Full wwPDB NMR Structure Validation Report (i)

Feb 8, 2022 – 04:26 PM EST

PDB ID	:	1CFP
Title	:	S100B (S100BETA) NMR DATA WAS COLLECTED FROM A SAMPLE OF CALCIUM FREE PROTEIN AT PH 6.3 AND A TEMPERATURE OF 311 K AND 1.7-6.9 MM CONCENTRATION, 25 STRUCTURES
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Deposited on	:	1996-06-04

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

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

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

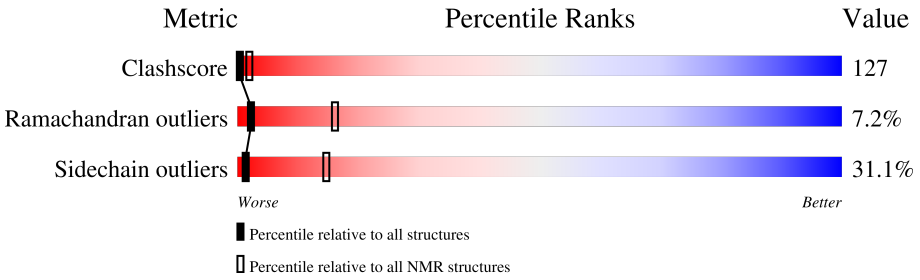
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	92	72% 18% 9%
1	B	92	73% 17% 9%

2 Ensemble composition and analysis

This entry contains 25 models. Model 23 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:0-A:83, B:0-B:83 (168)	0.73	23

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. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 11, 14, 15, 17, 18, 19, 20, 21, 22, 23
2	12, 16
3	10, 25
4	13, 24

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2912 atoms, of which 1420 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called S100B.

Mol	Chain	Residues	Atoms						Trace
1	A	92	Total	C	H	N	O	S	0
			1456	470	710	118	152	6	
1	B	92	Total	C	H	N	O	S	0
			1456	470	710	118	152	6	

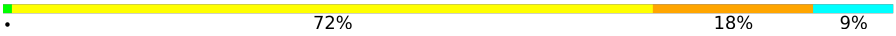
4 Residue-property plots

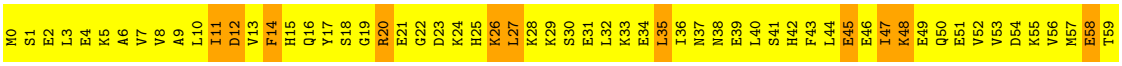
4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: S100B

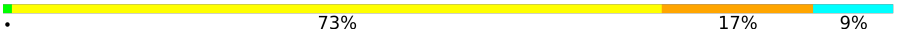
Chain A:

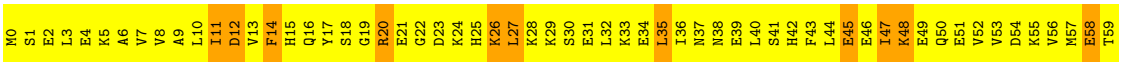




• Molecule 1: S100B

Chain B:





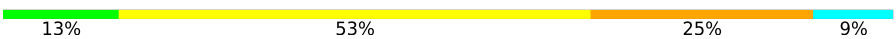
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

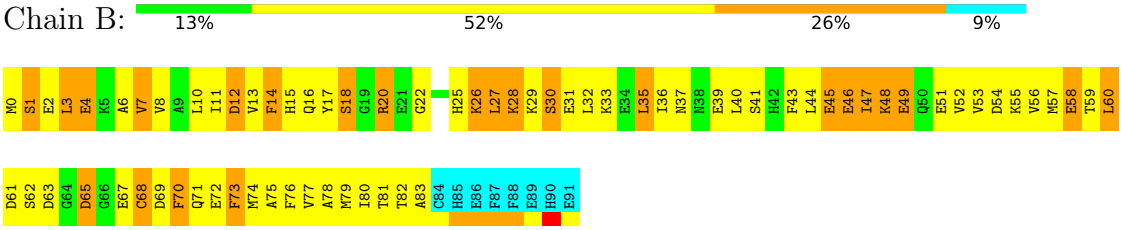
• Molecule 1: S100B

Chain A:



• Molecule 1: S100B

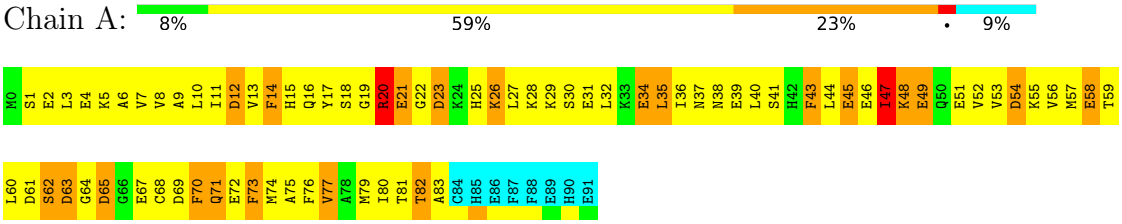
Chain B:



4.2.2 Score per residue for model 2

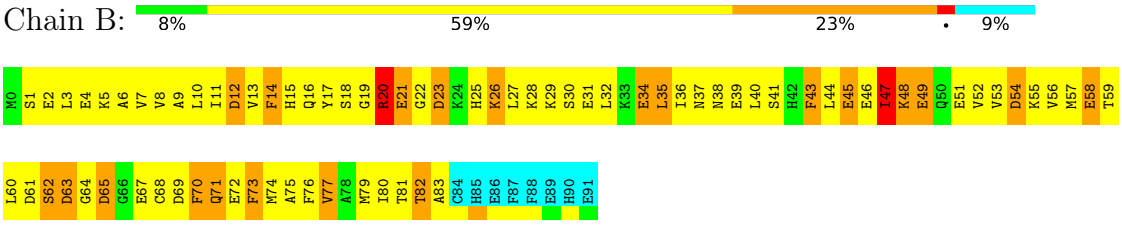
• Molecule 1: S100B

Chain A:



• Molecule 1: S100B

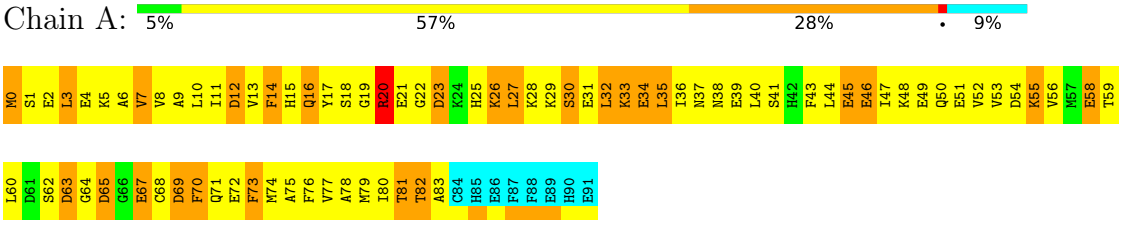
Chain B:



4.2.3 Score per residue for model 3

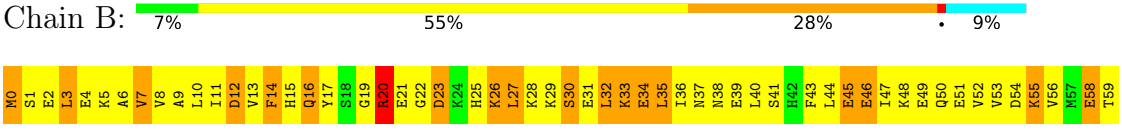
• Molecule 1: S100B

Chain A:



• Molecule 1: S100B

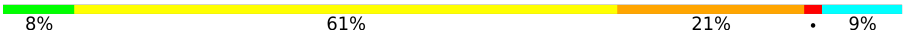
Chain B:

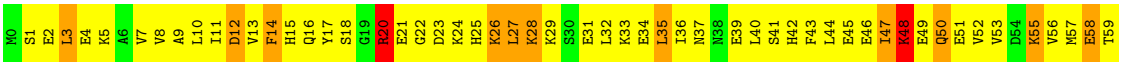


4.2.4 Score per residue for model 4

• Molecule 1: S100B

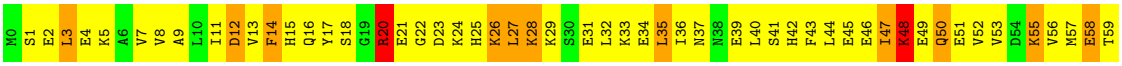
Chain A:





• Molecule 1: S100B

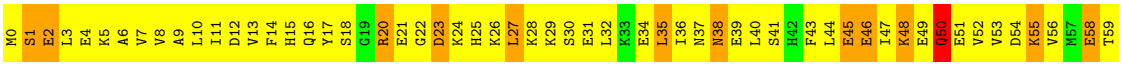
Chain B:



4.2.5 Score per residue for model 5

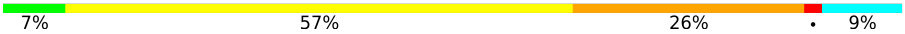
• Molecule 1: S100B

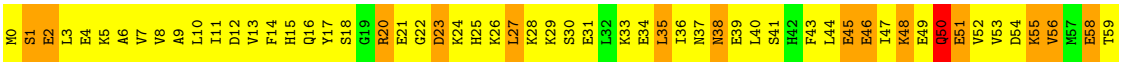
Chain A:



• Molecule 1: S100B

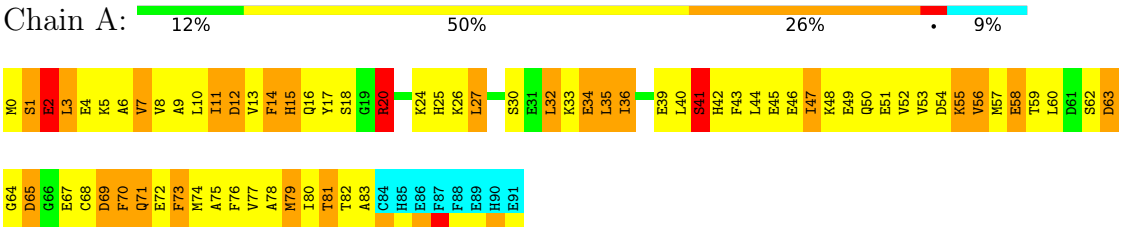
Chain B:



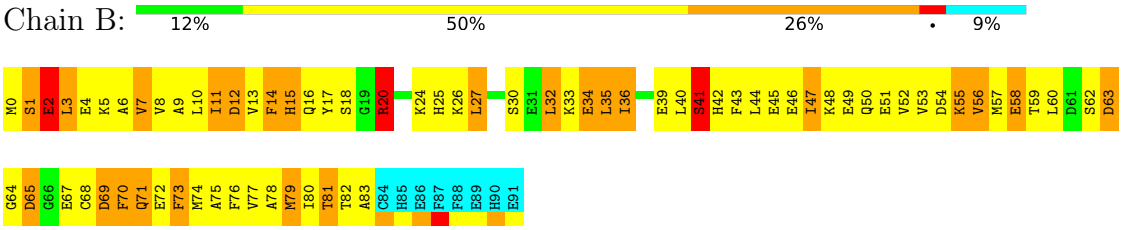


4.2.6 Score per residue for model 6

• Molecule 1: S100B

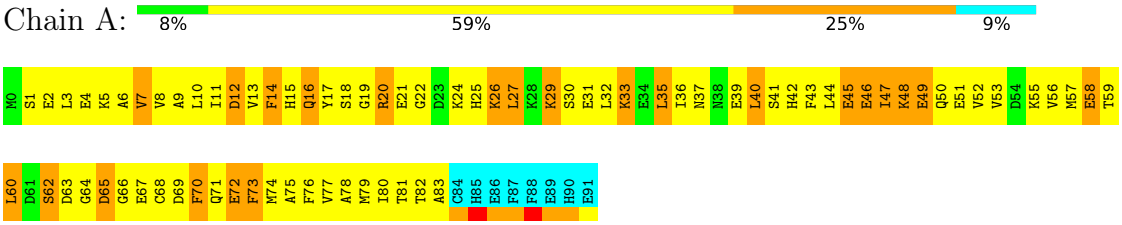


• Molecule 1: S100B

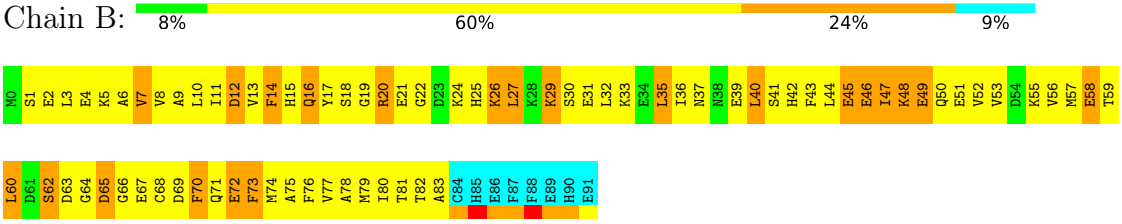


4.2.7 Score per residue for model 7

• Molecule 1: S100B

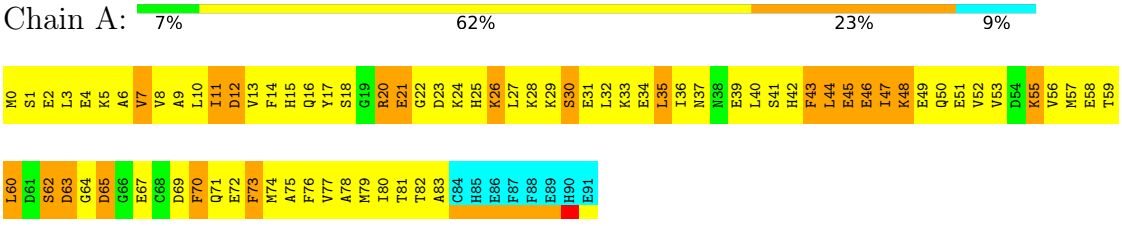


• Molecule 1: S100B



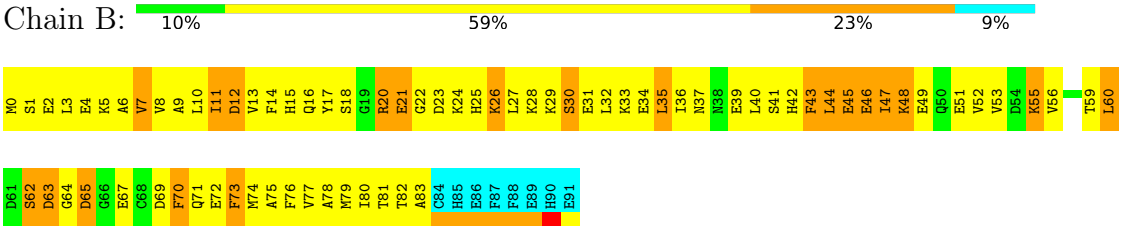
4.2.8 Score per residue for model 8

• Molecule 1: S100B



• Molecule 1: S100B

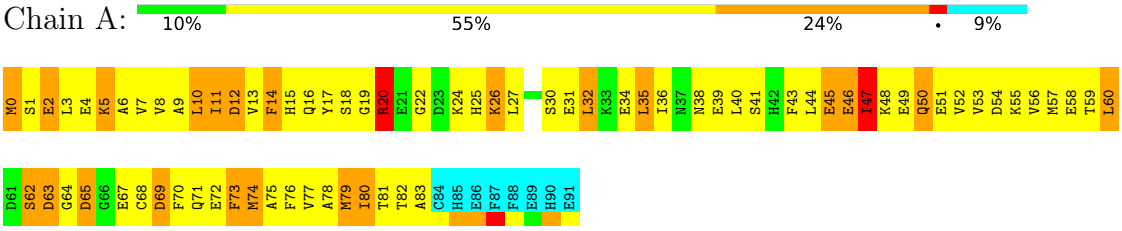
Chain B:



4.2.9 Score per residue for model 9

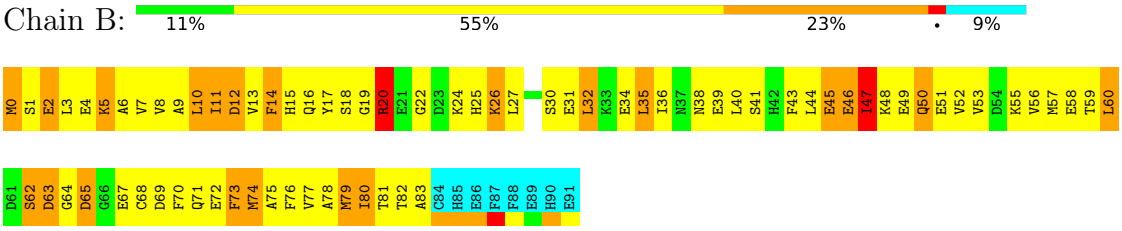
• Molecule 1: S100B

Chain A:



• Molecule 1: S100B

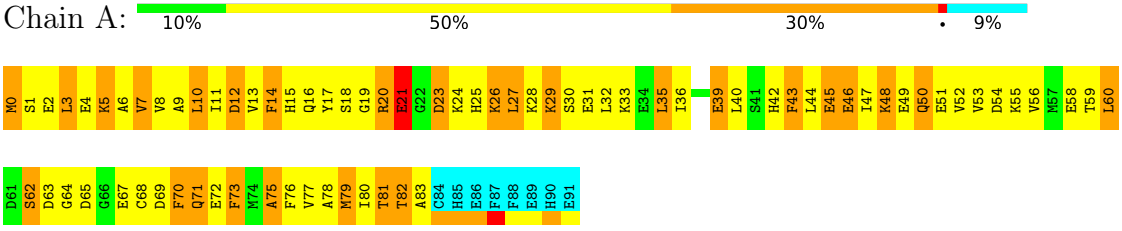
Chain B:



4.2.10 Score per residue for model 10

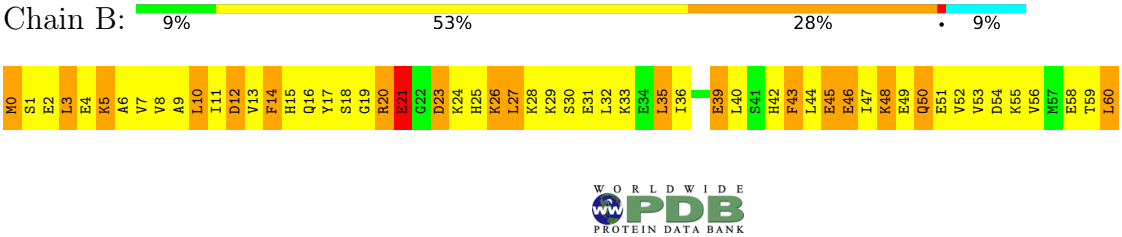
• Molecule 1: S100B

Chain A:



• Molecule 1: S100B

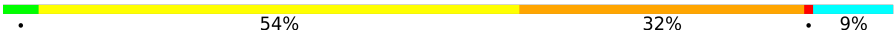
Chain B:

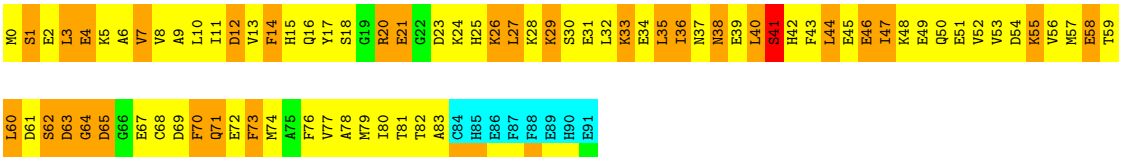


4.2.11 Score per residue for model 11

• Molecule 1: S100B

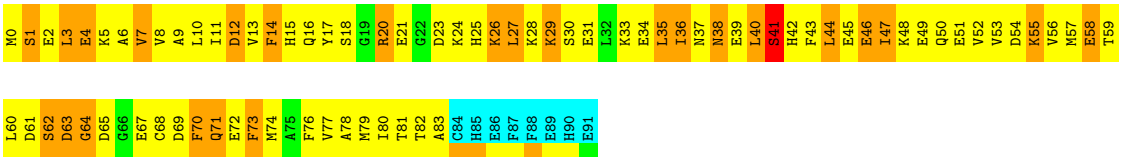
Chain A:





• Molecule 1: S100B

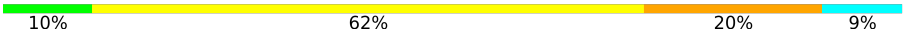
Chain B:

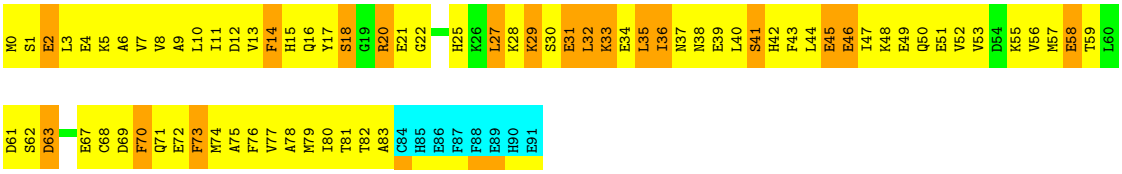


4.2.12 Score per residue for model 12

• Molecule 1: S100B

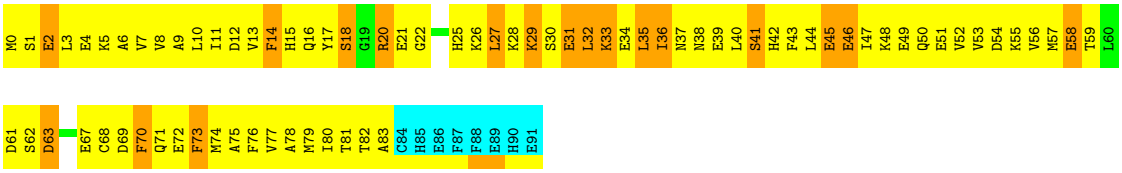
Chain A:





• Molecule 1: S100B

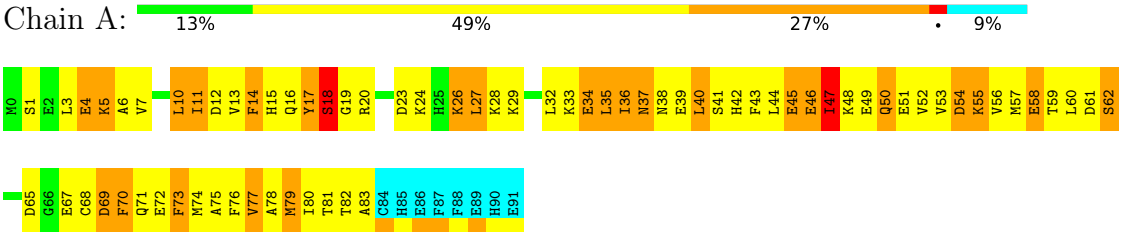
Chain B:



4.2.13 Score per residue for model 13

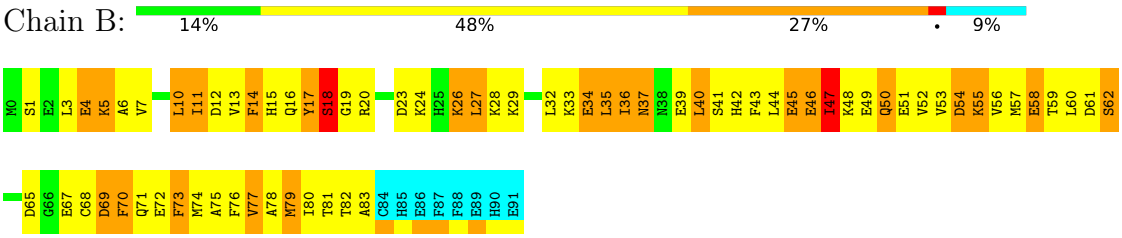
• Molecule 1: S100B

Chain A:



• Molecule 1: S100B

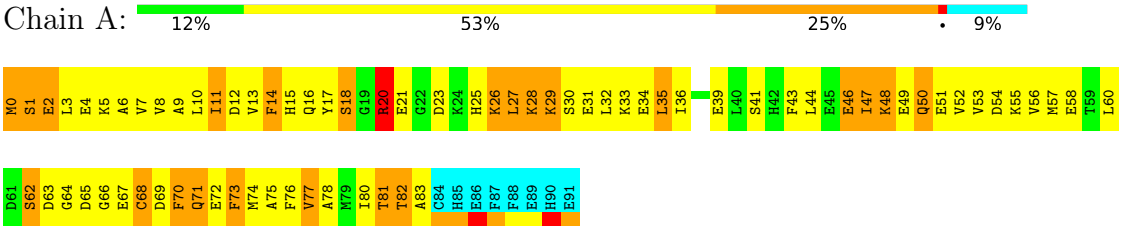
Chain B:



4.2.14 Score per residue for model 14

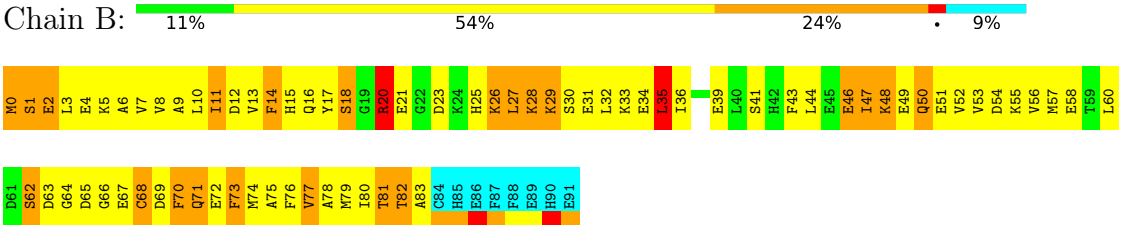
• Molecule 1: S100B

Chain A:



• Molecule 1: S100B

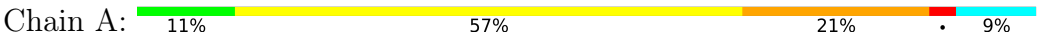
Chain B:

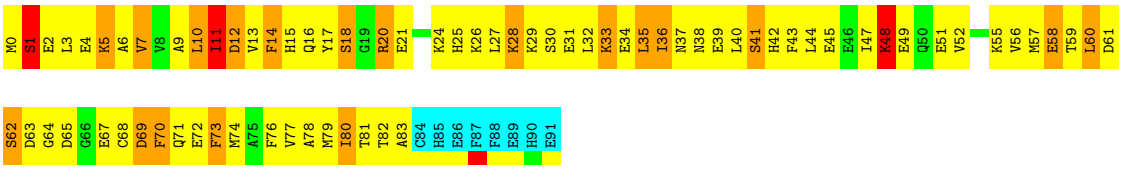


4.2.15 Score per residue for model 15

• Molecule 1: S100B

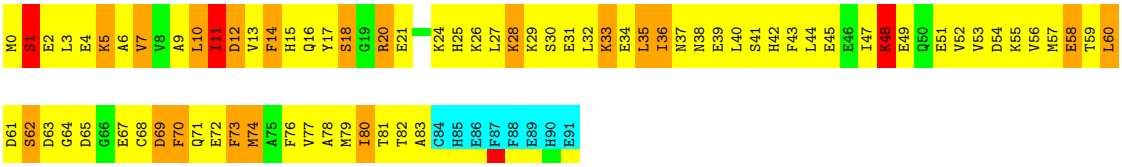
Chain A:





• Molecule 1: S100B

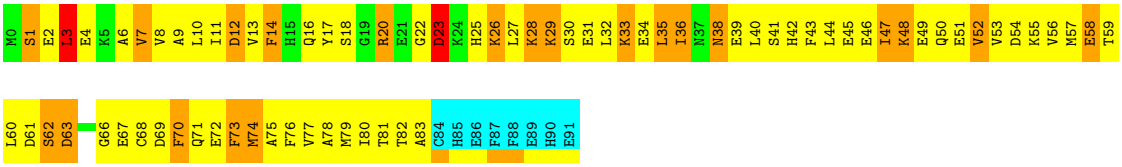
Chain B: 9% 59% 21% • 9%



4.2.16 Score per residue for model 16

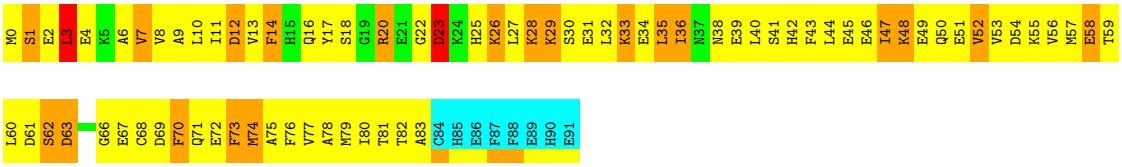
• Molecule 1: S100B

Chain A: 10% 57% 23% • 9%



• Molecule 1: S100B

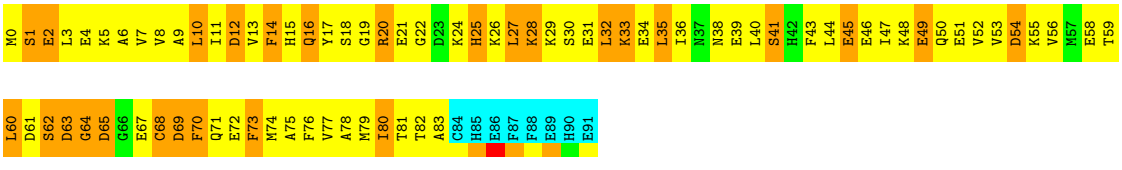
Chain B: 9% 59% 22% • 9%



4.2.17 Score per residue for model 17

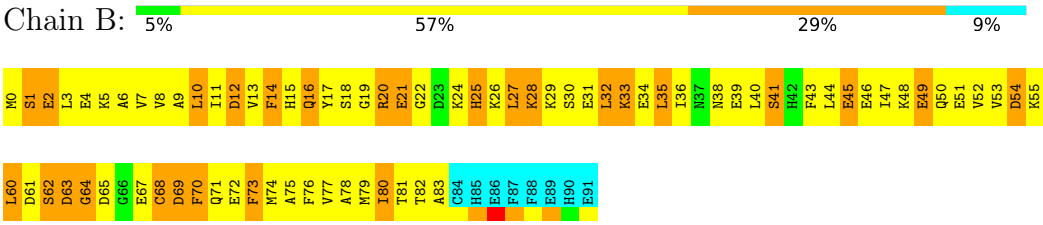
• Molecule 1: S100B

Chain A: 5% 57% 29% 9%



• Molecule 1: S100B

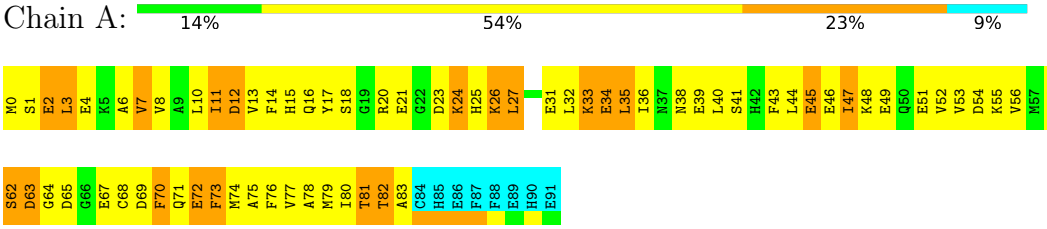
Chain B:



4.2.18 Score per residue for model 18

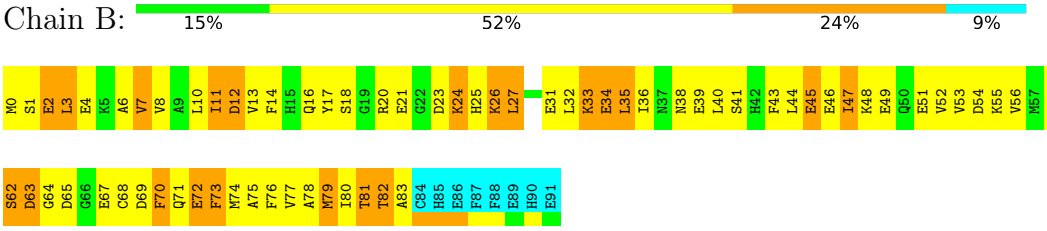
- Molecule 1: S100B

Chain A:



- Molecule 1: S100B

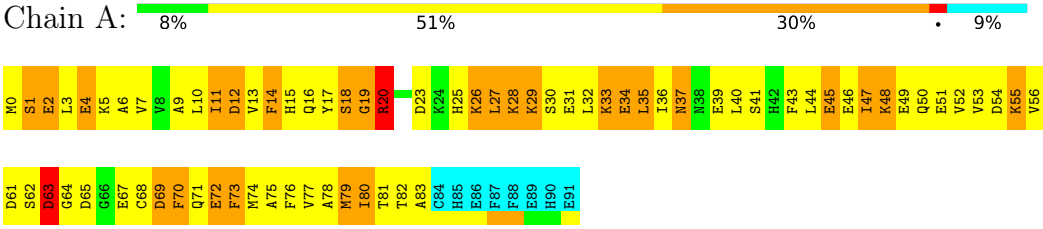
Chain B:



4.2.19 Score per residue for model 19

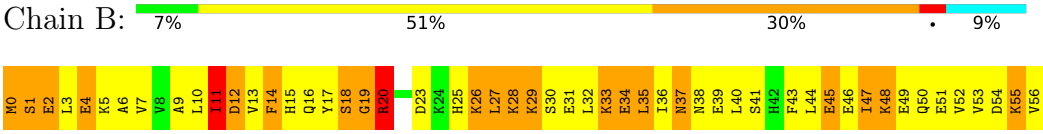
- Molecule 1: S100B

Chain A:



- Molecule 1: S100B

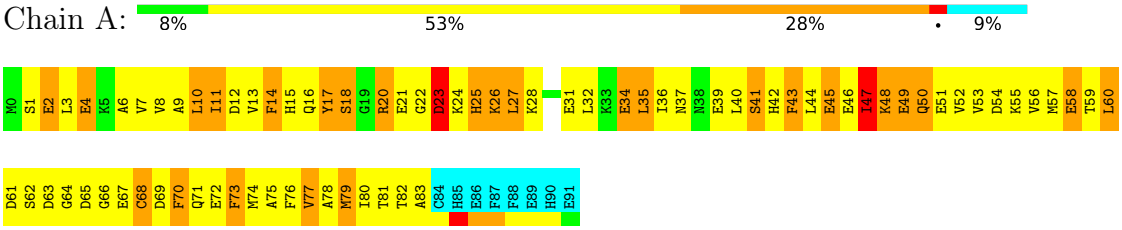
Chain B:



4.2.20 Score per residue for model 20

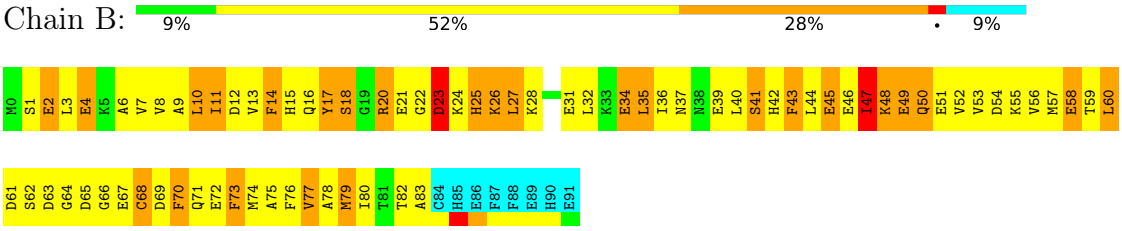
• Molecule 1: S100B

Chain A:



• Molecule 1: S100B

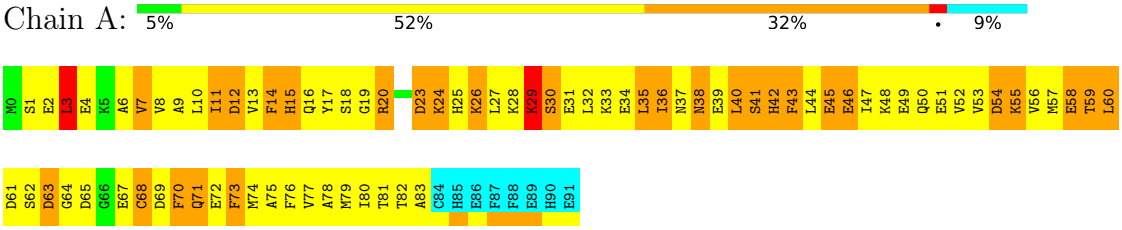
Chain B:



4.2.21 Score per residue for model 21

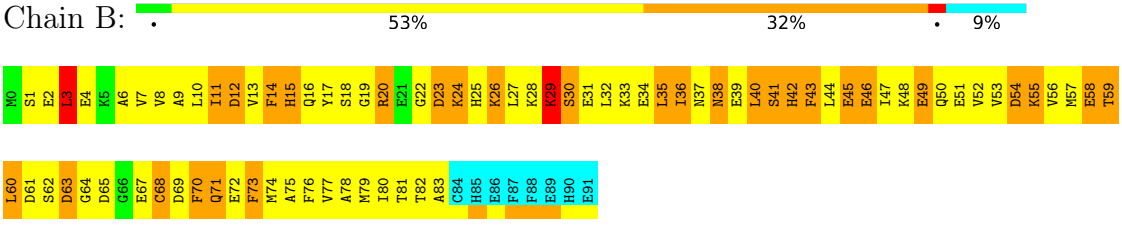
• Molecule 1: S100B

Chain A:



• Molecule 1: S100B

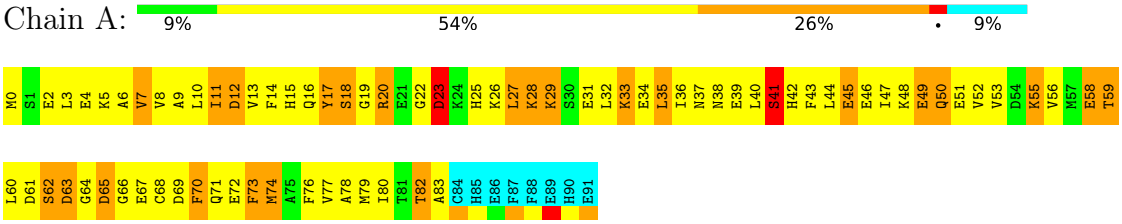
Chain B:



4.2.22 Score per residue for model 22

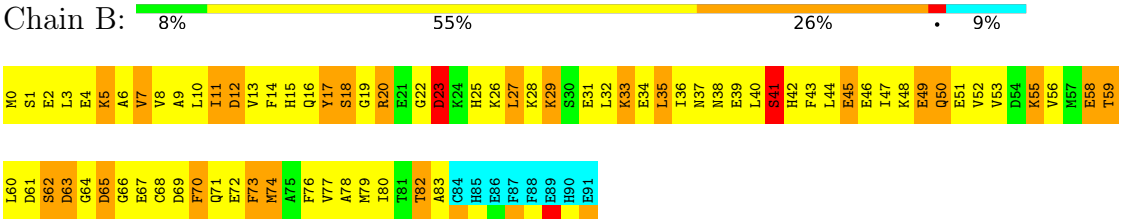
• Molecule 1: S100B

Chain A:



• Molecule 1: S100B

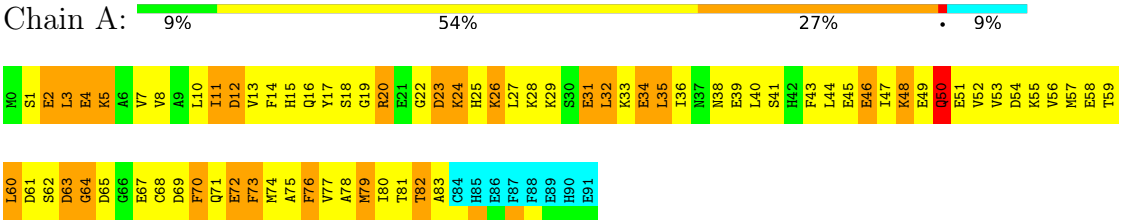
Chain B:



4.2.23 Score per residue for model 23 (medoid)

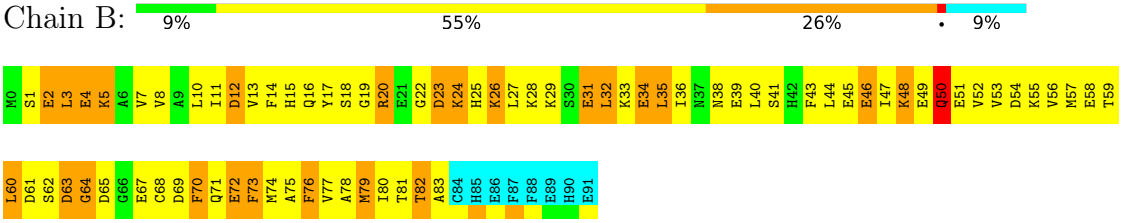
• Molecule 1: S100B

Chain A:



• Molecule 1: S100B

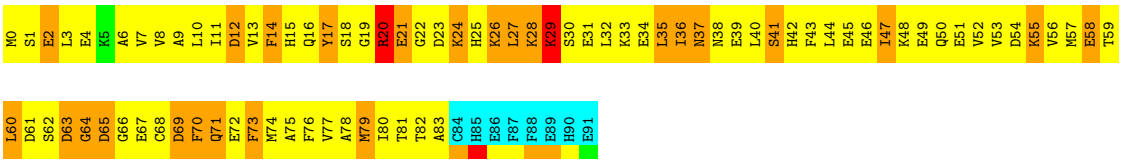
Chain B:



4.2.24 Score per residue for model 24

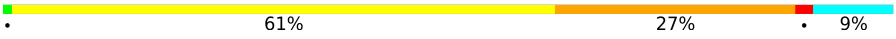
• Molecule 1: S100B

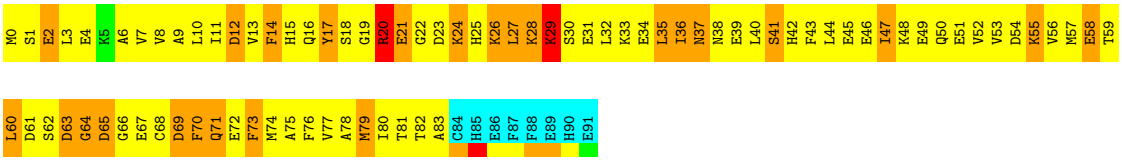
Chain A:



• Molecule 1: S100B

Chain B:

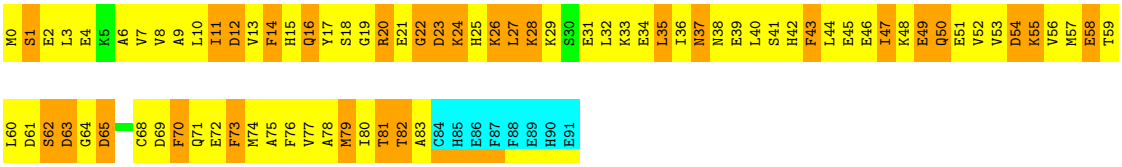




4.2.25 Score per residue for model 25

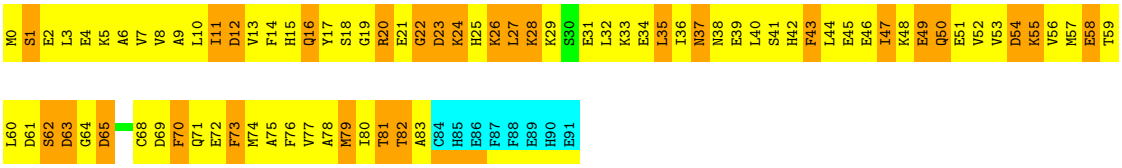
• Molecule 1: S100B

Chain A:



• Molecule 1: S100B

Chain B:



5 Refinement protocol and experimental data overview

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

Of the 91 calculated structures, 25 were deposited, based on the following criterion: *TOTAL ENERGY*.

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

Software name	Classification	Version
X-PLOR	refinement	3.841
X-PLOR	structure solution	3.841

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.9±0.3
1	B	0.0±0.0	0.9±0.3
All	All	0	46

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	20	ARG	Sidechain	23
1	B	20	ARG	Sidechain	23

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	671	655	655	190±17
1	B	671	655	655	189±17
All	All	33550	32750	32750	8428

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 127.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:VAL:HG13	1:A:83:ALA:HB3	1.10	1.14	24	8
1:A:81:THR:HG23	1:B:7:VAL:HG13	1.09	1.11	23	8
1:A:17:TYR:CD2	1:A:35:LEU:HD12	1.09	1.82	19	15
1:A:76:PHE:CE1	1:A:80:ILE:HD11	1.08	1.83	21	15
1:B:56:VAL:HG22	1:B:80:ILE:HG23	1.08	1.18	10	4
1:B:76:PHE:CZ	1:B:80:ILE:HD11	1.08	1.83	10	16
1:A:13:VAL:HG11	1:B:3:LEU:HD21	1.08	1.24	7	10
1:B:76:PHE:CE1	1:B:80:ILE:HD11	1.07	1.83	21	15
1:A:3:LEU:HD21	1:B:13:VAL:HG11	1.07	1.22	7	12
1:B:17:TYR:CD2	1:B:35:LEU:HD12	1.07	1.83	19	15
1:A:56:VAL:HG13	1:A:80:ILE:HD12	1.06	1.13	3	9
1:A:76:PHE:CZ	1:A:80:ILE:HD11	1.06	1.84	6	16
1:A:56:VAL:HG22	1:A:80:ILE:HG23	1.06	1.18	10	4
1:B:35:LEU:HD11	1:B:73:PHE:CE2	1.06	1.86	8	3
1:B:56:VAL:HG13	1:B:80:ILE:HD12	1.05	1.14	3	9
1:A:35:LEU:HD11	1:A:73:PHE:CE2	1.04	1.86	8	3
1:B:52:VAL:HG13	1:B:83:ALA:CB	1.04	1.83	6	14
1:B:52:VAL:HG13	1:B:83:ALA:HB3	1.03	1.13	24	8
1:A:32:LEU:HD11	1:A:76:PHE:CE2	1.03	1.89	13	1
1:A:52:VAL:HG13	1:A:83:ALA:CB	1.02	1.83	6	14
1:B:32:LEU:HD11	1:B:76:PHE:CE2	1.02	1.89	13	1
1:A:3:LEU:HD11	1:B:35:LEU:CD2	1.02	1.85	21	2
1:A:17:TYR:CD1	1:A:35:LEU:HD12	1.02	1.89	5	9
1:A:52:VAL:CG1	1:A:83:ALA:HB1	1.02	1.85	4	8
1:B:52:VAL:HG13	1:B:83:ALA:HB1	1.02	1.31	14	14
1:B:52:VAL:CG1	1:B:83:ALA:HB1	1.02	1.85	4	8
1:B:17:TYR:CD1	1:B:35:LEU:HD12	1.01	1.90	5	9
1:A:7:VAL:HG13	1:B:81:THR:HG23	1.01	1.21	2	8
1:B:36:ILE:HD12	1:B:80:ILE:CD1	1.01	1.85	13	4
1:A:35:LEU:CD2	1:B:3:LEU:HD11	1.01	1.86	21	2
1:A:36:ILE:HD12	1:A:80:ILE:CD1	1.01	1.85	13	4
1:A:52:VAL:HG12	1:A:56:VAL:HG23	1.00	1.31	5	16
1:B:3:LEU:HD13	1:B:4:GLU:N	1.00	1.72	3	4
1:B:56:VAL:HG13	1:B:80:ILE:CD1	1.00	1.87	6	10
1:A:13:VAL:CG1	1:B:3:LEU:HD21	0.99	1.86	23	8
1:A:3:LEU:HD13	1:A:4:GLU:N	0.99	1.72	3	4
1:B:17:TYR:CE2	1:B:35:LEU:HD12	0.99	1.93	11	9
1:A:56:VAL:HG13	1:A:80:ILE:CD1	0.99	1.87	25	10
1:A:56:VAL:HG22	1:A:80:ILE:HD12	0.99	1.31	18	7
1:A:17:TYR:CE2	1:A:35:LEU:HD12	0.99	1.93	11	9
1:A:36:ILE:CG2	1:A:40:LEU:HD12	0.99	1.88	8	2
1:A:52:VAL:HG13	1:A:83:ALA:HB1	0.98	1.33	14	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:VAL:O	1:A:11:ILE:HG23	0.98	1.59	8	17
1:B:56:VAL:HG22	1:B:80:ILE:HD12	0.98	1.32	18	7
1:B:35:LEU:HD21	1:B:73:PHE:CE1	0.98	1.94	3	22
1:B:36:ILE:HG23	1:B:40:LEU:CD1	0.98	1.89	8	1
1:B:36:ILE:CG2	1:B:40:LEU:HD12	0.98	1.88	8	2
1:A:35:LEU:HD21	1:A:73:PHE:CE1	0.97	1.94	3	22
1:A:36:ILE:HG23	1:A:40:LEU:CD1	0.97	1.88	8	1
1:A:78:ALA:O	1:A:82:THR:HG23	0.97	1.59	16	5
1:B:7:VAL:O	1:B:11:ILE:HG23	0.97	1.59	8	17
1:A:14:PHE:CE1	1:A:27:LEU:HD13	0.97	1.93	13	1
1:B:78:ALA:O	1:B:82:THR:HG23	0.97	1.60	16	5
1:B:14:PHE:CE1	1:B:27:LEU:HD13	0.97	1.92	13	1
1:A:3:LEU:HD23	1:B:73:PHE:CZ	0.96	1.95	18	3
1:B:36:ILE:HG23	1:B:40:LEU:HD12	0.96	0.98	8	1
1:A:36:ILE:HG23	1:A:40:LEU:HD12	0.96	0.96	8	1
1:A:7:VAL:CG1	1:B:81:THR:HG23	0.95	1.90	23	3
1:A:14:PHE:CE1	1:A:27:LEU:HD23	0.95	1.95	23	4
1:B:52:VAL:HG12	1:B:56:VAL:HG23	0.95	1.38	3	16
1:B:14:PHE:CE1	1:B:27:LEU:HD23	0.95	1.97	23	4
1:A:46:GLU:O	1:A:53:VAL:HG21	0.95	1.62	11	6
1:A:32:LEU:O	1:A:36:ILE:HD12	0.95	1.62	23	2
1:A:36:ILE:HD12	1:A:80:ILE:HD11	0.95	1.37	13	1
1:B:46:GLU:O	1:B:53:VAL:HG21	0.95	1.61	11	6
1:A:7:VAL:HG13	1:B:81:THR:CG2	0.94	1.92	23	10
1:B:36:ILE:HD12	1:B:80:ILE:HD11	0.94	1.38	13	1
1:B:32:LEU:O	1:B:36:ILE:HD12	0.94	1.62	23	2
1:B:32:LEU:HD23	1:B:60:LEU:CD2	0.94	1.92	22	2
1:A:32:LEU:HD23	1:A:60:LEU:CD2	0.94	1.92	22	2
1:A:76:PHE:CE2	1:A:80:ILE:HD11	0.93	1.98	2	10
1:A:56:VAL:CG2	1:A:80:ILE:HG23	0.93	1.92	10	1
1:A:35:LEU:HD11	1:A:73:PHE:CD2	0.93	1.99	4	2
1:B:76:PHE:CE2	1:B:80:ILE:HD11	0.93	1.98	2	9
1:A:10:LEU:HD13	1:A:74:MET:CE	0.93	1.93	25	4
1:A:81:THR:HG21	1:B:7:VAL:CG1	0.93	1.94	8	3
1:A:32:LEU:HD11	1:A:76:PHE:CD2	0.93	1.98	13	2
1:B:56:VAL:CG2	1:B:80:ILE:HG23	0.93	1.92	10	1
1:B:10:LEU:HD13	1:B:74:MET:CE	0.93	1.94	25	3
1:A:49:GLU:O	1:A:53:VAL:HG23	0.92	1.65	14	21
1:B:9:ALA:O	1:B:13:VAL:HG23	0.92	1.63	14	8
1:A:7:VAL:CG1	1:B:81:THR:HG21	0.92	1.93	8	3
1:B:35:LEU:HD11	1:B:73:PHE:CD2	0.92	1.98	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:32:LEU:HD11	1:B:76:PHE:CD2	0.91	1.98	13	2
1:B:49:GLU:O	1:B:53:VAL:HG23	0.91	1.66	14	21
1:A:82:THR:HG23	1:B:70:PHE:CD1	0.91	2.00	10	1
1:A:81:THR:HG23	1:B:7:VAL:CG1	0.91	1.96	4	2
1:A:3:LEU:HD21	1:B:13:VAL:CG1	0.91	1.96	22	9
1:A:9:ALA:O	1:A:13:VAL:HG23	0.90	1.66	25	8
1:B:32:LEU:HD21	1:B:76:PHE:CD2	0.90	2.02	16	6
1:B:46:GLU:HG3	1:B:53:VAL:HG22	0.90	1.41	8	9
1:A:32:LEU:HD11	1:A:68:CYS:SG	0.90	2.07	1	1
1:A:36:ILE:HG21	1:A:80:ILE:HG21	0.90	1.43	6	4
1:A:32:LEU:HD21	1:A:76:PHE:CD2	0.90	2.01	16	6
1:B:57:MET:CE	1:B:60:LEU:HD23	0.89	1.97	25	1
1:B:32:LEU:HD11	1:B:68:CYS:SG	0.89	2.06	1	1
1:A:52:VAL:HG11	1:A:83:ALA:O	0.89	1.67	1	1
1:A:10:LEU:HD21	1:B:3:LEU:HD23	0.89	1.41	3	1
1:A:27:LEU:HD13	1:A:31:GLU:HB2	0.89	1.44	11	5
1:A:10:LEU:HD13	1:A:74:MET:SD	0.89	2.08	6	12
1:A:3:LEU:HD23	1:B:10:LEU:HD21	0.89	1.42	3	1
1:B:36:ILE:HG21	1:B:80:ILE:HG21	0.89	1.44	6	4
1:A:3:LEU:HD11	1:B:73:PHE:CZ	0.88	2.02	11	1
1:B:6:ALA:O	1:B:10:LEU:HD12	0.88	1.68	10	4
1:B:10:LEU:HD13	1:B:74:MET:SD	0.88	2.07	6	12
1:B:27:LEU:HD13	1:B:31:GLU:HB2	0.88	1.45	11	5
1:A:73:PHE:CZ	1:B:3:LEU:HD11	0.88	2.03	11	2
1:A:57:MET:CE	1:A:60:LEU:HD23	0.88	1.98	25	1
1:B:32:LEU:HD23	1:B:60:LEU:CD1	0.88	1.99	2	2
1:A:46:GLU:CG	1:A:53:VAL:HG22	0.88	1.99	17	11
1:A:46:GLU:HG3	1:A:53:VAL:HG22	0.87	1.42	8	9
1:A:6:ALA:HB1	1:B:6:ALA:HB1	0.87	1.45	11	3
1:B:46:GLU:CG	1:B:53:VAL:HG22	0.87	1.99	17	11
1:B:52:VAL:HG11	1:B:83:ALA:O	0.87	1.67	1	1
1:A:56:VAL:HG22	1:A:80:ILE:HD13	0.87	1.47	15	5
1:A:11:ILE:HD12	1:A:12:ASP:N	0.86	1.85	16	2
1:B:57:MET:HE2	1:B:60:LEU:HD23	0.86	1.47	25	1
1:A:32:LEU:HD23	1:A:60:LEU:CD1	0.86	1.99	2	2
1:A:70:PHE:HB3	1:B:82:THR:HG21	0.86	1.47	11	8
1:B:52:VAL:O	1:B:56:VAL:HG23	0.86	1.71	16	4
1:B:17:TYR:CE1	1:B:35:LEU:HD12	0.86	2.06	17	3
1:B:11:ILE:HD12	1:B:12:ASP:N	0.86	1.86	16	3
1:B:56:VAL:HG22	1:B:80:ILE:HD13	0.86	1.48	15	6
1:B:13:VAL:HG12	1:B:17:TYR:CD2	0.86	2.06	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:THR:CG2	1:B:7:VAL:HG13	0.85	2.00	2	11
1:A:78:ALA:HB2	1:B:74:MET:SD	0.85	2.11	20	10
1:A:32:LEU:HD12	1:A:60:LEU:HD13	0.85	1.46	13	1
1:B:3:LEU:HD22	1:B:3:LEU:O	0.85	1.70	3	3
1:A:6:ALA:O	1:A:10:LEU:HD12	0.85	1.71	10	4
1:A:3:LEU:O	1:A:3:LEU:HD22	0.85	1.71	3	2
1:A:17:TYR:CE1	1:A:35:LEU:HD12	0.85	2.06	17	3
1:A:74:MET:SD	1:B:78:ALA:HB2	0.85	2.12	13	7
1:A:52:VAL:O	1:A:56:VAL:HG23	0.85	1.71	16	4
1:A:14:PHE:CE1	1:A:27:LEU:HD12	0.85	2.06	25	7
1:A:10:LEU:HD12	1:A:74:MET:HE2	0.84	1.48	21	1
1:A:47:ILE:HD13	1:A:47:ILE:O	0.84	1.72	9	15
1:A:70:PHE:CD1	1:B:82:THR:HG23	0.84	2.07	10	1
1:A:81:THR:HG21	1:B:7:VAL:HG13	0.84	1.48	20	9
1:A:57:MET:HE2	1:A:60:LEU:HD23	0.84	1.50	25	1
1:A:52:VAL:HG11	1:A:83:ALA:HB1	0.84	1.50	5	5
1:A:36:ILE:HG23	1:A:80:ILE:HD13	0.84	1.50	13	3
1:B:52:VAL:HG11	1:B:83:ALA:HB1	0.84	1.50	5	5
1:B:36:ILE:HG23	1:B:80:ILE:HD13	0.83	1.50	13	3
1:A:43:PHE:CE2	1:A:80:ILE:HG22	0.83	2.08	17	12
1:B:46:GLU:HG2	1:B:53:VAL:HG22	0.83	1.50	4	8
1:A:10:LEU:HD23	1:A:73:PHE:CZ	0.83	2.09	17	3
1:A:82:THR:HG21	1:B:70:PHE:HB3	0.83	1.49	11	8
1:B:14:PHE:CE1	1:B:27:LEU:HD12	0.82	2.09	25	6
1:B:47:ILE:HD13	1:B:47:ILE:O	0.82	1.72	9	15
1:B:10:LEU:HD23	1:B:73:PHE:CZ	0.82	2.10	17	3
1:A:17:TYR:HB3	1:A:27:LEU:HD21	0.82	1.51	18	12
1:A:13:VAL:HG12	1:A:17:TYR:CD1	0.82	2.10	16	6
1:B:63:ASP:O	1:B:65:ASP:N	0.82	2.12	5	9
1:A:13:VAL:HG11	1:B:3:LEU:HD12	0.82	1.49	11	3
1:B:32:LEU:HD12	1:B:60:LEU:HD13	0.82	1.47	13	1
1:B:43:PHE:CE2	1:B:80:ILE:HG22	0.82	2.09	17	12
1:A:3:LEU:HB2	1:B:13:VAL:HG11	0.82	1.52	16	2
1:A:10:LEU:HD13	1:A:74:MET:HE1	0.82	1.49	25	1
1:B:13:VAL:HG12	1:B:17:TYR:CD1	0.82	2.10	16	6
1:A:17:TYR:HB3	1:A:27:LEU:HD11	0.81	1.50	13	5
1:B:36:ILE:CG2	1:B:80:ILE:HG21	0.81	2.05	7	6
1:A:52:VAL:HG21	1:A:83:ALA:HB2	0.81	1.49	12	1
1:B:52:VAL:HG21	1:B:83:ALA:HB2	0.81	1.49	12	1
1:B:17:TYR:HB3	1:B:27:LEU:HD21	0.81	1.53	15	12
1:A:13:VAL:HG12	1:A:17:TYR:CD2	0.81	2.11	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:27:LEU:HD23	1:B:31:GLU:HB3	0.81	1.52	3	10
1:B:13:VAL:HG13	1:B:17:TYR:CD1	0.81	2.10	18	4
1:A:63:ASP:O	1:A:65:ASP:N	0.81	2.14	11	9
1:A:52:VAL:HG22	1:A:83:ALA:O	0.81	1.76	13	4
1:A:3:LEU:HD22	1:B:35:LEU:HD21	0.81	1.50	22	4
1:A:46:GLU:HG2	1:A:53:VAL:HG22	0.80	1.49	4	8
1:A:35:LEU:HD21	1:B:3:LEU:HD22	0.80	1.52	22	4
1:A:27:LEU:HD23	1:A:31:GLU:HB3	0.80	1.53	3	10
1:A:27:LEU:HD22	1:A:73:PHE:HB2	0.80	1.50	13	1
1:A:36:ILE:CG2	1:A:80:ILE:HG21	0.80	2.05	7	6
1:A:4:GLU:CD	1:B:40:LEU:HD13	0.80	1.97	21	1
1:A:75:ALA:HB2	1:B:75:ALA:HB2	0.80	1.52	13	1
1:B:36:ILE:HG22	1:B:43:PHE:CD2	0.80	2.12	15	3
1:B:71:GLN:O	1:B:75:ALA:HB2	0.80	1.77	10	17
1:B:52:VAL:HG22	1:B:83:ALA:O	0.80	1.77	13	4
1:A:36:ILE:HG22	1:A:43:PHE:CD2	0.79	2.12	15	3
1:B:27:LEU:HD22	1:B:73:PHE:HB2	0.79	1.52	13	1
1:B:36:ILE:HD11	1:B:76:PHE:CE1	0.79	2.12	14	2
1:A:40:LEU:HD13	1:B:4:GLU:CD	0.79	1.96	21	1
1:A:13:VAL:HG13	1:A:17:TYR:CD1	0.79	2.12	18	4
1:B:17:TYR:HB3	1:B:27:LEU:HD11	0.79	1.51	13	5
1:A:71:GLN:O	1:A:75:ALA:HB2	0.79	1.77	10	17
1:A:3:LEU:HD12	1:B:13:VAL:HG11	0.79	1.52	11	3
1:A:36:ILE:HD11	1:A:76:PHE:CE1	0.79	2.12	14	2
1:A:13:VAL:HG11	1:B:3:LEU:HB2	0.79	1.54	16	2
1:A:43:PHE:CZ	1:A:56:VAL:HG21	0.79	2.12	18	1
1:A:10:LEU:HD22	1:A:74:MET:SD	0.79	2.18	25	4
1:A:3:LEU:HD22	1:B:39:GLU:OE2	0.79	1.78	17	1
1:B:10:LEU:HD22	1:B:74:MET:SD	0.79	2.18	12	4
1:A:32:LEU:HD23	1:A:60:LEU:HD21	0.79	1.55	22	1
1:A:52:VAL:HG12	1:A:56:VAL:CG2	0.78	2.09	6	15
1:B:43:PHE:CZ	1:B:56:VAL:HG21	0.78	2.13	18	1
1:B:52:VAL:HG12	1:B:56:VAL:CG2	0.77	2.09	6	15
1:A:39:GLU:OE2	1:B:3:LEU:HD22	0.77	1.78	17	1
1:A:52:VAL:HG11	1:A:83:ALA:CB	0.77	2.10	3	5
1:B:10:LEU:HD13	1:B:10:LEU:N	0.77	1.95	9	1
1:A:43:PHE:CZ	1:A:80:ILE:HG21	0.77	2.15	10	1
1:A:82:THR:HG22	1:B:70:PHE:CD1	0.77	2.14	6	1
1:A:70:PHE:CD1	1:B:82:THR:HG22	0.76	2.14	6	2
1:A:43:PHE:CZ	1:A:80:ILE:HG22	0.76	2.15	16	4
1:A:10:LEU:N	1:A:10:LEU:HD13	0.76	1.95	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:PHE:CZ	1:B:80:ILE:HG22	0.76	2.15	16	4
1:A:4:GLU:O	1:A:8:VAL:HG23	0.76	1.81	2	3
1:A:75:ALA:HB2	1:B:75:ALA:CB	0.76	2.11	13	1
1:B:14:PHE:CD2	1:B:70:PHE:CD1	0.76	2.73	20	4
1:B:14:PHE:CE2	1:B:70:PHE:HA	0.76	2.16	7	22
1:A:70:PHE:HB3	1:B:82:THR:HG23	0.76	1.58	22	1
1:A:36:ILE:N	1:A:36:ILE:HD13	0.76	1.95	13	12
1:A:60:LEU:HD12	1:A:76:PHE:CZ	0.76	2.16	3	3
1:B:4:GLU:O	1:B:8:VAL:HG23	0.76	1.81	2	3
1:B:43:PHE:CE2	1:B:80:ILE:HG23	0.76	2.16	7	5
1:B:43:PHE:CZ	1:B:80:ILE:HG21	0.76	2.16	10	1
1:A:7:VAL:HG13	1:B:81:THR:OG1	0.76	1.80	13	1
1:A:49:GLU:HG3	1:A:53:VAL:HG23	0.75	1.59	23	5
1:B:36:ILE:HD13	1:B:36:ILE:N	0.75	1.94	13	12
1:A:4:GLU:OE1	1:B:40:LEU:HD21	0.75	1.81	3	2
1:A:13:VAL:HG21	1:B:3:LEU:HB2	0.75	1.58	3	3
1:B:32:LEU:HD23	1:B:60:LEU:HD21	0.75	1.55	22	1
1:A:13:VAL:HG11	1:B:3:LEU:CD2	0.75	2.10	23	8
1:A:73:PHE:CE1	1:B:3:LEU:HD22	0.75	2.17	7	2
1:B:46:GLU:OE1	1:B:56:VAL:HG11	0.75	1.81	25	2
1:A:6:ALA:O	1:A:9:ALA:HB3	0.75	1.82	9	14
1:A:60:LEU:HD23	1:A:65:ASP:OD2	0.75	1.80	20	1
1:B:52:VAL:HG11	1:B:83:ALA:CB	0.75	2.11	3	5
1:B:60:LEU:HD12	1:B:76:PHE:CZ	0.75	2.16	3	3
1:B:27:LEU:HD22	1:B:31:GLU:HB3	0.75	1.58	21	2
1:A:70:PHE:CD2	1:B:82:THR:CG2	0.75	2.69	25	5
1:A:3:LEU:HD22	1:B:73:PHE:CE1	0.75	2.16	7	1
1:A:43:PHE:CE2	1:A:80:ILE:HG23	0.75	2.16	7	5
1:A:27:LEU:HD22	1:A:31:GLU:HB3	0.75	1.57	21	2
1:A:10:LEU:HD23	1:A:73:PHE:CE2	0.74	2.16	10	2
1:A:77:VAL:HG23	1:B:4:GLU:OE2	0.74	1.82	16	1
1:A:7:VAL:HG22	1:B:81:THR:OG1	0.74	1.81	4	8
1:B:46:GLU:OE1	1:B:53:VAL:HG13	0.74	1.81	4	1
1:A:69:ASP:O	1:A:71:GLN:N	0.74	2.20	22	6
1:B:60:LEU:HD23	1:B:65:ASP:OD2	0.74	1.81	20	1
1:A:2:GLU:O	1:A:6:ALA:HB2	0.74	1.82	8	8
1:A:3:LEU:CD2	1:B:13:VAL:HG11	0.74	2.11	14	10
1:A:81:THR:OG1	1:B:7:VAL:HG13	0.74	1.81	13	1
1:A:14:PHE:CE2	1:A:70:PHE:HA	0.74	2.17	12	22
1:A:3:LEU:HD21	1:B:73:PHE:CZ	0.74	2.17	21	6
1:B:2:GLU:O	1:B:6:ALA:HB2	0.74	1.82	8	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:10:LEU:HD23	1:B:73:PHE:CE2	0.74	2.17	10	2
1:A:25:HIS:CD2	1:A:70:PHE:CD1	0.74	2.76	19	1
1:B:69:ASP:O	1:B:71:GLN:N	0.74	2.20	22	6
1:B:35:LEU:HD13	1:B:73:PHE:CD1	0.74	2.17	21	1
1:A:75:ALA:CB	1:B:75:ALA:HB2	0.74	2.11	13	1
1:A:46:GLU:OE1	1:A:53:VAL:HG13	0.74	1.81	4	1
1:A:73:PHE:CZ	1:B:3:LEU:HD21	0.73	2.18	21	6
1:A:10:LEU:HD21	1:B:6:ALA:CB	0.73	2.13	16	1
1:B:25:HIS:CD2	1:B:70:PHE:CD1	0.73	2.76	19	1
1:A:52:VAL:HG11	1:A:83:ALA:HB2	0.73	1.59	16	1
1:B:49:GLU:HG3	1:B:53:VAL:HG23	0.73	1.58	23	4
1:A:37:ASN:OD1	1:A:44:LEU:HD13	0.73	1.84	4	3
1:A:81:THR:OG1	1:B:7:VAL:HG22	0.73	1.83	4	8
1:A:3:LEU:HD22	1:A:3:LEU:C	0.73	2.04	3	2
1:B:35:LEU:HD21	1:B:73:PHE:CD1	0.73	2.19	14	10
1:A:3:LEU:HB2	1:B:13:VAL:HG21	0.73	1.58	3	3
1:A:56:VAL:HG22	1:A:80:ILE:CD1	0.73	2.13	12	7
1:B:6:ALA:O	1:B:9:ALA:HB3	0.73	1.83	9	14
1:A:35:LEU:HD21	1:A:73:PHE:CD1	0.73	2.19	5	10
1:A:7:VAL:HG13	1:B:81:THR:HG21	0.73	1.60	21	6
1:A:46:GLU:OE1	1:A:56:VAL:HG11	0.72	1.83	25	2
1:A:3:LEU:HD12	1:B:13:VAL:CG1	0.72	2.14	11	2
1:A:13:VAL:CG1	1:B:3:LEU:HD12	0.72	2.13	11	2
1:B:56:VAL:HG22	1:B:80:ILE:CD1	0.72	2.13	12	6
1:B:25:HIS:CD2	1:B:70:PHE:CE1	0.72	2.77	11	3
1:A:14:PHE:CD2	1:A:70:PHE:CD1	0.72	2.78	20	5
1:A:35:LEU:HD13	1:A:73:PHE:CD1	0.72	2.18	21	1
1:A:70:PHE:CD2	1:B:82:THR:HG23	0.72	2.18	25	2
1:A:82:THR:HG23	1:B:70:PHE:HB3	0.72	1.60	22	1
1:A:25:HIS:CD2	1:A:70:PHE:CE1	0.72	2.78	11	3
1:A:36:ILE:HG23	1:A:80:ILE:HG21	0.72	1.61	7	2
1:A:60:LEU:HD12	1:A:76:PHE:CE2	0.72	2.20	16	1
1:B:37:ASN:OD1	1:B:44:LEU:HD13	0.72	1.83	4	3
1:A:13:VAL:HG13	1:B:3:LEU:HD11	0.72	1.62	2	1
1:A:3:LEU:O	1:A:6:ALA:HB3	0.72	1.85	3	5
1:A:7:VAL:HG22	1:B:81:THR:HG23	0.72	1.61	5	1
1:A:6:ALA:CB	1:B:10:LEU:HD21	0.72	2.15	16	1
1:A:3:LEU:HB3	1:B:13:VAL:HG21	0.71	1.62	8	1
1:B:52:VAL:HG11	1:B:83:ALA:HB2	0.71	1.61	16	1
1:A:7:VAL:HG22	1:B:81:THR:CG2	0.71	2.15	5	1
1:A:39:GLU:OE2	1:B:3:LEU:HD12	0.71	1.85	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:PHE:CE1	1:A:56:VAL:HG11	0.71	2.21	10	1
1:B:14:PHE:CZ	1:B:27:LEU:HD23	0.71	2.20	22	1
1:A:10:LEU:CD2	1:B:3:LEU:HD23	0.71	2.14	3	2
1:B:36:ILE:HG23	1:B:80:ILE:HG21	0.71	1.60	7	2
1:A:7:VAL:HA	1:A:10:LEU:HD12	0.71	1.62	25	2
1:B:39:GLU:HG3	1:B:40:LEU:HD12	0.71	1.61	13	4
1:A:10:LEU:HD11	1:B:10:LEU:HD11	0.71	1.61	12	1
1:A:35:LEU:HD23	1:B:3:LEU:HD11	0.71	1.62	21	1
1:A:3:LEU:HD23	1:B:10:LEU:CD2	0.71	2.15	3	2
1:A:7:VAL:HG11	1:B:81:THR:OG1	0.71	1.85	21	2
1:B:3:LEU:O	1:B:6:ALA:HB3	0.71	1.84	3	5
1:A:4:GLU:OE2	1:B:77:VAL:HG23	0.71	1.85	16	2
1:A:47:ILE:HG23	1:A:48:LYS:HD3	0.71	1.63	23	2
1:A:13:VAL:HG21	1:B:3:LEU:CB	0.71	2.16	3	2
1:B:3:LEU:HD22	1:B:3:LEU:C	0.70	2.06	6	2
1:B:13:VAL:HG13	1:B:17:TYR:CD2	0.70	2.21	5	5
1:A:39:GLU:CD	1:B:3:LEU:HD12	0.70	2.07	7	2
1:B:6:ALA:O	1:B:10:LEU:HD22	0.70	1.86	9	1
1:B:43:PHE:CE1	1:B:56:VAL:HG11	0.70	2.21	10	1
1:A:27:LEU:HD13	1:A:31:GLU:CB	0.70	2.16	11	5
1:A:39:GLU:HG3	1:A:40:LEU:HD12	0.70	1.62	13	4
1:A:70:PHE:CD1	1:B:82:THR:CG2	0.70	2.75	18	3
1:A:3:LEU:HD12	1:B:39:GLU:CD	0.70	2.07	7	2
1:A:35:LEU:HD21	1:B:3:LEU:HD11	0.70	1.62	15	2
1:A:82:THR:HG23	1:B:70:PHE:CD2	0.70	2.21	25	1
1:B:27:LEU:HD13	1:B:31:GLU:CB	0.70	2.17	11	5
1:A:81:THR:CG2	1:B:7:VAL:HG22	0.70	2.17	5	2
1:A:81:THR:OG1	1:B:7:VAL:HG11	0.70	1.86	21	2
1:B:14:PHE:CZ	1:B:27:LEU:HD12	0.70	2.22	9	2
1:A:3:LEU:HD11	1:B:13:VAL:HG13	0.70	1.61	2	1
1:A:52:VAL:HG21	1:A:83:ALA:CB	0.70	2.16	12	1
1:B:52:VAL:HG21	1:B:83:ALA:CB	0.70	2.16	12	1
1:A:14:PHE:CZ	1:A:27:LEU:HD23	0.70	2.21	22	1
1:A:49:GLU:OE1	1:A:52:VAL:HG11	0.70	1.87	14	5
1:B:49:GLU:OE1	1:B:52:VAL:HG11	0.70	1.86	14	5
1:A:13:VAL:HG13	1:A:17:TYR:CD2	0.70	2.22	5	5
1:A:81:THR:HG23	1:B:7:VAL:HG22	0.70	1.64	5	2
1:A:6:ALA:O	1:A:10:LEU:HD22	0.70	1.86	9	1
1:B:25:HIS:CD2	1:B:25:HIS:O	0.70	2.45	19	2
1:B:77:VAL:HA	1:B:80:ILE:HD12	0.70	1.64	24	1
1:B:14:PHE:CZ	1:B:70:PHE:HA	0.70	2.22	19	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:36:ILE:CG2	1:B:80:ILE:HD13	0.70	2.16	13	3
1:A:32:LEU:HD13	1:A:60:LEU:CD1	0.70	2.17	6	1
1:A:3:LEU:HD12	1:B:39:GLU:OE2	0.70	1.87	24	2
1:A:13:VAL:HG21	1:B:3:LEU:HB3	0.70	1.62	8	1
1:B:14:PHE:CD1	1:B:73:PHE:CD2	0.70	2.80	13	4
1:B:47:ILE:HG23	1:B:48:LYS:HD3	0.70	1.63	23	2
1:A:14:PHE:CZ	1:A:27:LEU:HD12	0.70	2.22	9	2
1:A:14:PHE:CD1	1:A:73:PHE:CD2	0.70	2.80	13	4
1:B:14:PHE:CE2	1:B:70:PHE:N	0.70	2.60	24	4
1:B:60:LEU:HD12	1:B:76:PHE:CE2	0.70	2.22	16	1
1:B:7:VAL:HA	1:B:10:LEU:HD12	0.69	1.62	25	2
1:A:40:LEU:HD21	1:B:4:GLU:OE1	0.69	1.87	3	2
1:B:32:LEU:HD13	1:B:60:LEU:CD1	0.69	2.17	6	1
1:A:13:VAL:HG11	1:B:3:LEU:HD11	0.69	1.64	19	1
1:A:36:ILE:CG2	1:A:80:ILE:HD13	0.69	2.16	13	3
1:A:14:PHE:CD1	1:A:70:PHE:CD1	0.69	2.80	19	3
1:A:13:VAL:HG11	1:B:3:LEU:CD1	0.69	2.16	11	2
1:A:82:THR:CG2	1:B:70:PHE:CD2	0.69	2.74	25	6
1:B:45:GLU:HB3	1:B:47:ILE:HG22	0.69	1.65	21	4
1:A:44:LEU:HD12	1:A:44:LEU:O	0.69	1.86	8	1
1:A:13:VAL:CG1	1:A:17:TYR:CD1	0.69	2.76	8	6
1:A:3:LEU:HD11	1:B:35:LEU:HD21	0.69	1.62	15	2
1:B:44:LEU:O	1:B:44:LEU:HD12	0.69	1.87	8	1
1:A:39:GLU:HG3	1:B:3:LEU:HD13	0.69	1.64	15	1
1:A:73:PHE:CZ	1:B:3:LEU:HD23	0.69	2.22	18	3
1:A:35:LEU:CD2	1:B:3:LEU:HD13	0.69	2.16	20	2
1:A:43:PHE:CD2	1:A:80:ILE:HG22	0.69	2.23	17	1
1:A:14:PHE:CZ	1:A:70:PHE:HA	0.69	2.23	19	19
1:A:43:PHE:CE2	1:A:80:ILE:CG2	0.69	2.75	12	13
1:B:14:PHE:CD1	1:B:70:PHE:CD1	0.69	2.80	19	3
1:A:3:LEU:CD1	1:B:13:VAL:HG11	0.69	2.17	11	2
1:B:13:VAL:CG1	1:B:17:TYR:CD1	0.69	2.76	8	6
1:A:3:LEU:CB	1:B:13:VAL:HG21	0.69	2.18	3	2
1:A:32:LEU:HD12	1:A:68:CYS:SG	0.69	2.28	3	2
1:A:25:HIS:CD2	1:A:25:HIS:O	0.69	2.45	19	2
1:A:14:PHE:CE2	1:A:70:PHE:N	0.69	2.60	24	4
1:A:35:LEU:CD1	1:A:73:PHE:CD1	0.69	2.76	21	2
1:B:36:ILE:CD1	1:B:80:ILE:HD11	0.69	2.17	13	1
1:A:3:LEU:HD13	1:B:39:GLU:HG3	0.69	1.63	15	1
1:B:13:VAL:HG13	1:B:17:TYR:CE1	0.68	2.23	18	5
1:A:14:PHE:CD2	1:A:73:PHE:CD2	0.68	2.81	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:14:PHE:CD2	1:B:73:PHE:CD2	0.68	2.81	9	3
1:B:43:PHE:CE2	1:B:80:ILE:CG2	0.68	2.75	12	13
1:A:11:ILE:HD12	1:A:11:ILE:C	0.68	2.08	12	2
1:A:13:VAL:HG13	1:A:17:TYR:CE2	0.68	2.23	23	8
1:B:35:LEU:CD1	1:B:73:PHE:CD1	0.68	2.76	21	2
1:A:3:LEU:C	1:A:3:LEU:HD22	0.68	2.09	21	2
1:B:32:LEU:HD12	1:B:68:CYS:SG	0.68	2.28	3	2
1:A:82:THR:CG2	1:B:70:PHE:CD1	0.68	2.76	6	2
1:A:52:VAL:HG21	1:A:83:ALA:O	0.68	1.88	10	4
1:A:70:PHE:CG	1:B:82:THR:CG2	0.68	2.77	25	3
1:A:13:VAL:HG13	1:A:17:TYR:CE1	0.68	2.24	18	4
1:B:43:PHE:CZ	1:B:80:ILE:CG2	0.68	2.77	16	6
1:B:14:PHE:CD1	1:B:70:PHE:CE1	0.68	2.82	12	5
1:B:43:PHE:HE1	1:B:56:VAL:HG11	0.68	1.49	10	1
1:B:26:LYS:O	1:B:27:LEU:HD12	0.68	1.88	24	1
1:A:73:PHE:CD1	1:A:73:PHE:C	0.68	2.67	19	24
1:A:35:LEU:HG	1:B:3:LEU:HD22	0.68	1.64	9	2
1:A:82:THR:HG23	1:B:70:PHE:CG	0.68	2.23	10	1
1:A:3:LEU:HD11	1:B:13:VAL:HG11	0.67	1.65	19	1
1:A:26:LYS:O	1:A:27:LEU:HD12	0.67	1.89	24	1
1:B:35:LEU:CD2	1:B:73:PHE:CE1	0.67	2.77	1	8
1:A:14:PHE:CE2	1:A:73:PHE:CG	0.67	2.82	8	3
1:B:13:VAL:CG1	1:B:17:TYR:CE2	0.67	2.77	14	2
1:B:13:VAL:HG12	1:B:17:TYR:HD1	0.67	1.49	16	1
1:A:43:PHE:CZ	1:A:80:ILE:CG2	0.67	2.77	16	6
1:A:72:GLU:O	1:A:75:ALA:HB3	0.67	1.89	13	5
1:A:17:TYR:CE1	1:B:3:LEU:HD11	0.67	2.25	9	3
1:A:43:PHE:CZ	1:A:80:ILE:HD13	0.67	2.25	10	1
1:B:52:VAL:HG21	1:B:83:ALA:O	0.67	1.89	10	4
1:A:13:VAL:HG21	1:B:3:LEU:CD1	0.67	2.19	17	2
1:A:3:LEU:HD11	1:B:35:LEU:HD23	0.67	1.61	21	1
1:A:77:VAL:HA	1:A:80:ILE:HD12	0.67	1.65	24	1
1:B:14:PHE:CE2	1:B:73:PHE:CG	0.67	2.83	8	3
1:B:11:ILE:HD12	1:B:11:ILE:C	0.67	2.08	12	8
1:B:13:VAL:HG13	1:B:17:TYR:CE2	0.67	2.24	23	7
1:A:52:VAL:HG22	1:A:56:VAL:HG23	0.67	1.64	12	1
1:B:32:LEU:HD22	1:B:68:CYS:SG	0.67	2.30	18	1
1:B:3:LEU:C	1:B:3:LEU:HD22	0.67	2.09	21	2
1:B:32:LEU:HD13	1:B:68:CYS:SG	0.67	2.30	21	2
1:A:43:PHE:CE2	1:A:56:VAL:HG21	0.67	2.24	21	4
1:A:3:LEU:CD1	1:B:13:VAL:HG21	0.67	2.19	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:VAL:CG1	1:A:83:ALA:HB2	0.67	2.20	16	1
1:A:74:MET:O	1:A:77:VAL:HG12	0.67	1.90	13	13
1:B:17:TYR:CD2	1:B:35:LEU:CD1	0.67	2.78	14	6
1:A:13:VAL:CG1	1:A:17:TYR:CE2	0.67	2.78	3	2
1:B:72:GLU:O	1:B:75:ALA:HB3	0.67	1.89	13	4
1:A:43:PHE:CE2	1:A:80:ILE:HG21	0.67	2.25	10	2
1:A:52:VAL:CG2	1:A:83:ALA:HB2	0.67	2.20	12	1
1:B:36:ILE:HG23	1:B:80:ILE:CD1	0.67	2.20	13	1
1:A:6:ALA:HB3	1:B:10:LEU:HD21	0.67	1.64	16	1
1:B:52:VAL:HG22	1:B:56:VAL:HG23	0.67	1.65	12	1
1:A:36:ILE:CD1	1:A:80:ILE:HD11	0.67	2.16	13	1
1:B:43:PHE:CD2	1:B:80:ILE:HG22	0.67	2.23	17	1
1:A:35:LEU:CD2	1:A:73:PHE:CE1	0.67	2.77	1	8
1:B:73:PHE:CD1	1:B:73:PHE:C	0.67	2.67	19	24
1:A:14:PHE:CD1	1:A:70:PHE:CE1	0.67	2.83	12	6
1:A:36:ILE:HG23	1:A:80:ILE:CD1	0.67	2.20	13	1
1:B:3:LEU:HD13	1:B:3:LEU:C	0.66	2.11	1	3
1:B:76:PHE:CE1	1:B:80:ILE:CD1	0.66	2.78	3	8
1:A:17:TYR:CD2	1:A:35:LEU:CD1	0.66	2.77	3	5
1:B:43:PHE:CE2	1:B:56:VAL:HG21	0.66	2.25	21	4
1:A:3:LEU:HD11	1:B:17:TYR:CE1	0.66	2.26	9	3
1:A:81:THR:OG1	1:B:7:VAL:HG21	0.66	1.90	15	3
1:B:40:LEU:N	1:B:40:LEU:HD23	0.66	2.04	3	1
1:A:3:LEU:HD13	1:A:3:LEU:C	0.66	2.10	3	3
1:A:14:PHE:CE1	1:A:27:LEU:CD1	0.66	2.79	25	5
1:A:76:PHE:CE1	1:A:80:ILE:CD1	0.66	2.78	3	8
1:B:35:LEU:HD21	1:B:73:PHE:CE2	0.66	2.25	2	2
1:A:32:LEU:HD13	1:A:68:CYS:SG	0.66	2.30	21	2
1:B:52:VAL:CG2	1:B:83:ALA:HB2	0.66	2.20	12	1
1:B:43:PHE:CZ	1:B:80:ILE:HD13	0.66	2.26	10	1
1:A:32:LEU:HD22	1:A:68:CYS:SG	0.66	2.30	18	1
1:A:7:VAL:HG21	1:B:77:VAL:HG22	0.66	1.68	21	2
1:A:45:GLU:HB3	1:A:47:ILE:HG22	0.66	1.65	21	4
1:A:3:LEU:C	1:A:3:LEU:HD23	0.66	2.11	11	2
1:B:36:ILE:HD12	1:B:80:ILE:HD12	0.66	1.67	2	2
1:A:7:VAL:HG21	1:B:81:THR:OG1	0.66	1.91	15	2
1:A:59:THR:HG21	1:A:79:MET:HG3	0.66	1.67	8	1
1:A:32:LEU:HD12	1:A:76:PHE:CD2	0.66	2.26	10	1
1:B:43:PHE:CE2	1:B:80:ILE:HG21	0.66	2.26	10	2
1:B:10:LEU:HD13	1:B:74:MET:HE1	0.66	1.65	25	1
1:A:76:PHE:CZ	1:A:80:ILE:CD1	0.66	2.79	14	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:GLU:CB	1:B:4:GLU:HB2	0.66	2.21	8	7
1:A:3:LEU:HD22	1:B:35:LEU:HG	0.66	1.65	9	2
1:A:73:PHE:CG	1:A:74:MET:N	0.66	2.64	13	4
1:B:3:LEU:C	1:B:3:LEU:HD23	0.66	2.11	11	2
1:A:32:LEU:CD2	1:A:36:ILE:HD11	0.66	2.21	12	1
1:B:32:LEU:CD2	1:B:36:ILE:HD11	0.66	2.21	12	1
1:B:41:SER:HA	1:B:44:LEU:HD23	0.65	1.66	8	1
1:B:74:MET:O	1:B:77:VAL:HG12	0.65	1.90	13	11
1:B:43:PHE:CD2	1:B:80:ILE:CG2	0.65	2.80	8	1
1:B:76:PHE:CD2	1:B:80:ILE:HD11	0.65	2.26	24	3
1:A:10:LEU:HD21	1:B:6:ALA:HB3	0.65	1.65	16	1
1:A:3:LEU:HD11	1:B:17:TYR:CE2	0.65	2.26	20	5
1:A:41:SER:HA	1:A:44:LEU:HD23	0.65	1.67	8	1
1:B:59:THR:HG21	1:B:79:MET:HG3	0.65	1.69	8	1
1:A:10:LEU:HD12	1:A:74:MET:HE3	0.65	1.66	11	2
1:B:46:GLU:HG2	1:B:53:VAL:HG13	0.65	1.68	10	4
1:A:40:LEU:N	1:A:40:LEU:HD23	0.65	2.05	3	1
1:A:47:ILE:HG23	1:A:48:LYS:HD2	0.65	1.68	5	1
1:A:10:LEU:HD12	1:A:74:MET:CE	0.65	2.22	11	3
1:A:3:LEU:HD11	1:B:13:VAL:HG21	0.65	1.67	17	2
1:B:73:PHE:CG	1:B:74:MET:N	0.65	2.64	13	4
1:A:14:PHE:CZ	1:A:70:PHE:N	0.65	2.65	13	2
1:B:14:PHE:CE2	1:B:73:PHE:CD2	0.65	2.84	8	3
1:A:82:THR:HG21	1:B:71:GLN:HB3	0.65	1.68	22	1
1:A:43:PHE:CD2	1:A:80:ILE:CG2	0.65	2.80	8	1
1:B:35:LEU:HD11	1:B:73:PHE:CE1	0.65	2.27	13	1
1:A:60:LEU:CD1	1:A:76:PHE:CZ	0.65	2.80	3	2
1:B:10:LEU:HD12	1:B:74:MET:HE3	0.65	1.67	11	2
1:B:14:PHE:CZ	1:B:70:PHE:N	0.65	2.65	13	2
1:B:27:LEU:HD22	1:B:31:GLU:CB	0.65	2.22	15	2
1:A:0:MET:HE2	1:A:3:LEU:HD12	0.65	1.69	9	1
1:B:10:LEU:HD12	1:B:74:MET:CE	0.65	2.22	11	3
1:A:13:VAL:HG12	1:A:17:TYR:HD1	0.65	1.48	16	1
1:A:36:ILE:HD12	1:A:80:ILE:HD12	0.64	1.67	2	2
1:B:32:LEU:HD12	1:B:76:PHE:CD2	0.64	2.27	10	1
1:A:27:LEU:HD22	1:A:31:GLU:CB	0.64	2.22	15	2
1:A:82:THR:HG22	1:B:70:PHE:HB3	0.64	1.69	17	2
1:A:70:PHE:HB3	1:B:82:THR:HG22	0.64	1.69	17	2
1:A:3:LEU:HD11	1:B:13:VAL:CG1	0.64	2.22	2	2
1:A:11:ILE:C	1:A:11:ILE:HD12	0.64	2.13	25	9
1:A:32:LEU:HD13	1:A:60:LEU:HD13	0.64	1.68	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:PHE:CE2	1:A:80:ILE:CD1	0.64	2.81	9	4
1:A:13:VAL:HG21	1:B:3:LEU:HD11	0.64	1.68	17	1
1:A:46:GLU:HG2	1:A:53:VAL:HG13	0.64	1.69	10	4
1:B:60:LEU:CD1	1:B:76:PHE:CZ	0.64	2.81	3	2
1:A:56:VAL:HG22	1:A:80:ILE:HA	0.64	1.68	24	3
1:A:71:GLN:HA	1:B:78:ALA:HB3	0.64	1.70	13	1
1:B:14:PHE:CE1	1:B:27:LEU:CD1	0.64	2.80	25	5
1:B:76:PHE:CZ	1:B:80:ILE:CD1	0.64	2.79	14	9
1:B:32:LEU:HD13	1:B:60:LEU:HD13	0.64	1.68	6	1
1:A:14:PHE:CE2	1:A:73:PHE:CD2	0.64	2.84	8	3
1:B:52:VAL:CG1	1:B:83:ALA:HB2	0.64	2.21	16	1
1:A:76:PHE:CD2	1:A:80:ILE:HD11	0.64	2.26	24	3
1:B:14:PHE:CE2	1:B:73:PHE:HB3	0.64	2.28	4	15
1:B:10:LEU:CD1	1:B:74:MET:SD	0.64	2.85	15	10
1:B:56:VAL:HG22	1:B:80:ILE:HA	0.64	1.68	24	3
1:B:76:PHE:CE2	1:B:80:ILE:CD1	0.64	2.81	9	4
1:A:43:PHE:HE1	1:A:56:VAL:HG11	0.64	1.49	10	1
1:A:35:LEU:HD11	1:A:73:PHE:CE1	0.64	2.27	13	1
1:B:13:VAL:CG1	1:B:17:TYR:CD2	0.64	2.81	14	8
1:A:4:GLU:HB2	1:B:39:GLU:CB	0.63	2.22	8	7
1:A:3:LEU:CD1	1:B:73:PHE:CZ	0.63	2.81	16	2
1:A:73:PHE:CZ	1:B:3:LEU:CD1	0.63	2.80	16	2
1:A:14:PHE:CE2	1:A:73:PHE:HB3	0.63	2.28	4	15
1:B:47:ILE:HG23	1:B:48:LYS:HD2	0.63	1.69	5	1
1:B:44:LEU:HD12	1:B:44:LEU:C	0.63	2.14	8	1
1:A:37:ASN:OD1	1:A:44:LEU:HD12	0.63	1.93	5	1
1:A:60:LEU:CD2	1:A:76:PHE:CE2	0.63	2.81	9	2
1:A:14:PHE:CE2	1:A:73:PHE:CB	0.63	2.82	8	3
1:A:44:LEU:HD12	1:A:44:LEU:C	0.63	2.14	8	1
1:B:60:LEU:CD2	1:B:76:PHE:CE2	0.63	2.81	9	2
1:B:46:GLU:HG3	1:B:53:VAL:HG21	0.63	1.70	18	2
1:A:29:LYS:O	1:A:60:LEU:HD11	0.63	1.93	13	1
1:A:71:GLN:HB3	1:B:82:THR:HG21	0.63	1.69	22	1
1:A:32:LEU:HD22	1:A:76:PHE:CD2	0.63	2.29	15	2
1:A:35:LEU:CG	1:B:3:LEU:HD11	0.63	2.23	15	1
1:A:43:PHE:CD1	1:A:43:PHE:C	0.63	2.72	8	2
1:B:32:LEU:CD1	1:B:60:LEU:HD22	0.63	2.24	13	1
1:B:25:HIS:NE2	1:B:70:PHE:CZ	0.62	2.67	11	1
1:A:7:VAL:HG12	1:A:8:VAL:N	0.62	2.09	10	10
1:A:25:HIS:NE2	1:A:70:PHE:CZ	0.62	2.67	11	1
1:A:11:ILE:CD1	1:A:12:ASP:N	0.62	2.62	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:32:LEU:HD22	1:B:76:PHE:CD2	0.62	2.29	15	2
1:A:52:VAL:CG1	1:A:56:VAL:HG23	0.62	2.21	14	7
1:A:32:LEU:HD23	1:A:60:LEU:HD12	0.62	1.71	2	1
1:B:0:MET:HE2	1:B:3:LEU:HD12	0.62	1.70	9	1
1:A:14:PHE:CD1	1:A:27:LEU:HD23	0.62	2.29	23	2
1:A:39:GLU:CG	1:A:40:LEU:HD12	0.62	2.25	13	1
1:B:29:LYS:O	1:B:60:LEU:HD11	0.62	1.93	13	1
1:A:35:LEU:HD21	1:A:73:PHE:CE2	0.62	2.28	2	2
1:B:32:LEU:HD23	1:B:60:LEU:HD12	0.62	1.72	2	2
1:A:73:PHE:CZ	1:B:3:LEU:CD2	0.62	2.83	20	6
1:B:32:LEU:HD21	1:B:76:PHE:CG	0.62	2.30	22	2
1:B:7:VAL:HG12	1:B:8:VAL:N	0.62	2.10	10	10
1:B:74:MET:O	1:B:78:ALA:HB2	0.62	1.95	5	5
1:A:13:VAL:CG1	1:B:3:LEU:HD11	0.62	2.25	2	2
1:B:14:PHE:CE2	1:B:73:PHE:CB	0.62	2.83	8	3
1:B:62:SER:O	1:B:63:ASP:O	0.62	2.17	4	8
1:A:3:LEU:HD22	1:B:35:LEU:CD2	0.62	2.25	22	5
1:B:43:PHE:CD1	1:B:43:PHE:C	0.62	2.72	8	2
1:A:32:LEU:CD1	1:A:60:LEU:HD22	0.62	2.24	13	1
1:A:78:ALA:HB3	1:B:71:GLN:HA	0.62	1.69	13	1
1:B:43:PHE:CE2	1:B:56:VAL:HG11	0.62	2.30	21	1
1:A:17:TYR:CE2	1:A:35:LEU:HG	0.62	2.30	3	5
1:A:46:GLU:HG3	1:A:53:VAL:HG21	0.61	1.70	18	2
1:B:39:GLU:CG	1:B:40:LEU:HD12	0.61	2.24	13	1
1:A:32:LEU:HD21	1:A:76:PHE:CG	0.61	2.30	22	2
1:A:35:LEU:HD23	1:B:3:LEU:HD13	0.61	1.71	20	2
1:A:70:PHE:CG	1:B:82:THR:HG23	0.61	2.30	10	1
1:B:11:ILE:CD1	1:B:12:ASP:N	0.61	2.62	16	2
1:B:47:ILE:HD13	1:B:47:ILE:C	0.61	2.15	25	14
1:B:43:PHE:HE2	1:B:80:ILE:HG22	0.61	1.55	3	3
1:A:77:VAL:HG22	1:B:7:VAL:HG21	0.61	1.71	21	2
1:B:37:ASN:OD1	1:B:44:LEU:HD12	0.61	1.94	5	1
1:A:56:VAL:HG22	1:A:80:ILE:CG2	0.61	2.11	10	2
1:A:32:LEU:O	1:A:36:ILE:HD13	0.61	1.96	21	2
1:A:3:LEU:HD11	1:B:35:LEU:CG	0.61	2.25	15	1
1:A:70:PHE:CB	1:B:82:THR:CG2	0.61	2.79	14	3
1:A:47:ILE:HD13	1:A:47:ILE:C	0.61	2.16	19	14
1:B:40:LEU:HD13	1:B:80:ILE:HG21	0.61	1.71	18	1
1:A:43:PHE:CE2	1:A:56:VAL:HG11	0.61	2.31	21	1
1:A:13:VAL:HG12	1:A:17:TYR:CE2	0.61	2.31	3	1
1:A:39:GLU:CB	1:B:4:GLU:CB	0.61	2.78	11	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:67:GLU:O	1:B:67:GLU:CG	0.61	2.49	22	5
1:B:10:LEU:CD1	1:B:74:MET:CE	0.61	2.79	23	6
1:B:17:TYR:HH	1:B:39:GLU:CD	0.61	1.98	17	1
1:A:67:GLU:CG	1:A:67:GLU:O	0.61	2.49	22	3
1:A:4:GLU:CB	1:B:39:GLU:CB	0.61	2.79	11	5
1:A:4:GLU:CD	1:B:40:LEU:HD21	0.61	2.16	8	1
1:A:60:LEU:CD2	1:A:76:PHE:CZ	0.61	2.84	23	1
1:B:32:LEU:O	1:B:36:ILE:HD13	0.60	1.96	21	2
1:A:3:LEU:HD22	1:B:39:GLU:CD	0.60	2.16	17	1
1:A:17:TYR:HH	1:A:39:GLU:CD	0.60	1.99	17	1
1:A:3:LEU:CB	1:B:13:VAL:HG11	0.60	2.26	21	1
1:A:14:PHE:CD2	1:A:18:SER:CB	0.60	2.84	24	2
1:B:27:LEU:CD1	1:B:31:GLU:CB	0.60	2.80	23	4
1:A:36:ILE:CG2	1:A:43:PHE:CD2	0.60	2.84	15	3
1:A:82:THR:CG2	1:B:70:PHE:CB	0.60	2.79	19	2
1:A:10:LEU:CD1	1:A:74:MET:CE	0.60	2.79	23	5
1:A:77:VAL:CG1	1:B:74:MET:HE1	0.60	2.26	15	3
1:A:43:PHE:O	1:A:46:GLU:N	0.60	2.35	8	10
1:A:27:LEU:CD1	1:A:31:GLU:CB	0.60	2.79	23	4
1:B:10:LEU:O	1:B:13:VAL:N	0.60	2.34	19	13
1:B:62:SER:O	1:B:63:ASP:CB	0.60	2.50	20	3
1:B:8:VAL:O	1:B:11:ILE:CG1	0.60	2.50	21	13
1:A:16:GLN:O	1:A:20:ARG:N	0.60	2.35	24	23
1:A:15:HIS:C	1:A:15:HIS:CD2	0.60	2.75	21	4
1:A:7:VAL:HG22	1:B:81:THR:HG21	0.60	1.74	11	1
1:B:43:PHE:O	1:B:46:GLU:N	0.60	2.35	8	10
1:B:69:ASP:HB2	1:B:72:GLU:HG3	0.60	1.73	12	2
1:B:60:LEU:CD2	1:B:76:PHE:CZ	0.60	2.84	23	1
1:A:39:GLU:CD	1:B:3:LEU:HD22	0.60	2.16	17	1
1:B:14:PHE:CD2	1:B:18:SER:CB	0.60	2.84	24	2
1:A:35:LEU:HD21	1:A:73:PHE:HE1	0.60	1.57	13	3
1:B:25:HIS:O	1:B:25:HIS:CG	0.60	2.55	19	2
1:B:36:ILE:CG2	1:B:43:PHE:CD2	0.60	2.84	15	3
1:A:70:PHE:CG	1:B:82:THR:HG22	0.60	2.31	14	2
1:B:75:ALA:O	1:B:78:ALA:HB3	0.60	1.97	1	5
1:A:13:VAL:CG1	1:A:17:TYR:CD2	0.60	2.83	14	7
1:A:74:MET:HE2	1:B:77:VAL:CG1	0.60	2.27	24	2
1:A:40:LEU:HD21	1:B:4:GLU:CD	0.60	2.17	8	1
1:B:41:SER:CA	1:B:44:LEU:HD23	0.60	2.27	8	1
1:A:59:THR:HG22	1:A:63:ASP:HB2	0.59	1.74	4	1
1:A:41:SER:CA	1:A:44:LEU:HD23	0.59	2.27	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:40:LEU:HD12	1:B:40:LEU:N	0.59	2.12	15	1
1:A:8:VAL:O	1:A:11:ILE:CG1	0.59	2.50	21	13
1:B:13:VAL:HG12	1:B:17:TYR:HD2	0.59	1.57	3	1
1:A:81:THR:HG21	1:B:7:VAL:HG22	0.59	1.74	11	1
1:B:60:LEU:O	1:B:65:ASP:CB	0.59	2.50	21	1
1:A:75:ALA:O	1:A:78:ALA:HB3	0.59	1.97	1	5
1:A:43:PHE:HE2	1:A:80:ILE:HG22	0.59	1.56	3	3
1:B:16:GLN:O	1:B:20:ARG:N	0.59	2.35	24	21
1:B:76:PHE:HE1	1:B:80:ILE:HD11	0.59	1.52	3	2
1:A:74:MET:O	1:A:78:ALA:HB2	0.59	1.96	5	5
1:A:25:HIS:O	1:A:25:HIS:CG	0.59	2.55	19	2
1:A:40:LEU:HD13	1:A:80:ILE:HG21	0.59	1.72	18	1
1:B:36:ILE:CD1	1:B:80:ILE:CD1	0.59	2.80	24	3
1:B:74:MET:HA	1:B:77:VAL:HG12	0.59	1.74	5	4
1:A:76:PHE:CE1	1:A:80:ILE:HG13	0.59	2.33	18	4
1:A:3:LEU:CD2	1:B:73:PHE:CZ	0.59	2.85	5	5
1:B:25:HIS:NE2	1:B:70:PHE:CE1	0.59	2.70	11	1
1:A:69:ASP:HB2	1:A:72:GLU:HG3	0.59	1.74	12	2
1:B:32:LEU:HD12	1:B:60:LEU:CD1	0.59	2.24	13	1
1:A:77:VAL:HG21	1:B:3:LEU:HD21	0.59	1.74	1	2
1:B:35:LEU:HD21	1:B:73:PHE:HE1	0.59	1.56	13	2
1:A:35:LEU:CD2	1:B:3:LEU:HD22	0.59	2.26	22	3
1:B:52:VAL:HG12	1:B:56:VAL:HG21	0.59	1.74	6	3
1:B:14:PHE:CZ	1:B:27:LEU:HD13	0.59	2.33	13	1
1:B:14:PHE:CD1	1:B:27:LEU:HD23	0.59	2.33	23	2
1:B:15:HIS:C	1:B:15:HIS:CD2	0.59	2.75	21	4
1:B:11:ILE:O	1:B:15:HIS:CB	0.59	2.50	19	3
1:A:43:PHE:O	1:A:43:PHE:CD1	0.59	2.56	10	1
1:A:11:ILE:O	1:A:15:HIS:CB	0.59	2.51	19	3
1:B:36:ILE:CG2	1:B:80:ILE:CG2	0.59	2.81	7	2
1:B:43:PHE:O	1:B:43:PHE:CD1	0.59	2.56	10	1
1:B:14:PHE:CE1	1:B:73:PHE:CD2	0.59	2.91	25	6
1:A:13:VAL:HG11	1:B:3:LEU:CB	0.59	2.26	21	1
1:A:36:ILE:CD1	1:A:80:ILE:CD1	0.59	2.80	24	4
1:A:74:MET:HA	1:A:77:VAL:HG12	0.59	1.74	5	4
1:A:62:SER:O	1:A:63:ASP:CB	0.59	2.51	20	3
1:A:60:LEU:O	1:A:65:ASP:CB	0.59	2.51	21	1
1:A:4:GLU:OE2	1:B:35:LEU:HD23	0.58	1.98	3	1
1:B:76:PHE:CZ	1:B:80:ILE:HG13	0.58	2.33	23	3
1:A:17:TYR:CE2	1:B:3:LEU:HD11	0.58	2.33	13	4
1:A:3:LEU:HD21	1:B:77:VAL:HG21	0.58	1.73	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ILE:N	1:A:36:ILE:HD12	0.58	2.12	25	7
1:A:69:ASP:O	1:A:70:PHE:C	0.58	2.42	13	22
1:B:76:PHE:CE1	1:B:80:ILE:HG13	0.58	2.34	18	4
1:A:36:ILE:HD11	1:A:76:PHE:CZ	0.58	2.33	14	2
1:B:3:LEU:CD1	1:B:4:GLU:N	0.58	2.63	1	3
1:B:69:ASP:O	1:B:70:PHE:C	0.58	2.41	13	22
1:A:52:VAL:HG12	1:A:56:VAL:HG21	0.58	1.74	6	3
1:A:7:VAL:HA	1:A:10:LEU:CD2	0.58	2.28	9	1
1:B:36:ILE:HD12	1:B:36:ILE:N	0.58	2.12	25	3
1:B:36:ILE:CD1	1:B:36:ILE:N	0.58	2.66	3	5
1:A:3:LEU:HD12	1:A:4:GLU:N	0.58	2.14	8	1
1:B:40:LEU:HD13	1:B:80:ILE:CG2	0.58	2.28	18	1
1:B:69:ASP:O	1:B:72:GLU:N	0.58	2.36	16	17
1:A:76:PHE:CZ	1:A:80:ILE:HG13	0.58	2.33	23	3
1:A:40:LEU:N	1:A:40:LEU:HD12	0.58	2.13	15	2
1:A:75:ALA:HB1	1:B:71:GLN:HG3	0.58	1.75	13	1
1:B:36:ILE:HD11	1:B:76:PHE:CZ	0.58	2.33	14	2
1:B:14:PHE:CD2	1:B:18:SER:OG	0.58	2.51	20	4
1:A:10:LEU:HD22	1:A:73:PHE:CZ	0.58	2.34	18	2
1:A:40:LEU:HD13	1:A:80:ILE:CG2	0.58	2.29	18	1
1:A:36:ILE:N	1:A:36:ILE:CD1	0.58	2.66	3	18
1:B:14:PHE:CZ	1:B:73:PHE:HB3	0.58	2.34	4	3
1:A:71:GLN:O	1:A:75:ALA:CB	0.58	2.51	16	5
1:B:10:LEU:HD22	1:B:73:PHE:CZ	0.58	2.33	18	2
1:A:27:LEU:CD1	1:A:32:LEU:N	0.58	2.66	20	1
1:A:73:PHE:CE1	1:B:3:LEU:HD23	0.58	2.33	5	3
1:B:71:GLN:O	1:B:75:ALA:CB	0.58	2.52	16	5
1:A:47:ILE:HG23	1:A:48:LYS:N	0.58	2.14	10	7
1:A:35:LEU:HD21	1:A:73:PHE:CZ	0.58	2.34	8	1
1:A:14:PHE:CE1	1:A:73:PHE:CD2	0.58	2.92	15	6
1:B:32:LEU:CD2	1:B:76:PHE:CD2	0.58	2.84	16	4
1:A:62:SER:O	1:A:63:ASP:O	0.58	2.22	5	8
1:A:64:GLY:O	1:A:65:ASP:CB	0.58	2.51	17	4
1:A:14:PHE:CD2	1:A:18:SER:OG	0.58	2.55	24	5
1:A:32:LEU:HD12	1:A:60:LEU:CD1	0.58	2.24	13	1
1:B:32:LEU:HD12	1:B:60:LEU:HD22	0.58	1.75	13	1
1:A:62:SER:O	1:A:65:ASP:N	0.58	2.34	7	7
1:A:32:LEU:HD12	1:A:60:LEU:HD22	0.58	1.76	13	1
1:A:71:GLN:HG3	1:B:75:ALA:HB1	0.58	1.74	13	1
1:A:71:GLN:NE2	1:A:72:GLU:HG2	0.58	2.14	24	6
1:B:32:LEU:HD23	1:B:60:LEU:HD13	0.58	1.76	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:GLU:CG	1:A:59:THR:N	0.58	2.67	23	4
1:B:43:PHE:CZ	1:B:49:GLU:OE2	0.58	2.57	13	2
1:A:20:ARG:CG	1:A:20:ARG:O	0.57	2.52	2	1
1:B:20:ARG:CG	1:B:20:ARG:O	0.57	2.52	2	1
1:B:3:LEU:HD12	1:B:4:GLU:N	0.57	2.14	8	1
1:A:78:ALA:HA	1:A:81:THR:OG1	0.57	1.99	14	1
1:B:14:PHE:CE1	1:B:70:PHE:CD1	0.57	2.91	17	3
1:B:80:ILE:O	1:B:83:ALA:HB3	0.57	1.99	22	2
1:A:10:LEU:CD1	1:A:74:MET:HE1	0.57	2.28	25	2
1:A:14:PHE:CE1	1:A:70:PHE:CD1	0.57	2.92	17	3
1:A:69:ASP:O	1:A:72:GLU:N	0.57	2.36	16	18
1:B:17:TYR:CE2	1:B:35:LEU:CD1	0.57	2.81	11	5
1:B:35:LEU:CD1	1:B:73:PHE:CD2	0.57	2.82	4	2
1:B:35:LEU:HD21	1:B:73:PHE:CZ	0.57	2.34	8	1
1:B:56:VAL:HG22	1:B:80:ILE:CG2	0.57	2.12	10	2
1:B:43:PHE:CE1	1:B:49:GLU:OE2	0.57	2.58	12	7
1:A:18:SER:HB2	1:A:25:HIS:HA	0.57	1.76	11	4
1:B:77:VAL:O	1:B:81:THR:OG1	0.57	2.22	14	7
1:A:3:LEU:HD23	1:B:73:PHE:CE1	0.57	2.35	5	3
1:A:1:SER:CB	1:B:39:GLU:CG	0.57	2.82	8	1
1:A:43:PHE:CZ	1:A:49:GLU:OE2	0.57	2.57	13	2
1:B:27:LEU:CD1	1:B:32:LEU:N	0.57	2.67	20	1
1:A:43:PHE:CD1	1:A:49:GLU:OE2	0.57	2.57	5	2
1:A:14:PHE:O	1:A:18:SER:N	0.57	2.36	14	3
1:A:56:VAL:HG13	1:A:80:ILE:HD11	0.57	1.75	15	1
1:A:14:PHE:CZ	1:A:73:PHE:HB3	0.57	2.34	4	3
1:B:14:PHE:CZ	1:B:70:PHE:CA	0.57	2.87	19	13
1:B:71:GLN:NE2	1:B:72:GLU:HG2	0.57	2.15	24	6
1:A:43:PHE:CE1	1:A:49:GLU:OE2	0.57	2.57	15	7
1:A:35:LEU:HD23	1:B:4:GLU:OE2	0.57	1.99	3	1
1:B:43:PHE:CD1	1:B:49:GLU:OE2	0.57	2.58	17	2
1:B:47:ILE:HG23	1:B:48:LYS:N	0.57	2.13	10	8
1:A:17:TYR:CE2	1:A:35:LEU:CD1	0.57	2.81	11	5
1:A:77:VAL:O	1:A:81:THR:OG1	0.57	2.22	14	8
1:A:10:LEU:O	1:A:13:VAL:N	0.57	2.37	15	13
1:A:27:LEU:HD23	1:A:31:GLU:CB	0.57	2.29	5	4
1:B:35:LEU:CD1	1:B:73:PHE:CE2	0.57	2.78	8	1
1:A:25:HIS:NE2	1:A:70:PHE:CE1	0.57	2.72	11	1
1:A:64:GLY:O	1:A:65:ASP:C	0.57	2.43	25	8
1:B:18:SER:HB2	1:B:25:HIS:HA	0.57	1.75	11	4
1:B:58:GLU:CG	1:B:59:THR:N	0.57	2.67	23	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LEU:CD1	1:A:31:GLU:HB2	0.57	2.29	22	5
1:A:27:LEU:CB	1:A:68:CYS:O	0.57	2.53	22	6
1:A:3:LEU:HD11	1:B:10:LEU:CD2	0.57	2.30	14	1
1:B:76:PHE:CD1	1:B:76:PHE:C	0.57	2.79	18	3
1:B:17:TYR:CE2	1:B:35:LEU:HG	0.56	2.34	3	5
1:A:14:PHE:CZ	1:A:73:PHE:CB	0.56	2.88	8	2
1:A:35:LEU:HG	1:B:3:LEU:HD21	0.56	1.75	16	1
1:A:73:PHE:HZ	1:B:3:LEU:HD23	0.56	1.60	23	1
1:B:14:PHE:O	1:B:18:SER:N	0.56	2.36	14	5
1:A:74:MET:CE	1:B:77:VAL:CG1	0.56	2.83	24	4
1:A:24:LYS:O	1:A:25:HIS:CD2	0.56	2.57	24	2
1:A:4:GLU:OE2	1:B:40:LEU:HD11	0.56	1.99	8	1
1:A:81:THR:CG2	1:B:7:VAL:CG1	0.56	2.80	8	4
1:B:7:VAL:HA	1:B:10:LEU:CD2	0.56	2.30	9	1
1:B:78:ALA:HA	1:B:81:THR:OG1	0.56	2.00	14	1
1:A:16:GLN:O	1:A:20:ARG:CD	0.56	2.53	19	1
1:A:7:VAL:CG2	1:B:81:THR:OG1	0.56	2.54	19	10
1:A:27:LEU:N	1:A:68:CYS:O	0.56	2.39	24	12
1:A:82:THR:HG22	1:B:70:PHE:CD2	0.56	2.36	14	2
1:B:27:LEU:HD23	1:B:31:GLU:CB	0.56	2.30	5	4
1:B:35:LEU:CD2	1:B:73:PHE:CD1	0.56	2.88	18	9
1:A:36:ILE:CG2	1:A:80:ILE:CG2	0.56	2.81	7	2
1:A:41:SER:HA	1:A:44:LEU:CD2	0.56	2.30	8	1
1:B:14:PHE:CE2	1:B:18:SER:OG	0.56	2.56	15	1
1:B:16:GLN:O	1:B:20:ARG:CD	0.56	2.53	19	1
1:A:80:ILE:O	1:A:83:ALA:HB3	0.56	2.00	22	2
1:A:55:LYS:N	1:A:55:LYS:CD	0.56	2.69	4	4
1:B:40:LEU:O	1:B:43:PHE:N	0.56	2.36	22	3
1:A:7:VAL:CG1	1:B:81:THR:CG2	0.56	2.79	8	3
1:B:27:LEU:CB	1:B:68:CYS:O	0.56	2.53	22	6
1:B:17:TYR:CE1	1:B:35:LEU:HG	0.56	2.36	20	6
1:B:41:SER:HA	1:B:44:LEU:CD2	0.56	2.30	8	1
1:B:14:PHE:CE2	1:B:18:SER:HB3	0.56	2.35	24	3
1:A:82:THR:CG2	1:B:70:PHE:CG	0.56	2.89	25	1
1:A:4:GLU:CB	1:B:39:GLU:HB3	0.56	2.31	11	9
1:B:35:LEU:O	1:B:39:GLU:OE1	0.56	2.24	24	10
1:B:49:GLU:O	1:B:53:VAL:CG2	0.56	2.53	16	7
1:B:64:GLY:O	1:B:65:ASP:C	0.56	2.43	25	8
1:A:46:GLU:O	1:A:53:VAL:CG2	0.56	2.54	14	10
1:A:40:LEU:O	1:A:43:PHE:N	0.56	2.36	22	3
1:A:8:VAL:O	1:A:11:ILE:HG13	0.56	2.00	2	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:PHE:CZ	1:A:70:PHE:CA	0.56	2.88	19	13
1:B:36:ILE:N	1:B:36:ILE:CD1	0.56	2.65	24	10
1:B:37:ASN:HB3	1:B:44:LEU:HD12	0.56	1.77	7	1
1:A:73:PHE:HE1	1:B:3:LEU:HD21	0.56	1.60	17	2
1:A:3:LEU:CD1	1:B:10:LEU:CD2	0.56	2.83	14	1
1:B:14:PHE:CD2	1:B:18:SER:HB3	0.56	2.36	24	2
1:A:80:ILE:O	1:A:83:ALA:N	0.56	2.39	10	13
1:B:8:VAL:O	1:B:11:ILE:HG13	0.56	2.01	2	17
1:A:35:LEU:CD1	1:A:73:PHE:CD2	0.56	2.82	4	2
1:B:55:LYS:N	1:B:55:LYS:CD	0.56	2.69	4	4
1:A:73:PHE:CE1	1:B:3:LEU:CD2	0.56	2.89	14	2
1:A:39:GLU:CG	1:B:1:SER:CB	0.56	2.84	8	1
1:A:10:LEU:O	1:A:14:PHE:N	0.56	2.39	19	4
1:A:14:PHE:CE2	1:A:70:PHE:CA	0.56	2.89	13	3
1:A:76:PHE:CD1	1:A:76:PHE:C	0.56	2.79	18	3
1:A:3:LEU:HD23	1:B:13:VAL:HG21	0.56	1.76	21	1
1:B:25:HIS:HB3	1:B:70:PHE:CZ	0.56	2.36	18	8
1:B:80:ILE:O	1:B:83:ALA:N	0.56	2.39	4	13
1:A:63:ASP:O	1:A:64:GLY:C	0.56	2.44	5	11
1:A:35:LEU:CD2	1:A:73:PHE:CD1	0.56	2.88	18	9
1:A:74:MET:O	1:B:74:MET:CB	0.56	2.54	24	3
1:A:36:ILE:HG13	1:A:40:LEU:HD12	0.56	1.78	10	1
1:A:32:LEU:CD1	1:A:76:PHE:CE2	0.56	2.81	13	1
1:A:68:CYS:HA	1:A:72:GLU:CB	0.56	2.31	22	2
1:A:39:GLU:HB3	1:B:4:GLU:CB	0.55	2.31	11	9
1:A:43:PHE:CE1	1:A:49:GLU:CD	0.55	2.80	5	8
1:B:43:PHE:CE1	1:B:49:GLU:CD	0.55	2.79	5	8
1:A:10:LEU:CD1	1:A:74:MET:SD	0.55	2.94	22	9
1:A:47:ILE:CG2	1:A:48:LYS:N	0.55	2.69	22	17
1:B:52:VAL:CG1	1:B:56:VAL:HG23	0.55	2.22	14	8
1:B:47:ILE:CG2	1:B:48:LYS:N	0.55	2.69	22	18
1:A:79:MET:HA	1:A:82:THR:OG1	0.55	2.02	24	7
1:B:6:ALA:O	1:B:10:LEU:CD2	0.55	2.55	13	4
1:B:10:LEU:O	1:B:14:PHE:N	0.55	2.39	15	4
1:A:7:VAL:CG1	1:B:81:THR:OG1	0.55	2.54	21	2
1:A:14:PHE:CE2	1:A:18:SER:HB3	0.55	2.35	24	3
1:A:81:THR:OG1	1:B:7:VAL:CG2	0.55	2.55	1	10
1:B:76:PHE:CE1	1:B:80:ILE:CG1	0.55	2.89	3	4
1:B:27:LEU:CD1	1:B:31:GLU:HB2	0.55	2.31	17	6
1:B:43:PHE:CD1	1:B:49:GLU:CD	0.55	2.80	5	1
1:A:36:ILE:HG21	1:A:80:ILE:HD12	0.55	1.78	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:ALA:CB	1:B:74:MET:SD	0.55	2.94	16	5
1:A:35:LEU:CG	1:B:3:LEU:HD22	0.55	2.30	9	1
1:A:14:PHE:CD2	1:A:18:SER:HB3	0.55	2.36	24	2
1:B:14:PHE:CE2	1:B:27:LEU:HD23	0.55	2.37	22	1
1:A:77:VAL:CG1	1:B:74:MET:CE	0.55	2.84	24	4
1:A:71:GLN:CG	1:A:72:GLU:N	0.55	2.69	13	1
1:B:14:PHE:CE2	1:B:70:PHE:CA	0.55	2.89	13	4
1:A:43:PHE:CZ	1:A:49:GLU:CD	0.55	2.79	14	1
1:A:14:PHE:CE2	1:A:70:PHE:CD1	0.55	2.95	25	2
1:A:76:PHE:CE1	1:A:80:ILE:CG1	0.55	2.89	3	4
1:A:43:PHE:CD1	1:A:49:GLU:CD	0.55	2.80	5	1
1:A:6:ALA:O	1:A:10:LEU:CD2	0.55	2.55	13	4
1:A:17:TYR:CZ	1:B:3:LEU:HD11	0.55	2.36	20	2
1:A:45:GLU:O	1:A:47:ILE:N	0.55	2.40	18	16
1:B:62:SER:O	1:B:63:ASP:C	0.55	2.45	3	15
1:A:76:PHE:HE1	1:A:80:ILE:HD11	0.55	1.52	3	2
1:A:10:LEU:O	1:A:13:VAL:HB	0.55	2.01	23	5
1:A:74:MET:CB	1:B:74:MET:O	0.55	2.54	24	4
1:A:76:PHE:O	1:A:80:ILE:CG1	0.55	2.55	9	1
1:B:36:ILE:CG1	1:B:80:ILE:CD1	0.55	2.84	9	1
1:B:43:PHE:CZ	1:B:49:GLU:CD	0.55	2.80	14	1
1:B:78:ALA:O	1:B:82:THR:CG2	0.55	2.52	24	2
1:A:60:LEU:HD22	1:A:76:PHE:CE2	0.55	2.36	23	1
1:A:49:GLU:O	1:A:53:VAL:CG2	0.55	2.55	12	7
1:B:46:GLU:O	1:B:53:VAL:CG2	0.55	2.54	14	10
1:B:14:PHE:CZ	1:B:73:PHE:CB	0.55	2.90	8	2
1:B:71:GLN:CG	1:B:72:GLU:N	0.55	2.69	13	1
1:A:46:GLU:O	1:A:53:VAL:HG22	0.55	2.02	14	1
1:A:13:VAL:HG21	1:B:3:LEU:HD23	0.55	1.79	21	1
1:A:62:SER:O	1:A:63:ASP:C	0.55	2.45	18	18
1:B:62:SER:O	1:B:65:ASP:N	0.55	2.39	15	7
1:B:27:LEU:N	1:B:68:CYS:O	0.55	2.39	25	12
1:A:49:GLU:OE2	1:A:56:VAL:HG21	0.55	2.01	4	2
1:B:76:PHE:O	1:B:79:MET:N	0.55	2.40	24	11
1:A:10:LEU:HD23	1:A:73:PHE:HE1	0.55	1.61	8	1
1:A:3:LEU:HD22	1:B:35:LEU:CG	0.55	2.31	9	1
1:A:70:PHE:HB3	1:B:82:THR:CG2	0.55	2.30	14	6
1:A:52:VAL:CG2	1:A:83:ALA:O	0.55	2.55	19	6
1:B:52:VAL:CG2	1:B:83:ALA:O	0.55	2.55	14	7
1:A:52:VAL:CG1	1:A:83:ALA:CB	0.55	2.85	3	7
1:B:51:GLU:O	1:B:55:LYS:CD	0.55	2.55	17	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:MET:SD	1:B:78:ALA:CB	0.55	2.95	16	5
1:B:13:VAL:HG12	1:B:17:TYR:CE2	0.55	2.37	3	1
1:A:73:PHE:CE1	1:B:3:LEU:HD21	0.55	2.36	10	2
1:B:20:ARG:CG	1:B:21:GLU:N	0.55	2.70	10	2
1:B:56:VAL:HG13	1:B:80:ILE:HD11	0.55	1.76	15	1
1:A:51:GLU:O	1:A:55:LYS:CD	0.55	2.55	17	13
1:B:45:GLU:O	1:B:47:ILE:N	0.55	2.40	18	16
1:A:62:SER:O	1:A:64:GLY:N	0.55	2.40	25	4
1:A:7:VAL:CG1	1:A:8:VAL:N	0.55	2.70	16	7
1:A:36:ILE:CG1	1:A:80:ILE:CD1	0.55	2.85	9	1
1:A:20:ARG:O	1:A:21:GLU:CB	0.55	2.54	11	1
1:A:3:LEU:HD21	1:B:73:PHE:HE1	0.55	1.61	17	1
1:B:77:VAL:CG1	1:B:78:ALA:N	0.54	2.69	6	20
1:A:10:LEU:HD13	1:A:74:MET:CG	0.54	2.33	22	2
1:A:32:LEU:CD2	1:A:76:PHE:CD2	0.54	2.84	16	4
1:A:70:PHE:CD2	1:B:82:THR:HG22	0.54	2.37	14	3
1:A:73:PHE:CZ	1:B:3:LEU:HG	0.54	2.37	19	2
1:B:27:LEU:HD23	1:B:31:GLU:OE1	0.54	2.02	21	1
1:B:60:LEU:HD22	1:B:76:PHE:CE2	0.54	2.38	23	1
1:A:17:TYR:CE1	1:A:35:LEU:HG	0.54	2.37	20	6
1:A:25:HIS:HB3	1:A:70:PHE:CZ	0.54	2.37	23	8
1:B:59:THR:O	1:B:63:ASP:N	0.54	2.40	19	12
1:B:24:LYS:O	1:B:25:HIS:CD2	0.54	2.60	24	2
1:B:36:ILE:HG21	1:B:80:ILE:HD12	0.54	1.77	7	1
1:B:64:GLY:O	1:B:65:ASP:CB	0.54	2.55	24	4
1:A:14:PHE:CZ	1:A:27:LEU:HD13	0.54	2.34	13	1
1:A:3:LEU:HD13	1:B:35:LEU:HD21	0.54	1.79	24	1
1:A:77:VAL:CG1	1:A:78:ALA:N	0.54	2.70	6	20
1:B:24:LYS:C	1:B:25:HIS:CD2	0.54	2.81	6	1
1:A:40:LEU:HD11	1:B:4:GLU:OE2	0.54	2.03	8	1
1:A:81:THR:OG1	1:B:7:VAL:CG1	0.54	2.55	21	2
1:A:35:LEU:HG	1:B:3:LEU:HD11	0.54	1.79	15	1
1:A:65:ASP:O	1:A:67:GLU:N	0.54	2.41	24	1
1:A:37:ASN:OD1	1:A:37:ASN:N	0.54	2.40	7	5
1:A:73:PHE:O	1:A:77:VAL:CG1	0.54	2.56	16	7
1:B:2:GLU:O	1:B:6:ALA:CB	0.54	2.56	7	8
1:B:36:ILE:O	1:B:40:LEU:N	0.54	2.40	15	4
1:B:10:LEU:HD23	1:B:73:PHE:HE1	0.54	1.62	8	1
1:A:52:VAL:CG1	1:A:53:VAL:N	0.54	2.70	12	1
1:B:52:VAL:CG1	1:B:53:VAL:N	0.54	2.70	12	1
1:A:3:LEU:HD21	1:B:35:LEU:HG	0.54	1.78	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:68:CYS:HA	1:B:72:GLU:CB	0.54	2.31	22	2
1:B:65:ASP:O	1:B:67:GLU:N	0.54	2.41	24	1
1:B:10:LEU:O	1:B:11:ILE:C	0.54	2.46	15	10
1:A:19:GLY:O	1:A:21:GLU:N	0.54	2.40	2	2
1:B:54:ASP:O	1:B:58:GLU:CB	0.54	2.56	17	4
1:A:3:LEU:HD22	1:B:73:PHE:CZ	0.54	2.37	7	1
1:B:43:PHE:HE2	1:B:56:VAL:HG21	0.54	1.63	21	3
1:A:3:LEU:HD11	1:B:35:LEU:O	0.54	2.03	8	1
1:B:36:ILE:HG13	1:B:40:LEU:HD12	0.54	1.77	10	1
1:A:3:LEU:CD1	1:A:4:GLU:N	0.54	2.63	1	3
1:B:0:MET:O	1:B:2:GLU:N	0.54	2.41	1	4
1:A:32:LEU:HD23	1:A:60:LEU:HD13	0.54	1.77	2	1
1:B:59:THR:O	1:B:63:ASP:CB	0.54	2.56	3	1
1:A:3:LEU:CD1	1:B:35:LEU:O	0.54	2.56	8	1
1:A:32:LEU:O	1:A:36:ILE:CD1	0.54	2.56	9	2
1:B:43:PHE:CE2	1:B:49:GLU:OE2	0.54	2.61	14	1
1:B:75:ALA:O	1:B:78:ALA:N	0.54	2.40	10	2
1:A:24:LYS:C	1:A:25:HIS:CD2	0.54	2.81	6	1
1:A:36:ILE:O	1:A:40:LEU:N	0.54	2.40	15	5
1:A:57:MET:O	1:A:61:ASP:CB	0.54	2.56	24	4
1:A:35:LEU:HD11	1:B:3:LEU:HD11	0.54	1.79	16	1
1:B:52:VAL:HG22	1:B:83:ALA:C	0.54	2.23	17	1
1:A:0:MET:O	1:A:3:LEU:HD12	0.54	2.01	18	1
1:A:14:PHE:CE2	1:A:27:LEU:HD23	0.54	2.37	22	1
1:B:73:PHE:O	1:B:77:VAL:HG12	0.54	2.02	21	6
1:A:59:THR:O	1:A:63:ASP:N	0.54	2.41	19	12
1:A:77:VAL:O	1:A:81:THR:CB	0.54	2.56	5	4
1:A:78:ALA:HB2	1:B:74:MET:CB	0.54	2.33	15	3
1:B:7:VAL:CG1	1:B:8:VAL:N	0.54	2.70	16	6
1:B:37:ASN:OD1	1:B:38:ASN:N	0.54	2.41	11	3
1:B:8:VAL:O	1:B:11:ILE:HG12	0.54	2.03	10	3
1:A:76:PHE:O	1:A:79:MET:N	0.54	2.41	24	11
1:A:21:GLU:CG	1:A:22:GLY:N	0.54	2.71	8	1
1:B:4:GLU:OE2	1:B:5:LYS:CE	0.54	2.56	14	1
1:B:10:LEU:HD13	1:B:74:MET:CG	0.54	2.33	22	2
1:B:76:PHE:CZ	1:B:80:ILE:HG12	0.54	2.37	24	1
1:B:37:ASN:N	1:B:37:ASN:OD1	0.54	2.40	7	4
1:B:73:PHE:O	1:B:77:VAL:CG1	0.54	2.56	24	7
1:A:54:ASP:O	1:A:58:GLU:CB	0.54	2.55	17	4
1:A:59:THR:O	1:A:63:ASP:CB	0.54	2.55	3	1
1:A:3:LEU:HG	1:B:73:PHE:CZ	0.54	2.38	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:79:MET:HA	1:B:82:THR:OG1	0.54	2.02	24	6
1:A:68:CYS:CB	1:A:72:GLU:OE1	0.54	2.56	7	1
1:A:73:PHE:CZ	1:B:3:LEU:HD22	0.54	2.37	7	2
1:A:4:GLU:O	1:A:7:VAL:N	0.54	2.41	8	3
1:A:27:LEU:O	1:A:68:CYS:CB	0.54	2.56	17	4
1:B:35:LEU:HD11	1:B:73:PHE:CD1	0.54	2.38	13	2
1:B:14:PHE:CE2	1:B:70:PHE:CD1	0.54	2.96	15	2
1:A:52:VAL:HG11	1:A:83:ALA:CA	0.54	2.32	16	1
1:A:53:VAL:O	1:A:57:MET:CG	0.54	2.56	19	10
1:B:63:ASP:O	1:B:64:GLY:C	0.54	2.45	11	14
1:A:3:LEU:CD2	1:B:73:PHE:CE1	0.54	2.90	5	2
1:A:43:PHE:CE2	1:A:49:GLU:OE2	0.54	2.61	14	1
1:A:79:MET:O	1:A:83:ALA:CB	0.54	2.56	15	1
1:A:52:VAL:HG22	1:A:83:ALA:C	0.54	2.23	17	1
1:A:29:LYS:CA	1:A:65:ASP:OD1	0.54	2.56	21	1
1:A:0:MET:O	1:A:2:GLU:N	0.53	2.41	1	4
1:A:11:ILE:HG13	1:A:12:ASP:N	0.53	2.17	21	16
1:A:13:VAL:HG11	1:A:73:PHE:CZ	0.53	2.38	24	4
1:B:72:GLU:O	1:B:75:ALA:N	0.53	2.41	24	3
1:B:62:SER:O	1:B:64:GLY:N	0.53	2.41	25	4
1:B:64:GLY:O	1:B:67:GLU:CB	0.53	2.56	5	1
1:A:77:VAL:CG1	1:B:74:MET:HE2	0.53	2.33	24	2
1:B:68:CYS:CB	1:B:72:GLU:OE1	0.53	2.56	7	1
1:B:79:MET:O	1:B:83:ALA:CB	0.53	2.56	15	1
1:A:27:LEU:O	1:A:67:GLU:CB	0.53	2.56	1	1
1:A:47:ILE:O	1:A:49:GLU:N	0.53	2.41	20	12
1:B:77:VAL:O	1:B:81:THR:CB	0.53	2.57	4	4
1:A:2:GLU:O	1:A:6:ALA:CB	0.53	2.56	7	9
1:A:39:GLU:OE1	1:B:3:LEU:CB	0.53	2.56	20	6
1:A:76:PHE:CZ	1:A:80:ILE:HG12	0.53	2.38	24	1
1:A:75:ALA:O	1:A:78:ALA:N	0.53	2.41	10	2
1:B:41:SER:O	1:B:44:LEU:N	0.53	2.41	11	13
1:B:52:VAL:CG1	1:B:83:ALA:CB	0.53	2.85	3	7
1:B:52:VAL:O	1:B:55:LYS:N	0.53	2.42	21	17
1:A:37:ASN:OD1	1:A:38:ASN:N	0.53	2.41	11	3
1:A:32:LEU:O	1:A:35:LEU:CB	0.53	2.56	4	5
1:B:73:PHE:HE1	1:B:77:VAL:HG21	0.53	1.63	18	3
1:A:37:ASN:HB3	1:A:44:LEU:HD12	0.53	1.78	7	1
1:B:32:LEU:CD2	1:B:63:ASP:OD2	0.53	2.57	8	2
1:A:0:MET:O	1:B:39:GLU:CG	0.53	2.56	19	4
1:B:43:PHE:CE1	1:B:49:GLU:CG	0.53	2.92	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LYS:HA	1:A:60:LEU:HD21	0.53	1.81	24	1
1:A:36:ILE:HD12	1:A:80:ILE:HD13	0.53	1.79	24	1
1:A:35:LEU:O	1:A:39:GLU:OE1	0.53	2.25	24	9
1:A:72:GLU:O	1:A:75:ALA:N	0.53	2.41	24	3
1:B:25:HIS:O	1:B:26:LYS:CE	0.53	2.57	23	8
1:B:4:GLU:O	1:B:7:VAL:N	0.53	2.41	8	3
1:B:76:PHE:O	1:B:80:ILE:CG1	0.53	2.55	9	1
1:A:27:LEU:HD23	1:A:31:GLU:OE1	0.53	2.04	21	1
1:A:73:PHE:O	1:A:77:VAL:HG12	0.53	2.03	21	6
1:B:27:LEU:O	1:B:67:GLU:CA	0.53	2.57	1	1
1:B:46:GLU:O	1:B:48:LYS:N	0.53	2.42	13	8
1:B:53:VAL:O	1:B:57:MET:CG	0.53	2.57	19	10
1:B:19:GLY:O	1:B:21:GLU:N	0.53	2.41	2	2
1:A:35:LEU:HD11	1:A:73:PHE:CD1	0.53	2.38	13	2
1:B:18:SER:O	1:B:23:ASP:CB	0.53	2.57	14	1
1:B:46:GLU:O	1:B:53:VAL:HG22	0.53	2.02	14	1
1:B:52:VAL:HG11	1:B:83:ALA:CA	0.53	2.33	16	1
1:A:70:PHE:HB2	1:B:82:THR:CG2	0.53	2.34	19	1
1:A:82:THR:CG2	1:B:70:PHE:HB2	0.53	2.32	19	1
1:A:10:LEU:CD1	1:A:74:MET:HE2	0.53	2.30	21	1
1:B:27:LEU:CB	1:B:31:GLU:HB2	0.53	2.33	4	1
1:A:70:PHE:O	1:A:72:GLU:N	0.53	2.42	10	2
1:A:17:TYR:OH	1:B:3:LEU:CD1	0.53	2.57	23	5
1:B:20:ARG:O	1:B:21:GLU:CB	0.53	2.55	11	1
1:A:4:GLU:OE2	1:A:5:LYS:CE	0.53	2.56	14	1
1:A:77:VAL:HG23	1:B:4:GLU:CD	0.53	2.23	16	1
1:B:37:ASN:HA	1:B:44:LEU:HD13	0.53	1.80	21	1
1:A:10:LEU:O	1:A:11:ILE:C	0.53	2.45	9	11
1:B:76:PHE:O	1:B:80:ILE:HG13	0.53	2.04	17	6
1:B:0:MET:CG	1:B:1:SER:N	0.53	2.71	12	3
1:B:10:LEU:N	1:B:10:LEU:CD1	0.53	2.67	9	1
1:B:37:ASN:HB2	1:B:44:LEU:HD12	0.53	1.81	19	3
1:A:51:GLU:O	1:A:55:LYS:CG	0.53	2.56	13	1
1:B:51:GLU:O	1:B:55:LYS:CG	0.53	2.56	13	1
1:B:39:GLU:HG3	1:B:40:LEU:N	0.53	2.19	13	11
1:B:32:LEU:O	1:B:36:ILE:CD1	0.53	2.56	9	2
1:A:37:ASN:HB2	1:A:44:LEU:HD12	0.53	1.81	19	3
1:A:14:PHE:CE2	1:A:18:SER:OG	0.53	2.57	15	1
1:A:74:MET:HB3	1:B:78:ALA:CB	0.53	2.34	22	1
1:A:16:GLN:O	1:A:20:ARG:CB	0.53	2.57	19	15
1:A:25:HIS:O	1:A:26:LYS:CE	0.53	2.57	23	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LYS:O	1:A:30:SER:N	0.53	2.42	19	10
1:A:41:SER:O	1:A:44:LEU:N	0.53	2.41	11	12
1:A:52:VAL:O	1:A:55:LYS:N	0.53	2.42	5	17
1:B:11:ILE:HG13	1:B:12:ASP:N	0.53	2.18	4	16
1:B:13:VAL:HG11	1:B:73:PHE:CZ	0.53	2.39	24	3
1:B:16:GLN:O	1:B:20:ARG:CB	0.53	2.57	22	16
1:B:26:LYS:HD2	1:B:27:LEU:N	0.53	2.19	3	4
1:B:32:LEU:O	1:B:35:LEU:CB	0.53	2.56	4	5
1:A:32:LEU:CD2	1:A:63:ASP:OD2	0.53	2.57	8	2
1:B:74:MET:O	1:B:78:ALA:CB	0.53	2.57	5	3
1:B:40:LEU:O	1:B:42:HIS:N	0.53	2.42	6	8
1:A:39:GLU:CB	1:B:4:GLU:OE1	0.53	2.57	11	1
1:B:14:PHE:O	1:B:15:HIS:C	0.53	2.48	11	20
1:B:52:VAL:O	1:B:56:VAL:N	0.53	2.42	5	20
1:A:4:GLU:N	1:B:39:GLU:HB2	0.53	2.19	4	8
1:A:76:PHE:O	1:A:80:ILE:HG13	0.53	2.04	19	6
1:B:1:SER:O	1:B:5:LYS:CG	0.53	2.57	17	7
1:A:50:GLN:O	1:A:53:VAL:N	0.53	2.42	14	9
1:B:49:GLU:OE2	1:B:56:VAL:HG21	0.53	2.02	4	2
1:A:40:LEU:O	1:A:42:HIS:N	0.53	2.42	22	8
1:B:10:LEU:O	1:B:12:ASP:N	0.53	2.42	15	4
1:A:27:LEU:O	1:A:67:GLU:CA	0.52	2.57	1	1
1:A:4:GLU:HB3	1:B:39:GLU:CG	0.52	2.34	3	1
1:B:17:TYR:CG	1:B:35:LEU:HD12	0.52	2.36	19	4
1:A:26:LYS:CG	1:A:69:ASP:OD1	0.52	2.57	10	3
1:A:32:LEU:HD22	1:A:63:ASP:OD2	0.52	2.04	5	1
1:B:57:MET:O	1:B:61:ASP:CB	0.52	2.56	24	4
1:A:35:LEU:HD21	1:B:3:LEU:HD13	0.52	1.81	24	1
1:B:32:LEU:HD22	1:B:76:PHE:HD2	0.52	1.63	1	2
1:B:71:GLN:N	1:B:71:GLN:OE1	0.52	2.42	1	1
1:A:26:LYS:HD2	1:A:27:LEU:N	0.52	2.19	3	4
1:A:77:VAL:HG13	1:A:78:ALA:N	0.52	2.19	24	7
1:A:43:PHE:HE2	1:A:80:ILE:HG23	0.52	1.63	7	1
1:A:3:LEU:CB	1:B:39:GLU:OE1	0.52	2.58	22	4
1:B:29:LYS:CA	1:B:65:ASP:OD1	0.52	2.57	21	1
1:A:52:VAL:O	1:A:56:VAL:N	0.52	2.42	5	20
1:B:1:SER:O	1:B:3:LEU:N	0.52	2.42	12	18
1:A:39:GLU:HG3	1:A:40:LEU:N	0.52	2.19	20	11
1:B:16:GLN:O	1:B:20:ARG:CG	0.52	2.57	25	7
1:B:14:PHE:O	1:B:18:SER:OG	0.52	2.26	20	5
1:A:69:ASP:O	1:A:72:GLU:CB	0.52	2.58	10	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:PHE:CE1	1:B:49:GLU:OE1	0.52	2.62	5	2
1:B:47:ILE:O	1:B:49:GLU:N	0.52	2.42	20	12
1:B:18:SER:OG	1:B:26:LYS:N	0.52	2.42	2	3
1:A:73:PHE:HE1	1:A:77:VAL:HG21	0.52	1.64	18	3
1:B:70:PHE:O	1:B:72:GLU:N	0.52	2.42	10	2
1:A:0:MET:HE2	1:A:3:LEU:CD1	0.52	2.33	9	1
1:B:10:LEU:HG	1:B:74:MET:CG	0.52	2.34	9	1
1:A:69:ASP:N	1:A:72:GLU:HG3	0.52	2.19	10	11
1:B:16:GLN:O	1:B:20:ARG:HB3	0.52	2.05	19	20
1:B:55:LYS:O	1:B:58:GLU:N	0.52	2.43	5	15
1:B:69:ASP:O	1:B:72:GLU:CB	0.52	2.58	10	8
1:A:46:GLU:OE2	1:A:57:MET:CG	0.52	2.58	2	1
1:B:15:HIS:O	1:B:19:GLY:N	0.52	2.43	3	3
1:A:81:THR:CB	1:B:7:VAL:HG22	0.52	2.35	5	1
1:A:0:MET:CG	1:A:1:SER:N	0.52	2.71	12	3
1:A:1:SER:CB	1:B:39:GLU:HG3	0.52	2.34	8	1
1:A:16:GLN:CG	1:A:20:ARG:HD2	0.52	2.35	24	3
1:A:1:SER:O	1:A:3:LEU:N	0.52	2.42	12	18
1:A:32:LEU:HD22	1:A:76:PHE:HD2	0.52	1.62	1	2
1:B:27:LEU:O	1:B:67:GLU:CB	0.52	2.57	1	1
1:A:1:SER:O	1:A:5:LYS:CG	0.52	2.58	17	8
1:B:13:VAL:CG1	1:B:17:TYR:CE1	0.52	2.93	10	3
1:B:79:MET:O	1:B:82:THR:OG1	0.52	2.27	24	12
1:A:74:MET:O	1:A:78:ALA:CB	0.52	2.58	5	3
1:A:35:LEU:CD1	1:A:73:PHE:CE2	0.52	2.79	8	1
1:B:0:MET:HE2	1:B:3:LEU:CD1	0.52	2.34	9	1
1:B:43:PHE:CZ	1:B:80:ILE:HG23	0.52	2.39	18	2
1:A:39:GLU:CG	1:B:0:MET:O	0.52	2.58	19	3
1:A:28:LYS:O	1:A:31:GLU:N	0.52	2.43	19	1
1:A:37:ASN:HA	1:A:44:LEU:HD13	0.52	1.80	21	1
1:A:13:VAL:HG13	1:B:3:LEU:HD21	0.52	1.78	23	1
1:A:14:PHE:O	1:A:15:HIS:C	0.52	2.48	11	21
1:A:46:GLU:O	1:A:48:LYS:N	0.52	2.42	13	8
1:A:16:GLN:O	1:A:20:ARG:CG	0.52	2.58	24	7
1:A:34:GLU:O	1:A:38:ASN:N	0.52	2.42	5	8
1:A:39:GLU:HB2	1:B:4:GLU:N	0.52	2.20	4	9
1:B:34:GLU:O	1:B:38:ASN:N	0.52	2.42	5	7
1:B:32:LEU:CD1	1:B:68:CYS:SG	0.52	2.97	3	1
1:B:50:GLN:O	1:B:53:VAL:N	0.52	2.43	16	8
1:A:27:LEU:CB	1:A:31:GLU:HB2	0.52	2.34	4	1
1:B:69:ASP:O	1:B:72:GLU:CG	0.52	2.58	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LEU:HG	1:A:74:MET:CG	0.52	2.35	9	1
1:A:60:LEU:HD23	1:A:76:PHE:CZ	0.52	2.40	23	2
1:B:27:LEU:O	1:B:68:CYS:CB	0.52	2.57	14	4
1:B:32:LEU:HD13	1:B:32:LEU:C	0.52	2.25	13	1
1:B:28:LYS:O	1:B:31:GLU:N	0.52	2.42	19	1
1:A:32:LEU:HG	1:A:76:PHE:CE2	0.52	2.40	22	3
1:A:40:LEU:CB	1:A:43:PHE:CD1	0.52	2.92	22	1
1:A:18:SER:OG	1:A:26:LYS:N	0.52	2.42	2	4
1:A:79:MET:O	1:A:82:THR:OG1	0.52	2.27	24	9
1:A:32:LEU:CD1	1:A:68:CYS:SG	0.52	2.98	3	2
1:A:7:VAL:HG22	1:B:81:THR:CB	0.52	2.35	5	1
1:A:3:LEU:HD11	1:B:35:LEU:HG	0.52	1.81	15	1
1:A:78:ALA:HB2	1:B:74:MET:HB3	0.52	1.81	15	2
1:B:69:ASP:OD2	1:B:71:GLN:CG	0.52	2.58	19	1
1:A:35:LEU:HD23	1:B:3:LEU:CD1	0.52	2.34	21	1
1:A:43:PHE:CE1	1:A:49:GLU:CG	0.52	2.92	23	1
1:B:39:GLU:OE2	1:B:77:VAL:CG2	0.52	2.58	25	1
1:B:69:ASP:N	1:B:72:GLU:HG3	0.52	2.18	10	11
1:B:26:LYS:CG	1:B:69:ASP:OD1	0.52	2.57	10	3
1:B:77:VAL:HG13	1:B:78:ALA:N	0.52	2.20	24	7
1:A:10:LEU:O	1:A:12:ASP:N	0.52	2.43	15	4
1:A:20:ARG:CG	1:A:21:GLU:N	0.52	2.72	10	2
1:A:13:VAL:HG23	1:A:14:PHE:N	0.52	2.20	21	1
1:B:40:LEU:CB	1:B:43:PHE:CD1	0.52	2.93	22	1
1:A:3:LEU:HD22	1:A:3:LEU:O	0.52	2.05	1	1
1:A:43:PHE:CE1	1:A:49:GLU:OE1	0.52	2.63	5	2
1:A:7:VAL:C	1:A:11:ILE:HG23	0.52	2.24	9	1
1:A:46:GLU:O	1:A:46:GLU:CG	0.52	2.58	11	2
1:A:68:CYS:O	1:A:68:CYS:SG	0.52	2.68	16	2
1:B:32:LEU:HG	1:B:76:PHE:CE2	0.52	2.40	22	3
1:A:28:LYS:O	1:A:29:LYS:C	0.51	2.49	12	20
1:A:55:LYS:O	1:A:58:GLU:N	0.51	2.43	12	15
1:B:1:SER:O	1:B:2:GLU:C	0.51	2.49	6	22
1:B:28:LYS:O	1:B:30:SER:N	0.51	2.43	16	10
1:B:7:VAL:O	1:B:10:LEU:N	0.51	2.44	14	3
1:A:15:HIS:O	1:A:19:GLY:N	0.51	2.43	3	3
1:A:35:LEU:O	1:B:3:LEU:CD1	0.51	2.57	8	1
1:A:39:GLU:HG3	1:B:1:SER:CB	0.51	2.35	8	1
1:A:3:LEU:CD1	1:B:17:TYR:OH	0.51	2.58	13	4
1:A:8:VAL:HA	1:A:11:ILE:HG12	0.51	1.82	16	2
1:A:69:ASP:OD2	1:A:71:GLN:CG	0.51	2.58	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:VAL:CG1	1:A:17:TYR:CE1	0.51	2.93	10	2
1:B:52:VAL:O	1:B:56:VAL:CG2	0.51	2.57	18	4
1:B:14:PHE:CZ	1:B:27:LEU:HB2	0.51	2.40	20	1
1:A:78:ALA:O	1:A:82:THR:CG2	0.51	2.53	24	2
1:A:3:LEU:HD21	1:B:13:VAL:CG2	0.51	2.34	24	1
1:A:71:GLN:N	1:A:71:GLN:OE1	0.51	2.43	1	1
1:A:74:MET:HA	1:A:77:VAL:CG1	0.51	2.36	18	14
1:A:70:PHE:CB	1:B:82:THR:HG21	0.51	2.35	14	3
1:B:52:VAL:CG1	1:B:83:ALA:HB3	0.51	2.25	6	1
1:A:43:PHE:HE2	1:A:56:VAL:HG21	0.51	1.65	13	3
1:A:60:LEU:HD23	1:A:76:PHE:CE2	0.51	2.41	9	1
1:B:7:VAL:C	1:B:11:ILE:HG23	0.51	2.24	9	1
1:B:46:GLU:O	1:B:46:GLU:CG	0.51	2.58	11	2
1:A:3:LEU:O	1:B:10:LEU:HD21	0.51	2.06	16	1
1:B:10:LEU:HD22	1:B:74:MET:HG2	0.51	1.83	17	1
1:B:34:GLU:O	1:B:38:ASN:ND2	0.51	2.44	18	1
1:A:1:SER:O	1:A:2:GLU:C	0.51	2.48	6	23
1:A:39:GLU:CG	1:B:4:GLU:HB3	0.51	2.34	3	2
1:A:69:ASP:O	1:A:72:GLU:CG	0.51	2.58	7	1
1:B:17:TYR:OH	1:B:39:GLU:OE2	0.51	2.28	7	1
1:A:82:THR:CG2	1:B:70:PHE:HB3	0.51	2.35	15	5
1:B:16:GLN:CG	1:B:20:ARG:HD2	0.51	2.35	24	3
1:A:32:LEU:HD13	1:A:32:LEU:C	0.51	2.26	13	1
1:A:13:VAL:CG2	1:B:3:LEU:HD21	0.51	2.36	24	1
1:B:39:GLU:CG	1:B:40:LEU:N	0.51	2.73	13	6
1:A:17:TYR:CZ	1:A:35:LEU:HG	0.51	2.41	6	8
1:B:10:LEU:HD22	1:B:74:MET:CG	0.51	2.35	8	1
1:A:14:PHE:CD2	1:A:73:PHE:HD2	0.51	2.23	19	2
1:A:14:PHE:CD1	1:A:18:SER:HB3	0.51	2.41	11	4
1:A:17:TYR:CG	1:A:35:LEU:HD12	0.51	2.36	19	3
1:A:74:MET:CE	1:B:74:MET:SD	0.51	2.98	18	2
1:A:10:LEU:HD21	1:B:3:LEU:O	0.51	2.06	16	1
1:B:68:CYS:SG	1:B:68:CYS:O	0.51	2.69	16	1
1:B:25:HIS:CG	1:B:70:PHE:CZ	0.51	2.98	20	1
1:A:77:VAL:HG13	1:B:74:MET:HE1	0.51	1.82	22	1
1:A:39:GLU:OE2	1:A:77:VAL:CG2	0.51	2.59	25	1
1:A:17:TYR:OH	1:A:39:GLU:OE2	0.51	2.28	7	1
1:A:35:LEU:O	1:B:3:LEU:HD11	0.51	2.06	8	1
1:B:60:LEU:HD23	1:B:76:PHE:CZ	0.51	2.40	23	2
1:A:18:SER:O	1:A:23:ASP:CB	0.51	2.58	14	1
1:A:43:PHE:CE1	1:A:49:GLU:HB3	0.51	2.41	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:GLU:OE2	1:A:40:LEU:HD12	0.51	2.05	20	1
1:A:78:ALA:CB	1:B:74:MET:HB3	0.51	2.35	22	1
1:B:39:GLU:OE2	1:B:77:VAL:HG23	0.51	2.05	25	1
1:A:16:GLN:O	1:A:20:ARG:HB3	0.51	2.06	19	21
1:B:46:GLU:OE2	1:B:57:MET:CG	0.51	2.58	2	1
1:A:52:VAL:O	1:A:56:VAL:CG2	0.51	2.57	18	4
1:B:0:MET:O	1:B:3:LEU:HD12	0.51	2.05	18	1
1:A:0:MET:O	1:B:39:GLU:HG2	0.51	2.06	24	3
1:A:69:ASP:OD1	1:A:70:PHE:N	0.51	2.42	1	2
1:B:28:LYS:O	1:B:29:LYS:C	0.51	2.49	21	20
1:B:74:MET:HA	1:B:77:VAL:CG1	0.51	2.36	23	12
1:B:80:ILE:O	1:B:82:THR:N	0.51	2.44	18	4
1:A:43:PHE:CZ	1:A:49:GLU:OE1	0.51	2.64	4	1
1:A:82:THR:HG21	1:B:70:PHE:CB	0.51	2.32	11	2
1:B:40:LEU:O	1:B:41:SER:C	0.51	2.49	22	15
1:A:47:ILE:O	1:A:47:ILE:CD1	0.51	2.56	14	3
1:A:3:LEU:HD11	1:B:17:TYR:CZ	0.51	2.41	9	3
1:A:64:GLY:CA	1:A:72:GLU:OE1	0.51	2.59	10	1
1:A:17:TYR:O	1:A:19:GLY:N	0.51	2.44	13	2
1:A:43:PHE:CZ	1:A:80:ILE:HG23	0.51	2.40	18	2
1:B:43:PHE:CZ	1:B:56:VAL:CG2	0.51	2.92	18	1
1:B:13:VAL:HG23	1:B:14:PHE:N	0.51	2.20	21	1
1:B:32:LEU:CD2	1:B:60:LEU:CD2	0.51	2.81	22	1
1:B:29:LYS:HA	1:B:60:LEU:HD21	0.51	1.81	24	1
1:A:25:HIS:HB3	1:A:70:PHE:CE1	0.51	2.41	1	7
1:A:10:LEU:CD2	1:B:3:LEU:CD2	0.51	2.88	3	1
1:A:18:SER:CB	1:A:25:HIS:HA	0.51	2.36	16	4
1:A:49:GLU:OE1	1:A:52:VAL:CG1	0.51	2.59	4	2
1:B:49:GLU:OE1	1:B:52:VAL:CG1	0.51	2.59	4	2
1:A:27:LEU:O	1:A:68:CYS:N	0.51	2.44	21	3
1:B:37:ASN:O	1:B:37:ASN:ND2	0.51	2.43	8	1
1:B:47:ILE:O	1:B:47:ILE:CD1	0.51	2.56	14	3
1:A:7:VAL:HA	1:A:10:LEU:HD23	0.51	1.83	9	1
1:B:14:PHE:CD2	1:B:73:PHE:HD2	0.51	2.23	19	2
1:B:14:PHE:CD1	1:B:18:SER:HB3	0.51	2.41	11	3
1:A:15:HIS:O	1:A:19:GLY:CA	0.51	2.59	23	4
1:B:58:GLU:O	1:B:62:SER:N	0.51	2.43	20	1
1:B:55:LYS:N	1:B:55:LYS:HD3	0.51	2.21	7	1
1:A:16:GLN:HG3	1:A:20:ARG:CB	0.51	2.36	9	1
1:A:43:PHE:CD1	1:A:49:GLU:HG2	0.51	2.41	19	1
1:B:16:GLN:HG2	1:B:20:ARG:CD	0.50	2.36	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:60:LEU:HD23	1:B:76:PHE:CE2	0.50	2.41	9	1
1:A:30:SER:OG	1:A:31:GLU:N	0.50	2.44	10	1
1:B:7:VAL:O	1:B:11:ILE:CG2	0.50	2.55	16	3
1:A:3:LEU:HD12	1:B:73:PHE:CZ	0.50	2.41	16	1
1:B:52:VAL:CG2	1:B:83:ALA:C	0.50	2.80	17	1
1:A:43:PHE:CZ	1:A:56:VAL:CG2	0.50	2.91	18	1
1:B:43:PHE:CD1	1:B:49:GLU:HG2	0.50	2.41	19	1
1:B:17:TYR:CE1	1:B:35:LEU:HA	0.50	2.41	21	7
1:A:27:LEU:HB2	1:A:68:CYS:O	0.50	2.06	12	10
1:B:17:TYR:CE2	1:B:35:LEU:CG	0.50	2.94	24	5
1:B:64:GLY:O	1:B:65:ASP:O	0.50	2.29	9	3
1:B:36:ILE:HG12	1:B:76:PHE:CE2	0.50	2.41	5	4
1:B:64:GLY:CA	1:B:72:GLU:OE1	0.50	2.59	10	1
1:A:9:ALA:O	1:A:12:ASP:N	0.50	2.44	12	1
1:A:36:ILE:HG13	1:A:76:PHE:CE1	0.50	2.42	18	1
1:A:58:GLU:O	1:A:62:SER:N	0.50	2.44	20	1
1:A:3:LEU:CD1	1:B:35:LEU:HD23	0.50	2.33	21	1
1:B:36:ILE:HD12	1:B:80:ILE:HD13	0.50	1.78	24	1
1:A:17:TYR:CE1	1:A:35:LEU:HA	0.50	2.40	21	7
1:B:27:LEU:HB2	1:B:68:CYS:O	0.50	2.05	12	10
1:B:43:PHE:CZ	1:B:49:GLU:OE1	0.50	2.65	4	1
1:A:52:VAL:CG1	1:A:83:ALA:HB3	0.50	2.26	6	1
1:B:17:TYR:OH	1:B:38:ASN:ND2	0.50	2.45	24	1
1:B:58:GLU:HG3	1:B:59:THR:N	0.50	2.21	23	21
1:A:39:GLU:CA	1:B:4:GLU:HB2	0.50	2.36	5	3
1:B:27:LEU:O	1:B:68:CYS:N	0.50	2.44	21	3
1:A:11:ILE:O	1:A:15:HIS:HB2	0.50	2.07	13	5
1:B:16:GLN:O	1:B:19:GLY:N	0.50	2.44	9	3
1:B:21:GLU:CG	1:B:22:GLY:N	0.50	2.71	8	1
1:B:16:GLN:HG3	1:B:20:ARG:CB	0.50	2.36	9	1
1:B:10:LEU:CD1	1:B:74:MET:HE1	0.50	2.35	13	1
1:A:39:GLU:HG2	1:B:0:MET:O	0.50	2.07	24	3
1:B:25:HIS:HB3	1:B:70:PHE:CE1	0.50	2.42	1	7
1:B:69:ASP:OD1	1:B:70:PHE:N	0.50	2.43	1	2
1:A:64:GLY:O	1:A:65:ASP:O	0.50	2.29	9	3
1:A:74:MET:CB	1:B:78:ALA:HB2	0.50	2.36	12	3
1:B:9:ALA:O	1:B:12:ASP:N	0.50	2.43	12	2
1:B:17:TYR:CZ	1:B:35:LEU:HG	0.50	2.41	22	9
1:A:39:GLU:CG	1:A:40:LEU:N	0.50	2.73	13	6
1:A:48:LYS:CD	1:A:48:LYS:N	0.50	2.75	5	1
1:A:7:VAL:HG11	1:B:81:THR:CB	0.50	2.37	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:51:GLU:O	1:B:55:LYS:HG2	0.50	2.06	13	2
1:B:78:ALA:O	1:B:81:THR:N	0.50	2.44	13	1
1:B:10:LEU:HD22	1:B:73:PHE:HZ	0.50	1.65	16	1
1:A:14:PHE:HE1	1:A:73:PHE:CB	0.50	2.19	24	2
1:B:32:LEU:CG	1:B:76:PHE:CD2	0.50	2.95	22	3
1:A:74:MET:HE1	1:B:77:VAL:HG13	0.50	1.83	22	1
1:A:3:LEU:HD21	1:B:13:VAL:HG22	0.50	1.84	24	1
1:A:4:GLU:HB2	1:B:39:GLU:HB3	0.50	1.82	14	5
1:A:17:TYR:CE2	1:A:35:LEU:CG	0.50	2.95	10	6
1:A:4:GLU:OE1	1:B:40:LEU:CD2	0.50	2.58	3	2
1:A:16:GLN:O	1:A:19:GLY:N	0.50	2.44	9	4
1:B:7:VAL:HA	1:B:10:LEU:HG	0.50	1.84	19	6
1:B:17:TYR:CE1	1:B:35:LEU:CG	0.50	2.95	25	5
1:A:74:MET:SD	1:B:74:MET:CE	0.50	3.00	9	2
1:A:73:PHE:CZ	1:B:3:LEU:HD12	0.50	2.41	16	1
1:A:52:VAL:CG2	1:A:83:ALA:C	0.50	2.80	17	1
1:B:52:VAL:HG22	1:B:83:ALA:HB1	0.50	1.83	17	1
1:A:14:PHE:CZ	1:A:27:LEU:HB2	0.50	2.42	20	1
1:A:17:TYR:CB	1:A:27:LEU:HD21	0.50	2.33	3	1
1:A:17:TYR:CE1	1:A:35:LEU:CG	0.50	2.95	25	5
1:A:55:LYS:N	1:A:55:LYS:HD3	0.50	2.20	7	1
1:A:37:ASN:O	1:A:37:ASN:ND2	0.50	2.44	8	1
1:A:73:PHE:CE2	1:B:3:LEU:HD12	0.50	2.41	16	1
1:A:32:LEU:CG	1:A:76:PHE:CD2	0.50	2.95	22	3
1:A:39:GLU:OE2	1:A:77:VAL:HG23	0.50	2.07	25	1
1:B:67:GLU:CG	1:B:69:ASP:OD1	0.50	2.60	8	2
1:A:39:GLU:CB	1:B:4:GLU:HB3	0.50	2.37	3	1
1:B:36:ILE:N	1:B:36:ILE:HD12	0.50	2.22	3	4
1:A:8:VAL:O	1:A:11:ILE:HG12	0.50	2.07	10	3
1:A:10:LEU:N	1:A:10:LEU:HD23	0.50	2.21	20	5
1:B:11:ILE:O	1:B:15:HIS:HB2	0.50	2.07	13	5
1:A:16:GLN:HG2	1:A:20:ARG:CD	0.50	2.36	24	2
1:A:16:GLN:CA	1:A:20:ARG:HB3	0.50	2.37	18	5
1:B:7:VAL:HA	1:B:10:LEU:HD23	0.50	1.84	9	1
1:B:8:VAL:HA	1:B:11:ILE:HG12	0.50	1.83	12	2
1:A:0:MET:CG	1:A:2:GLU:OE1	0.50	2.60	17	1
1:A:39:GLU:CB	1:B:3:LEU:HB2	0.50	2.37	17	2
1:A:34:GLU:O	1:A:38:ASN:ND2	0.50	2.43	18	1
1:A:49:GLU:O	1:A:53:VAL:CB	0.50	2.60	23	3
1:A:76:PHE:O	1:A:77:VAL:C	0.50	2.50	16	23
1:B:18:SER:CB	1:B:25:HIS:HA	0.50	2.36	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:14:PHE:CZ	1:B:73:PHE:HB2	0.50	2.42	8	1
1:B:69:ASP:OD1	1:B:69:ASP:N	0.50	2.45	9	3
1:A:19:GLY:O	1:A:20:ARG:C	0.50	2.50	24	3
1:A:7:VAL:O	1:A:11:ILE:CG2	0.50	2.54	16	2
1:A:48:LYS:CB	1:A:49:GLU:OE2	0.50	2.59	20	1
1:B:32:LEU:HD23	1:B:60:LEU:HG	0.50	1.84	21	2
1:A:6:ALA:O	1:A:10:LEU:HG	0.49	2.07	7	12
1:B:3:LEU:O	1:B:7:VAL:N	0.49	2.42	18	6
1:A:10:LEU:HD22	1:A:74:MET:CG	0.49	2.36	8	1
1:A:76:PHE:CE2	1:A:80:ILE:HD13	0.49	2.41	9	1
1:B:10:LEU:HD22	1:B:10:LEU:H	0.49	1.67	9	1
1:B:30:SER:OG	1:B:31:GLU:N	0.49	2.44	10	1
1:A:20:ARG:O	1:A:21:GLU:CG	0.49	2.60	11	1
1:A:27:LEU:CB	1:A:68:CYS:HB3	0.49	2.37	16	2
1:A:3:LEU:HD11	1:B:35:LEU:HD11	0.49	1.83	16	1
1:B:43:PHE:CE1	1:B:49:GLU:HB3	0.49	2.41	19	1
1:A:56:VAL:HG13	1:A:80:ILE:HD13	0.49	1.78	25	1
1:B:6:ALA:O	1:B:10:LEU:HG	0.49	2.07	7	12
1:A:20:ARG:O	1:A:20:ARG:HG3	0.49	2.07	2	1
1:A:7:VAL:HA	1:A:10:LEU:HG	0.49	1.84	19	6
1:B:78:ALA:O	1:B:82:THR:OG1	0.49	2.30	6	9
1:B:48:LYS:N	1:B:48:LYS:CD	0.49	2.75	5	1
1:B:10:LEU:O	1:B:13:VAL:HB	0.49	2.08	12	6
1:A:32:LEU:O	1:A:35:LEU:N	0.49	2.46	7	3
1:A:14:PHE:CZ	1:A:73:PHE:HB2	0.49	2.41	8	1
1:B:76:PHE:CE2	1:B:80:ILE:HD13	0.49	2.41	9	1
1:A:52:VAL:HG13	1:A:53:VAL:N	0.49	2.21	12	1
1:A:74:MET:O	1:B:74:MET:SD	0.49	2.70	13	1
1:A:69:ASP:OD1	1:A:71:GLN:CG	0.49	2.61	19	1
1:A:32:LEU:HD23	1:A:60:LEU:HG	0.49	1.83	21	2
1:A:21:GLU:O	1:A:23:ASP:N	0.49	2.45	24	1
1:A:29:LYS:HE3	1:A:63:ASP:HA	0.49	1.83	24	1
1:A:78:ALA:O	1:A:82:THR:OG1	0.49	2.31	6	7
1:B:3:LEU:O	1:B:6:ALA:N	0.49	2.46	5	3
1:B:10:LEU:CD2	1:B:74:MET:SD	0.49	3.01	5	2
1:A:18:SER:HB3	1:A:25:HIS:HA	0.49	1.84	21	3
1:A:39:GLU:CG	1:B:1:SER:HA	0.49	2.38	21	4
1:A:69:ASP:N	1:A:69:ASP:OD1	0.49	2.44	9	3
1:A:78:ALA:O	1:A:81:THR:N	0.49	2.45	13	1
1:B:17:TYR:O	1:B:19:GLY:N	0.49	2.45	13	2
1:A:3:LEU:HD12	1:B:73:PHE:CE2	0.49	2.41	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:LEU:CG	1:B:73:PHE:CZ	0.49	2.95	19	1
1:B:14:PHE:HE1	1:B:73:PHE:CB	0.49	2.19	24	2
1:B:20:ARG:NH2	1:B:34:GLU:OE2	0.49	2.45	20	1
1:B:47:ILE:C	1:B:47:ILE:CD1	0.49	2.81	7	11
1:A:7:VAL:O	1:A:10:LEU:N	0.49	2.46	14	3
1:A:13:VAL:O	1:A:14:PHE:C	0.49	2.50	17	14
1:A:36:ILE:HG12	1:A:76:PHE:CE2	0.49	2.42	5	4
1:B:18:SER:O	1:B:24:LYS:O	0.49	2.31	25	11
1:A:78:ALA:HB2	1:B:74:MET:CE	0.49	2.36	6	2
1:A:32:LEU:CD1	1:A:60:LEU:HD13	0.49	2.31	13	1
1:B:32:LEU:CD1	1:B:60:LEU:HD13	0.49	2.32	13	1
1:A:32:LEU:HG	1:A:76:PHE:CD2	0.49	2.43	20	3
1:B:17:TYR:CB	1:B:27:LEU:HD21	0.49	2.31	3	2
1:B:49:GLU:O	1:B:53:VAL:CB	0.49	2.60	23	3
1:A:27:LEU:CB	1:A:72:GLU:OE2	0.49	2.61	7	1
1:A:74:MET:HB3	1:B:74:MET:O	0.49	2.08	7	4
1:B:27:LEU:CB	1:B:72:GLU:OE2	0.49	2.61	7	1
1:B:27:LEU:HB2	1:B:72:GLU:OE2	0.49	2.08	7	1
1:B:27:LEU:CB	1:B:68:CYS:HB3	0.49	2.38	16	2
1:A:74:MET:SD	1:B:74:MET:O	0.49	2.70	13	1
1:A:10:LEU:HD22	1:A:74:MET:HG2	0.49	1.83	17	1
1:B:36:ILE:HG13	1:B:76:PHE:CE1	0.49	2.42	18	1
1:B:69:ASP:OD1	1:B:71:GLN:CG	0.49	2.60	19	1
1:A:26:LYS:CB	1:A:67:GLU:OE1	0.49	2.60	1	1
1:A:47:ILE:C	1:A:47:ILE:CD1	0.49	2.81	9	11
1:A:4:GLU:HB2	1:B:39:GLU:CA	0.49	2.38	25	4
1:A:51:GLU:O	1:A:55:LYS:HG2	0.49	2.07	13	3
1:A:67:GLU:O	1:A:72:GLU:OE2	0.49	2.30	24	4
1:B:46:GLU:HG2	1:B:53:VAL:CG2	0.49	2.38	16	2
1:A:20:ARG:NH2	1:A:34:GLU:OE2	0.49	2.45	20	1
1:A:3:LEU:HD21	1:B:73:PHE:CE2	0.49	2.42	21	1
1:A:79:MET:SD	1:B:71:GLN:CB	0.49	3.01	23	1
1:A:78:ALA:HB2	1:B:74:MET:HE3	0.49	1.85	25	1
1:A:39:GLU:HB3	1:B:4:GLU:HB2	0.49	1.85	21	6
1:A:16:GLN:O	1:A:17:TYR:C	0.49	2.51	10	16
1:A:40:LEU:O	1:A:41:SER:C	0.49	2.49	22	16
1:A:11:ILE:C	1:A:11:ILE:CD1	0.49	2.80	25	4
1:A:74:MET:CE	1:B:77:VAL:HG13	0.49	2.38	6	3
1:A:74:MET:O	1:B:74:MET:HB3	0.49	2.08	24	4
1:A:36:ILE:HG13	1:A:80:ILE:CD1	0.49	2.38	9	1
1:B:20:ARG:O	1:B:21:GLU:CG	0.49	2.60	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:CYS:CA	1:A:72:GLU:HB2	0.49	2.38	13	2
1:B:10:LEU:HA	1:B:13:VAL:CG2	0.49	2.38	21	2
1:B:73:PHE:O	1:B:77:VAL:HB	0.49	2.08	12	17
1:A:67:GLU:CG	1:A:69:ASP:OD1	0.49	2.61	8	2
1:B:69:ASP:N	1:B:72:GLU:HB2	0.49	2.23	16	7
1:B:27:LEU:HB3	1:B:31:GLU:CB	0.49	2.38	4	1
1:B:25:HIS:HB3	1:B:70:PHE:CE2	0.49	2.43	9	2
1:A:32:LEU:HD11	1:A:76:PHE:HD2	0.49	1.68	16	1
1:A:49:GLU:O	1:A:53:VAL:N	0.49	2.41	23	2
1:A:64:GLY:O	1:A:65:ASP:HB3	0.49	2.06	4	4
1:A:39:GLU:CD	1:B:3:LEU:CD1	0.49	2.80	7	1
1:A:81:THR:CB	1:B:7:VAL:HG11	0.49	2.38	8	1
1:B:3:LEU:CD2	1:B:4:GLU:N	0.49	2.76	11	1
1:B:52:VAL:HG13	1:B:53:VAL:N	0.49	2.22	12	1
1:B:7:VAL:HA	1:B:10:LEU:CD1	0.49	2.38	15	2
1:B:68:CYS:CA	1:B:72:GLU:HB2	0.49	2.38	13	2
1:A:4:GLU:CD	1:B:77:VAL:HG23	0.49	2.28	16	1
1:A:36:ILE:HG22	1:A:40:LEU:HD12	0.49	1.85	16	1
1:B:48:LYS:CB	1:B:49:GLU:OE2	0.49	2.61	20	1
1:B:43:PHE:CZ	1:B:56:VAL:HG11	0.49	2.43	21	1
1:B:21:GLU:O	1:B:23:ASP:N	0.49	2.46	24	1
1:B:29:LYS:HE3	1:B:63:ASP:HA	0.49	1.83	24	1
1:A:3:LEU:C	1:A:3:LEU:CD2	0.49	2.81	21	4
1:A:32:LEU:HD12	1:A:63:ASP:OD2	0.49	2.08	1	1
1:B:16:GLN:O	1:B:17:TYR:C	0.49	2.51	10	14
1:A:77:VAL:HG13	1:B:74:MET:CE	0.49	2.38	6	2
1:B:14:PHE:CE2	1:B:70:PHE:O	0.49	2.66	9	1
1:A:3:LEU:CD2	1:A:4:GLU:N	0.49	2.75	11	1
1:A:14:PHE:O	1:A:18:SER:OG	0.49	2.28	19	6
1:A:72:GLU:HA	1:A:75:ALA:CB	0.49	2.38	13	1
1:A:10:LEU:HD22	1:A:73:PHE:HZ	0.49	1.66	16	1
1:A:60:LEU:HD11	1:A:76:PHE:CZ	0.49	2.43	21	1
1:A:34:GLU:O	1:A:37:ASN:OD1	0.49	2.31	22	1
1:B:33:LYS:CE	1:B:46:GLU:OE2	0.49	2.61	22	1
1:A:10:LEU:HD12	1:A:74:MET:SD	0.49	2.48	23	1
1:A:60:LEU:HG	1:A:76:PHE:CZ	0.48	2.43	1	3
1:A:60:LEU:O	1:A:63:ASP:OD2	0.48	2.31	14	3
1:B:72:GLU:O	1:B:73:PHE:C	0.48	2.52	24	6
1:B:27:LEU:CD1	1:B:31:GLU:HB3	0.48	2.38	23	3
1:B:64:GLY:O	1:B:67:GLU:HB3	0.48	2.08	5	3
1:A:3:LEU:O	1:A:6:ALA:N	0.48	2.46	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LEU:CD2	1:A:74:MET:SD	0.48	3.01	5	2
1:A:25:HIS:HB3	1:A:70:PHE:CE2	0.48	2.43	9	2
1:B:36:ILE:CG2	1:B:43:PHE:CE1	0.48	2.96	8	1
1:A:3:LEU:CB	1:B:39:GLU:HG2	0.48	2.38	10	1
1:B:72:GLU:HA	1:B:75:ALA:CB	0.48	2.38	13	1
1:A:52:VAL:HG22	1:A:83:ALA:HB1	0.48	1.83	17	1
1:A:73:PHE:CZ	1:B:3:LEU:CG	0.48	2.95	19	1
1:A:65:ASP:O	1:A:66:GLY:C	0.48	2.51	20	2
1:A:35:LEU:HD11	1:A:73:PHE:HD2	0.48	1.64	2	2
1:A:49:GLU:HB2	1:A:52:VAL:CG2	0.48	2.38	17	8
1:A:36:ILE:CG2	1:A:43:PHE:CE1	0.48	2.96	8	1
1:A:44:LEU:C	1:A:44:LEU:CD1	0.48	2.79	8	1
1:B:16:GLN:CA	1:B:20:ARG:HB3	0.48	2.38	18	5
1:B:32:LEU:HD11	1:B:76:PHE:HD2	0.48	1.67	16	1
1:A:3:LEU:CD1	1:B:13:VAL:CG2	0.48	2.91	17	1
1:B:0:MET:CG	1:B:2:GLU:OE1	0.48	2.60	17	1
1:A:25:HIS:O	1:A:69:ASP:OD1	0.48	2.31	14	4
1:A:46:GLU:O	1:A:47:ILE:C	0.48	2.51	2	14
1:A:58:GLU:HG3	1:A:59:THR:N	0.48	2.22	23	20
1:A:27:LEU:C	1:A:28:LYS:CG	0.48	2.82	21	2
1:B:20:ARG:O	1:B:20:ARG:HG3	0.48	2.07	2	1
1:B:3:LEU:C	1:B:3:LEU:CD2	0.48	2.75	3	2
1:A:4:GLU:HB2	1:B:39:GLU:HB2	0.48	1.85	18	4
1:A:74:MET:CE	1:B:78:ALA:HB2	0.48	2.39	6	2
1:B:10:LEU:N	1:B:10:LEU:HD23	0.48	2.23	20	5
1:B:44:LEU:C	1:B:44:LEU:CD1	0.48	2.79	8	1
1:A:10:LEU:HD22	1:A:10:LEU:H	0.48	1.67	9	1
1:A:39:GLU:OE1	1:B:3:LEU:CD2	0.48	2.60	19	2
1:B:4:GLU:OE2	1:B:5:LYS:HE3	0.48	2.08	14	1
1:A:3:LEU:CG	1:A:4:GLU:N	0.48	2.76	16	1
1:A:3:LEU:HB2	1:B:39:GLU:CB	0.48	2.37	17	2
1:B:15:HIS:O	1:B:19:GLY:CA	0.48	2.61	23	4
1:A:33:LYS:CE	1:A:46:GLU:OE2	0.48	2.62	22	1
1:A:4:GLU:HG3	1:B:40:LEU:HD23	0.48	1.86	1	1
1:A:74:MET:SD	1:B:78:ALA:HB1	0.48	2.47	1	1
1:A:27:LEU:HB2	1:A:72:GLU:OE2	0.48	2.08	7	1
1:B:69:ASP:O	1:B:73:PHE:N	0.48	2.42	8	1
1:A:10:LEU:HD13	1:A:10:LEU:H	0.48	1.67	9	1
1:A:14:PHE:CE2	1:A:70:PHE:O	0.48	2.66	9	1
1:B:36:ILE:HG13	1:B:80:ILE:CD1	0.48	2.38	9	1
1:A:48:LYS:HD3	1:A:48:LYS:N	0.48	2.23	21	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:48:LYS:HD3	1:B:48:LYS:N	0.48	2.23	21	3
1:A:3:LEU:CD2	1:B:39:GLU:OE1	0.48	2.61	19	1
1:B:65:ASP:O	1:B:66:GLY:C	0.48	2.52	22	2
1:A:28:LYS:O	1:A:32:LEU:N	0.48	2.46	21	1
1:A:55:LYS:O	1:A:56:VAL:C	0.48	2.52	12	22
1:B:4:GLU:CA	1:B:4:GLU:OE1	0.48	2.61	15	2
1:B:60:LEU:HB2	1:B:76:PHE:CZ	0.48	2.43	6	1
1:B:35:LEU:O	1:B:39:GLU:OE2	0.48	2.32	13	4
1:A:17:TYR:HE1	1:B:3:LEU:HD11	0.48	1.69	12	1
1:A:46:GLU:HG2	1:A:53:VAL:CG2	0.48	2.38	16	2
1:B:32:LEU:CD2	1:B:68:CYS:SG	0.48	3.01	18	1
1:A:80:ILE:O	1:A:81:THR:C	0.48	2.52	10	9
1:A:17:TYR:CE2	1:A:35:LEU:HA	0.48	2.44	12	6
1:B:46:GLU:OE1	1:B:53:VAL:CG1	0.48	2.59	4	1
1:A:4:GLU:CA	1:A:4:GLU:OE1	0.48	2.61	15	2
1:B:19:GLY:O	1:B:20:ARG:C	0.48	2.50	24	3
1:A:25:HIS:NE2	1:A:70:PHE:CE2	0.48	2.81	11	1
1:A:39:GLU:HB2	1:B:4:GLU:HB3	0.48	1.85	12	1
1:A:10:LEU:HA	1:A:13:VAL:CG2	0.48	2.38	21	2
1:B:34:GLU:O	1:B:37:ASN:OD1	0.48	2.31	22	1
1:A:73:PHE:O	1:A:77:VAL:HB	0.48	2.08	24	16
1:B:25:HIS:O	1:B:69:ASP:OD1	0.48	2.31	14	3
1:A:27:LEU:CD1	1:A:31:GLU:HB3	0.48	2.38	23	3
1:B:41:SER:O	1:B:44:LEU:CB	0.48	2.62	20	5
1:A:27:LEU:HB3	1:A:31:GLU:CB	0.48	2.38	4	1
1:A:46:GLU:OE1	1:A:53:VAL:CG1	0.48	2.59	4	1
1:A:1:SER:HA	1:B:39:GLU:CG	0.48	2.38	21	4
1:A:3:LEU:HD13	1:B:35:LEU:HD23	0.48	1.86	8	1
1:B:67:GLU:OE2	1:B:69:ASP:OD2	0.48	2.32	12	2
1:B:15:HIS:O	1:B:19:GLY:O	0.48	2.32	13	2
1:A:45:GLU:CB	1:A:48:LYS:HE2	0.48	2.39	20	1
1:A:3:LEU:HB2	1:B:13:VAL:CG1	0.48	2.39	21	1
1:A:78:ALA:HB1	1:B:74:MET:SD	0.48	2.49	1	1
1:B:17:TYR:OH	1:B:39:GLU:OE1	0.48	2.32	1	2
1:B:18:SER:O	1:B:23:ASP:O	0.48	2.31	10	5
1:A:49:GLU:O	1:A:49:GLU:HG2	0.48	2.09	5	1
1:A:0:MET:HG3	1:A:1:SER:N	0.48	2.23	15	3
1:A:10:LEU:HD23	1:B:3:LEU:HD23	0.48	1.85	6	1
1:A:3:LEU:CD1	1:B:39:GLU:CD	0.48	2.81	7	1
1:A:35:LEU:O	1:A:39:GLU:OE2	0.48	2.32	13	6
1:B:42:HIS:CD2	1:B:48:LYS:HB3	0.48	2.44	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:THR:HG21	1:B:7:VAL:HG11	0.48	1.82	8	1
1:A:67:GLU:OE2	1:A:69:ASP:OD2	0.48	2.32	12	2
1:A:15:HIS:O	1:A:19:GLY:O	0.48	2.32	13	2
1:A:74:MET:O	1:B:74:MET:HE1	0.48	2.09	15	1
1:A:3:LEU:HG	1:B:73:PHE:CE1	0.48	2.44	19	1
1:B:46:GLU:O	1:B:47:ILE:C	0.48	2.51	9	14
1:B:51:GLU:O	1:B:55:LYS:HD2	0.48	2.09	25	16
1:B:55:LYS:O	1:B:56:VAL:C	0.48	2.52	12	22
1:B:56:VAL:CG1	1:B:80:ILE:CD1	0.48	2.80	1	4
1:A:60:LEU:HD12	1:A:76:PHE:HZ	0.48	1.65	3	1
1:B:56:VAL:HA	1:B:80:ILE:HD13	0.48	1.85	3	1
1:B:67:GLU:O	1:B:72:GLU:CD	0.48	2.52	20	3
1:A:32:LEU:CD1	1:A:60:LEU:CD1	0.48	2.91	6	1
1:B:0:MET:HG3	1:B:1:SER:N	0.48	2.22	15	3
1:A:40:LEU:CD2	1:B:4:GLU:CD	0.48	2.82	8	1
1:B:32:LEU:HG	1:B:76:PHE:CD2	0.48	2.43	20	3
1:B:45:GLU:CB	1:B:48:LYS:HE2	0.48	2.38	20	1
1:A:43:PHE:CZ	1:A:56:VAL:HG11	0.48	2.43	21	1
1:A:3:LEU:O	1:A:7:VAL:HG23	0.48	2.08	22	1
1:B:41:SER:O	1:B:44:LEU:HB2	0.48	2.08	20	14
1:B:60:LEU:HG	1:B:76:PHE:CZ	0.48	2.44	1	4
1:B:73:PHE:CD1	1:B:73:PHE:O	0.48	2.67	21	3
1:B:32:LEU:O	1:B:35:LEU:HB2	0.48	2.09	21	2
1:B:64:GLY:O	1:B:65:ASP:HB3	0.48	2.07	11	4
1:A:39:GLU:HB2	1:B:4:GLU:CA	0.48	2.39	5	1
1:B:17:TYR:CE1	1:B:35:LEU:CD1	0.48	2.92	17	3
1:B:49:GLU:O	1:B:49:GLU:HG2	0.48	2.09	5	1
1:A:3:LEU:CD1	1:B:39:GLU:OE2	0.48	2.62	7	1
1:B:18:SER:HB3	1:B:25:HIS:HA	0.48	1.84	21	3
1:A:32:LEU:CD1	1:A:36:ILE:HD11	0.48	2.38	9	1
1:B:68:CYS:HB3	1:B:72:GLU:CB	0.48	2.39	11	2
1:B:68:CYS:CB	1:B:72:GLU:HB2	0.48	2.39	13	1
1:B:36:ILE:HG22	1:B:40:LEU:HD12	0.48	1.86	16	1
1:A:35:LEU:CD2	1:B:3:LEU:HD23	0.48	2.39	19	1
1:A:73:PHE:CE1	1:B:3:LEU:HG	0.48	2.44	19	1
1:A:32:LEU:CD2	1:A:60:LEU:CD2	0.48	2.81	22	1
1:A:64:GLY:O	1:A:65:ASP:HB2	0.48	2.08	24	1
1:A:42:HIS:N	1:A:42:HIS:CD2	0.48	2.82	25	1
1:B:13:VAL:O	1:B:14:PHE:C	0.47	2.50	17	15
1:A:18:SER:O	1:A:23:ASP:O	0.47	2.32	10	5
1:B:32:LEU:O	1:B:35:LEU:N	0.47	2.46	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:GLU:CD	1:B:40:LEU:CD2	0.47	2.81	8	1
1:B:32:LEU:CD1	1:B:36:ILE:HD11	0.47	2.39	9	1
1:A:68:CYS:CB	1:A:72:GLU:HB2	0.47	2.39	13	1
1:A:78:ALA:CB	1:B:74:MET:CB	0.47	2.92	15	2
1:A:14:PHE:CD1	1:A:70:PHE:HE1	0.47	2.27	21	2
1:B:27:LEU:HD11	1:B:32:LEU:N	0.47	2.24	20	1
1:A:17:TYR:OH	1:A:38:ASN:ND2	0.47	2.46	24	1
1:A:22:GLY:O	1:A:23:ASP:O	0.47	2.32	20	6
1:A:69:ASP:N	1:A:72:GLU:HB2	0.47	2.24	16	7
1:B:22:GLY:O	1:B:23:ASP:O	0.47	2.32	16	7
1:B:27:LEU:C	1:B:28:LYS:CG	0.47	2.82	21	2
1:A:4:GLU:CB	1:B:39:GLU:HG2	0.47	2.39	3	2
1:B:17:TYR:CE2	1:B:35:LEU:HA	0.47	2.44	12	6
1:B:60:LEU:HB2	1:B:76:PHE:CE1	0.47	2.44	4	2
1:A:18:SER:O	1:A:24:LYS:O	0.47	2.32	5	10
1:A:35:LEU:O	1:A:39:GLU:CD	0.47	2.51	14	6
1:B:36:ILE:HG22	1:B:43:PHE:CE1	0.47	2.44	8	1
1:A:0:MET:HE3	1:A:0:MET:C	0.47	2.29	9	1
1:B:16:GLN:HG3	1:B:20:ARG:HB3	0.47	1.87	9	4
1:B:45:GLU:OE1	1:B:45:GLU:N	0.47	2.47	19	1
1:B:26:LYS:CB	1:B:67:GLU:OE1	0.47	2.61	1	1
1:B:45:GLU:O	1:B:46:GLU:CB	0.47	2.63	5	9
1:B:47:ILE:C	1:B:49:GLU:N	0.47	2.67	17	12
1:B:76:PHE:O	1:B:80:ILE:HG12	0.47	2.09	16	8
1:B:46:GLU:CD	1:B:53:VAL:HG13	0.47	2.30	4	1
1:A:64:GLY:O	1:A:67:GLU:CB	0.47	2.62	5	1
1:B:3:LEU:O	1:B:4:GLU:C	0.47	2.52	14	4
1:A:74:MET:HE1	1:B:74:MET:SD	0.47	2.49	9	1
1:B:34:GLU:HG2	1:B:38:ASN:ND2	0.47	2.25	9	1
1:B:67:GLU:OE2	1:B:69:ASP:OD1	0.47	2.32	12	1
1:A:39:GLU:OE1	1:B:3:LEU:HD23	0.47	2.08	14	1
1:B:69:ASP:OD2	1:B:71:GLN:HG2	0.47	2.10	19	1
1:B:60:LEU:HD11	1:B:76:PHE:CZ	0.47	2.44	21	1
1:B:46:GLU:CD	1:B:56:VAL:HG11	0.47	2.29	25	1
1:A:17:TYR:CE1	1:A:35:LEU:CA	0.47	2.98	1	4
1:A:76:PHE:O	1:A:80:ILE:HG12	0.47	2.10	16	11
1:B:49:GLU:HB2	1:B:52:VAL:CG2	0.47	2.39	17	8
1:B:26:LYS:CE	1:B:67:GLU:HA	0.47	2.39	5	2
1:B:59:THR:O	1:B:62:SER:N	0.47	2.48	4	1
1:A:36:ILE:HG22	1:A:43:PHE:CE1	0.47	2.44	8	1
1:A:43:PHE:CD1	1:A:44:LEU:N	0.47	2.83	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:LEU:HD21	1:B:73:PHE:CE1	0.47	2.43	10	2
1:A:10:LEU:CD1	1:A:74:MET:HE3	0.47	2.39	11	1
1:A:3:LEU:HD11	1:B:17:TYR:HE1	0.47	1.70	12	1
1:A:69:ASP:CG	1:A:70:PHE:N	0.47	2.67	15	2
1:A:10:LEU:CD2	1:B:3:LEU:HA	0.47	2.39	16	1
1:A:32:LEU:CD2	1:A:68:CYS:SG	0.47	3.02	18	1
1:A:60:LEU:O	1:A:65:ASP:HB3	0.47	2.10	20	1
1:A:64:GLY:O	1:A:72:GLU:OE1	0.47	2.32	20	2
1:A:56:VAL:CG1	1:A:80:ILE:CD1	0.47	2.82	3	4
1:A:77:VAL:O	1:A:81:THR:HB	0.47	2.09	10	5
1:A:80:ILE:O	1:A:82:THR:N	0.47	2.47	3	4
1:B:50:GLN:O	1:B:51:GLU:C	0.47	2.53	4	13
1:A:42:HIS:CD2	1:A:48:LYS:HB3	0.47	2.44	7	1
1:A:1:SER:CA	1:B:39:GLU:HG2	0.47	2.40	8	1
1:B:26:LYS:HB3	1:B:67:GLU:CG	0.47	2.39	11	1
1:A:4:GLU:HB3	1:B:39:GLU:HB2	0.47	1.86	12	1
1:B:18:SER:OG	1:B:25:HIS:HA	0.47	2.09	14	1
1:B:67:GLU:O	1:B:72:GLU:OE2	0.47	2.31	24	4
1:A:25:HIS:CG	1:A:70:PHE:CZ	0.47	3.03	20	1
1:A:13:VAL:CG1	1:B:3:LEU:HB2	0.47	2.40	21	1
1:A:40:LEU:HD13	1:B:4:GLU:OE1	0.47	2.09	21	1
1:A:45:GLU:O	1:A:46:GLU:CB	0.47	2.62	5	10
1:B:32:LEU:HD12	1:B:63:ASP:OD2	0.47	2.09	1	1
1:A:20:ARG:O	1:A:21:GLU:O	0.47	2.32	2	1
1:A:39:GLU:HB3	1:B:4:GLU:HB3	0.47	1.85	3	2
1:B:11:ILE:C	1:B:11:ILE:CD1	0.47	2.80	14	4
1:B:13:VAL:O	1:B:17:TYR:N	0.47	2.47	21	2
1:A:47:ILE:HG22	1:A:48:LYS:CE	0.47	2.40	11	1
1:A:74:MET:HB3	1:B:78:ALA:HB2	0.47	1.86	15	2
1:B:46:GLU:HG2	1:B:53:VAL:CG1	0.47	2.39	16	2
1:B:64:GLY:O	1:B:65:ASP:HB2	0.47	2.08	24	1
1:A:41:SER:O	1:A:44:LEU:HB2	0.47	2.09	20	14
1:B:60:LEU:O	1:B:63:ASP:OD2	0.47	2.32	7	3
1:B:80:ILE:O	1:B:81:THR:C	0.47	2.52	10	10
1:A:3:LEU:CD2	1:B:10:LEU:CD2	0.47	2.90	3	1
1:A:40:LEU:N	1:A:40:LEU:CD2	0.47	2.71	3	1
1:B:77:VAL:O	1:B:81:THR:HB	0.47	2.10	10	5
1:B:70:PHE:O	1:B:71:GLN:C	0.47	2.53	10	2
1:A:16:GLN:CG	1:A:20:ARG:HB3	0.47	2.39	10	3
1:B:0:MET:C	1:B:0:MET:HE3	0.47	2.30	9	1
1:B:16:GLN:CG	1:B:20:ARG:HB3	0.47	2.40	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LYS:HB3	1:A:67:GLU:CG	0.47	2.39	11	1
1:A:14:PHE:O	1:A:18:SER:HB2	0.47	2.10	14	1
1:B:14:PHE:O	1:B:18:SER:HB2	0.47	2.09	14	1
1:B:36:ILE:CD1	1:B:76:PHE:CE1	0.47	2.97	23	2
1:A:25:HIS:CD2	1:A:70:PHE:CZ	0.47	3.03	15	1
1:A:74:MET:HE1	1:B:77:VAL:CG1	0.47	2.40	22	2
1:B:14:PHE:CD1	1:B:70:PHE:HE1	0.47	2.25	21	2
1:A:13:VAL:CG2	1:B:3:LEU:CD1	0.47	2.91	17	1
1:A:45:GLU:N	1:A:45:GLU:OE1	0.47	2.47	19	1
1:B:14:PHE:CG	1:B:18:SER:OG	0.47	2.65	20	1
1:B:64:GLY:O	1:B:72:GLU:OE1	0.47	2.33	20	2
1:A:13:VAL:HG22	1:B:3:LEU:HD21	0.47	1.85	24	1
1:B:37:ASN:OD1	1:B:37:ASN:O	0.47	2.33	24	1
1:A:17:TYR:CD1	1:A:35:LEU:CD1	0.47	2.93	25	1
1:A:46:GLU:CD	1:A:56:VAL:HG11	0.47	2.29	25	1
1:B:42:HIS:N	1:B:42:HIS:CD2	0.47	2.82	25	1
1:B:56:VAL:HG13	1:B:80:ILE:HD13	0.47	1.79	25	1
1:A:26:LYS:CG	1:A:69:ASP:OD2	0.47	2.62	3	1
1:A:37:ASN:OD1	1:A:37:ASN:C	0.47	2.53	3	5
1:B:37:ASN:C	1:B:37:ASN:OD1	0.47	2.53	3	2
1:A:17:TYR:OH	1:A:35:LEU:HA	0.47	2.10	4	10
1:A:60:LEU:HB2	1:A:76:PHE:CZ	0.47	2.43	6	1
1:B:56:VAL:CG1	1:B:80:ILE:HD12	0.47	2.23	6	1
1:A:26:LYS:CE	1:A:67:GLU:HB2	0.47	2.40	7	1
1:B:9:ALA:C	1:B:13:VAL:HG23	0.47	2.30	9	1
1:B:34:GLU:CG	1:B:38:ASN:ND2	0.47	2.78	9	1
1:B:20:ARG:HG3	1:B:21:GLU:N	0.47	2.23	10	1
1:A:48:LYS:N	1:A:48:LYS:HD3	0.47	2.25	11	2
1:B:14:PHE:CE1	1:B:73:PHE:CB	0.47	2.98	24	2
1:B:3:LEU:CG	1:B:4:GLU:N	0.47	2.78	16	1
1:A:17:TYR:OH	1:A:38:ASN:CB	0.47	2.63	21	1
1:B:17:TYR:OH	1:B:38:ASN:CB	0.47	2.62	21	1
1:B:10:LEU:HD12	1:B:74:MET:SD	0.47	2.50	23	1
1:A:51:GLU:O	1:A:55:LYS:HD2	0.47	2.10	18	15
1:B:3:LEU:HD13	1:B:4:GLU:CA	0.47	2.40	3	3
1:B:76:PHE:O	1:B:77:VAL:C	0.47	2.50	16	21
1:B:25:HIS:O	1:B:26:LYS:HE3	0.47	2.10	8	6
1:B:73:PHE:CD1	1:B:74:MET:N	0.47	2.83	13	2
1:A:4:GLU:HB3	1:B:39:GLU:CB	0.47	2.39	3	1
1:A:46:GLU:CD	1:A:53:VAL:HG13	0.47	2.29	4	1
1:B:62:SER:C	1:B:63:ASP:O	0.47	2.53	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:60:LEU:O	1:B:61:ASP:C	0.47	2.53	5	1
1:A:55:LYS:O	1:A:57:MET:N	0.47	2.47	6	2
1:B:7:VAL:CA	1:B:10:LEU:HG	0.47	2.40	13	4
1:B:26:LYS:CE	1:B:67:GLU:HB2	0.47	2.40	7	1
1:B:14:PHE:CG	1:B:70:PHE:CD1	0.47	3.02	9	1
1:A:39:GLU:HG2	1:B:3:LEU:CB	0.47	2.40	10	1
1:B:68:CYS:C	1:B:69:ASP:OD1	0.47	2.53	11	2
1:B:4:GLU:HG3	1:B:5:LYS:N	0.47	2.25	12	2
1:A:3:LEU:HD23	1:B:35:LEU:CD2	0.47	2.39	19	1
1:A:26:LYS:HA	1:A:68:CYS:O	0.47	2.10	19	1
1:B:18:SER:O	1:B:26:LYS:O	0.47	2.33	19	1
1:A:27:LEU:HD11	1:A:32:LEU:N	0.47	2.25	20	1
1:A:47:ILE:O	1:A:50:GLN:OE1	0.47	2.33	23	1
1:A:41:SER:O	1:A:44:LEU:CB	0.47	2.63	20	5
1:B:49:GLU:O	1:B:53:VAL:N	0.47	2.42	23	2
1:A:25:HIS:O	1:A:26:LYS:HE3	0.47	2.10	8	6
1:A:56:VAL:HA	1:A:80:ILE:HD13	0.47	1.86	3	1
1:A:63:ASP:C	1:A:65:ASP:N	0.47	2.68	7	8
1:B:55:LYS:O	1:B:57:MET:N	0.47	2.48	6	2
1:A:39:GLU:OE2	1:B:3:LEU:CD1	0.47	2.61	7	1
1:A:13:VAL:O	1:A:17:TYR:N	0.47	2.47	21	2
1:B:79:MET:O	1:B:79:MET:SD	0.47	2.73	24	2
1:A:34:GLU:CG	1:A:38:ASN:ND2	0.47	2.78	9	1
1:A:67:GLU:O	1:A:72:GLU:OE1	0.47	2.33	16	3
1:A:77:VAL:CG2	1:B:4:GLU:OE1	0.47	2.63	16	1
1:A:37:ASN:CB	1:A:44:LEU:HD12	0.47	2.40	19	1
1:B:26:LYS:HA	1:B:68:CYS:O	0.47	2.10	19	1
1:A:10:LEU:HA	1:A:13:VAL:HG22	0.47	1.86	21	1
1:A:3:LEU:O	1:A:7:VAL:CG2	0.47	2.63	22	1
1:A:49:GLU:CG	1:A:53:VAL:HG23	0.47	2.36	23	1
1:A:1:SER:HA	1:B:39:GLU:CB	0.47	2.40	24	1
1:A:29:LYS:HE3	1:A:64:GLY:N	0.47	2.26	24	1
1:A:17:TYR:OH	1:A:39:GLU:OE1	0.46	2.33	1	2
1:A:1:SER:O	1:A:5:LYS:HG3	0.46	2.10	2	8
1:B:26:LYS:CG	1:B:69:ASP:OD2	0.46	2.63	3	1
1:A:1:SER:O	1:A:4:GLU:N	0.46	2.47	6	1
1:A:26:LYS:CG	1:A:69:ASP:CG	0.46	2.84	6	3
1:B:50:GLN:HG3	1:B:51:GLU:N	0.46	2.24	21	2
1:B:69:ASP:O	1:B:72:GLU:HG3	0.46	2.10	7	4
1:A:79:MET:O	1:A:79:MET:SD	0.46	2.73	8	2
1:B:43:PHE:CD1	1:B:44:LEU:N	0.46	2.83	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:GLU:HG2	1:A:38:ASN:ND2	0.46	2.25	9	1
1:B:47:ILE:HG22	1:B:48:LYS:CE	0.46	2.40	11	1
1:A:49:GLU:HG3	1:A:52:VAL:CG1	0.46	2.39	12	1
1:A:7:VAL:CA	1:A:10:LEU:HG	0.46	2.40	13	4
1:A:16:GLN:CG	1:A:20:ARG:NE	0.46	2.78	18	1
1:A:69:ASP:OD2	1:A:71:GLN:HG2	0.46	2.10	19	1
1:B:10:LEU:HA	1:B:13:VAL:HG22	0.46	1.85	21	1
1:B:0:MET:O	1:B:1:SER:C	0.46	2.54	1	4
1:A:56:VAL:CG1	1:A:80:ILE:HD12	0.46	2.23	6	1
1:B:1:SER:O	1:B:4:GLU:N	0.46	2.47	6	1
1:A:52:VAL:HA	1:A:83:ALA:HB1	0.46	1.85	24	2
1:A:20:ARG:HG3	1:A:21:GLU:N	0.46	2.25	10	1
1:A:46:GLU:C	1:A:53:VAL:CG2	0.46	2.84	13	2
1:B:70:PHE:C	1:B:72:GLU:N	0.46	2.68	10	1
1:A:29:LYS:CD	1:A:63:ASP:HA	0.46	2.40	16	2
1:B:49:GLU:HG3	1:B:52:VAL:CG1	0.46	2.40	12	1
1:B:71:GLN:O	1:B:72:GLU:C	0.46	2.54	13	1
1:A:4:GLU:OE2	1:A:5:LYS:HE3	0.46	2.10	14	1
1:A:35:LEU:CG	1:B:3:LEU:HD21	0.46	2.41	16	1
1:B:3:LEU:O	1:B:7:VAL:HG23	0.46	2.10	22	1
1:B:17:TYR:CD1	1:B:35:LEU:CD1	0.46	2.91	22	2
1:B:77:VAL:O	1:B:80:ILE:HB	0.46	2.10	22	1
1:A:39:GLU:CB	1:B:1:SER:HA	0.46	2.40	24	1
1:B:16:GLN:O	1:B:20:ARG:HG2	0.46	2.11	24	10
1:B:55:LYS:N	1:B:55:LYS:HD2	0.46	2.25	23	3
1:B:20:ARG:O	1:B:21:GLU:O	0.46	2.32	2	1
1:B:64:GLY:O	1:B:65:ASP:OD1	0.46	2.34	3	1
1:A:32:LEU:O	1:A:35:LEU:HB2	0.46	2.10	21	2
1:A:4:GLU:CA	1:B:39:GLU:HB2	0.46	2.40	5	1
1:A:50:GLN:HG3	1:A:51:GLU:N	0.46	2.24	6	2
1:A:50:GLN:CG	1:A:51:GLU:N	0.46	2.78	21	2
1:B:32:LEU:CD1	1:B:60:LEU:CD1	0.46	2.91	6	1
1:B:52:VAL:HA	1:B:83:ALA:HB1	0.46	1.86	24	2
1:A:70:PHE:O	1:A:71:GLN:C	0.46	2.54	10	2
1:A:74:MET:HE2	1:B:78:ALA:HB2	0.46	1.86	15	1
1:B:69:ASP:CG	1:B:70:PHE:N	0.46	2.68	15	2
1:B:60:LEU:O	1:B:65:ASP:HB3	0.46	2.10	20	1
1:A:40:LEU:HB2	1:A:43:PHE:CD1	0.46	2.46	22	1
1:A:3:LEU:N	1:A:3:LEU:HD23	0.46	2.25	24	1
1:B:29:LYS:HE3	1:B:64:GLY:N	0.46	2.26	24	1
1:A:47:ILE:C	1:A:49:GLU:N	0.46	2.67	2	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:63:ASP:C	1:B:65:ASP:N	0.46	2.68	7	11
1:A:27:LEU:O	1:A:68:CYS:HB2	0.46	2.10	11	4
1:A:39:GLU:HG2	1:B:4:GLU:CB	0.46	2.40	3	2
1:B:65:ASP:O	1:B:65:ASP:CG	0.46	2.54	3	4
1:B:26:LYS:CG	1:B:69:ASP:CG	0.46	2.84	6	4
1:A:9:ALA:C	1:A:13:VAL:HG23	0.46	2.30	9	1
1:A:75:ALA:O	1:B:71:GLN:CB	0.46	2.63	13	1
1:A:36:ILE:CD1	1:A:76:PHE:CE1	0.46	2.95	14	2
1:B:25:HIS:CD2	1:B:70:PHE:CZ	0.46	3.03	15	1
1:A:46:GLU:HG2	1:A:53:VAL:CG1	0.46	2.40	16	2
1:A:36:ILE:HD13	1:A:60:LEU:HD11	0.46	1.88	17	1
1:A:76:PHE:CD1	1:A:77:VAL:N	0.46	2.84	23	1
1:A:3:LEU:O	1:A:7:VAL:N	0.46	2.42	18	6
1:A:4:GLU:HB3	1:B:39:GLU:HB3	0.46	1.87	3	2
1:A:26:LYS:CD	1:A:27:LEU:N	0.46	2.79	3	2
1:A:64:GLY:O	1:A:67:GLU:HB3	0.46	2.11	5	3
1:B:50:GLN:CG	1:B:51:GLU:N	0.46	2.78	21	2
1:A:27:LEU:HB3	1:A:72:GLU:OE1	0.46	2.10	7	1
1:B:27:LEU:HB3	1:B:72:GLU:OE1	0.46	2.10	7	1
1:B:29:LYS:CD	1:B:63:ASP:HA	0.46	2.40	16	2
1:A:27:LEU:O	1:A:68:CYS:O	0.46	2.33	13	1
1:A:18:SER:HA	1:A:26:LYS:O	0.46	2.11	19	2
1:B:18:SER:O	1:B:23:ASP:HB3	0.46	2.11	14	1
1:A:35:LEU:HG	1:B:3:LEU:CD1	0.46	2.40	15	1
1:B:3:LEU:O	1:B:6:ALA:CB	0.46	2.63	21	2
1:A:16:GLN:O	1:A:20:ARG:HG2	0.46	2.11	24	10
1:A:46:GLU:CD	1:A:57:MET:CE	0.46	2.84	1	1
1:B:27:LEU:O	1:B:67:GLU:HA	0.46	2.10	9	2
1:A:36:ILE:O	1:A:39:GLU:HG2	0.46	2.10	12	4
1:B:57:MET:O	1:B:61:ASP:HB2	0.46	2.11	24	4
1:B:4:GLU:OE1	1:B:4:GLU:HA	0.46	2.11	15	3
1:A:69:ASP:O	1:A:72:GLU:HG3	0.46	2.09	7	3
1:A:69:ASP:N	1:A:72:GLU:HG2	0.46	2.26	7	1
1:A:18:SER:HB2	1:A:26:LYS:N	0.46	2.26	24	2
1:B:32:LEU:CD1	1:B:76:PHE:CE2	0.46	2.81	13	1
1:A:18:SER:OG	1:A:25:HIS:HA	0.46	2.10	14	1
1:A:3:LEU:O	1:A:6:ALA:CB	0.46	2.64	21	1
1:A:17:TYR:CZ	1:A:35:LEU:HD23	0.46	2.45	21	1
1:B:47:ILE:O	1:B:50:GLN:OE1	0.46	2.33	23	1
1:B:59:THR:HG22	1:B:63:ASP:OD1	0.46	2.11	25	1
1:A:72:GLU:O	1:A:73:PHE:C	0.46	2.52	24	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:17:TYR:CE1	1:B:35:LEU:CA	0.46	2.98	1	6
1:A:73:PHE:CD1	1:A:74:MET:N	0.46	2.84	13	2
1:B:1:SER:O	1:B:5:LYS:HG3	0.46	2.10	2	10
1:A:67:GLU:O	1:A:72:GLU:CD	0.46	2.53	20	5
1:B:27:LEU:O	1:B:68:CYS:HB2	0.46	2.10	11	4
1:B:34:GLU:HA	1:B:37:ASN:OD1	0.46	2.11	11	2
1:A:50:GLN:O	1:A:51:GLU:C	0.46	2.54	12	12
1:B:14:PHE:CG	1:B:70:PHE:CE1	0.46	3.04	8	2
1:A:14:PHE:CG	1:A:70:PHE:CD1	0.46	3.03	9	1
1:B:18:SER:HA	1:B:26:LYS:O	0.46	2.11	19	3
1:A:3:LEU:HB2	1:B:39:GLU:OE1	0.46	2.11	19	2
1:A:77:VAL:O	1:A:80:ILE:HB	0.46	2.11	22	1
1:A:37:ASN:OD1	1:A:37:ASN:O	0.46	2.33	24	1
1:A:59:THR:HG22	1:A:63:ASP:OD1	0.46	2.11	25	1
1:A:59:THR:O	1:A:62:SER:N	0.46	2.48	11	2
1:A:17:TYR:CE1	1:A:35:LEU:CD1	0.46	2.92	17	3
1:B:3:LEU:HD12	1:B:4:GLU:HG2	0.46	1.88	8	1
1:B:10:LEU:HD22	1:B:74:MET:HG3	0.46	1.86	8	1
1:A:68:CYS:C	1:A:69:ASP:OD1	0.46	2.54	11	2
1:A:4:GLU:HG3	1:A:5:LYS:N	0.46	2.25	12	2
1:B:67:GLU:O	1:B:72:GLU:OE1	0.46	2.33	16	3
1:B:79:MET:C	1:B:82:THR:OG1	0.46	2.54	24	3
1:A:18:SER:O	1:A:26:LYS:O	0.46	2.33	19	1
1:A:3:LEU:HD13	1:A:4:GLU:CA	0.46	2.41	1	3
1:A:27:LEU:O	1:A:67:GLU:HA	0.46	2.10	9	2
1:A:54:ASP:O	1:A:58:GLU:HB3	0.46	2.11	20	4
1:A:3:LEU:HD22	1:B:35:LEU:HD23	0.46	1.87	4	1
1:A:4:GLU:OE2	1:B:40:LEU:CD1	0.46	2.64	8	1
1:A:38:ASN:O	1:A:39:GLU:OE1	0.46	2.34	15	1
1:A:3:LEU:CD1	1:B:35:LEU:CD2	0.46	2.77	21	1
1:A:17:TYR:O	1:A:31:GLU:OE1	0.46	2.33	2	2
1:A:39:GLU:HG3	1:A:40:LEU:CD1	0.46	2.41	9	4
1:A:78:ALA:HB1	1:B:74:MET:HB2	0.46	1.86	5	1
1:A:26:LYS:CE	1:A:67:GLU:HG3	0.46	2.41	6	1
1:B:39:GLU:HB2	1:B:40:LEU:HD12	0.46	1.88	15	2
1:B:68:CYS:HB2	1:B:72:GLU:OE1	0.46	2.11	7	1
1:A:1:SER:HA	1:B:39:GLU:HG2	0.46	1.87	8	2
1:B:27:LEU:CD2	1:B:31:GLU:CB	0.46	2.94	8	1
1:A:73:PHE:CD1	1:A:73:PHE:O	0.46	2.69	21	2
1:B:46:GLU:C	1:B:53:VAL:CG2	0.46	2.84	13	2
1:B:46:GLU:HG3	1:B:53:VAL:CG2	0.46	2.41	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:VAL:O	1:A:53:VAL:C	0.45	2.55	13	16
1:A:54:ASP:OD2	1:A:55:LYS:NZ	0.45	2.44	1	1
1:A:56:VAL:HA	1:A:80:ILE:CD1	0.45	2.41	16	3
1:B:56:VAL:HA	1:B:80:ILE:CD1	0.45	2.41	11	3
1:A:62:SER:O	1:A:63:ASP:CG	0.45	2.55	7	2
1:B:32:LEU:CD1	1:B:36:ILE:CD1	0.45	2.94	9	1
1:A:49:GLU:CG	1:A:52:VAL:CG1	0.45	2.94	12	1
1:B:35:LEU:CD2	1:B:77:VAL:CG2	0.45	2.94	13	1
1:A:3:LEU:CD1	1:B:35:LEU:HG	0.45	2.42	15	1
1:A:64:GLY:HA3	1:A:72:GLU:OE1	0.45	2.11	15	1
1:B:63:ASP:OD1	1:B:64:GLY:N	0.45	2.49	15	1
1:A:3:LEU:HA	1:B:10:LEU:CD2	0.45	2.41	16	1
1:B:36:ILE:HD11	1:B:76:PHE:CE2	0.45	2.47	17	1
1:B:25:HIS:C	1:B:26:LYS:CD	0.45	2.84	18	2
1:A:3:LEU:HB3	1:B:39:GLU:OE1	0.45	2.11	23	1
1:A:27:LEU:HA	1:A:31:GLU:OE1	0.45	2.11	23	1
1:A:3:LEU:C	1:A:3:LEU:CD1	0.45	2.80	3	3
1:A:55:LYS:O	1:A:58:GLU:HG3	0.45	2.12	12	12
1:B:3:LEU:C	1:B:3:LEU:CD1	0.45	2.80	3	2
1:B:39:GLU:HG3	1:B:40:LEU:CD1	0.45	2.41	9	4
1:B:17:TYR:CZ	1:B:35:LEU:HA	0.45	2.47	14	2
1:B:26:LYS:CD	1:B:27:LEU:N	0.45	2.79	3	2
1:A:26:LYS:CE	1:A:67:GLU:HA	0.45	2.40	5	2
1:A:60:LEU:HB2	1:A:76:PHE:CE1	0.45	2.46	4	2
1:B:17:TYR:OH	1:B:35:LEU:HA	0.45	2.11	4	11
1:B:35:LEU:HD11	1:B:73:PHE:HD2	0.45	1.60	4	1
1:A:74:MET:HB2	1:B:78:ALA:HB1	0.45	1.88	5	1
1:A:4:GLU:OE1	1:A:4:GLU:HA	0.45	2.10	15	4
1:A:39:GLU:CD	1:B:0:MET:O	0.45	2.55	6	1
1:A:52:VAL:HG21	1:A:83:ALA:HB1	0.45	1.89	8	1
1:A:16:GLN:HG3	1:A:20:ARG:HB3	0.45	1.87	9	4
1:B:48:LYS:N	1:B:48:LYS:HD3	0.45	2.25	24	2
1:B:27:LEU:O	1:B:68:CYS:O	0.45	2.33	13	1
1:B:51:GLU:O	1:B:55:LYS:HD3	0.45	2.10	23	2
1:B:17:TYR:CZ	1:B:35:LEU:HD23	0.45	2.45	21	1
1:B:59:THR:HB	1:B:76:PHE:CD1	0.45	2.46	21	1
1:A:3:LEU:HD23	1:B:73:PHE:HZ	0.45	1.72	23	1
1:B:3:LEU:N	1:B:3:LEU:HD23	0.45	2.26	24	1
1:A:0:MET:O	1:A:1:SER:C	0.45	2.54	1	4
1:A:43:PHE:O	1:A:44:LEU:C	0.45	2.54	2	14
1:A:47:ILE:O	1:A:48:LYS:C	0.45	2.55	15	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:55:LYS:O	1:B:58:GLU:HG3	0.45	2.12	12	12
1:A:65:ASP:O	1:A:65:ASP:CG	0.45	2.54	3	3
1:B:35:LEU:O	1:B:39:GLU:CD	0.45	2.54	14	6
1:A:10:LEU:HD22	1:A:74:MET:HG3	0.45	1.88	8	1
1:A:27:LEU:CD2	1:A:31:GLU:CB	0.45	2.95	8	1
1:A:70:PHE:C	1:A:72:GLU:N	0.45	2.68	10	2
1:A:39:GLU:CB	1:B:4:GLU:HG2	0.45	2.41	10	1
1:A:49:GLU:CD	1:A:52:VAL:HG11	0.45	2.32	10	1
1:B:25:HIS:NE2	1:B:70:PHE:CE2	0.45	2.84	11	1
1:A:67:GLU:OE2	1:A:69:ASP:CG	0.45	2.55	12	2
1:A:67:GLU:OE2	1:A:69:ASP:OD1	0.45	2.33	12	1
1:B:67:GLU:OE2	1:B:69:ASP:CG	0.45	2.55	12	2
1:B:29:LYS:HA	1:B:60:LEU:CD1	0.45	2.41	13	1
1:A:17:TYR:CZ	1:A:35:LEU:HA	0.45	2.46	14	1
1:A:39:GLU:OE2	1:B:3:LEU:HB3	0.45	2.11	15	1
1:B:10:LEU:HB2	1:B:74:MET:HE3	0.45	1.89	16	1
1:B:37:ASN:CB	1:B:44:LEU:HD12	0.45	2.41	19	1
1:A:27:LEU:HB3	1:A:68:CYS:O	0.45	2.11	20	1
1:A:4:GLU:OE1	1:B:40:LEU:HD13	0.45	2.09	21	1
1:B:36:ILE:O	1:B:40:LEU:HB2	0.45	2.11	21	1
1:B:76:PHE:CD1	1:B:77:VAL:N	0.45	2.84	23	1
1:B:17:TYR:O	1:B:31:GLU:OE1	0.45	2.34	2	2
1:B:36:ILE:O	1:B:39:GLU:HG2	0.45	2.11	12	4
1:A:12:ASP:O	1:A:15:HIS:HB3	0.45	2.12	3	5
1:A:57:MET:O	1:A:61:ASP:HB2	0.45	2.12	16	4
1:A:45:GLU:O	1:A:46:GLU:HB3	0.45	2.12	19	3
1:A:48:LYS:C	1:A:49:GLU:OE1	0.45	2.55	7	1
1:A:74:MET:SD	1:B:74:MET:HE1	0.45	2.51	9	1
1:B:18:SER:HB2	1:B:26:LYS:N	0.45	2.26	24	2
1:A:3:LEU:HD23	1:A:4:GLU:N	0.45	2.25	11	1
1:A:76:PHE:CZ	1:A:80:ILE:CG1	0.45	3.00	11	2
1:B:14:PHE:CE1	1:B:18:SER:HB3	0.45	2.46	11	1
1:A:3:LEU:HD13	1:B:35:LEU:HG	0.45	1.89	13	1
1:A:29:LYS:HA	1:A:60:LEU:CD1	0.45	2.41	13	1
1:A:57:MET:O	1:A:61:ASP:N	0.45	2.48	13	3
1:B:3:LEU:O	1:B:7:VAL:CG2	0.45	2.64	22	1
1:A:37:ASN:C	1:A:37:ASN:ND2	0.45	2.69	25	1
1:B:43:PHE:O	1:B:44:LEU:C	0.45	2.54	2	15
1:B:14:PHE:CE2	1:B:73:PHE:HD2	0.45	2.30	9	5
1:B:26:LYS:CE	1:B:67:GLU:HG3	0.45	2.41	6	1
1:A:29:LYS:CE	1:A:66:GLY:O	0.45	2.65	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:ALA:O	1:A:9:ALA:CB	0.45	2.61	9	1
1:A:32:LEU:CD1	1:A:36:ILE:CD1	0.45	2.94	9	1
1:A:35:LEU:HG	1:B:3:LEU:CD2	0.45	2.39	9	3
1:A:3:LEU:O	1:A:4:GLU:C	0.45	2.53	14	4
1:B:3:LEU:HD23	1:B:4:GLU:N	0.45	2.26	11	1
1:B:34:GLU:O	1:B:36:ILE:N	0.45	2.50	14	1
1:B:38:ASN:O	1:B:39:GLU:OE1	0.45	2.34	15	1
1:A:0:MET:O	1:B:39:GLU:HG3	0.45	2.12	17	1
1:B:36:ILE:HD13	1:B:60:LEU:HD11	0.45	1.87	17	1
1:B:17:TYR:C	1:B:27:LEU:HD11	0.45	2.32	24	1
1:B:37:ASN:C	1:B:37:ASN:ND2	0.45	2.69	25	1
1:A:55:LYS:N	1:A:55:LYS:HD2	0.45	2.25	23	3
1:A:59:THR:CG2	1:A:76:PHE:CD1	0.45	3.00	1	1
1:B:58:GLU:O	1:B:62:SER:CB	0.45	2.65	3	2
1:A:26:LYS:HG2	1:A:69:ASP:CG	0.45	2.32	6	2
1:A:74:MET:SD	1:B:74:MET:SD	0.45	3.14	6	1
1:B:69:ASP:O	1:B:72:GLU:HB2	0.45	2.11	10	5
1:A:68:CYS:HB2	1:A:72:GLU:OE1	0.45	2.12	7	1
1:B:48:LYS:C	1:B:49:GLU:OE1	0.45	2.55	7	1
1:B:10:LEU:HD13	1:B:10:LEU:H	0.45	1.67	9	1
1:B:76:PHE:CZ	1:B:80:ILE:CG1	0.45	2.99	11	3
1:A:46:GLU:HG3	1:A:53:VAL:CG2	0.45	2.41	12	1
1:B:68:CYS:O	1:B:68:CYS:SG	0.45	2.74	12	1
1:A:71:GLN:O	1:A:72:GLU:C	0.45	2.54	13	1
1:A:3:LEU:HB3	1:B:39:GLU:OE2	0.45	2.12	15	1
1:A:36:ILE:O	1:A:40:LEU:HB2	0.45	2.11	21	2
1:A:63:ASP:OD1	1:A:64:GLY:N	0.45	2.49	15	1
1:A:79:MET:O	1:A:83:ALA:N	0.45	2.50	22	2
1:A:48:LYS:CB	1:A:49:GLU:OE1	0.45	2.65	16	1
1:A:17:TYR:O	1:A:31:GLU:OE2	0.45	2.34	21	1
1:B:17:TYR:O	1:B:31:GLU:OE2	0.45	2.33	21	1
1:A:40:LEU:HD23	1:B:4:GLU:HG3	0.45	1.87	1	1
1:A:39:GLU:O	1:B:4:GLU:HB2	0.45	2.12	9	6
1:A:4:GLU:O	1:A:7:VAL:HB	0.45	2.12	3	5
1:A:34:GLU:HA	1:A:37:ASN:OD1	0.45	2.11	11	2
1:A:51:GLU:O	1:A:55:LYS:HD3	0.45	2.11	23	3
1:A:64:GLY:O	1:A:65:ASP:OD1	0.45	2.34	3	1
1:A:35:LEU:HD23	1:B:3:LEU:HD22	0.45	1.88	4	1
1:A:67:GLU:O	1:A:67:GLU:CG	0.45	2.64	13	2
1:B:62:SER:O	1:B:63:ASP:CG	0.45	2.55	7	2
1:A:14:PHE:CG	1:A:70:PHE:CE1	0.45	3.05	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:GLU:HG2	1:B:1:SER:CA	0.45	2.42	8	1
1:A:47:ILE:CD1	1:A:47:ILE:C	0.45	2.85	8	2
1:A:39:GLU:HB3	1:B:4:GLU:CG	0.45	2.41	11	1
1:B:49:GLU:CG	1:B:52:VAL:CG1	0.45	2.94	12	1
1:B:64:GLY:HA3	1:B:72:GLU:OE1	0.45	2.11	15	1
1:A:10:LEU:HB2	1:A:74:MET:HE3	0.45	1.88	16	1
1:A:77:VAL:CG2	1:B:4:GLU:CD	0.45	2.85	16	1
1:B:28:LYS:HB3	1:B:31:GLU:OE2	0.45	2.12	23	1
1:A:3:LEU:CD2	1:B:13:VAL:CG2	0.45	2.95	24	1
1:A:65:ASP:O	1:A:65:ASP:OD2	0.45	2.35	3	2
1:A:67:GLU:HG3	1:A:69:ASP:OD1	0.45	2.12	6	2
1:B:26:LYS:HG2	1:B:69:ASP:CG	0.45	2.32	6	3
1:B:29:LYS:CE	1:B:66:GLY:O	0.45	2.65	7	1
1:B:69:ASP:N	1:B:72:GLU:HG2	0.45	2.26	7	1
1:B:25:HIS:O	1:B:26:LYS:HE2	0.45	2.11	19	4
1:A:68:CYS:HB3	1:A:72:GLU:CB	0.45	2.40	11	1
1:A:8:VAL:C	1:A:11:ILE:CG1	0.45	2.86	16	2
1:A:6:ALA:O	1:A:10:LEU:N	0.45	2.49	14	1
1:A:61:ASP:O	1:A:62:SER:C	0.45	2.55	24	2
1:A:82:THR:HG22	1:B:70:PHE:CB	0.45	2.42	19	1
1:B:27:LEU:HB3	1:B:68:CYS:O	0.45	2.12	20	1
1:A:73:PHE:CE2	1:B:3:LEU:HD21	0.45	2.45	21	1
1:B:27:LEU:HA	1:B:31:GLU:OE1	0.45	2.11	23	1
1:A:71:GLN:NE2	1:A:72:GLU:CG	0.45	2.79	24	1
1:A:4:GLU:CB	1:B:39:GLU:CG	0.45	2.95	3	1
1:A:49:GLU:OE1	1:A:83:ALA:O	0.45	2.35	3	1
1:B:4:GLU:O	1:B:7:VAL:HB	0.45	2.11	11	5
1:A:32:LEU:HD21	1:A:63:ASP:OD2	0.45	2.12	4	1
1:B:50:GLN:O	1:B:52:VAL:N	0.45	2.50	14	4
1:A:32:LEU:CD2	1:A:63:ASP:CG	0.45	2.85	5	1
1:A:39:GLU:OE2	1:B:0:MET:O	0.45	2.34	10	2
1:A:79:MET:CA	1:A:82:THR:OG1	0.45	2.65	24	3
1:A:69:ASP:O	1:A:72:GLU:HB2	0.45	2.11	10	4
1:A:14:PHE:CE1	1:A:18:SER:HB3	0.45	2.46	11	1
1:B:14:PHE:HE1	1:B:27:LEU:HD23	0.45	1.70	11	1
1:B:30:SER:O	1:B:33:LYS:CB	0.45	2.65	14	1
1:A:79:MET:C	1:A:82:THR:OG1	0.45	2.54	24	3
1:A:59:THR:HB	1:A:76:PHE:CD1	0.45	2.46	21	1
1:B:47:ILE:O	1:B:48:LYS:C	0.45	2.55	2	9
1:A:0:MET:HG2	1:A:1:SER:N	0.45	2.27	3	1
1:A:11:ILE:CG1	1:A:12:ASP:N	0.45	2.80	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:0:MET:O	1:B:0:MET:CE	0.45	2.65	9	1
1:A:39:GLU:CD	1:B:3:LEU:CD2	0.45	2.85	14	1
1:A:65:ASP:CG	1:A:65:ASP:O	0.45	2.56	19	2
1:A:25:HIS:C	1:A:26:LYS:CD	0.45	2.85	18	2
1:B:60:LEU:HA	1:B:65:ASP:OD2	0.45	2.12	20	1
1:B:65:ASP:O	1:B:65:ASP:OD2	0.44	2.35	3	2
1:A:32:LEU:HD12	1:A:76:PHE:HD2	0.44	1.71	10	1
1:A:78:ALA:O	1:A:79:MET:C	0.44	2.55	13	2
1:A:7:VAL:HA	1:A:10:LEU:CD1	0.44	2.42	15	2
1:A:35:LEU:CD2	1:A:77:VAL:CG2	0.44	2.95	13	1
1:B:57:MET:O	1:B:61:ASP:N	0.44	2.50	24	3
1:B:13:VAL:O	1:B:17:TYR:HB2	0.44	2.13	14	1
1:A:39:GLU:HG3	1:B:0:MET:O	0.44	2.12	17	1
1:A:60:LEU:HG	1:A:76:PHE:CE2	0.44	2.47	18	1
1:B:70:PHE:CD1	1:B:70:PHE:N	0.44	2.85	19	1
1:B:17:TYR:CD1	1:B:35:LEU:HG	0.44	2.47	21	1
1:B:59:THR:CG2	1:B:76:PHE:CD1	0.44	3.00	1	1
1:A:4:GLU:HB2	1:B:39:GLU:O	0.44	2.12	18	8
1:A:40:LEU:CD2	1:B:4:GLU:OE1	0.44	2.63	3	2
1:B:11:ILE:CG1	1:B:12:ASP:N	0.44	2.80	4	2
1:A:60:LEU:O	1:A:61:ASP:C	0.44	2.55	5	1
1:A:39:GLU:HB2	1:B:4:GLU:HB2	0.44	1.88	23	3
1:A:1:SER:O	1:A:5:LYS:HG2	0.44	2.13	17	3
1:A:4:GLU:HB2	1:B:39:GLU:C	0.44	2.32	18	4
1:B:20:ARG:O	1:B:21:GLU:HG2	0.44	2.13	11	1
1:B:58:GLU:CA	1:B:58:GLU:OE1	0.44	2.65	14	1
1:B:62:SER:O	1:B:66:GLY:N	0.44	2.50	14	1
1:A:27:LEU:HB2	1:A:68:CYS:HB3	0.44	1.90	16	1
1:A:49:GLU:O	1:A:50:GLN:C	0.44	2.55	22	1
1:A:18:SER:O	1:A:24:LYS:C	0.44	2.56	24	1
1:A:29:LYS:HE3	1:A:63:ASP:CA	0.44	2.43	24	1
1:A:46:GLU:C	1:A:48:LYS:N	0.44	2.71	2	4
1:A:34:GLU:O	1:A:35:LEU:C	0.44	2.56	14	5
1:A:69:ASP:N	1:A:72:GLU:CG	0.44	2.81	23	6
1:A:39:GLU:OE1	1:B:1:SER:C	0.44	2.56	6	1
1:A:13:VAL:HG11	1:B:3:LEU:HG	0.44	1.89	9	1
1:B:37:ASN:OD1	1:B:37:ASN:C	0.44	2.55	11	3
1:A:36:ILE:HG21	1:A:43:PHE:CD2	0.44	2.48	13	1
1:A:71:GLN:CB	1:B:75:ALA:O	0.44	2.65	13	1
1:B:33:LYS:O	1:B:36:ILE:N	0.44	2.49	15	1
1:A:35:LEU:CD2	1:B:3:LEU:HD21	0.44	2.42	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:GLU:OE1	1:B:3:LEU:HB2	0.44	2.12	19	3
1:A:3:LEU:CG	1:B:13:VAL:HG11	0.44	2.43	21	1
1:B:40:LEU:HB2	1:B:43:PHE:CD1	0.44	2.46	22	1
1:A:12:ASP:HB3	1:B:2:GLU:OE1	0.44	2.12	23	1
1:B:49:GLU:CG	1:B:53:VAL:HG23	0.44	2.35	23	1
1:B:12:ASP:O	1:B:15:HIS:HB3	0.44	2.12	3	4
1:B:34:GLU:O	1:B:35:LEU:C	0.44	2.55	14	5
1:A:0:MET:O	1:B:39:GLU:CD	0.44	2.55	6	1
1:B:79:MET:CA	1:B:82:THR:OG1	0.44	2.65	24	4
1:A:69:ASP:O	1:A:73:PHE:N	0.44	2.42	8	1
1:B:1:SER:O	1:B:5:LYS:HG2	0.44	2.13	9	3
1:A:18:SER:HB3	1:A:26:LYS:N	0.44	2.27	15	1
1:B:46:GLU:HG2	1:B:53:VAL:HG21	0.44	1.90	16	1
1:A:3:LEU:HD11	1:B:13:VAL:CG2	0.44	2.41	17	1
1:A:40:LEU:HD12	1:A:80:ILE:HD12	0.44	1.89	17	1
1:B:60:LEU:HG	1:B:76:PHE:CE2	0.44	2.47	18	1
1:A:59:THR:O	1:A:62:SER:HB3	0.44	2.13	21	2
1:B:37:ASN:HB3	1:B:44:LEU:HD13	0.44	1.89	20	1
1:A:17:TYR:CD1	1:A:35:LEU:HG	0.44	2.47	21	1
1:B:71:GLN:NE2	1:B:72:GLU:CG	0.44	2.80	24	1
1:A:23:ASP:OD2	1:A:31:GLU:OE2	0.44	2.36	25	1
1:B:52:VAL:O	1:B:53:VAL:C	0.44	2.54	5	16
1:B:54:ASP:O	1:B:58:GLU:HB3	0.44	2.12	20	4
1:A:1:SER:C	1:B:39:GLU:OE1	0.44	2.56	6	1
1:A:9:ALA:O	1:A:12:ASP:CB	0.44	2.66	19	3
1:A:14:PHE:CZ	1:A:27:LEU:CD1	0.44	2.99	9	1
1:A:16:GLN:CG	1:A:20:ARG:CD	0.44	2.95	24	2
1:B:6:ALA:O	1:B:9:ALA:CB	0.44	2.62	9	1
1:B:77:VAL:CA	1:B:80:ILE:HG13	0.44	2.43	17	2
1:A:1:SER:O	1:A:4:GLU:HG3	0.44	2.12	13	2
1:B:1:SER:O	1:B:4:GLU:HG3	0.44	2.12	13	2
1:A:26:LYS:HG3	1:A:69:ASP:OD2	0.44	2.12	11	1
1:B:26:LYS:HG3	1:B:69:ASP:OD2	0.44	2.12	11	1
1:A:30:SER:O	1:A:33:LYS:CB	0.44	2.66	14	1
1:A:39:GLU:C	1:B:4:GLU:HB2	0.44	2.33	15	2
1:B:48:LYS:CB	1:B:49:GLU:OE1	0.44	2.65	16	1
1:B:39:GLU:OE2	1:B:40:LEU:HD12	0.44	2.12	20	1
1:A:36:ILE:O	1:A:40:LEU:CB	0.44	2.66	21	1
1:B:28:LYS:O	1:B:32:LEU:N	0.44	2.46	21	1
1:B:79:MET:O	1:B:83:ALA:N	0.44	2.50	22	1
1:B:46:GLU:CD	1:B:57:MET:CE	0.44	2.86	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:45:GLU:O	1:B:46:GLU:HB3	0.44	2.12	19	4
1:B:47:ILE:CD1	1:B:47:ILE:C	0.44	2.86	14	2
1:A:78:ALA:HB2	1:B:74:MET:HG3	0.44	1.89	12	2
1:A:62:SER:O	1:A:66:GLY:N	0.44	2.50	14	1
1:B:59:THR:OG1	1:B:79:MET:SD	0.44	2.76	20	1
1:B:10:LEU:HD12	1:B:74:MET:HE1	0.44	1.90	21	1
1:B:33:LYS:O	1:B:37:ASN:CG	0.44	2.56	21	1
1:B:36:ILE:O	1:B:40:LEU:CB	0.44	2.66	21	1
1:A:3:LEU:HD11	1:B:17:TYR:OH	0.44	2.13	23	1
1:B:60:LEU:CD1	1:B:60:LEU:O	0.44	2.65	23	1
1:B:29:LYS:HE3	1:B:63:ASP:CA	0.44	2.42	24	1
1:A:74:MET:CE	1:B:74:MET:CE	0.44	2.95	2	1
1:A:78:ALA:CB	1:B:74:MET:HB2	0.44	2.43	5	1
1:B:43:PHE:CG	1:B:49:GLU:OE2	0.44	2.70	5	1
1:A:3:LEU:HD23	1:B:10:LEU:HD23	0.44	1.88	6	1
1:A:15:HIS:CG	1:A:16:GLN:N	0.44	2.86	6	2
1:A:73:PHE:O	1:A:77:VAL:CB	0.44	2.65	24	4
1:A:0:MET:CE	1:A:0:MET:O	0.44	2.66	9	1
1:A:3:LEU:CB	1:B:39:GLU:CG	0.44	2.96	10	1
1:A:78:ALA:HA	1:A:81:THR:HB	0.44	1.90	10	1
1:A:77:VAL:O	1:A:81:THR:N	0.44	2.51	11	1
1:A:26:LYS:HG2	1:A:69:ASP:OD2	0.44	2.13	13	1
1:A:18:SER:O	1:A:23:ASP:HB3	0.44	2.12	14	1
1:A:18:SER:OG	1:A:25:HIS:C	0.44	2.56	14	1
1:B:40:LEU:HD12	1:B:80:ILE:HD12	0.44	1.89	17	1
1:A:39:GLU:HB3	1:B:3:LEU:CD1	0.44	2.43	18	1
1:A:70:PHE:CD1	1:A:70:PHE:N	0.44	2.85	19	2
1:B:29:LYS:O	1:B:33:LYS:HG2	0.44	2.12	21	1
1:B:18:SER:O	1:B:24:LYS:C	0.44	2.55	24	1
1:B:52:VAL:CG2	1:B:83:ALA:HB1	0.44	2.43	25	1
1:A:22:GLY:O	1:A:23:ASP:C	0.44	2.55	22	4
1:A:59:THR:O	1:A:60:LEU:C	0.44	2.56	11	5
1:A:58:GLU:O	1:A:62:SER:OG	0.44	2.34	23	2
1:B:33:LYS:O	1:B:34:GLU:C	0.44	2.56	6	9
1:B:15:HIS:CG	1:B:16:GLN:N	0.44	2.85	6	2
1:B:14:PHE:HD1	1:B:18:SER:HG	0.44	1.54	7	2
1:A:81:THR:CG2	1:B:7:VAL:HG11	0.44	2.42	8	1
1:A:35:LEU:O	1:A:39:GLU:CG	0.44	2.65	20	2
1:B:16:GLN:CG	1:B:20:ARG:CD	0.44	2.96	24	2
1:B:78:ALA:HA	1:B:81:THR:HB	0.44	1.88	10	1
1:A:14:PHE:O	1:A:16:GLN:N	0.44	2.51	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:MET:HG3	1:B:78:ALA:HB2	0.44	1.90	12	1
1:B:36:ILE:HG21	1:B:43:PHE:CD2	0.44	2.48	13	1
1:B:6:ALA:O	1:B:10:LEU:N	0.44	2.51	14	1
1:A:29:LYS:O	1:A:33:LYS:HG2	0.44	2.13	21	1
1:A:71:GLN:CB	1:B:79:MET:CE	0.44	2.96	22	1
1:B:43:PHE:CE1	1:B:49:GLU:HG2	0.44	2.48	23	1
1:B:10:LEU:C	1:B:12:ASP:N	0.44	2.71	19	6
1:B:60:LEU:HA	1:B:63:ASP:OD1	0.44	2.13	14	2
1:A:74:MET:HE2	1:B:74:MET:CE	0.44	2.43	2	1
1:B:7:VAL:O	1:B:8:VAL:C	0.44	2.56	6	6
1:B:11:ILE:C	1:B:11:ILE:HD12	0.44	2.32	19	3
1:B:69:ASP:N	1:B:72:GLU:CG	0.44	2.81	14	6
1:A:39:GLU:HB2	1:A:40:LEU:HD12	0.44	1.88	15	2
1:B:32:LEU:O	1:B:33:LYS:C	0.44	2.57	19	9
1:A:43:PHE:CD2	1:A:80:ILE:HG23	0.44	2.48	8	1
1:B:57:MET:O	1:B:61:ASP:HB3	0.44	2.13	13	1
1:B:40:LEU:N	1:B:40:LEU:CD1	0.44	2.81	15	1
1:A:46:GLU:OE2	1:A:53:VAL:CG1	0.44	2.66	16	1
1:A:17:TYR:CE2	1:A:35:LEU:CA	0.44	3.01	19	3
1:B:16:GLN:CG	1:B:20:ARG:NE	0.44	2.80	18	1
1:A:55:LYS:O	1:A:58:GLU:HB3	0.44	2.13	20	1
1:B:59:THR:O	1:B:62:SER:HB3	0.44	2.13	21	1
1:A:4:GLU:CD	1:B:39:GLU:O	0.43	2.56	2	1
1:A:17:TYR:CD2	1:A:35:LEU:HD11	0.43	2.47	3	1
1:B:0:MET:HG2	1:B:1:SER:N	0.43	2.28	3	1
1:B:9:ALA:O	1:B:12:ASP:CB	0.43	2.66	19	3
1:B:3:LEU:O	1:B:7:VAL:HB	0.43	2.14	10	2
1:B:78:ALA:O	1:B:79:MET:C	0.43	2.55	13	2
1:A:20:ARG:O	1:A:21:GLU:HG2	0.43	2.14	11	1
1:B:14:PHE:O	1:B:16:GLN:N	0.43	2.51	11	1
1:B:25:HIS:CD2	1:B:25:HIS:C	0.43	2.90	19	2
1:B:47:ILE:CG2	1:B:48:LYS:HD3	0.43	2.43	16	4
1:A:36:ILE:HA	1:A:39:GLU:CG	0.43	2.42	12	2
1:A:57:MET:O	1:A:61:ASP:HB3	0.43	2.12	13	1
1:A:17:TYR:CE1	1:B:3:LEU:HD13	0.43	2.48	16	1
1:A:32:LEU:O	1:A:35:LEU:HB3	0.43	2.13	17	1
1:A:70:PHE:CG	1:B:82:THR:HG21	0.43	2.47	18	1
1:A:25:HIS:CD2	1:A:25:HIS:C	0.43	2.91	19	1
1:A:70:PHE:CB	1:B:82:THR:HG22	0.43	2.43	19	1
1:A:14:PHE:CG	1:A:18:SER:OG	0.43	2.69	20	1
1:A:64:GLY:O	1:A:67:GLU:C	0.43	2.57	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LYS:HB2	1:A:49:GLU:OE2	0.43	2.12	20	2
1:A:58:GLU:O	1:A:62:SER:CB	0.43	2.65	3	2
1:A:50:GLN:O	1:A:52:VAL:N	0.43	2.51	5	5
1:A:7:VAL:HG11	1:B:81:THR:CG2	0.43	2.41	8	1
1:A:13:VAL:HG11	1:B:3:LEU:CG	0.43	2.42	21	2
1:A:25:HIS:O	1:A:26:LYS:HE2	0.43	2.12	19	4
1:A:39:GLU:O	1:B:4:GLU:HB3	0.43	2.13	12	2
1:A:75:ALA:O	1:A:76:PHE:C	0.43	2.56	10	1
1:A:47:ILE:CG2	1:A:48:LYS:HD3	0.43	2.43	19	4
1:B:77:VAL:O	1:B:81:THR:N	0.43	2.51	11	1
1:A:14:PHE:CE1	1:A:73:PHE:CB	0.43	3.01	13	2
1:A:60:LEU:HA	1:A:65:ASP:OD2	0.43	2.13	20	1
1:B:8:VAL:HA	1:B:11:ILE:HG23	0.43	1.89	20	1
1:A:79:MET:SD	1:B:71:GLN:HB2	0.43	2.53	23	1
1:B:33:LYS:NZ	1:B:46:GLU:OE2	0.43	2.48	24	1
1:A:39:GLU:CG	1:B:4:GLU:CB	0.43	2.96	3	2
1:B:49:GLU:OE1	1:B:83:ALA:O	0.43	2.36	3	1
1:B:40:LEU:N	1:B:40:LEU:HD12	0.43	2.28	6	1
1:B:67:GLU:HG2	1:B:69:ASP:OD1	0.43	2.13	8	1
1:A:3:LEU:HB2	1:B:39:GLU:HB3	0.43	1.89	23	3
1:A:35:LEU:O	1:A:39:GLU:HG2	0.43	2.13	9	4
1:A:77:VAL:CA	1:A:80:ILE:HG13	0.43	2.43	17	2
1:B:35:LEU:O	1:B:39:GLU:HG2	0.43	2.14	18	4
1:B:26:LYS:HB3	1:B:67:GLU:OE2	0.43	2.13	11	1
1:B:21:GLU:HG3	1:B:22:GLY:N	0.43	2.28	12	1
1:B:35:LEU:CD2	1:B:77:VAL:HG23	0.43	2.43	13	1
1:A:3:LEU:HA	1:B:10:LEU:HD23	0.43	1.90	16	1
1:A:34:GLU:O	1:A:38:ASN:HB2	0.43	2.13	17	4
1:B:8:VAL:HA	1:B:11:ILE:CG2	0.43	2.42	20	1
1:A:73:PHE:HZ	1:B:3:LEU:HD21	0.43	1.67	21	1
1:A:13:VAL:CG2	1:B:3:LEU:CD2	0.43	2.96	24	1
1:A:14:PHE:CD2	1:A:70:PHE:CE1	0.43	3.06	24	2
1:B:14:PHE:CB	1:B:18:SER:HG	0.43	2.26	24	1
1:A:27:LEU:HD23	1:A:31:GLU:HB2	0.43	1.90	25	1
1:A:15:HIS:O	1:A:19:GLY:HA3	0.43	2.14	25	3
1:A:33:LYS:O	1:A:34:GLU:C	0.43	2.56	4	8
1:A:32:LEU:O	1:A:33:LYS:C	0.43	2.57	6	12
1:A:3:LEU:HD12	1:A:4:GLU:HG2	0.43	1.90	8	1
1:A:39:GLU:HG2	1:B:1:SER:HA	0.43	1.89	8	2
1:A:25:HIS:O	1:A:26:LYS:HG3	0.43	2.14	19	4
1:A:27:LEU:HB3	1:A:68:CYS:HB3	0.43	1.90	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:GLU:CA	1:B:4:GLU:HB3	0.43	2.43	12	1
1:B:36:ILE:O	1:B:39:GLU:CG	0.43	2.66	12	1
1:A:39:GLU:CD	1:B:3:LEU:HB2	0.43	2.33	14	1
1:A:3:LEU:HG	1:A:4:GLU:N	0.43	2.28	16	1
1:A:34:GLU:O	1:A:38:ASN:CB	0.43	2.66	17	1
1:B:25:HIS:O	1:B:26:LYS:HG3	0.43	2.13	19	3
1:A:4:GLU:CB	1:B:39:GLU:HB2	0.43	2.43	22	1
1:A:43:PHE:CE1	1:A:49:GLU:HG2	0.43	2.49	23	1
1:A:10:LEU:C	1:A:12:ASP:N	0.43	2.71	19	6
1:B:54:ASP:OD2	1:B:55:LYS:NZ	0.43	2.43	1	1
1:B:48:LYS:HB2	1:B:49:GLU:OE2	0.43	2.13	20	2
1:B:9:ALA:O	1:B:12:ASP:HB2	0.43	2.13	12	4
1:A:57:MET:O	1:A:58:GLU:C	0.43	2.57	14	2
1:A:11:ILE:HD12	1:A:11:ILE:O	0.43	2.13	25	2
1:B:27:LEU:HD23	1:B:32:LEU:N	0.43	2.29	6	1
1:A:3:LEU:CD2	1:B:35:LEU:HG	0.43	2.44	12	3
1:A:4:GLU:HB3	1:B:39:GLU:CA	0.43	2.44	12	1
1:B:8:VAL:C	1:B:11:ILE:CG1	0.43	2.86	16	2
1:B:69:ASP:CB	1:B:72:GLU:HG3	0.43	2.41	12	1
1:A:58:GLU:CA	1:A:58:GLU:OE1	0.43	2.65	14	2
1:B:27:LEU:HB2	1:B:68:CYS:HB3	0.43	1.90	16	1
1:A:37:ASN:HB3	1:A:44:LEU:HD13	0.43	1.89	20	1
1:B:64:GLY:O	1:B:68:CYS:N	0.43	2.51	21	1
1:B:14:PHE:HD2	1:B:70:PHE:CE1	0.43	2.31	24	1
1:A:7:VAL:O	1:A:8:VAL:C	0.43	2.56	9	6
1:A:39:GLU:O	1:B:4:GLU:CD	0.43	2.57	2	1
1:B:63:ASP:OD2	1:B:72:GLU:O	0.43	2.37	2	1
1:A:39:GLU:HB3	1:B:3:LEU:HB2	0.43	1.91	9	4
1:B:36:ILE:HG22	1:B:44:LEU:CD1	0.43	2.44	10	1
1:A:52:VAL:O	1:A:56:VAL:HB	0.43	2.13	11	1
1:B:10:LEU:CD1	1:B:74:MET:HE3	0.43	2.40	11	1
1:B:49:GLU:HB2	1:B:52:VAL:CG1	0.43	2.43	12	1
1:B:73:PHE:O	1:B:77:VAL:CB	0.43	2.66	24	3
1:B:68:CYS:HB3	1:B:73:PHE:N	0.43	2.28	13	1
1:A:35:LEU:HD21	1:A:73:PHE:HD1	0.43	1.68	14	1
1:A:46:GLU:HG2	1:A:53:VAL:HG21	0.43	1.89	16	1
1:A:49:GLU:O	1:A:53:VAL:HB	0.43	2.13	16	2
1:B:34:GLU:HA	1:B:37:ASN:ND2	0.43	2.29	19	1
1:A:60:LEU:HD12	1:A:76:PHE:CE1	0.43	2.49	21	1
1:B:45:GLU:O	1:B:46:GLU:C	0.43	2.57	21	1
1:B:64:GLY:O	1:B:67:GLU:C	0.43	2.57	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LYS:HB3	1:A:31:GLU:OE2	0.43	2.12	23	1
1:A:43:PHE:C	1:A:45:GLU:N	0.43	2.71	20	2
1:B:43:PHE:C	1:B:45:GLU:N	0.43	2.71	20	2
1:A:9:ALA:O	1:A:12:ASP:HB2	0.43	2.12	7	4
1:B:58:GLU:O	1:B:62:SER:OG	0.43	2.33	23	2
1:B:67:GLU:HG3	1:B:69:ASP:OD1	0.43	2.13	6	2
1:B:17:TYR:CE2	1:B:35:LEU:CA	0.43	3.02	18	4
1:B:63:ASP:CG	1:B:68:CYS:SG	0.43	2.97	9	2
1:A:32:LEU:HD22	1:A:36:ILE:HD11	0.43	1.88	12	1
1:B:9:ALA:O	1:B:10:LEU:C	0.43	2.56	16	2
1:A:35:LEU:CD2	1:A:77:VAL:HG23	0.43	2.44	13	1
1:A:34:GLU:O	1:A:36:ILE:N	0.43	2.52	14	1
1:A:29:LYS:HG3	1:A:66:GLY:O	0.43	2.14	16	1
1:B:49:GLU:O	1:B:53:VAL:HB	0.43	2.13	16	2
1:A:3:LEU:HD23	1:B:35:LEU:HD21	0.43	1.90	19	1
1:A:60:LEU:CD2	1:A:65:ASP:OD2	0.43	2.61	20	1
1:B:17:TYR:HB3	1:B:27:LEU:CD2	0.43	2.44	20	2
1:A:4:GLU:CG	1:B:40:LEU:HG	0.43	2.43	24	1
1:B:31:GLU:O	1:B:32:LEU:C	0.43	2.57	24	1
1:A:14:PHE:CE2	1:A:73:PHE:HD2	0.43	2.30	9	6
1:B:69:ASP:H	1:B:72:GLU:CG	0.43	2.27	21	3
1:B:57:MET:O	1:B:58:GLU:C	0.43	2.57	14	2
1:B:59:THR:O	1:B:63:ASP:HB2	0.43	2.14	4	2
1:B:27:LEU:CB	1:B:72:GLU:CD	0.43	2.87	7	1
1:B:14:PHE:CZ	1:B:27:LEU:CD1	0.43	2.99	9	1
1:A:3:LEU:O	1:A:7:VAL:HB	0.43	2.13	10	2
1:A:4:GLU:HB3	1:B:39:GLU:O	0.43	2.13	10	2
1:A:11:ILE:HG22	1:B:81:THR:CG2	0.43	2.44	12	1
1:A:36:ILE:O	1:A:39:GLU:CG	0.43	2.66	12	1
1:A:49:GLU:HB2	1:A:52:VAL:CG1	0.43	2.44	12	1
1:A:68:CYS:HB3	1:A:73:PHE:N	0.43	2.29	13	1
1:B:17:TYR:O	1:B:18:SER:C	0.43	2.57	13	1
1:A:74:MET:C	1:A:77:VAL:HG12	0.43	2.34	24	2
1:B:34:GLU:O	1:B:38:ASN:HB2	0.43	2.13	17	3
1:A:17:TYR:HB3	1:A:27:LEU:CD2	0.43	2.44	20	2
1:A:33:LYS:O	1:A:37:ASN:CG	0.43	2.57	21	1
1:A:35:LEU:HD13	1:A:73:PHE:CE1	0.43	2.48	21	1
1:A:46:GLU:O	1:A:46:GLU:HG3	0.43	2.14	21	1
1:A:17:TYR:C	1:A:27:LEU:HD11	0.43	2.34	24	1
1:A:43:PHE:CG	1:A:49:GLU:OE2	0.43	2.71	5	1
1:A:0:MET:O	1:B:39:GLU:OE2	0.43	2.36	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:SER:C	1:A:3:LEU:N	0.43	2.72	15	4
1:B:26:LYS:HG2	1:B:69:ASP:OD2	0.43	2.13	13	1
1:A:40:LEU:N	1:A:40:LEU:CD1	0.43	2.81	15	1
1:A:3:LEU:HD13	1:B:17:TYR:CE1	0.43	2.48	16	1
1:A:64:GLY:O	1:A:68:CYS:N	0.43	2.51	21	1
1:B:14:PHE:CD2	1:B:70:PHE:CE1	0.43	3.06	24	1
1:B:18:SER:OG	1:B:26:LYS:O	0.43	2.37	25	1
1:B:53:VAL:O	1:B:57:MET:HB2	0.43	2.14	13	8
1:A:39:GLU:O	1:B:4:GLU:HG2	0.43	2.14	6	1
1:B:56:VAL:O	1:B:60:LEU:HB2	0.43	2.14	6	1
1:A:62:SER:C	1:A:63:ASP:CG	0.43	2.77	7	1
1:A:68:CYS:HB3	1:A:72:GLU:OE1	0.43	2.14	7	2
1:A:3:LEU:HG	1:B:13:VAL:HG11	0.43	1.90	9	1
1:B:63:ASP:CG	1:B:68:CYS:HG	0.43	2.18	9	1
1:A:4:GLU:CD	1:B:35:LEU:O	0.43	2.57	11	1
1:A:14:PHE:CE1	1:A:27:LEU:CD2	0.43	3.01	11	1
1:A:33:LYS:HG2	1:A:60:LEU:HD11	0.43	1.91	15	1
1:B:18:SER:HB3	1:B:26:LYS:N	0.43	2.28	15	2
1:B:32:LEU:O	1:B:35:LEU:HB3	0.43	2.13	17	1
1:B:27:LEU:C	1:B:28:LYS:HG3	0.43	2.35	21	1
1:B:68:CYS:HA	1:B:72:GLU:HB2	0.43	1.91	22	1
1:A:68:CYS:HA	1:A:72:GLU:CG	0.43	2.44	24	1
1:B:46:GLU:C	1:B:48:LYS:N	0.42	2.71	17	4
1:B:49:GLU:HB2	1:B:52:VAL:HB	0.42	1.91	5	1
1:B:41:SER:O	1:B:42:HIS:C	0.42	2.57	15	6
1:A:26:LYS:HB3	1:A:67:GLU:OE2	0.42	2.12	11	1
1:A:56:VAL:CG2	1:A:80:ILE:HD12	0.42	2.39	11	1
1:B:52:VAL:O	1:B:56:VAL:HB	0.42	2.14	11	1
1:A:21:GLU:HG3	1:A:22:GLY:N	0.42	2.29	12	1
1:A:3:LEU:HD11	1:B:10:LEU:HD22	0.42	1.90	14	1
1:A:10:LEU:HD22	1:B:3:LEU:HD11	0.42	1.89	14	1
1:A:26:LYS:CD	1:A:27:LEU:O	0.42	2.67	17	1
1:A:34:GLU:HA	1:A:37:ASN:ND2	0.42	2.29	19	1
1:A:45:GLU:HB3	1:A:48:LYS:CD	0.42	2.45	20	1
1:B:35:LEU:HD13	1:B:73:PHE:CE1	0.42	2.48	21	1
1:B:49:GLU:O	1:B:50:GLN:C	0.42	2.55	22	1
1:B:71:GLN:HG3	1:B:72:GLU:N	0.42	2.28	22	1
1:A:60:LEU:HA	1:A:63:ASP:OD1	0.42	2.14	1	2
1:B:22:GLY:O	1:B:23:ASP:C	0.42	2.55	22	4
1:A:4:GLU:HG2	1:B:39:GLU:O	0.42	2.14	6	1
1:A:27:LEU:HD23	1:A:32:LEU:N	0.42	2.29	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:GLU:HB2	1:B:4:GLU:CG	0.42	2.43	8	1
1:A:40:LEU:HD23	1:B:4:GLU:HB3	0.42	1.90	10	1
1:B:49:GLU:CD	1:B:52:VAL:HG11	0.42	2.33	10	1
1:B:27:LEU:HB3	1:B:68:CYS:HB3	0.42	1.90	12	1
1:B:36:ILE:HA	1:B:39:GLU:CG	0.42	2.43	12	1
1:A:10:LEU:HD22	1:B:3:LEU:CD1	0.42	2.44	14	1
1:A:33:LYS:O	1:A:36:ILE:N	0.42	2.49	15	1
1:A:3:LEU:O	1:B:10:LEU:CD2	0.42	2.67	16	1
1:B:46:GLU:OE2	1:B:53:VAL:CG1	0.42	2.67	16	1
1:A:37:ASN:ND2	1:A:44:LEU:CD1	0.42	2.82	20	1
1:B:37:ASN:ND2	1:B:44:LEU:CD1	0.42	2.82	20	1
1:A:45:GLU:O	1:A:46:GLU:C	0.42	2.57	21	1
1:A:14:PHE:HD2	1:A:70:PHE:CE1	0.42	2.32	24	1
1:A:74:MET:HE3	1:B:77:VAL:CG1	0.42	2.44	6	1
1:B:35:LEU:O	1:B:39:GLU:HG3	0.42	2.14	6	1
1:A:40:LEU:CD1	1:B:4:GLU:OE2	0.42	2.67	8	1
1:A:79:MET:O	1:A:79:MET:HE3	0.42	2.13	8	1
1:A:39:GLU:CG	1:B:3:LEU:HB3	0.42	2.44	10	1
1:A:4:GLU:OE1	1:B:39:GLU:CB	0.42	2.68	11	1
1:B:56:VAL:CG2	1:B:80:ILE:HD12	0.42	2.38	11	1
1:A:61:ASP:OD1	1:A:61:ASP:O	0.42	2.37	12	1
1:A:69:ASP:CB	1:A:72:GLU:HG3	0.42	2.41	12	1
1:A:17:TYR:O	1:A:18:SER:C	0.42	2.57	13	2
1:A:35:LEU:HG	1:B:3:LEU:HD13	0.42	1.90	13	1
1:B:56:VAL:O	1:B:60:LEU:HB3	0.42	2.15	13	1
1:B:18:SER:OG	1:B:25:HIS:C	0.42	2.57	14	1
1:B:29:LYS:HG3	1:B:66:GLY:O	0.42	2.15	16	1
1:B:26:LYS:CD	1:B:27:LEU:O	0.42	2.67	17	1
1:A:16:GLN:HA	1:A:20:ARG:HB3	0.42	1.91	19	2
1:A:39:GLU:CB	1:B:4:GLU:N	0.42	2.82	5	1
1:B:27:LEU:CD2	1:B:31:GLU:HB3	0.42	2.45	8	1
1:A:63:ASP:CG	1:A:68:CYS:SG	0.42	2.97	9	2
1:A:35:LEU:O	1:B:4:GLU:CD	0.42	2.58	11	1
1:A:10:LEU:HD23	1:B:3:LEU:HA	0.42	1.90	16	1
1:B:61:ASP:O	1:B:62:SER:C	0.42	2.56	24	2
1:A:36:ILE:HD11	1:A:76:PHE:CE2	0.42	2.48	17	1
1:A:39:GLU:HB2	1:B:4:GLU:CB	0.42	2.44	23	2
1:A:64:GLY:O	1:A:65:ASP:CG	0.42	2.58	3	1
1:B:64:GLY:O	1:B:65:ASP:CG	0.42	2.57	3	2
1:A:59:THR:O	1:A:63:ASP:HB2	0.42	2.14	19	4
1:B:64:GLY:O	1:B:67:GLU:N	0.42	2.52	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:SER:CA	1:B:39:GLU:CG	0.42	2.98	21	2
1:A:39:GLU:O	1:B:4:GLU:CB	0.42	2.67	9	1
1:B:49:GLU:OE1	1:B:52:VAL:HG21	0.42	2.15	10	1
1:A:81:THR:CG2	1:B:11:ILE:HG22	0.42	2.44	12	1
1:B:55:LYS:O	1:B:58:GLU:HB3	0.42	2.14	20	2
1:A:3:LEU:CD2	1:A:4:GLU:HG2	0.42	2.45	16	1
1:A:74:MET:HB3	1:B:74:MET:HB3	0.42	1.91	16	1
1:B:34:GLU:O	1:B:38:ASN:CB	0.42	2.67	17	1
1:B:65:ASP:CG	1:B:65:ASP:O	0.42	2.56	19	1
1:B:69:ASP:CG	1:B:71:GLN:CG	0.42	2.88	19	1
1:B:46:GLU:O	1:B:46:GLU:HG3	0.42	2.14	21	1
1:A:31:GLU:O	1:A:32:LEU:C	0.42	2.57	24	1
1:B:27:LEU:HB3	1:B:68:CYS:HB2	0.42	1.90	24	1
1:A:41:SER:O	1:A:42:HIS:C	0.42	2.57	20	6
1:A:27:LEU:CB	1:A:72:GLU:CD	0.42	2.88	7	1
1:B:60:LEU:HG	1:B:76:PHE:CE1	0.42	2.50	8	1
1:A:14:PHE:HE1	1:A:27:LEU:HD23	0.42	1.69	11	1
1:B:33:LYS:HD2	1:B:37:ASN:OD1	0.42	2.15	12	1
1:A:13:VAL:HG13	1:A:17:TYR:HE2	0.42	1.75	13	1
1:A:56:VAL:O	1:A:60:LEU:HB3	0.42	2.15	13	1
1:B:71:GLN:HG2	1:B:72:GLU:N	0.42	2.30	13	1
1:A:18:SER:OG	1:A:27:LEU:CD1	0.42	2.68	16	1
1:A:26:LYS:NZ	1:A:67:GLU:HA	0.42	2.30	17	1
1:A:35:LEU:HD21	1:B:3:LEU:HD23	0.42	1.91	19	1
1:A:69:ASP:CG	1:A:71:GLN:CG	0.42	2.88	19	1
1:B:68:CYS:HA	1:B:72:GLU:CG	0.42	2.44	24	1
1:B:27:LEU:O	1:B:28:LYS:HG2	0.42	2.15	2	1
1:B:54:ASP:OD1	1:B:54:ASP:C	0.42	2.57	18	3
1:B:62:SER:C	1:B:63:ASP:CG	0.42	2.78	7	1
1:A:4:GLU:CB	1:B:39:GLU:O	0.42	2.68	9	1
1:A:36:ILE:HG22	1:A:44:LEU:CD1	0.42	2.44	10	1
1:B:75:ALA:O	1:B:76:PHE:C	0.42	2.56	10	1
1:A:75:ALA:CB	1:B:71:GLN:HG3	0.42	2.43	13	1
1:A:78:ALA:CA	1:A:81:THR:OG1	0.42	2.67	14	1
1:B:39:GLU:OE1	1:B:39:GLU:CA	0.42	2.68	15	1
1:B:74:MET:C	1:B:77:VAL:HG12	0.42	2.35	24	2
1:A:14:PHE:CE1	1:A:70:PHE:CE1	0.42	3.07	17	1
1:A:43:PHE:CD1	1:A:49:GLU:CG	0.42	3.02	19	1
1:A:79:MET:HA	1:A:79:MET:CE	0.42	2.45	22	1
1:B:80:ILE:N	1:B:80:ILE:HD13	0.42	2.29	23	1
1:A:44:LEU:HD12	1:A:44:LEU:HA	0.42	1.73	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:LEU:CD2	1:B:35:LEU:HD21	0.42	2.44	25	1
1:B:23:ASP:OD2	1:B:31:GLU:OE2	0.42	2.38	25	1
1:A:4:GLU:CG	1:B:39:GLU:HB2	0.42	2.45	8	1
1:A:60:LEU:HG	1:A:76:PHE:CE1	0.42	2.50	8	1
1:B:79:MET:HA	1:B:82:THR:HG1	0.42	1.75	9	1
1:A:21:GLU:HG2	1:A:21:GLU:O	0.42	2.14	11	1
1:B:32:LEU:HD22	1:B:36:ILE:HD11	0.42	1.87	12	1
1:B:17:TYR:O	1:B:27:LEU:HG	0.42	2.15	14	1
1:A:39:GLU:OE1	1:A:39:GLU:CA	0.42	2.68	15	1
1:A:27:LEU:C	1:A:28:LYS:HG3	0.42	2.34	21	1
1:A:71:GLN:HB3	1:B:82:THR:CG2	0.42	2.44	22	1
1:B:62:SER:O	1:B:62:SER:OG	0.42	2.38	22	1
1:A:3:LEU:HD21	1:B:13:VAL:HG13	0.42	1.89	25	1
1:A:4:GLU:N	1:B:39:GLU:CB	0.42	2.82	5	1
1:A:4:GLU:O	1:A:5:LYS:C	0.42	2.58	8	1
1:A:27:LEU:CD2	1:A:31:GLU:HB3	0.42	2.45	8	2
1:A:28:LYS:C	1:A:30:SER:N	0.42	2.71	15	5
1:B:26:LYS:HG2	1:B:69:ASP:OD1	0.42	2.15	10	1
1:B:68:CYS:HA	1:B:72:GLU:OE2	0.42	2.15	11	1
1:A:49:GLU:CG	1:A:52:VAL:HG11	0.42	2.45	12	1
1:A:72:GLU:HA	1:A:75:ALA:HB3	0.42	1.91	13	1
1:B:26:LYS:NZ	1:B:67:GLU:HA	0.42	2.30	17	1
1:A:39:GLU:OE2	1:A:40:LEU:CD1	0.42	2.67	20	1
1:A:52:VAL:C	1:A:54:ASP:N	0.42	2.72	20	1
1:B:60:LEU:O	1:B:65:ASP:HB2	0.42	2.15	21	1
1:A:40:LEU:HG	1:B:4:GLU:CG	0.42	2.45	24	1
1:A:32:LEU:HD23	1:A:32:LEU:HA	0.42	1.71	1	2
1:A:27:LEU:HD12	1:A:31:GLU:HB2	0.42	1.91	2	1
1:A:27:LEU:O	1:A:28:LYS:HG2	0.42	2.15	2	1
1:A:60:LEU:HD12	1:A:60:LEU:O	0.42	2.15	2	1
1:B:55:LYS:O	1:B:58:GLU:HG2	0.42	2.14	4	1
1:A:14:PHE:CZ	1:A:69:ASP:C	0.42	2.93	9	1
1:B:1:SER:C	1:B:3:LEU:N	0.42	2.73	12	4
1:B:14:PHE:CZ	1:B:69:ASP:C	0.42	2.94	9	1
1:A:18:SER:OG	1:A:19:GLY:N	0.42	2.53	10	1
1:B:17:TYR:CZ	1:B:35:LEU:HD12	0.42	2.46	11	1
1:B:17:TYR:HA	1:B:20:ARG:CD	0.42	2.45	12	1
1:A:62:SER:O	1:A:65:ASP:CA	0.42	2.68	14	1
1:A:74:MET:CB	1:B:78:ALA:CB	0.42	2.97	15	1
1:A:74:MET:HE2	1:B:77:VAL:HG13	0.42	1.92	15	1
1:B:3:LEU:CD2	1:B:4:GLU:HG2	0.42	2.45	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:14:PHE:CE1	1:B:70:PHE:CE1	0.42	3.07	17	1
1:A:0:MET:CE	1:B:38:ASN:O	0.42	2.68	19	1
1:A:11:ILE:O	1:A:11:ILE:HD12	0.42	2.15	20	1
1:B:37:ASN:OD1	1:B:37:ASN:N	0.42	2.51	21	1
1:B:60:LEU:HD12	1:B:76:PHE:CE1	0.42	2.49	21	1
1:A:71:GLN:HG3	1:A:72:GLU:N	0.42	2.29	22	1
1:A:79:MET:CE	1:B:71:GLN:CB	0.42	2.98	22	1
1:A:69:ASP:H	1:A:72:GLU:CG	0.41	2.27	21	3
1:B:43:PHE:CD1	1:B:49:GLU:OE1	0.41	2.73	5	1
1:A:56:VAL:O	1:A:60:LEU:HB2	0.41	2.14	6	1
1:A:53:VAL:O	1:A:57:MET:HB2	0.41	2.15	23	8
1:B:43:PHE:HE2	1:B:80:ILE:HG23	0.41	1.64	7	1
1:B:52:VAL:HG21	1:B:83:ALA:HB1	0.41	1.90	8	1
1:A:4:GLU:O	1:A:7:VAL:CB	0.41	2.68	11	1
1:A:10:LEU:CD2	1:B:3:LEU:CD1	0.41	2.98	14	1
1:B:78:ALA:CA	1:B:81:THR:OG1	0.41	2.68	14	1
1:A:3:LEU:CD1	1:A:3:LEU:N	0.41	2.82	17	2
1:A:13:VAL:HG11	1:A:73:PHE:CE1	0.41	2.50	17	1
1:A:34:GLU:O	1:A:38:ASN:CG	0.41	2.58	17	1
1:B:3:LEU:CD1	1:B:3:LEU:N	0.41	2.82	17	2
1:A:71:GLN:HB2	1:B:79:MET:SD	0.41	2.55	18	1
1:A:3:LEU:CD2	1:B:13:VAL:HG21	0.41	2.43	21	1
1:A:17:TYR:C	1:A:27:LEU:HD21	0.41	2.36	21	1
1:B:62:SER:O	1:B:63:ASP:HB2	0.41	2.14	21	1
1:A:27:LEU:HB3	1:A:68:CYS:HB2	0.41	1.92	24	1
1:B:20:ARG:O	1:B:21:GLU:HB2	0.41	2.15	17	2
1:A:12:ASP:O	1:A:13:VAL:C	0.41	2.58	4	1
1:B:12:ASP:O	1:B:13:VAL:C	0.41	2.57	11	2
1:A:39:GLU:CG	1:B:3:LEU:CB	0.41	2.98	10	1
1:B:18:SER:OG	1:B:19:GLY:N	0.41	2.54	10	1
1:A:39:GLU:HB2	1:B:4:GLU:OE1	0.41	2.14	11	1
1:A:1:SER:O	1:A:4:GLU:HG2	0.41	2.14	12	1
1:A:33:LYS:HD2	1:A:37:ASN:OD1	0.41	2.15	12	1
1:A:81:THR:CG2	1:B:11:ILE:CG2	0.41	2.98	12	1
1:B:69:ASP:HB2	1:B:72:GLU:OE2	0.41	2.15	12	1
1:A:75:ALA:C	1:B:71:GLN:HG3	0.41	2.36	13	1
1:B:18:SER:OG	1:B:27:LEU:CD1	0.41	2.68	16	1
1:A:16:GLN:O	1:A:19:GLY:C	0.41	2.59	22	1
1:A:54:ASP:OD1	1:A:54:ASP:C	0.41	2.58	3	3
1:A:35:LEU:O	1:A:39:GLU:HG3	0.41	2.15	6	1
1:A:67:GLU:O	1:A:67:GLU:HG3	0.41	2.16	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:GLN:HG2	1:A:17:TYR:N	0.41	2.29	9	1
1:B:28:LYS:C	1:B:30:SER:N	0.41	2.72	15	3
1:B:8:VAL:C	1:B:11:ILE:HG13	0.41	2.35	12	1
1:B:33:LYS:HG2	1:B:60:LEU:HD11	0.41	1.92	15	1
1:A:13:VAL:CG2	1:B:3:LEU:HD11	0.41	2.41	17	1
1:A:34:GLU:O	1:A:38:ASN:OD1	0.41	2.38	17	1
1:B:13:VAL:HG11	1:B:73:PHE:CE1	0.41	2.50	17	1
1:A:11:ILE:O	1:A:15:HIS:HB3	0.41	2.16	19	1
1:A:41:SER:O	1:A:44:LEU:HB3	0.41	2.16	21	1
1:A:63:ASP:OD2	1:A:72:GLU:O	0.41	2.38	2	1
1:A:49:GLU:O	1:A:49:GLU:HG3	0.41	2.16	3	2
1:A:67:GLU:HG2	1:A:69:ASP:OD1	0.41	2.14	8	1
1:B:4:GLU:O	1:B:7:VAL:CB	0.41	2.68	11	1
1:B:32:LEU:HD12	1:B:60:LEU:CD2	0.41	2.44	13	1
1:A:56:VAL:CG2	1:A:80:ILE:HD13	0.41	2.32	15	1
1:A:4:GLU:OE1	1:B:77:VAL:CG2	0.41	2.69	16	1
1:B:46:GLU:HG2	1:B:53:VAL:HG11	0.41	1.93	16	1
1:B:43:PHE:CD1	1:B:49:GLU:CG	0.41	3.02	19	1
1:A:8:VAL:HA	1:A:11:ILE:HG23	0.41	1.92	20	1
1:B:41:SER:O	1:B:44:LEU:HB3	0.41	2.16	21	1
1:A:39:GLU:CG	1:B:0:MET:C	0.41	2.89	1	1
1:A:36:ILE:HG13	1:A:76:PHE:CE2	0.41	2.51	2	1
1:B:36:ILE:HG13	1:B:76:PHE:CE2	0.41	2.51	2	1
1:B:59:THR:O	1:B:60:LEU:C	0.41	2.58	2	2
1:B:60:LEU:HD12	1:B:60:LEU:O	0.41	2.15	2	1
1:A:74:MET:HB2	1:B:78:ALA:HB2	0.41	1.91	12	1
1:A:78:ALA:HB2	1:B:74:MET:HB2	0.41	1.92	12	1
1:A:61:ASP:C	1:A:63:ASP:N	0.41	2.72	16	2
1:A:54:ASP:C	1:A:54:ASP:OD1	0.41	2.57	18	1
1:B:52:VAL:C	1:B:54:ASP:N	0.41	2.72	20	1
1:B:16:GLN:O	1:B:19:GLY:C	0.41	2.58	22	1
1:B:60:LEU:HD13	1:B:76:PHE:CZ	0.41	2.50	25	1
1:B:27:LEU:HD12	1:B:31:GLU:HB2	0.41	1.91	2	1
1:B:70:PHE:N	1:B:70:PHE:CD1	0.41	2.87	3	1
1:B:60:LEU:O	1:B:63:ASP:HB2	0.41	2.16	6	1
1:B:17:TYR:HA	1:B:20:ARG:HG2	0.41	1.93	7	1
1:A:1:SER:HB3	1:B:39:GLU:HG3	0.41	1.92	8	1
1:A:3:LEU:HD13	1:B:35:LEU:CD2	0.41	2.45	8	1
1:A:8:VAL:C	1:A:11:ILE:HG13	0.41	2.35	12	1
1:A:40:LEU:C	1:A:42:HIS:N	0.41	2.73	13	2
1:B:46:GLU:CG	1:B:47:ILE:N	0.41	2.83	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:TYR:O	1:A:27:LEU:HG	0.41	2.15	14	1
1:B:61:ASP:C	1:B:63:ASP:N	0.41	2.73	16	2
1:B:17:TYR:C	1:B:27:LEU:HD21	0.41	2.35	21	1
1:B:79:MET:CE	1:B:79:MET:HA	0.41	2.46	22	1
1:A:20:ARG:O	1:A:21:GLU:HB2	0.41	2.16	2	1
1:A:53:VAL:O	1:A:57:MET:HG3	0.41	2.16	4	3
1:A:74:MET:HB2	1:B:78:ALA:CB	0.41	2.45	5	1
1:A:43:PHE:CZ	1:A:52:VAL:HG11	0.41	2.51	7	1
1:B:27:LEU:HD22	1:B:27:LEU:HA	0.41	1.73	7	1
1:A:39:GLU:CA	1:B:4:GLU:HG2	0.41	2.46	10	1
1:A:4:GLU:CG	1:B:39:GLU:HB3	0.41	2.46	11	1
1:A:4:GLU:CG	1:A:5:LYS:N	0.41	2.84	12	1
1:A:71:GLN:HG2	1:A:72:GLU:N	0.41	2.31	13	1
1:B:23:ASP:CG	1:B:31:GLU:OE1	0.41	2.59	14	1
1:A:3:LEU:HD21	1:B:35:LEU:CG	0.41	2.45	16	1
1:A:27:LEU:HB2	1:A:68:CYS:CB	0.41	2.46	16	1
1:A:38:ASN:OD1	1:B:0:MET:HG2	0.41	2.16	16	1
1:B:16:GLN:HA	1:B:20:ARG:HB3	0.41	1.91	19	3
1:A:27:LEU:CB	1:A:68:CYS:HB2	0.41	2.45	19	1
1:A:62:SER:O	1:A:62:SER:OG	0.41	2.38	22	1
1:A:71:GLN:CD	1:A:72:GLU:N	0.41	2.74	24	1
1:B:29:LYS:HA	1:B:60:LEU:CD2	0.41	2.45	24	1
1:B:27:LEU:HD23	1:B:31:GLU:HB2	0.41	1.92	25	1
1:A:17:TYR:HA	1:A:20:ARG:HG2	0.41	1.93	7	1
1:B:76:PHE:O	1:B:80:ILE:N	0.41	2.54	9	1
1:A:53:VAL:O	1:A:57:MET:HG2	0.41	2.15	11	1
1:A:69:ASP:HB2	1:A:72:GLU:OE2	0.41	2.15	12	1
1:B:61:ASP:OD1	1:B:61:ASP:O	0.41	2.38	12	1
1:A:9:ALA:O	1:A:10:LEU:C	0.41	2.56	16	1
1:A:29:LYS:HD2	1:A:63:ASP:HA	0.41	1.93	16	1
1:B:53:VAL:HA	1:B:56:VAL:HB	0.41	1.93	16	1
1:A:31:GLU:O	1:A:35:LEU:HB2	0.41	2.15	17	1
1:B:45:GLU:HB3	1:B:48:LYS:CD	0.41	2.45	20	1
1:A:39:GLU:CG	1:B:1:SER:CA	0.41	2.99	21	1
1:A:82:THR:HG22	1:B:70:PHE:CG	0.41	2.51	24	1
1:A:52:VAL:CG2	1:A:83:ALA:HB1	0.41	2.45	25	1
1:B:15:HIS:O	1:B:19:GLY:HA3	0.41	2.14	25	1
1:A:39:GLU:HG3	1:B:1:SER:N	0.41	2.31	1	1
1:A:46:GLU:OE1	1:A:57:MET:CE	0.41	2.69	1	1
1:A:14:PHE:CD1	1:A:18:SER:OG	0.41	2.73	3	1
1:A:60:LEU:CG	1:A:76:PHE:CZ	0.41	3.04	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:LYS:O	1:A:58:GLU:HG2	0.41	2.14	4	1
1:A:60:LEU:O	1:A:63:ASP:HB2	0.41	2.16	6	1
1:B:55:LYS:HD2	1:B:55:LYS:N	0.41	2.31	6	1
1:B:68:CYS:HB3	1:B:72:GLU:OE1	0.41	2.15	11	2
1:B:4:GLU:O	1:B:5:LYS:C	0.41	2.58	8	1
1:B:64:GLY:C	1:B:65:ASP:OD1	0.41	2.60	9	1
1:A:3:LEU:HB2	1:B:39:GLU:CD	0.41	2.36	10	1
1:A:49:GLU:OE1	1:A:52:VAL:HG21	0.41	2.16	10	1
1:A:51:GLU:O	1:A:54:ASP:HB3	0.41	2.16	10	1
1:B:16:GLN:C	1:B:20:ARG:HB3	0.41	2.36	10	1
1:B:21:GLU:HG2	1:B:21:GLU:O	0.41	2.14	11	1
1:B:40:LEU:C	1:B:42:HIS:N	0.41	2.74	13	2
1:B:53:VAL:O	1:B:57:MET:HG2	0.41	2.16	11	1
1:A:74:MET:HG3	1:B:78:ALA:CB	0.41	2.46	12	1
1:B:17:TYR:O	1:B:20:ARG:HG2	0.41	2.16	12	1
1:B:49:GLU:HB2	1:B:52:VAL:HG12	0.41	1.92	12	1
1:B:72:GLU:HA	1:B:75:ALA:HB3	0.41	1.92	13	1
1:A:23:ASP:CG	1:A:31:GLU:OE1	0.41	2.60	14	1
1:A:53:VAL:HA	1:A:56:VAL:HB	0.41	1.91	16	1
1:A:46:GLU:HG2	1:A:47:ILE:N	0.41	2.30	18	1
1:A:35:LEU:CD2	1:B:3:LEU:CD1	0.41	2.78	21	1
1:A:45:GLU:O	1:A:46:GLU:HG2	0.41	2.15	21	1
1:A:60:LEU:O	1:A:65:ASP:HB2	0.41	2.15	21	1
1:B:45:GLU:O	1:B:46:GLU:HG2	0.41	2.15	21	1
1:A:46:GLU:CG	1:A:53:VAL:HG13	0.41	2.45	22	1
1:B:40:LEU:HB3	1:B:43:PHE:CD1	0.41	2.51	22	1
1:A:39:GLU:OE1	1:B:3:LEU:HB3	0.41	2.16	23	1
1:A:43:PHE:CD1	1:A:49:GLU:OE1	0.41	2.74	5	1
1:A:58:GLU:OE1	1:A:58:GLU:HA	0.41	2.16	8	1
1:A:36:ILE:HG13	1:A:80:ILE:HD12	0.41	1.93	9	1
1:A:11:ILE:CG2	1:B:81:THR:CG2	0.41	2.99	12	1
1:A:69:ASP:CA	1:A:72:GLU:HG3	0.41	2.46	12	1
1:A:78:ALA:HB2	1:B:74:MET:CG	0.41	2.46	12	1
1:B:32:LEU:HG	1:B:68:CYS:HB2	0.41	1.93	12	1
1:A:3:LEU:HD22	1:B:39:GLU:CB	0.41	2.46	15	1
1:A:54:ASP:O	1:A:58:GLU:HB2	0.41	2.16	17	1
1:B:31:GLU:O	1:B:35:LEU:HB2	0.41	2.15	17	1
1:B:77:VAL:HA	1:B:80:ILE:HG13	0.41	1.93	17	1
1:B:27:LEU:CB	1:B:68:CYS:HB2	0.41	2.46	19	1
1:A:40:LEU:CD1	1:B:4:GLU:OE1	0.41	2.69	21	1
1:A:62:SER:O	1:A:63:ASP:HB2	0.41	2.15	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:28:LYS:HA	1:B:65:ASP:O	0.41	2.16	21	1
1:B:49:GLU:HG3	1:B:52:VAL:HB	0.41	1.93	21	1
1:A:80:ILE:N	1:A:80:ILE:HD13	0.41	2.29	23	1
1:B:44:LEU:HD12	1:B:44:LEU:HA	0.41	1.74	23	1
1:A:14:PHE:CB	1:A:18:SER:HG	0.41	2.29	24	1
1:A:33:LYS:NZ	1:A:46:GLU:OE2	0.41	2.49	24	1
1:B:51:GLU:CG	1:B:55:LYS:NZ	0.40	2.84	2	1
1:B:32:LEU:HD21	1:B:63:ASP:OD2	0.40	2.16	4	1
1:A:55:LYS:HD2	1:A:55:LYS:N	0.40	2.31	6	1
1:A:7:VAL:HG11	1:B:81:THR:HG21	0.40	1.81	8	1
1:A:3:LEU:HB3	1:B:39:GLU:CG	0.40	2.46	10	1
1:A:16:GLN:O	1:A:18:SER:N	0.40	2.54	10	1
1:A:36:ILE:CA	1:A:39:GLU:HG2	0.40	2.46	12	1
1:B:49:GLU:CG	1:B:52:VAL:HG11	0.40	2.45	12	1
1:B:52:VAL:CG1	1:B:56:VAL:CG2	0.40	2.99	17	1
1:A:74:MET:CA	1:A:77:VAL:HG12	0.40	2.46	21	1
1:A:78:ALA:HA	1:B:74:MET:SD	0.40	2.57	22	1
1:A:74:MET:HB2	1:B:74:MET:O	0.40	2.16	24	1
1:A:0:MET:C	1:B:39:GLU:CG	0.40	2.90	1	1
1:B:17:TYR:OH	1:B:39:GLU:HG3	0.40	2.16	6	1
1:B:16:GLN:HG2	1:B:17:TYR:N	0.40	2.30	9	1
1:A:46:GLU:CB	1:A:53:VAL:HG22	0.40	2.47	10	1
1:B:51:GLU:O	1:B:54:ASP:HB3	0.40	2.16	12	3
1:A:68:CYS:HA	1:A:72:GLU:OE2	0.40	2.16	11	1
1:A:17:TYR:O	1:A:20:ARG:HG2	0.40	2.16	12	1
1:B:1:SER:O	1:B:4:GLU:HG2	0.40	2.15	12	1
1:B:4:GLU:CG	1:B:5:LYS:N	0.40	2.84	12	1
1:B:36:ILE:CA	1:B:39:GLU:HG2	0.40	2.47	12	1
1:B:69:ASP:CA	1:B:72:GLU:HG3	0.40	2.46	12	1
1:A:71:GLN:HG3	1:B:75:ALA:CB	0.40	2.43	13	1
1:B:74:MET:O	1:B:75:ALA:C	0.40	2.59	13	1
1:B:3:LEU:HG	1:B:4:GLU:N	0.40	2.30	16	1
1:B:13:VAL:O	1:B:16:GLN:N	0.40	2.54	16	1
1:A:18:SER:HB3	1:A:27:LEU:CD2	0.40	2.46	17	1
1:B:34:GLU:O	1:B:38:ASN:CG	0.40	2.59	17	1
1:B:45:GLU:HB3	1:B:48:LYS:HD3	0.40	1.93	20	1
1:A:28:LYS:HA	1:A:65:ASP:O	0.40	2.15	21	1
1:B:26:LYS:HG3	1:B:69:ASP:CG	0.40	2.37	21	1
1:A:3:LEU:O	1:A:7:VAL:CB	0.40	2.70	22	1
1:A:29:LYS:HA	1:A:60:LEU:CD2	0.40	2.46	24	1
1:A:51:GLU:CG	1:A:55:LYS:NZ	0.40	2.85	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:6:ALA:O	1:B:9:ALA:N	0.40	2.54	3	1
1:B:35:LEU:O	1:B:39:GLU:CG	0.40	2.69	9	1
1:B:39:GLU:HG3	1:B:40:LEU:CG	0.40	2.47	9	1
1:A:16:GLN:C	1:A:20:ARG:HB3	0.40	2.36	10	1
1:A:32:LEU:HG	1:A:68:CYS:HB2	0.40	1.93	12	1
1:B:18:SER:N	1:B:27:LEU:HD11	0.40	2.31	12	1
1:A:71:GLN:HG3	1:B:75:ALA:C	0.40	2.37	13	1
1:A:3:LEU:HD22	1:B:39:GLU:HG3	0.40	1.93	15	1
1:A:4:GLU:CD	1:B:77:VAL:CG2	0.40	2.89	16	1
1:A:13:VAL:O	1:A:16:GLN:N	0.40	2.54	16	1
1:B:18:SER:HB3	1:B:27:LEU:CD2	0.40	2.46	17	1
1:B:14:PHE:CE1	1:B:70:PHE:HD1	0.40	2.35	19	1
1:B:14:PHE:CE1	1:B:73:PHE:HB3	0.40	2.51	20	1
1:A:13:VAL:HG11	1:B:3:LEU:HD23	0.40	1.92	21	1
1:B:18:SER:N	1:B:27:LEU:HD21	0.40	2.31	22	1
1:A:14:PHE:CE1	1:A:73:PHE:HD2	0.40	2.35	24	1
1:A:4:GLU:OE1	1:B:39:GLU:O	0.40	2.39	2	1
1:A:26:LYS:CB	1:A:69:ASP:OD1	0.40	2.70	5	1
1:A:17:TYR:OH	1:A:39:GLU:HG3	0.40	2.17	6	1
1:B:16:GLN:O	1:B:18:SER:N	0.40	2.55	10	1
1:A:17:TYR:HA	1:A:20:ARG:CD	0.40	2.46	12	1
1:A:18:SER:N	1:A:27:LEU:HD11	0.40	2.30	12	1
1:A:46:GLU:CG	1:A:47:ILE:N	0.40	2.84	12	1
1:A:78:ALA:CB	1:B:74:MET:HG3	0.40	2.45	12	1
1:B:4:GLU:HG3	1:B:5:LYS:HG3	0.40	1.93	12	1
1:A:71:GLN:OE1	1:B:79:MET:HB2	0.40	2.16	13	1
1:B:46:GLU:HG2	1:B:47:ILE:N	0.40	2.31	18	1
1:A:45:GLU:HB3	1:A:48:LYS:HD3	0.40	1.93	20	1
1:B:59:THR:OG1	1:B:79:MET:HG2	0.40	2.17	20	1
1:A:3:LEU:HD11	1:B:35:LEU:HD22	0.40	1.82	21	1
1:A:61:ASP:O	1:A:63:ASP:N	0.40	2.55	24	1
1:A:72:GLU:O	1:A:76:PHE:N	0.40	2.53	24	1
1:B:25:HIS:C	1:B:26:LYS:HE3	0.40	2.37	1	1
1:A:3:LEU:CD1	1:B:17:TYR:CZ	0.40	3.05	4	1
1:B:40:LEU:O	1:B:43:PHE:HB2	0.40	2.17	4	1
1:B:67:GLU:O	1:B:67:GLU:HG3	0.40	2.16	7	1
1:B:26:LYS:O	1:B:27:LEU:HG	0.40	2.17	8	1
1:A:4:GLU:HB3	1:B:40:LEU:HD23	0.40	1.92	10	1
1:B:1:SER:HB2	1:B:5:LYS:HD2	0.40	1.94	12	1
1:A:13:VAL:O	1:A:17:TYR:HB2	0.40	2.16	14	1
1:A:10:LEU:CD2	1:B:3:LEU:O	0.40	2.69	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:10:LEU:CD2	1:B:73:PHE:CE2	0.40	3.02	17	1
1:B:58:GLU:OE1	1:B:58:GLU:CA	0.40	2.67	20	1
1:A:18:SER:N	1:A:27:LEU:HD21	0.40	2.32	22	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	83/92 (90%)	57±3 (68±4%)	20±4 (24±4%)	6±2 (7±2%)	2	16
1	B	83/92 (90%)	57±3 (68±4%)	20±4 (24±5%)	6±2 (7±2%)	2	16
All	All	4150/4600 (90%)	2840 (68%)	1012 (24%)	298 (7%)	2	16

All 60 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	70	PHE	24
1	B	70	PHE	24
1	A	63	ASP	16
1	B	63	ASP	16
1	A	65	ASP	12
1	A	23	ASP	12
1	B	23	ASP	12
1	B	65	ASP	10
1	A	22	GLY	8
1	B	22	GLY	8
1	A	2	GLU	8
1	B	2	GLU	8
1	A	48	LYS	6
1	B	48	LYS	6
1	A	21	GLU	6
1	B	21	GLU	6
1	A	50	GLN	6
1	A	64	GLY	6

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Mol	Chain	Res	Type	Models (Total)
1	B	50	GLN	6
1	B	64	GLY	6
1	A	47	ILE	5
1	B	47	ILE	5
1	A	41	SER	5
1	A	29	LYS	5
1	A	1	SER	4
1	B	1	SER	4
1	B	41	SER	4
1	A	17	TYR	4
1	B	17	TYR	4
1	B	29	LYS	4
1	A	3	LEU	3
1	B	3	LEU	3
1	A	20	ARG	2
1	B	20	ARG	2
1	A	81	THR	2
1	B	81	THR	2
1	A	24	LYS	2
1	B	24	LYS	2
1	B	56	VAL	2
1	A	42	HIS	2
1	B	42	HIS	2
1	A	18	SER	2
1	A	46	GLU	2
1	B	18	SER	2
1	B	46	GLU	2
1	B	11	ILE	2
1	B	51	GLU	1
1	A	56	VAL	1
1	A	71	GLN	1
1	A	75	ALA	1
1	B	71	GLN	1
1	B	75	ALA	1
1	B	35	LEU	1
1	A	11	ILE	1
1	A	80	ILE	1
1	B	80	ILE	1
1	A	19	GLY	1
1	B	19	GLY	1
1	A	66	GLY	1
1	B	66	GLY	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	75/83 (90%)	52±4 (69±5%)	23±4 (31±5%)	1 14
1	B	75/83 (90%)	52±4 (69±5%)	23±4 (31±5%)	1 15
All	All	3750/4150 (90%)	2584 (69%)	1166 (31%)	1 15

All 136 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	35	LEU	25
1	A	73	PHE	25
1	B	35	LEU	25
1	B	73	PHE	25
1	A	12	ASP	22
1	B	12	ASP	22
1	A	14	PHE	20
1	A	26	LYS	20
1	A	45	GLU	20
1	B	26	LYS	20
1	B	45	GLU	20
1	B	14	PHE	19
1	A	27	LEU	18
1	A	58	GLU	18
1	B	27	LEU	18
1	B	58	GLU	18
1	A	47	ILE	15
1	A	60	LEU	15
1	B	47	ILE	15
1	B	60	LEU	15
1	A	62	SER	15
1	B	62	SER	15
1	A	33	LYS	13
1	A	79	MET	13
1	B	33	LYS	13
1	B	79	MET	13
1	A	54	ASP	13
1	A	11	ILE	13

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Mol	Chain	Res	Type	Models (Total)
1	A	7	VAL	12
1	B	54	ASP	12
1	A	55	LYS	12
1	B	55	LYS	12
1	B	11	ILE	12
1	A	28	LYS	11
1	A	30	SER	11
1	A	46	GLU	11
1	A	61	ASP	11
1	B	30	SER	11
1	B	46	GLU	11
1	B	61	ASP	11
1	B	7	VAL	10
1	B	28	LYS	10
1	A	34	GLU	10
1	A	82	THR	10
1	B	34	GLU	10
1	B	82	THR	10
1	A	48	LYS	10
1	B	0	MET	10
1	B	48	LYS	10
1	A	21	GLU	10
1	A	3	LEU	9
1	B	3	LEU	9
1	A	0	MET	9
1	A	5	LYS	9
1	A	69	ASP	9
1	B	5	LYS	9
1	B	21	GLU	9
1	A	50	GLN	9
1	B	50	GLN	9
1	A	49	GLU	8
1	B	49	GLU	8
1	B	69	ASP	8
1	A	36	ILE	8
1	B	36	ILE	8
1	A	18	SER	7
1	B	18	SER	7
1	A	71	GLN	7
1	B	71	GLN	7
1	A	1	SER	7
1	B	1	SER	7

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Mol	Chain	Res	Type	Models (Total)
1	A	41	SER	7
1	B	41	SER	7
1	A	29	LYS	7
1	B	29	LYS	7
1	A	24	LYS	7
1	B	24	LYS	7
1	A	4	GLU	6
1	B	4	GLU	6
1	A	43	PHE	6
1	A	77	VAL	6
1	B	43	PHE	6
1	B	77	VAL	6
1	A	20	ARG	6
1	A	32	LEU	6
1	B	20	ARG	6
1	B	32	LEU	6
1	A	23	ASP	6
1	B	23	ASP	6
1	A	10	LEU	6
1	B	10	LEU	6
1	A	68	CYS	5
1	B	68	CYS	5
1	A	72	GLU	5
1	B	72	GLU	5
1	A	16	GLN	4
1	A	67	GLU	4
1	B	16	GLN	4
1	B	67	GLU	4
1	A	65	ASP	4
1	B	65	ASP	4
1	A	38	ASN	4
1	B	38	ASN	4
1	A	2	GLU	4
1	A	81	THR	4
1	B	2	GLU	4
1	B	81	THR	4
1	A	40	LEU	4
1	B	40	LEU	4
1	B	74	MET	4
1	A	37	ASN	4
1	B	37	ASN	4
1	A	63	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	74	MET	3
1	A	80	ILE	3
1	B	63	ASP	3
1	B	80	ILE	3
1	A	42	HIS	2
1	B	42	HIS	2
1	A	15	HIS	2
1	B	15	HIS	2
1	A	44	LEU	2
1	B	44	LEU	2
1	A	31	GLU	2
1	B	31	GLU	2
1	A	57	MET	2
1	B	57	MET	2
1	A	25	HIS	2
1	B	25	HIS	2
1	A	59	THR	2
1	B	59	THR	2
1	A	39	GLU	1
1	B	39	GLU	1
1	A	52	VAL	1
1	B	52	VAL	1
1	A	76	PHE	1
1	B	76	PHE	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided