ALA:CB	1:A:22:VAL:CG1	0.45	2.95	1	15
1:B:73:PHE:CB	1:B:85:LEU:O	0.45	2.63	20	2
1:B:21:SER:OG	1:B:76:PHE:CE1	0.45	2.69	10	2
1:B:46:PHE:HA	1:B:50:TYR:HD2	0.45	1.72	18	2
1:A:31:LYS:C	1:A:32:TYR:CG	0.45	2.89	15	2
1:B:47:ASP:OD1	1:B:47:ASP:C	0.45	2.54	15	2
1:A:12:ASP:CB	1:A:72:HIS:CG	0.45	2.99	6	1
1:A:56:CYS:O	1:B:65:TYR:CB	0.45	2.64	14	1
1:A:62:PHE:O	1:B:35:GLU:CB	0.45	2.64	16	1
1:A:22:VAL:O	1:A:26:THR:OG1	0.45	2.33	4	5
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:A:43:LYS:CE	1:A:47:ASP:HB2	0.45	2.42	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:60:ARG:O	1:B:61:ASN:CB	0.45	2.63	11	3
1:A:62:PHE:CG	1:B:62:PHE:HB3	0.45	2.47	16	2
1:A:39:ALA:HB3	1:B:65:TYR:HB2	0.45	1.89	13	2
1:B:70:THR:C	1:B:72:HIS:N	0.45	2.68	15	2
1:B:47:ASP:CG	1:B:48:LYS:N	0.45	2.68	1	2
1:A:12:ASP:O	1:A:12:ASP:OD1	0.45	2.34	15	1
1:A:13:MET:CB	1:A:73:PHE:O	0.45	2.65	19	2
1:A:73:PHE:CD1	1:A:73:PHE:C	0.45	2.88	8	1
1:B:80:GLN:NE2	1:B:80:GLN:HA	0.45	2.26	20	1
1:B:55:HIS:CD2	1:B:88:SER:N	0.45	2.84	19	1
1:A:74:ILE:HG22	1:A:85:LEU:HB2	0.45	1.88	16	2
1:B:77:TYR:CA	1:B:81:VAL:O	0.45	2.65	3	3
1:A:78:LEU:C	1:A:80:GLN:N	0.45	2.70	17	2
1:A:88:SER:CB	1:B:88:SER:OG	0.45	2.64	17	1
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:34:ILE:O	1:B:38:ILE:CD1	0.45	2.64	7	1
1:B:4:ARG:NH1	1:B:4:ARG:CG	0.45	2.79	12	1
1:A:57:ILE:CG1	1:A:84:LEU:CD2	0.45	2.95	8	3
1:A:62:PHE:HB2	1:B:62:PHE:CD1	0.45	2.47	15	1
1:A:17:MET:CE	1:A:50:TYR:CE1	0.45	2.99	16	2
1:A:8:ILE:CA	1:A:75:TYR:O	0.45	2.62	8	1
1:A:39:ALA:CB	1:B:65:TYR:CB	0.45	2.95	20	1
1:B:43:LYS:HD3	1:B:44:LYS:N	0.45	2.27	19	1
1:A:5:LYS:C	1:A:78:LEU:HD13	0.45	2.32	18	2
1:A:35:GLU:CB	1:B:62:PHE:O	0.45	2.64	14	1
1:A:32:TYR:C	1:A:34:ILE:HD13	0.45	2.32	5	1
1:A:13:MET:HG3	1:A:72:HIS:CA	0.45	2.41	16	1
1:B:33:ASN:C	1:B:33:ASN:OD1	0.45	2.55	3	1
1:B:29:LEU:O	1:B:32:TYR:O	0.45	2.34	4	4
1:A:63:GLY:O	1:B:39:ALA:CB	0.45	2.65	19	3
1:B:62:PHE:HE2	1:B:64:SER:CB	0.45	2.24	10	2
1:B:74:ILE:CG2	1:B:76:PHE:HE1	0.45	2.25	5	2
1:A:6:ALA:HB3	1:A:22:VAL:CG1	0.45	2.41	14	5
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:77:TYR:HD1	1:A:78:LEU:O	0.45	1.95	12	1
1:B:54:TRP:CG	1:B:87:LYS:HG2	0.45	2.46	11	1
1:A:39:ALA:HA	1:A:56:CYS:SG	0.45	2.52	9	1
1:A:86:PHE:CE2	1:B:55:HIS:HD2	0.45	2.30	1	1
1:A:10:ASN:O	1:A:73:PHE:HE1	0.45	1.93	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:GLU:OE2	1:A:88:SER:CA	0.45	2.65	20	2
1:B:62:PHE:HE1	1:B:64:SER:CB	0.45	2.24	19	1
1:B:46:PHE:HB3	1:B:54:TRP:CD2	0.45	2.47	14	1
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:A:13:MET:CE	1:A:17:MET:SD	0.45	3.04	16	1
1:A:77:TYR:C	1:A:81:VAL:O	0.45	2.54	17	3
1:B:43:LYS:HE3	1:B:53:THR:HA	0.45	1.88	17	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:B:22:VAL:O	1:B:26:THR:OG1	0.45	2.32	10	1
1:A:15:GLU:C	1:A:17:MET:N	0.45	2.70	1	4
1:A:9:LYS:CE	1:A:76:PHE:C	0.45	2.84	2	1
1:A:7:VAL:O	1:A:9:LYS:CD	0.45	2.63	2	1
1:A:64:SER:N	1:B:57:ILE:HG23	0.45	2.26	2	1
1:A:24:CYS:SG	1:A:42:ILE:CG2	0.45	2.98	8	1
1:B:13:MET:CG	1:B:18:GLN:OE1	0.45	2.63	8	2
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:A:32:TYR:O	1:A:38:ILE:HG12	0.45	2.11	13	1
1:A:77:TYR:O	1:A:77:TYR:HD1	0.45	1.95	18	1
1:A:72:HIS:CB	1:A:87:LYS:CD	0.45	2.94	16	1
1:B:20:ASP:C	1:B:20:ASP:OD1	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:54:TRP:CD2	1:A:87:LYS:CD	0.45	2.99	1	3
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: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:46:PHE:HA	1:B:50:TYR:CD2	0.45	2.46	18	1
1:A:51:ASN:O	1:A:87:LYS:CE	0.45	2.64	16	2
1:A:32:TYR:O	1:A:38:ILE:HD11	0.45	2.11	16	1
1:A:64:SER:OG	1:A:75:TYR:CE1	0.45	2.70	4	4
1:A:28:ALA:CB	1:A:38:ILE:HA	0.45	2.36	17	1
1:A:13:MET:CG	1:A:17:MET:CB	0.45	2.95	18	7
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: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:46:PHE:C	1:A:54:TRP:CD1	0.45	2.91	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:LEU:CD2	1:B:57:ILE:CD1	0.45	2.95	16	2
1:A:65:TYR:HE2	1:B:43:LYS:CE	0.45	2.25	19	2
1:B:73:PHE:HD1	1:B:73:PHE:C	0.45	2.16	20	1
1:B:21:SER:HA	1:B:46:PHE:HE2	0.45	1.69	19	1
1:A:59:GLY:HA2	1:B:62:PHE:HA	0.45	1.89	14	1
1:A:43:LYS:CD	1:A:54:TRP:C	0.45	2.85	5	1
1:A:44:LYS:O	1:A:47:ASP:OD2	0.45	2.35	16	1
1:A:7:VAL:HB	1:A:9:LYS:HE2	0.45	1.87	16	1
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:A:17:MET:CE	1:A:50:TYR:CD2	0.44	3.00	17	2
1:B:4:ARG:HB3	1:B:22:VAL:HG11	0.44	1.89	4	1
1:A:54:TRP:CE3	1:A:87:LYS:HD2	0.44	2.46	16	2
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:A:62:PHE:O	1:B:35:GLU:OE1	0.44	2.35	11	1
1:A:62:PHE:CE2	1:B:57:ILE:HG21	0.44	2.47	15	1
1:B:12:ASP:OD1	1:B:72:HIS:CD2	0.44	2.70	15	1
1:A:65:TYR:CZ	1:B:40:ALA:HB2	0.44	2.46	15	2
1:B:21:SER:HB3	1:B:46:PHE:CZ	0.44	2.46	15	1
1:A:13:MET:CB	1:A:72:HIS:HA	0.44	2.41	1	3
1:A:74:ILE:O	1:A:76:PHE:HE1	0.44	1.95	8	1
1:A:65:TYR:O	1:B:56:CYS:O	0.44	2.35	19	1
1:B:7:VAL:CB	1:B:77:TYR:O	0.44	2.65	18	2
1:B:70:THR:HG21	1:B:87:LYS:HZ3	0.44	1.67	4	1
1:B:49:LYS:HB3	1:B:50:TYR:CE1	0.44	2.48	16	3
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:61:ASN:HD22	1:A:61:ASN:H	0.44	1.55	7	1
1:A:35:GLU:OE2	1:A:60:ARG:CD	0.44	2.65	11	1
1:A:57:ILE:HB	1:A:84:LEU:CD2	0.44	2.42	9	1
1:A:69:GLU:O	1:A:70:THR:CB	0.44	2.65	14	3
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:64:SER:OG	1:B:75:TYR:CE1	0.44	2.69	6	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
1:B:74:ILE:CG2	1:B:85:LEU:HB2	0.44	2.38	14	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:46:PHE:O	1:B:50:TYR:HD2	0.44	1.95	18	2
1:B:38:ILE:CB	1:B:58:VAL:HG11	0.44	2.39	11	2
1:A:28:ALA:CB	1:A:41:HIS:HB3	0.44	2.43	12	1
1:B:33:ASN:HD22	1:B:34:ILE:HD13	0.44	1.72	11	1
1:A:16:GLU:HA	1:A:19:GLN:HE21	0.44	1.72	8	1
1:B:12:ASP:OD2	1:B:68:HIS:NE2	0.44	2.50	5	1
1:B:73:PHE:HD2	1:B:86:PHE:CB	0.44	2.26	3	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:A:14:SER:O	1:A:18:GLN:CG	0.44	2.62	10	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:72:HIS:CD2	1:A:87:LYS:HD3	0.44	2.47	10	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:B:42:ILE:O	1:B:43:LYS:C	0.44	2.55	16	7
1:A:21:SER:HA	1:A:46:PHE:HE1	0.44	1.67	12	2
1:B:43:LYS:HD2	1:B:43:LYS:C	0.44	2.33	2	1
1:A:21:SER:HB3	1:A:46:PHE:CZ	0.44	2.47	5	2
1:B:4:ARG:CD	1:B:19:GLN:HG2	0.44	2.43	19	1
1:B:4:ARG:O	1:B:6:ALA:N	0.44	2.50	5	1
1:A:59:GLY:HA3	1:B:62:PHE:HA	0.44	1.90	18	3
1:B:53:THR:O	1:B:87:LYS:HB2	0.44	2.13	18	1
1:A:13:MET:SD	1:A:18:GLN:HB3	0.44	2.53	10	1
1:B:73:PHE:CD1	1:B:86:PHE:CB	0.44	3.00	2	2
1:A:14:SER:HB2	1:A:17:MET:HB2	0.44	1.89	11	1
1:A:43:LYS:C	1:A:43:LYS:CD	0.44	2.86	1	1
1:A:17:MET:HE1	1:A:50:TYR:CE1	0.44	2.48	2	1
1:A:25:ALA:CA	1:A:42:ILE:HG12	0.44	2.42	19	1
1:A:78:LEU:HD22	1:A:78:LEU:N	0.44	2.27	13	3
1:B:76:PHE:HE2	1:B:78:LEU:HD21	0.44	1.71	13	1
1:B:75:TYR:CD1	1:B:84:LEU:HD12	0.44	2.46	14	1
1:B:46:PHE:CE1	1:B:54:TRP:CZ3	0.44	3.06	3	1
1:A:35:GLU:CB	1:B:62:PHE:C	0.44	2.86	10	3
1:B:6:ALA:HA	1:B:77:TYR:O	0.44	2.13	7	1
1:A:31:LYS:HB3	1:A:32:TYR:CZ	0.44	2.47	11	1
1:A:32:TYR:CE1	1:A:41:HIS:CB	0.44	3.01	9	1
1:A:24:CYS:HB2	1:A:46:PHE:HE1	0.44	1.73	1	1
1:B:68:HIS:HB3	1:B:73:PHE:CB	0.44	2.43	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ASP:O	1:A:52:PRO:CD	0.44	2.65	16	2
1:A:57:ILE:HD13	1:B:64:SER:HB2	0.44	1.88	14	1
1:B:42:ILE:O	1:B:44:LYS:N	0.44	2.51	17	1
1:A:6:ALA:CB	1:A:78:LEU:CD2	0.44	2.96	4	1
1:A:62:PHE:HE1	1:A:64:SER:CB	0.44	2.25	12	2
1:A:14:SER:O	1:A:17:MET:CB	0.44	2.64	11	1
1:B:12:ASP:HB3	1:B:72:HIS:HB3	0.44	1.89	18	2
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: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:B:15:GLU:CA	1:B:18:GLN:OE1	0.44	2.65	20	1
1:B:5:LYS:O	1:B:6:ALA:HB3	0.44	2.12	20	1
1:A:69:GLU:HB2	1:A:87:LYS:O	0.44	2.12	19	1
1:B:56:CYS:HB2	1:B:84:LEU:O	0.44	2.13	13	1
1:A:44:LYS:CA	1:A:44:LYS:HE2	0.44	2.42	5	1
1:A:7:VAL:O	1:A:9:LYS:HE3	0.44	2.13	11	1
1:A:8:ILE:HD12	1:A:76:PHE:CB	0.44	2.41	1	2
1:B:68:HIS:CE1	1:B:70:THR:H	0.44	2.31	9	1
1:A:38:ILE:O	1:A:42:ILE:CD1	0.44	2.65	15	2
1:B:73:PHE:HD1	1:B:86:PHE:CB	0.44	2.26	2	1
1:B:54:TRP:CE3	1:B:87:LYS:HD2	0.44	2.48	19	1
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:B:73:PHE:HE1	1:B:84:LEU:CD1	0.44	2.26	12	1
1:A:65:TYR:CB	1:B:39:ALA:CB	0.44	2.96	9	2
1:B:45:GLU:O	1:B:49:LYS:N	0.44	2.51	16	4
1:A:31:LYS:HD3	1:A:41:HIS:CE1	0.44	2.47	1	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:A:86:PHE:HE2	1:B:55:HIS:HD1	0.44	1.55	6	1
1:B:68:HIS:C	1:B:68:HIS:HD1	0.44	2.16	6	1
1:B:49:LYS:HD3	1:B:50:TYR:CZ	0.44	2.47	13	2
1:A:46:PHE:CD2	1:A:54:TRP:CD2	0.44	3.06	20	1
1:A:78:LEU:CD2	1:A:83:ILE:HG12	0.44	2.42	19	1
1:B:58:VAL:CG2	1:B:81:VAL:CG1	0.44	2.96	19	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:75:TYR:CD1	1:B:83:ILE:O	0.43	2.71	3	1
1:A:11:ALA:CB	1:A:74:ILE:CG1	0.43	2.96	11	4
1:A:55:HIS:ND1	1:B:67:THR:O	0.43	2.50	4	2
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:B:32:TYR:C	1:B:34:ILE:HD12	0.43	2.34	7	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: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:34:ILE:O	1:A:37:ASP:CB	0.43	2.65	9	2
1:A:67:THR:CB	1:B:53:THR:CG2	0.43	2.96	15	1
1:A:8:ILE:HD11	1:A:22:VAL:HG21	0.43	1.89	2	1
1:B:9:LYS:O	1:B:10:ASN:HB2	0.43	2.12	20	1
1:A:57:ILE:CA	1:B:63:GLY:O	0.43	2.63	14	1
1:B:13:MET:CB	1:B:18:GLN:OE1	0.43	2.65	16	1
1:A:56:CYS:CA	1:A:84:LEU:O	0.43	2.63	8	3
1:A:64:SER:CA	1:B:57:ILE:CD1	0.43	2.94	14	4
1:A:32:TYR:HE1	1:A:41:HIS:CB	0.43	2.26	9	4
1:A:17:MET:CE	1:A:46:PHE:HE1	0.43	2.25	15	1
1:B:72:HIS:HB2	1:B:87:LYS:CB	0.43	2.36	2	1
1:B:78:LEU:HD23	1:B:83:ILE:CD1	0.43	2.42	6	1
1:A:70:THR:C	1:A:71:LYS:CG	0.43	2.85	20	1
1:A:10:ASN:O	1:A:73:PHE:CE2	0.43	2.71	19	1
1:A:66:VAL:CG1	1:B:86:PHE:HE2	0.43	2.25	14	1
1:A:43:LYS:HD2	1:A:55:HIS:N	0.43	2.28	5	1
1:B:53:THR:HG23	1:B:55:HIS:HE1	0.43	1.66	18	1
1:B:42:ILE:O	1:B:45:GLU:N	0.43	2.52	16	1
1:A:39:ALA:CB	1:B:63:GLY:O	0.43	2.66	16	4
1:B:21:SER:HB2	1:B:46:PHE:HZ	0.43	1.70	5	3
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:B:15:GLU:CA	1:B:18:GLN:HE22	0.43	2.27	11	1
1:B:68:HIS:NE2	1:B:87:LYS:N	0.43	2.66	9	1
1:A:16:GLU:C	1:A:19:GLN:HG2	0.43	2.34	1	1
1:A:29:LEU:HD23	1:A:38:ILE:HD13	0.43	1.90	5	1
1:A:39:ALA:H	1:A:58:VAL:CG1	0.43	2.26	18	1
1:A:12:ASP:HB3	1:A:72:HIS:HB3	0.43	1.89	17	2
1:A:11:ALA:O	1:A:12:ASP:CB	0.43	2.65	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:4:ARG:NH1	1:B:19:GLN:HE22	0.43	2.12	7	1
1:B:33:ASN:O	1:B:33:ASN:CG	0.43	2.57	12	1
1:B:24:CYS:SG	1:B:42:ILE:HA	0.43	2.53	11	1
1:B:68:HIS:HD2	1:B:86:PHE:CB	0.43	2.27	9	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: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:B:27:GLN:CG	1:B:28:ALA:N	0.43	2.78	18	1
1:A:13:MET:SD	1:A:73:PHE:N	0.43	2.91	16	1
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:9:LYS:CE	1:A:77:TYR:CB	0.43	2.95	2	2
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:14:SER:HB2	1:B:17:MET:HB2	0.43	1.89	11	1
1:B:46:PHE:HD2	1:B:54:TRP:CZ3	0.43	2.30	9	1
1:A:19:GLN:CG	1:A:20:ASP:N	0.43	2.81	1	2
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:66:VAL:CG1	1:B:55:HIS:CB	0.43	2.96	1	2
1:A:68:HIS:HD2	1:A:72:HIS:ND1	0.43	2.11	17	1
1:B:70:THR:HG21	1:B:87:LYS:HZ1	0.43	1.68	4	1
1:B:78:LEU:HD22	1:B:78:LEU:N	0.43	2.29	1	2
1:A:63:GLY:O	1:B:57:ILE:HA	0.43	2.14	7	1
1:A:78:LEU:N	1:A:78:LEU:HD22	0.43	2.29	11	2
1:B:23:GLU:O	1:B:27:GLN:CG	0.43	2.66	11	1
1:B:40:ALA:O	1:B:43:LYS:N	0.43	2.52	15	1
1:A:62:PHE:CE2	1:B:57:ILE:CG2	0.43	3.02	1	1
1:A:36:LYS:CB	1:A:36:LYS:NZ	0.43	2.76	2	1
1:A:43:LYS:HD3	1:A:54:TRP:C	0.43	2.33	6	2
1:B:54:TRP:CH2	1:B:87:LYS:HD2	0.43	2.48	19	1
1:A:55:HIS:CE1	1:A:88:SER:CB	0.43	3.02	13	1
1:A:60:ARG:HH11	1:A:60:ARG:HG3	0.43	1.74	18	1
1:A:66:VAL:CG1	1:B:55:HIS:CA	0.43	2.96	8	2
1:B:13:MET:CB	1:B:71:LYS:HG3	0.43	2.43	4	1
1:A:18:GLN:CB	1:A:74:ILE:CG1	0.43	2.96	10	1
1:A:77:TYR:CD1	1:A:77:TYR:C	0.43	2.92	9	2
1:B:70:THR:O	1:B:72:HIS:N	0.43	2.51	15	2
1:B:12:ASP:OD2	1:B:68:HIS:HD2	0.43	1.95	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:16:GLU:HA	1:A:16:GLU:OE1	0.43	2.14	12	1
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:B:57:ILE:HG12	1:B:84:LEU:CD2	0.43	2.32	9	2
1:B:15:GLU:O	1:B:18:GLN:HG3	0.43	2.13	15	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: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: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:72:HIS:N	1:A:72:HIS:CD2	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: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: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: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:A:27:GLN:HE21	1:A:41:HIS:CE1	0.43	2.32	15	1
1:A:67:THR:CG2	1:A:67:THR:O	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: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:86:PHE:HZ	1:B:86:PHE:HE2	0.43	1.56	5	1
1:A:13:MET:HE3	1:A:17:MET:SD	0.43	2.54	16	1
1:A:68:HIS:C	1:A:68:HIS:ND1	0.43	2.72	16	1
1:A:7:VAL:CB	1:A:9:LYS:HE2	0.43	2.44	16	1
1:A:55:HIS:NE2	1:A:87:LYS:C	0.42	2.73	3	1
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:A:64:SER:HB2	1:A:84:LEU:CD2	0.42	2.30	5	2
1:A:73:PHE:CB	1:A:85:LEU:O	0.42	2.66	12	2
1:A:57:ILE:CD1	1:B:64:SER:CA	0.42	2.96	12	3
1:A:28:ALA:CB	1:A:38:ILE:O	0.42	2.67	19	2
1:B:11:ALA:HB3	1:B:18:GLN:OE1	0.42	2.14	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ASP:O	1:A:71:LYS:CA	0.42	2.63	2	1
1:B:43:LYS:HD2	1:B:44:LYS:N	0.42	2.29	2	1
1:A:16:GLU:H	1:A:16:GLU:CD	0.42	2.17	6	1
1:A:62:PHE:CA	1:B:59:GLY:CA	0.42	2.96	19	2
1:B:43:LYS:N	1:B:56:CYS:SG	0.42	2.92	16	2
1:A:43:LYS:CD	1:A:43:LYS:C	0.42	2.86	16	4
1:B:68:HIS:HB2	1:B:73:PHE:CB	0.42	2.45	10	1
1:B:7:VAL:HB	1:B:77:TYR:HB3	0.42	1.91	12	1
1:B:56:CYS:SG	1:B:85:LEU:HD11	0.42	2.55	11	1
1:B:18:GLN:CA	1:B:74:ILE:CD1	0.42	2.95	9	3
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:A:51:ASN:HD22	1:A:51:ASN:N	0.42	2.12	20	1
1:A:5:LYS:O	1:A:78:LEU:HA	0.42	2.14	19	2
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:B:24:CYS:HB2	1:B:46:PHE:HE1	0.42	1.73	17	1
1:B:13:MET:O	1:B:14:SER:C	0.42	2.58	10	2
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:A:73:PHE:CA	1:A:85:LEU:O	0.42	2.67	12	1
1:B:51:ASN:O	1:B:52:PRO:O	0.42	2.37	9	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:B:75:TYR:CE1	1:B:84:LEU:HD13	0.42	2.48	20	1
1:A:65:TYR:CD2	1:B:43:LYS:CG	0.42	3.00	19	1
1:A:57:ILE:CD1	1:B:84:LEU:HD22	0.42	2.44	14	1
1:A:56:CYS:O	1:B:65:TYR:HB2	0.42	2.14	14	1
1:A:43:LYS:CE	1:B:65:TYR:HD2	0.42	2.27	14	1
1:B:43:LYS:O	1:B:47:ASP:CG	0.42	2.57	3	1
1:B:28:ALA:CB	1:B:38:ILE:O	0.42	2.67	17	1
1:A:57:ILE:HD12	1:A:84:LEU:CD2	0.42	2.45	14	2
1:B:62:PHE:HE1	1:B:82:ALA:O	0.42	1.97	11	1
1:B:4:ARG:CG	1:B:4:ARG:HH11	0.42	2.27	15	1
1:A:57:ILE:O	1:A:84:LEU:N	0.42	2.52	1	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:A:25:ALA:O	1:A:29:LEU:HG	0.42	2.13	5	1
1:B:46:PHE:O	1:B:50:TYR:CD2	0.42	2.73	18	1
1:B:6:ALA:C	1:B:7:VAL:CG2	0.42	2.88	18	1
1:B:11:ALA:CB	1:B:74:ILE:HG12	0.42	2.44	16	1
1:A:31:LYS:C	1:A:32:TYR:CD1	0.42	2.92	17	2
1:A:13:MET:CB	1:A:18:GLN:NE2	0.42	2.81	4	1
1:B:42:ILE:HG22	1:B:56:CYS:SG	0.42	2.55	11	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:38:ILE:C	1:A:42:ILE:HD12	0.42	2.34	20	1
1:B:10:ASN:CG	1:B:73:PHE:HZ	0.42	2.17	19	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:64:SER:HB2	1:B:84:LEU:CD2	0.42	2.43	2	3
1:B:13:MET:N	1:B:73:PHE:O	0.42	2.53	17	1
1:B:28:ALA:HA	1:B:32:TYR:CE1	0.42	2.50	10	2
1:A:63:GLY:O	1:B:58:VAL:N	0.42	2.51	10	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:35:GLU:O	1:A:36:LYS:C	0.42	2.57	1	2
1:A:65:TYR:N	1:B:57:ILE:CD1	0.42	2.83	5	2
1:A:80:GLN:CG	1:A:80:GLN:O	0.42	2.67	1	1
1:A:40:ALA:HB2	1:B:65:TYR:CD2	0.42	2.50	8	1
1:A:39:ALA:CB	1:A:56:CYS:SG	0.42	3.08	20	1
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:A:75:TYR:HD1	1:A:84:LEU:HA	0.42	1.74	1	2
1:B:42:ILE:CD1	1:B:56:CYS:SG	0.42	3.08	4	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:B:73:PHE:CA	1:B:85:LEU:O	0.42	2.63	5	4
1:A:77:TYR:CZ	1:A:80:GLN:HA	0.42	2.49	15	1
1:A:68:HIS:CB	1:A:73:PHE:CD2	0.42	3.02	1	2
1:A:55:HIS:HE1	1:A:88:SER:CB	0.42	2.28	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:B:13:MET:N	1:B:18:GLN:NE2	0.42	2.59	8	1
1:A:67:THR:HG22	1:B:53:THR:CG2	0.42	2.43	13	1
1:A:32:TYR:O	1:A:33:ASN:CG	0.42	2.58	18	1
1:A:72:HIS:CD2	1:A:87:LYS:HZ2	0.42	2.32	16	1
1:A:13:MET:SD	1:A:73:PHE:C	0.42	2.97	16	1
1:B:48:LYS:HA	1:B:48:LYS:HE2	0.42	1.91	16	1
1:B:67:THR:HG23	1:B:67:THR:O	0.42	2.14	16	1
1:A:17:MET:SD	1:A:50:TYR:CE2	0.42	3.12	17	1
1:B:18:GLN:H	1:B:18:GLN:HG2	0.42	1.38	17	3
1:B:46:PHE:HA	1:B:50:TYR:CE1	0.42	2.49	17	1
1:B:43:LYS:CD	1:B:54:TRP:H	0.42	2.28	17	1
1:B:71:LYS:HA	1:B:71:LYS:HE3	0.42	1.92	4	1
1:B:30:GLU:OE1	1:B:31:LYS:CD	0.42	2.68	10	1
1:A:61:ASN:OD1	1:A:61:ASN:O	0.42	2.37	12	1
1:B:37:ASP:O	1:B:41:HIS:NE2	0.42	2.53	12	1
1:A:56:CYS:HG	1:A:57:ILE:N	0.42	2.12	11	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:HD2	1:B:55:HIS:N	0.42	2.10	2	1
1:A:79:GLY:O	1:A:80:GLN:HB3	0.42	2.15	19	1
1:B:35:GLU:CD	1:B:35:GLU:H	0.42	2.18	13	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:37:ASP:C	1:B:41:HIS:NE2	0.42	2.72	18	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: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: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:47:ASP:CB	1:A:52:PRO:HB3	0.42	2.41	20	1
1:A:65:TYR:N	1:B:57:ILE:HG12	0.42	2.27	19	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
1:A:69:GLU:O	1:A:70:THR:CG2	0.42	2.67	16	1
1:B:78:LEU:C	1:B:80:GLN:N	0.42	2.74	7	2
1:B:51:ASN:O	1:B:87:LYS:CE	0.42	2.67	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:LYS:HB3	1:A:50:TYR:CD1	0.42	2.50	13	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:70:THR:HG23	1:A:71:LYS:N	0.42	2.28	14	1
1:A:61:ASN:O	1:B:35:GLU:CD	0.42	2.59	14	1
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:13:MET:HB2	1:B:73:PHE:H	0.41	1.74	17	2
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:A:35:GLU:CB	1:B:63:GLY:N	0.41	2.83	2	1
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:14:SER:OG	1:B:17:MET:HG3	0.41	2.14	17	1
1:A:63:GLY:CA	1:B:58:VAL:O	0.41	2.68	17	1
1:A:77:TYR:C	1:A:77:TYR:CD1	0.41	2.93	4	1
1:A:62:PHE:CG	1:B:62:PHE:CB	0.41	3.03	9	2
1:A:88:SER:CB	1:B:69:GLU:OE2	0.41	2.67	12	1
1:A:15:GLU:H	1:A:15:GLU:HG2	0.41	1.45	11	1
1:B:17:MET:CE	1:B:46:PHE:CE2	0.41	3.03	9	1
1:B:10:ASN:O	1:B:75:TYR:HB3	0.41	2.15	2	1
1:A:65:TYR:CE1	1:B:43:LYS:HD2	0.41	2.51	8	1
1:A:66:VAL:HA	1:B:55:HIS:CB	0.41	2.43	14	1
1:A:9:LYS:N	1:A:75:TYR:O	0.41	2.52	14	1
1:B:46:PHE:CD1	1:B:54:TRP:CH2	0.41	3.08	14	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:A:43:LYS:CD	1:B:65:TYR:HE2	0.41	2.26	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:86:PHE:CZ	1:B:86:PHE:CE2	0.41	3.08	12	1
1:A:40:ALA:CA	1:B:65:TYR:CD1	0.41	3.03	9	1
1:A:74:ILE:HG12	1:A:75:TYR:N	0.41	2.30	13	1
1:A:7:VAL:O	1:A:9:LYS:HD3	0.41	2.14	13	1
1:B:72:HIS:HB2	1:B:87:LYS:CG	0.41	2.44	13	1
1:B:35:GLU:OE2	1:B:60:ARG:NH2	0.41	2.53	10	1
1:A:39:ALA:CA	1:A:56:CYS:SG	0.41	3.08	20	1
1:A:50:TYR:C	1:A:51:ASN:OD1	0.41	2.58	14	1
1:A:43:LYS:HD2	1:A:55:HIS:C	0.41	2.35	5	1
1:B:11:ALA:HB2	1:B:74:ILE:HA	0.41	1.90	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:ILE:CA	1:A:76:PHE:CB	0.41	2.97	16	1
1:B:72:HIS:C	1:B:73:PHE:CD1	0.41	2.94	4	2
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:35:GLU:CG	1:B:61:ASN:O	0.41	2.69	7	1
1:B:84:LEU:HD21	1:B:86:PHE:CE2	0.41	2.50	11	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:A:88:SER:OG	1:B:88:SER:HB3	0.41	2.15	1	1
1:B:53:THR:CG2	1:B:53:THR:O	0.41	2.68	16	2
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: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:9:LYS:HE2	1:A:77:TYR:HB2	0.41	1.85	2	1
1:A:17:MET:SD	1:A:72:HIS:CE1	0.41	3.14	14	1
1:A:13:MET:HB2	1:A:72:HIS:N	0.41	2.30	7	1
1:B:44:LYS:CA	1:B:47:ASP:OD2	0.41	2.68	7	1
1:A:55:HIS:CA	1:B:66:VAL:HA	0.41	2.45	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: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:B:62:PHE:CZ	1:B:75:TYR:CE2	0.41	3.08	19	1
1:A:13:MET:CB	1:A:18:GLN:OE1	0.41	2.68	18	1
1:A:8:ILE:HG13	1:A:76:PHE:CB	0.41	2.39	18	1
1:B:86:PHE:O	1:B:86:PHE:CD2	0.41	2.74	18	1
1:A:57:ILE:HG23	1:B:63:GLY:C	0.41	2.36	4	1
1:B:5:LYS:HE3	1:B:5:LYS:HA	0.41	1.92	4	1
1:B:45:GLU:O	1:B:48:LYS:CG	0.41	2.67	7	1
1:A:59:GLY:CA	1:A:62:PHE:CE1	0.41	3.04	9	1
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:A:7:VAL:CB	1:A:77:TYR:O	0.41	2.69	6	1
1:A:61:ASN:OD1	1:B:60:ARG:NE	0.41	2.53	8	1
1:B:28:ALA:O	1:B:32:TYR:O	0.41	2.38	3	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:MET:CG	1:A:17:MET:CG	0.41	2.95	10	1
1:B:77:TYR:C	1:B:77:TYR:CD1	0.41	2.94	7	1
1:A:71:LYS:C	1:A:72:HIS:CG	0.41	2.94	7	1
1:A:21:SER:CB	1:A:46:PHE:HZ	0.41	2.29	12	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:B:26:THR:O	1:B:29:LEU:HB2	0.41	2.16	9	2
1:B:7:VAL:CG2	1:B:77:TYR:O	0.41	2.67	9	1
1:B:33:ASN:O	1:B:34:ILE:HD13	0.41	2.16	15	1
1:B:29:LEU:CD2	1:B:81:VAL:CG2	0.41	2.98	1	1
1:B:21:SER:HB3	1:B:74:ILE:HG21	0.41	1.92	1	1
1:A:8:ILE:C	1:A:9:LYS:CD	0.41	2.88	2	1
1:B:86:PHE:C	1:B:86:PHE:CD1	0.41	2.93	6	2
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:17:MET:HE2	1:A:46:PHE:CE2	0.41	2.51	8	1
1:A:84:LEU:HD11	1:A:86:PHE:CD1	0.41	2.51	8	1
1:A:71:LYS:O	1:A:72:HIS:HB2	0.41	2.15	8	1
1:B:53:THR:HG23	1:B:53:THR:O	0.41	2.15	20	1
1:B:62:PHE:CD1	1:B:62:PHE:C	0.41	2.94	19	1
1:A:43:LYS:CE	1:B:65:TYR:CD2	0.41	3.04	14	1
1:A:64:SER:HG	1:A:75:TYR:HE1	0.41	1.58	5	2
1:A:87:LYS:HZ3	1:A:87:LYS:HB3	0.41	1.75	5	1
1:B:67:THR:O	1:B:67:THR:CG2	0.41	2.68	16	1
1:B:9:LYS:HE3	1:B:77:TYR:CB	0.41	2.45	4	1
1:A:42:ILE:O	1:A:43:LYS:C	0.41	2.59	12	1
1:A:54:TRP:CZ2	1:A:87:LYS:CD	0.41	3.03	11	1
1:A:45:GLU:O	1:A:46:PHE:C	0.41	2.60	9	1
1:A:20:ASP:CB	1:A:50:TYR:OH	0.41	2.66	6	1
1:B:64:SER:HG	1:B:75:TYR:HE2	0.41	1.59	19	1
1:A:50:TYR:CD1	1:A:50:TYR:N	0.41	2.89	13	1
1:B:6:ALA:CB	1:B:78:LEU:CD2	0.40	2.97	18	2
1:B:68:HIS:CD2	1:B:87:LYS:O	0.40	2.74	9	1
1:A:46:PHE:CE1	1:A:50:TYR:CE2	0.40	3.08	15	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:A:58:VAL:HG23	1:A:81:VAL:HG11	0.40	1.91	14	1
1:B:8:ILE:CD1	1:B:22:VAL:HG21	0.40	2.45	5	1
1:B:73:PHE:HD2	1:B:86:PHE:HB2	0.40	1.77	3	1
1:A:9:LYS:HE3	1:A:77:TYR:HB2	0.40	1.92	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:ILE:CD1	1:A:22:VAL:CG2	0.40	2.99	4	1
1:A:13:MET:SD	1:A:18:GLN:CB	0.40	3.10	10	1
1:A:75:TYR:C	1:A:76:PHE:HD1	0.40	2.19	12	1
1:B:24:CYS:CA	1:B:27:GLN:HG3	0.40	2.45	11	1
1:A:15:GLU:HG3	1:A:15:GLU:H	0.40	1.57	2	1
1:B:71:LYS:HD2	1:B:72:HIS:CD2	0.40	2.52	2	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: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: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:B:44:LYS:HE2	1:B:44:LYS:O	0.40	2.15	18	1
1:B:53:THR:CG2	1:B:55:HIS:HE1	0.40	2.28	18	1
1:A:37:ASP:C	1:A:41:HIS:NE2	0.40	2.74	16	1
1:A:75:TYR:HD1	1:A:84:LEU:CB	0.40	2.29	3	1
1:B:4:ARG:HD3	1:B:19:GLN:NE2	0.40	2.32	17	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:5:LYS:O	1:B:5:LYS:CG	0.40	2.69	11	1
1:B:54:TRP:C	1:B:55:HIS:CD2	0.40	2.94	9	1
1:A:46:PHE:CD1	1:A:54:TRP:CE3	0.40	3.09	15	1
1:B:54:TRP:CD1	1:B:87:LYS:HE3	0.40	2.51	1	1
1:A:68:HIS:CB	1:A:72:HIS:O	0.40	2.69	6	1
1:A:14:SER:OG	1:A:17:MET:HB2	0.40	2.15	20	1
1:B:13:MET:SD	1:B:17:MET:HG3	0.40	2.55	13	1
1:B:82:ALA:C	1:B:83:ILE:CD1	0.40	2.87	14	1
1:B:72:HIS:HB3	1:B:87:LYS:HG3	0.40	1.93	14	1
1:B:36:LYS:HG2	1:B:36:LYS:H	0.40	1.38	5	1
1:B:35:GLU:OE1	1:B:35:GLU:HA	0.40	2.16	17	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:A:61:ASN:HB3	1:B:60:ARG:HE	0.40	1.76	10	1
1:A:71:LYS:C	1:A:72:HIS:ND1	0.40	2.75	7	1
1:A:21:SER:CB	1:A:46:PHE:CZ	0.40	3.03	15	2
1:A:68:HIS:O	1:A:69:GLU:CB	0.40	2.68	12	1
1:B:32:TYR:CD2	1:B:41:HIS:CE1	0.40	3.09	11	1
1:A:24:CYS:HB3	1:A:42:ILE:HG23	0.40	1.93	9	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:VAL:CG2	1:A:83:ILE:CD1	0.40	2.99	6	1
1:A:46:PHE:CD1	1:A:85:LEU:HD21	0.40	2.52	8	1
1:B:7:VAL:H	1:B:77:TYR:N	0.40	2.14	20	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:A:70:THR:HB	1:A:71:LYS:H	0.40	1.54	5	1
1:B:6:ALA:O	1:B:7:VAL:CG2	0.40	2.69	18	1
1:A:57:ILE:HD13	1:B:64:SER:HB3	0.40	1.92	4	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:55:HIS:HD2	1:A:86:PHE:O	0.40	2.00	2	1
1:A:16:GLU:N	1:A:16:GLU:CD	0.40	2.75	6	1
1:B:18:GLN:HB3	1:B:18:GLN:HE21	0.40	1.50	20	1
1:A:27:GLN:O	1:A:31:LYS:CG	0.40	2.70	18	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	7
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	B	51	ASN	20
1	A	35	GLU	20
1	A	51	ASN	20
1	B	79	GLY	19
1	B	60	ARG	17
1	B	8	ILE	15

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Mol	Chain	Res	Type	Models (Total)
1	B	61	ASN	14
1	B	70	THR	14
1	A	79	GLY	14
1	A	61	ASN	14
1	A	71	LYS	12
1	B	7	VAL	12
1	A	70	THR	12
1	B	71	LYS	11
1	B	73	PHE	10
1	A	72	HIS	10
1	A	8	ILE	10
1	B	72	HIS	9
1	A	15	GLU	9
1	A	73	PHE	9
1	A	78	LEU	8
1	B	10	ASN	8
1	B	6	ALA	7
1	A	60	ARG	7
1	B	68	HIS	7
1	B	4	ARG	6
1	A	68	HIS	6
1	A	58	VAL	5
1	A	42	ILE	5
1	A	10	ASN	5
1	A	6	ALA	5
1	A	5	LYS	5
1	B	5	LYS	4
1	A	12	ASP	4
1	A	69	GLU	4
1	A	74	ILE	4
1	B	35	GLU	4
1	B	69	GLU	4
1	B	58	VAL	3
1	B	52	PRO	3
1	B	11	ALA	3
1	A	11	ALA	3
1	A	33	ASN	2
1	A	67	THR	2
1	A	16	GLU	2
1	B	42	ILE	2
1	A	7	VAL	2
1	B	14	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	52	PRO	1
1	B	12	ASP	1
1	A	55	HIS	1
1	B	74	ILE	1
1	B	33	ASN	1
1	A	65	TYR	1
1	A	86	PHE	1
1	B	43	LYS	1
1	A	66	VAL	1
1	A	88	SER	1
1	A	9	LYS	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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	B	32	TYR	20
1	B	83	ILE	20
1	B	18	GLN	20
1	A	83	ILE	20
1	A	32	TYR	20
1	A	41	HIS	19
1	A	18	GLN	19
1	B	41	HIS	18
1	A	60	ARG	18
1	A	36	LYS	18
1	B	46	PHE	18
1	B	36	LYS	17
1	A	88	SER	17

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Mol	Chain	Res	Type	Models (Total)
1	A	85	LEU	16
1	A	48	LYS	16
1	B	10	ASN	16
1	A	8	ILE	16
1	B	88	SER	15
1	B	17	MET	15
1	B	4	ARG	15
1	A	76	PHE	15
1	B	5	LYS	15
1	B	48	LYS	15
1	A	49	LYS	15
1	B	69	GLU	15
1	B	49	LYS	15
1	A	55	HIS	15
1	B	74	ILE	15
1	A	10	ASN	14
1	A	47	ASP	14
1	B	84	LEU	14
1	B	14	SER	14
1	A	17	MET	14
1	B	87	LYS	14
1	B	21	SER	14
1	B	8	ILE	13
1	B	30	GLU	13
1	A	43	LYS	13
1	B	47	ASP	13
1	B	20	ASP	12
1	A	5	LYS	12
1	A	37	ASP	12
1	B	60	ARG	12
1	B	85	LEU	12
1	A	44	LYS	12
1	A	20	ASP	11
1	B	71	LYS	11
1	A	80	GLN	11
1	A	70	THR	11
1	A	87	LYS	11
1	A	46	PHE	11
1	A	68	HIS	11
1	A	14	SER	10
1	A	74	ILE	10
1	A	61	ASN	10

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Mol	Chain	Res	Type	Models (Total)
1	B	70	THR	10
1	A	69	GLU	10
1	A	16	GLU	10
1	A	30	GLU	10
1	B	61	ASN	10
1	A	78	LEU	10
1	A	56	CYS	10
1	A	84	LEU	10
1	B	43	LYS	10
1	B	68	HIS	10
1	A	15	GLU	9
1	B	16	GLU	9
1	A	21	SER	9
1	B	56	CYS	9
1	B	80	GLN	9
1	B	76	PHE	9
1	B	78	LEU	9
1	B	44	LYS	9
1	A	71	LYS	8
1	B	33	ASN	8
1	A	9	LYS	8
1	A	51	ASN	8
1	B	45	GLU	8
1	A	62	PHE	8
1	B	86	PHE	8
1	B	9	LYS	8
1	B	55	HIS	7
1	A	24	CYS	7
1	A	31	LYS	7
1	B	75	TYR	7
1	A	12	ASP	7
1	B	73	PHE	7
1	B	12	ASP	7
1	B	37	ASP	7
1	A	13	MET	7
1	A	27	GLN	7
1	A	19	GLN	6
1	A	33	ASN	6
1	B	27	GLN	6
1	A	73	PHE	6
1	A	45	GLU	5
1	B	13	MET	5

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

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 76% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4912

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1920
Number of shifts mapped to atoms	1920
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	178	-0.89 ± 0.14	Should be applied
$^{13}\text{C}_\beta$	168	-0.63 ± 0.17	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	174	-0.82 ± 0.22	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 76%, i.e. 1653 atoms were assigned a chemical shift out of a possible 2178. 18 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	672/846 (79%)	336/338 (99%)	170/340 (50%)	166/168 (99%)
Sidechain	867/1074 (81%)	551/631 (87%)	300/398 (75%)	16/45 (36%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	114/258 (44%)	112/134 (84%)	0/106 (0%)	2/18 (11%)
Overall	1653/2178 (76%)	999/1103 (91%)	470/844 (56%)	184/231 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 1716 atoms were assigned a chemical shift out of a possible 2266. 18 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	704/886 (79%)	352/354 (99%)	178/356 (50%)	174/176 (99%)
Sidechain	898/1122 (80%)	572/660 (87%)	310/414 (75%)	16/48 (33%)
Aromatic	114/258 (44%)	112/134 (84%)	0/106 (0%)	2/18 (11%)
Overall	1716/2266 (76%)	1036/1148 (90%)	488/876 (56%)	192/242 (79%)

7.1.4 Statistically unusual chemical shifts ⓘ

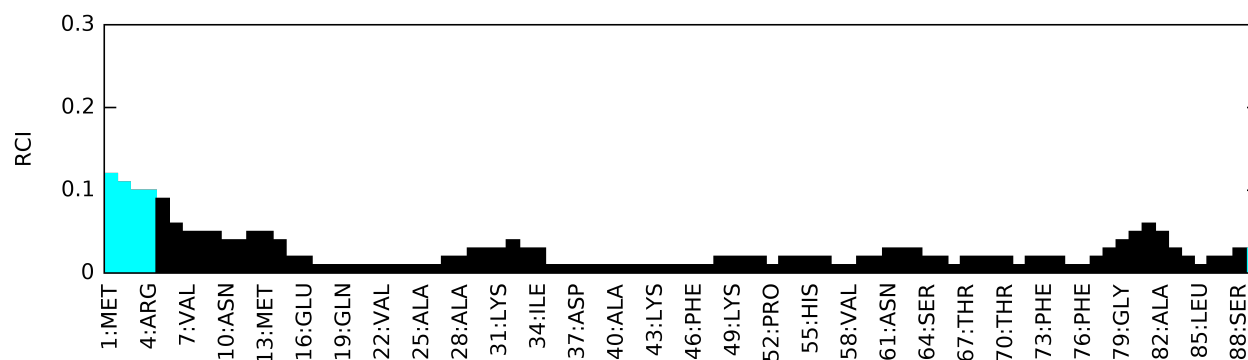
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	52	PRO	CD	26.96	55.31 – 45.41	-23.6
1	B	52	PRO	CD	26.96	55.31 – 45.41	-23.6
1	A	87	LYS	HB3	-0.15	3.10 – 0.40	-7.0
1	B	87	LYS	HB3	-0.15	3.10 – 0.40	-7.0
1	B	46	PHE	HB3	0.73	4.85 – 1.05	-5.8
1	A	46	PHE	HB3	0.73	4.85 – 1.05	-5.8
1	B	83	ILE	HB	0.22	3.24 – 0.34	-5.4
1	A	83	ILE	HB	0.22	3.24 – 0.34	-5.4
1	B	87	LYS	HG3	-0.15	2.76 – -0.04	-5.4
1	A	87	LYS	HG3	-0.15	2.76 – -0.04	-5.4

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

