Full wwPDB NMR Structure Validation Report (i)

Jun 7, 2020 – 04:35 am BST

PDB ID	:	6OC9
Title	:	S8 phosphorylated beta amyloid 40 fibrils
Authors	:	Qiang, W.; Hu, Z.W.
Deposited on	:	2019-03-22

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 (1)) were used in the production of this report:

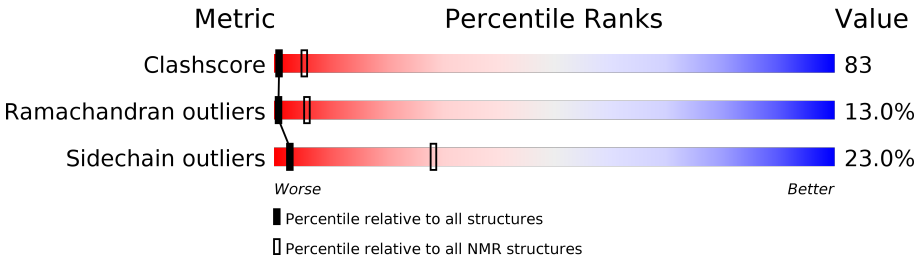
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 3%.

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	40	20% 50% 13% 18%
1	B	40	20% 63% 18%
1	C	40	18% 40% 10% 33%
1	D	40	13% 38% 10% 40%
1	E	40	20% 28% 10% 43%
1	F	40	33% 38% 10% 20%
1	G	40	25% 58% 18%
1	H	40	25% 58% 18%
1	I	40	18% 70% 13%

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Mol	Chain	Length	Quality of chain
1	J	40	

2 Ensemble composition and analysis

This entry contains 10 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:8-A:40, B:1-B:40, C:1-C:3, C:17-C:40, D:17-D:40, E:18-E:40, F:9-F:40, G:1-G:40, H:1-H:40, I:1-I:40, J:1-J:40 (339)	1.75	10

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 1 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 5, 6, 8, 9, 10
Single-model clusters	3; 7

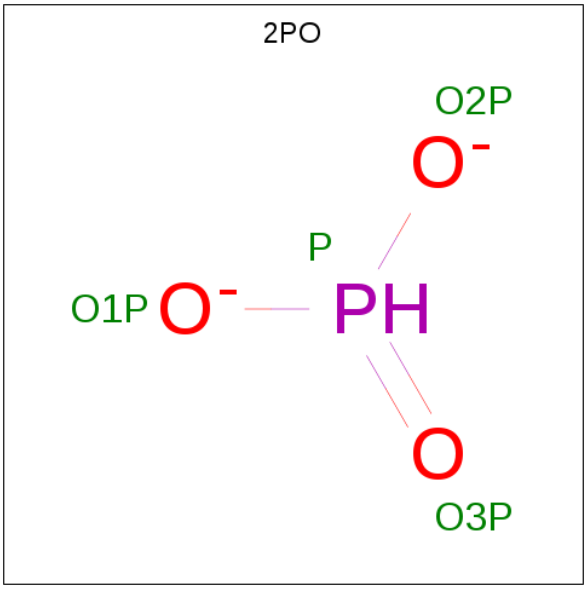
3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6010 atoms, of which 2910 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Amyloid-beta precursor protein.

Mol	Chain	Residues	Atoms						Trace
1	A	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	B	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	C	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	D	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	E	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	F	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	G	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	H	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	I	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	J	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	

- Molecule 2 is PHOSPHONATE (three-letter code: 2PO) (formula: HO_3P).



Mol	Chain	Residues	Atoms		
2	A	1	Total	O	P
			4	3	1
2	B	1	Total	O	P
			4	3	1
2	C	1	Total	O	P
			4	3	1
2	D	1	Total	O	P
			4	3	1
2	E	1	Total	O	P
			4	3	1
2	F	1	Total	O	P
			4	3	1
2	G	1	Total	O	P
			4	3	1
2	H	1	Total	O	P
			4	3	1
2	I	1	Total	O	P
			4	3	1
2	J	1	Total	O	P
			4	3	1

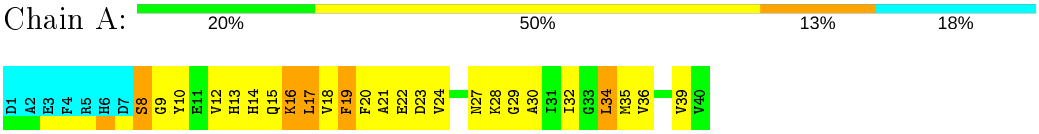
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

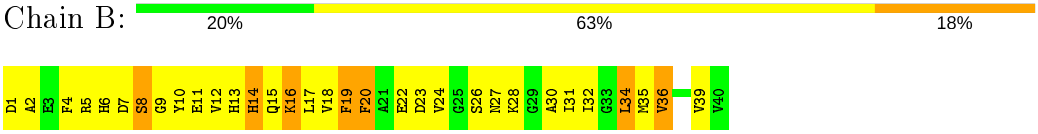
• Molecule 1: Amyloid-beta precursor protein

Chain A:



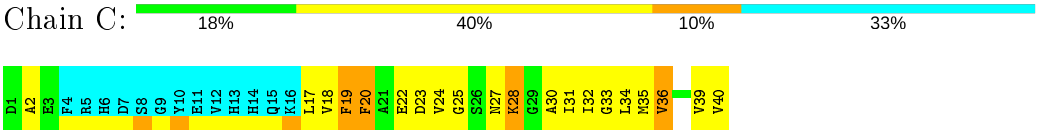
• Molecule 1: Amyloid-beta precursor protein

Chain B:



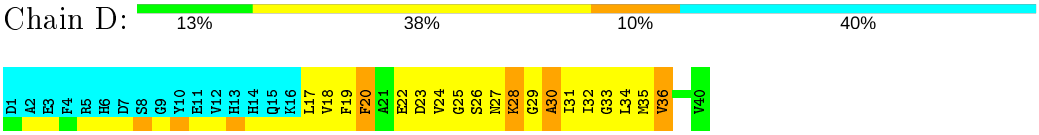
• Molecule 1: Amyloid-beta precursor protein

Chain C:



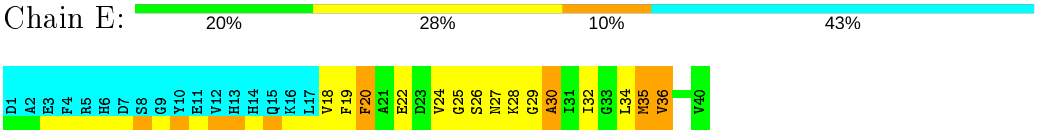
• Molecule 1: Amyloid-beta precursor protein

Chain D:



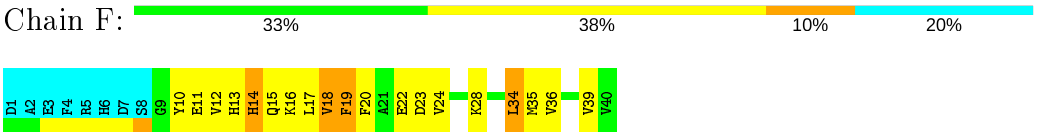
• Molecule 1: Amyloid-beta precursor protein

Chain E:



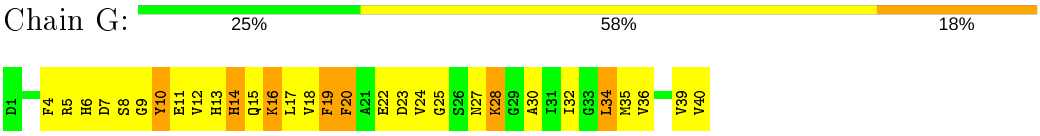
• Molecule 1: Amyloid-beta precursor protein

Chain F:



• Molecule 1: Amyloid-beta precursor protein

Chain G:

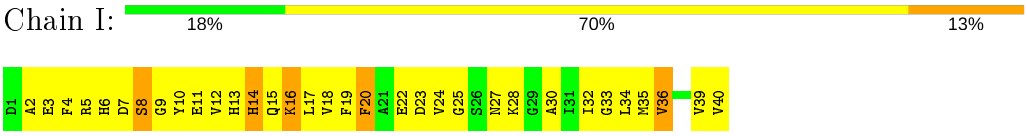


• Molecule 1: Amyloid-beta precursor protein

Chain H:

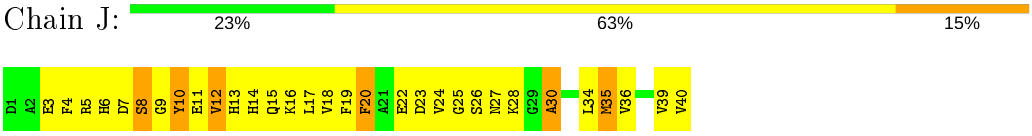
• Molecule 1: Amyloid-beta precursor protein

Chain I:



• Molecule 1: Amyloid-beta precursor protein

Chain J:



• Molecule 1: Amyloid-beta precursor protein

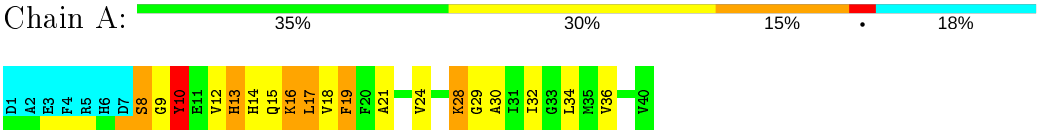
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

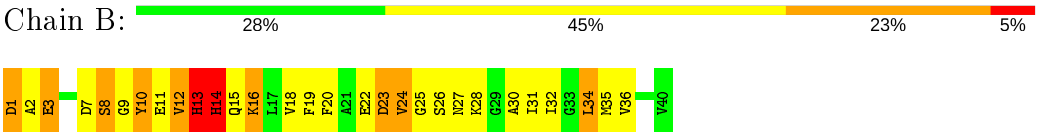
• Molecule 1: Amyloid-beta precursor protein

Chain A:



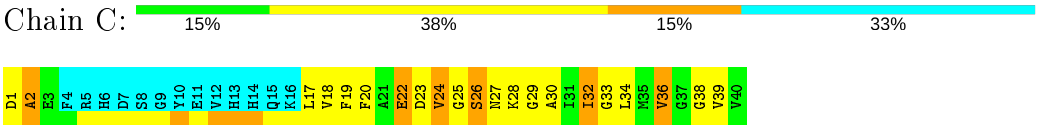
• Molecule 1: Amyloid-beta precursor protein

Chain B:



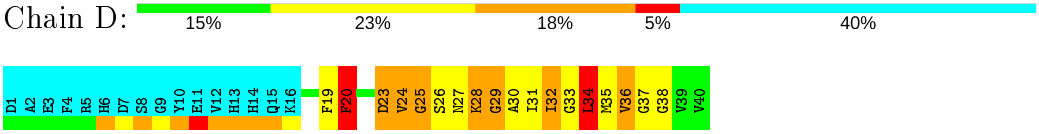
• Molecule 1: Amyloid-beta precursor protein

Chain C:



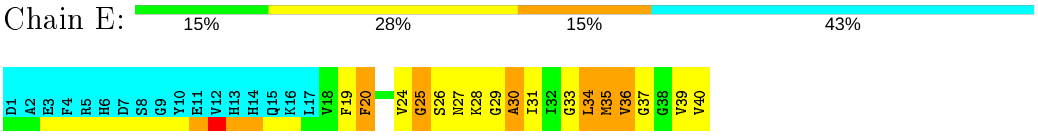
• Molecule 1: Amyloid-beta precursor protein

Chain D:



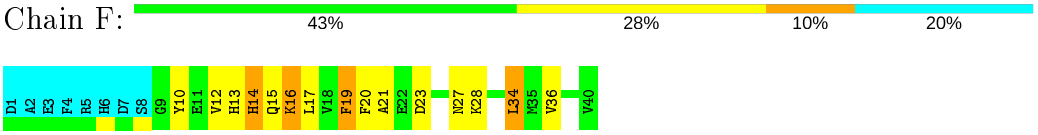
• Molecule 1: Amyloid-beta precursor protein

Chain E:



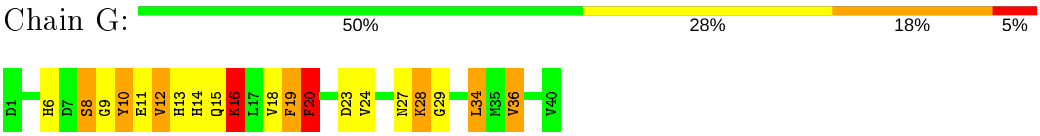
• Molecule 1: Amyloid-beta precursor protein

Chain F:



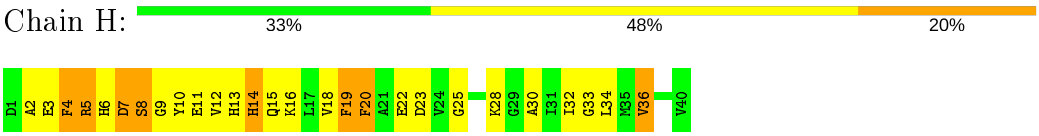
• Molecule 1: Amyloid-beta precursor protein

Chain G:



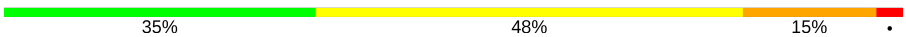
• Molecule 1: Amyloid-beta precursor protein

Chain H:



• Molecule 1: Amyloid-beta precursor protein

Chain I:



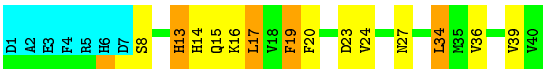
• Molecule 1: Amyloid-beta precursor protein

Chain J:

4.2.2 Score per residue for model 2

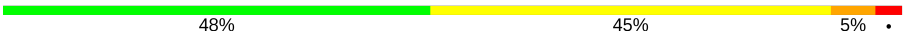
• Molecule 1: Amyloid-beta precursor protein

Chain A:



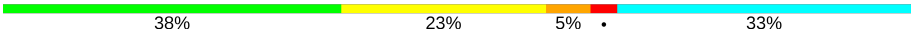
• Molecule 1: Amyloid-beta precursor protein

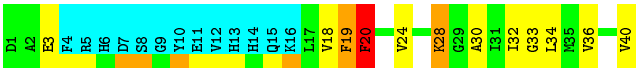
Chain B:



• Molecule 1: Amyloid-beta precursor protein

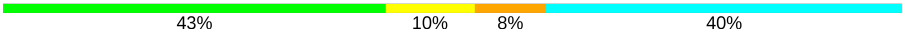
Chain C:





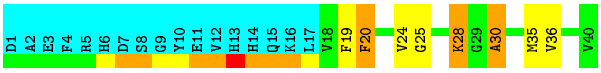
• Molecule 1: Amyloid-beta precursor protein

Chain D:



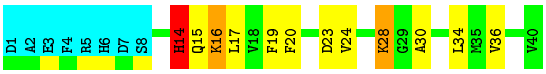
• Molecule 1: Amyloid-beta precursor protein

Chain E:



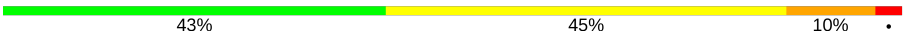
• Molecule 1: Amyloid-beta precursor protein

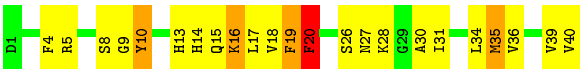
Chain F:



• Molecule 1: Amyloid-beta precursor protein

Chain G:



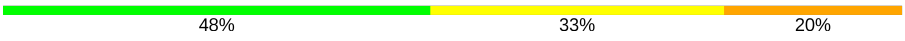


• Molecule 1: Amyloid-beta precursor protein

Chain H:

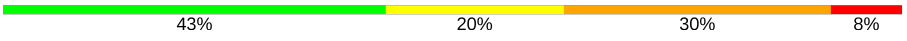
• Molecule 1: Amyloid-beta precursor protein

Chain I:



• Molecule 1: Amyloid-beta precursor protein

Chain J:



4.2.3 Score per residue for model 3

• Molecule 1: Amyloid-beta precursor protein

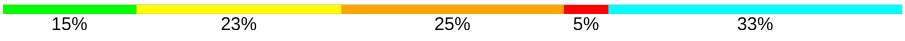
Chain A:

• Molecule 1: Amyloid-beta precursor protein

Chain B:

• Molecule 1: Amyloid-beta precursor protein

Chain C:



• Molecule 1: Amyloid-beta precursor protein

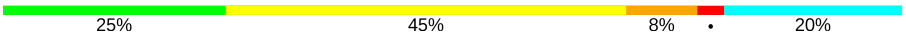
Chain D:

• Molecule 1: Amyloid-beta precursor protein

Chain E:

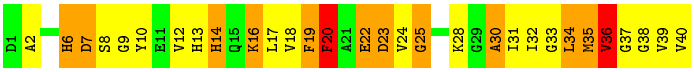
• Molecule 1: Amyloid-beta precursor protein

Chain F:



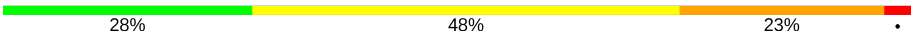
• Molecule 1: Amyloid-beta precursor protein

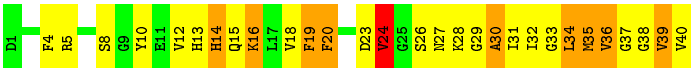
Chain G:



• Molecule 1: Amyloid-beta precursor protein

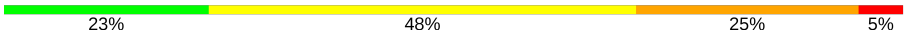
Chain H:

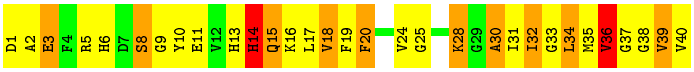




• Molecule 1: Amyloid-beta precursor protein

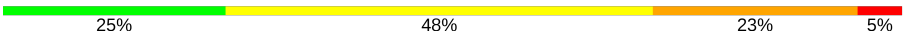
Chain I:





• Molecule 1: Amyloid-beta precursor protein

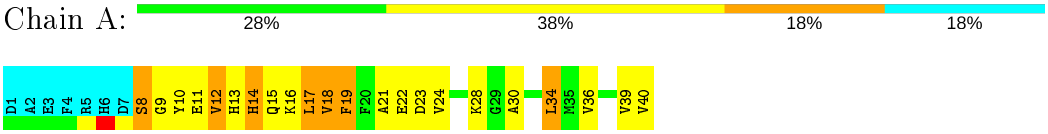
Chain J:



4.2.4 Score per residue for model 4

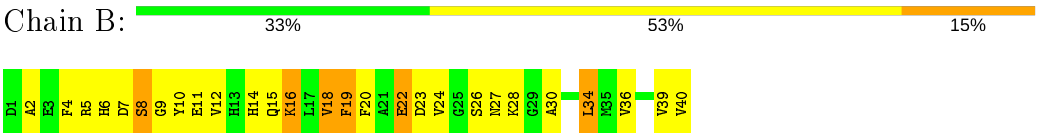
• Molecule 1: Amyloid-beta precursor protein

Chain A:



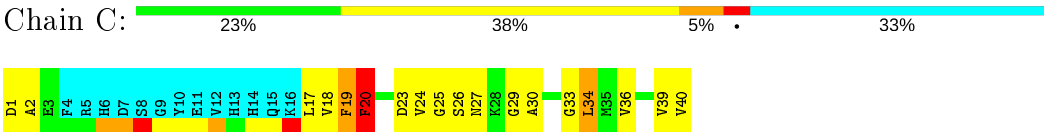
• Molecule 1: Amyloid-beta precursor protein

Chain B:



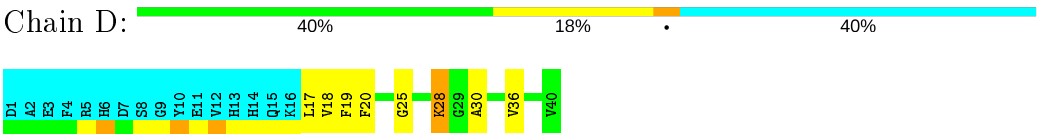
• Molecule 1: Amyloid-beta precursor protein

Chain C:



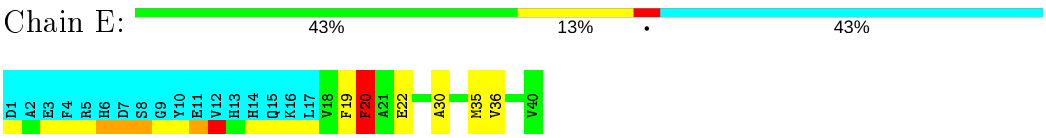
• Molecule 1: Amyloid-beta precursor protein

Chain D:



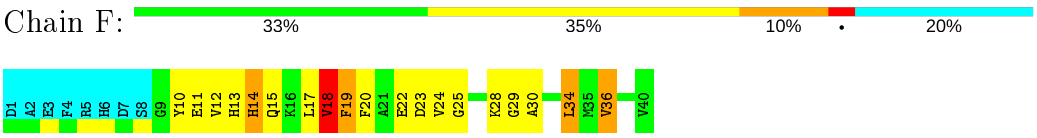
• Molecule 1: Amyloid-beta precursor protein

Chain E:



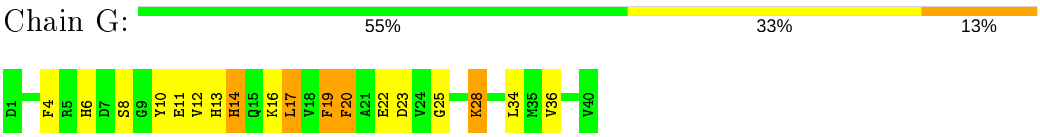
• Molecule 1: Amyloid-beta precursor protein

Chain F:



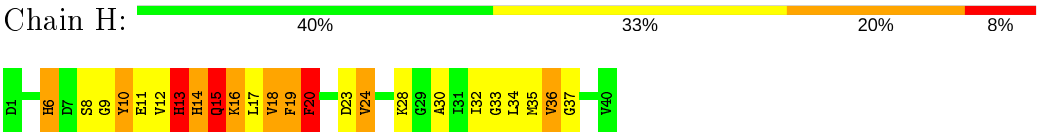
• Molecule 1: Amyloid-beta precursor protein

Chain G:



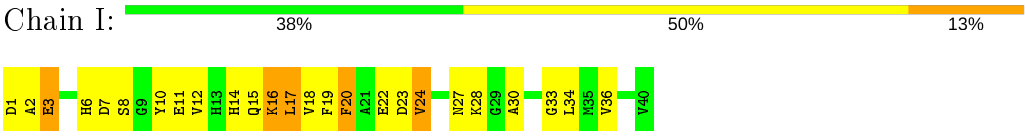
• Molecule 1: Amyloid-beta precursor protein

Chain H:



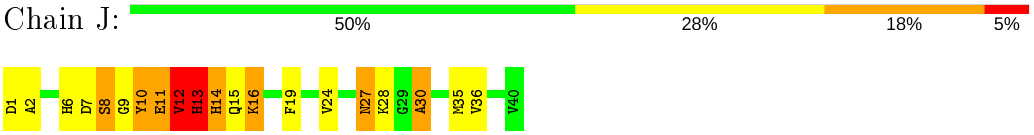
• Molecule 1: Amyloid-beta precursor protein

Chain I:



• Molecule 1: Amyloid-beta precursor protein

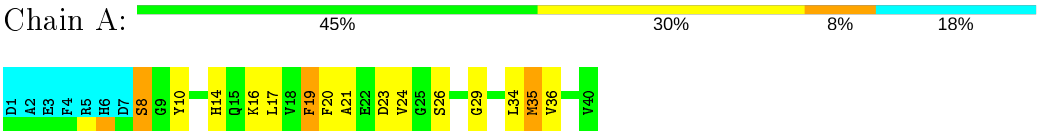
Chain J:



4.2.5 Score per residue for model 5

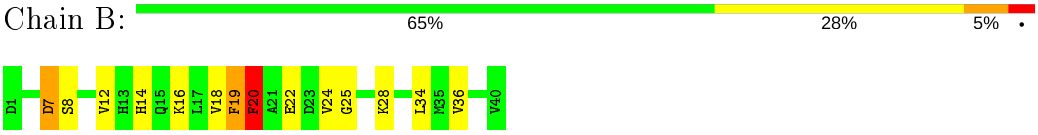
• Molecule 1: Amyloid-beta precursor protein

Chain A:



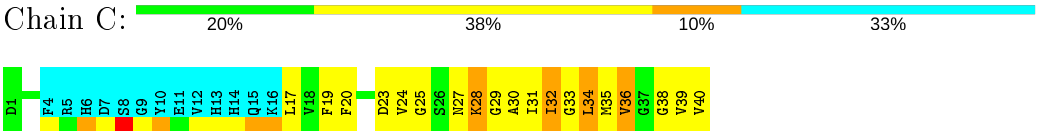
• Molecule 1: Amyloid-beta precursor protein

Chain B:



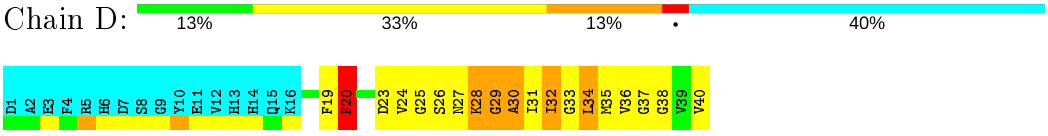
• Molecule 1: Amyloid-beta precursor protein

Chain C:



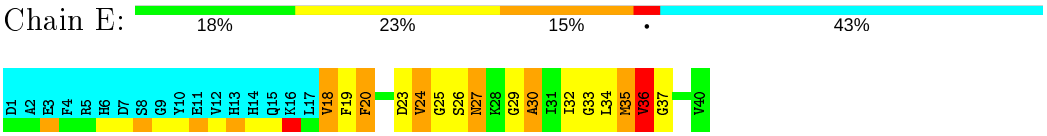
• Molecule 1: Amyloid-beta precursor protein

Chain D:



• Molecule 1: Amyloid-beta precursor protein

Chain E:

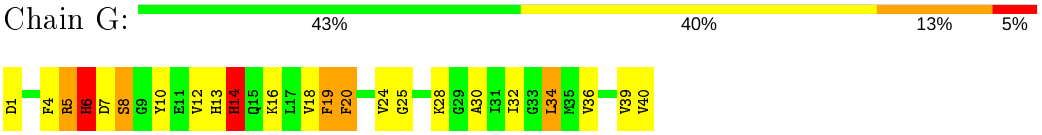


• Molecule 1: Amyloid-beta precursor protein

Chain F:

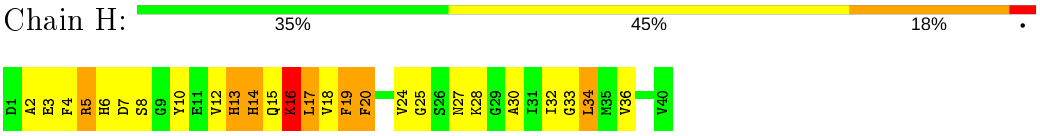
• Molecule 1: Amyloid-beta precursor protein

Chain G:



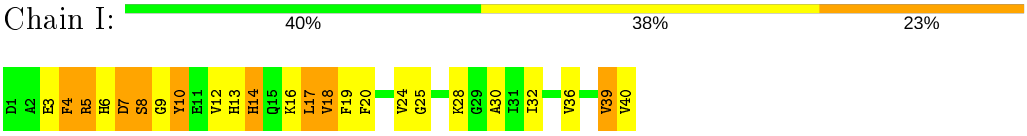
• Molecule 1: Amyloid-beta precursor protein

Chain H:



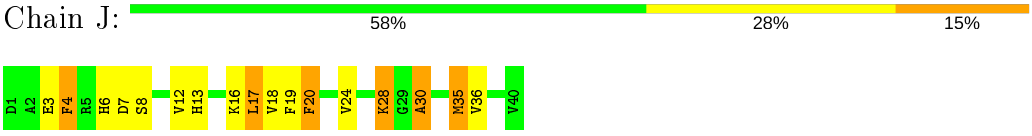
• Molecule 1: Amyloid-beta precursor protein

Chain I:



• Molecule 1: Amyloid-beta precursor protein

Chain J:



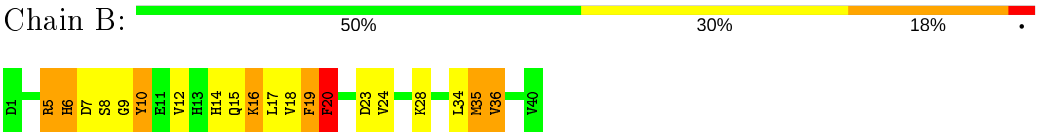
4.2.6 Score per residue for model 6

• Molecule 1: Amyloid-beta precursor protein

Chain A:

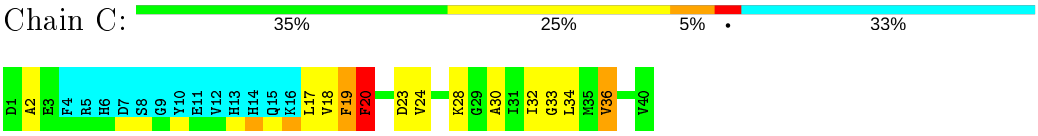
• Molecule 1: Amyloid-beta precursor protein

Chain B:



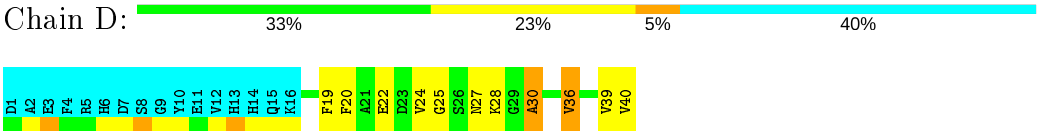
• Molecule 1: Amyloid-beta precursor protein

Chain C:



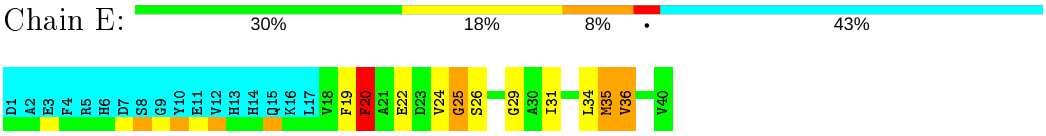
• Molecule 1: Amyloid-beta precursor protein

Chain D:



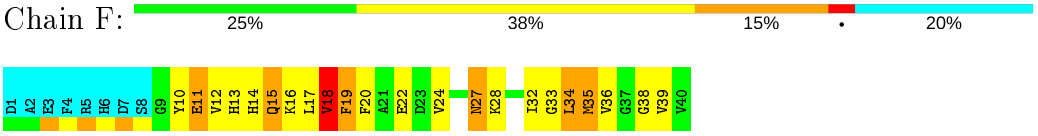
• Molecule 1: Amyloid-beta precursor protein

Chain E:



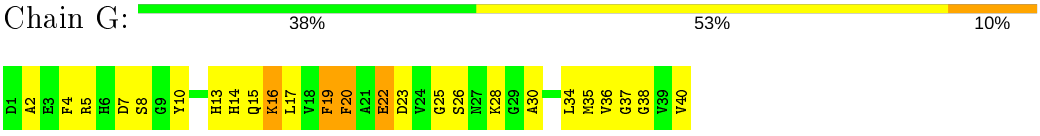
• Molecule 1: Amyloid-beta precursor protein

Chain F:



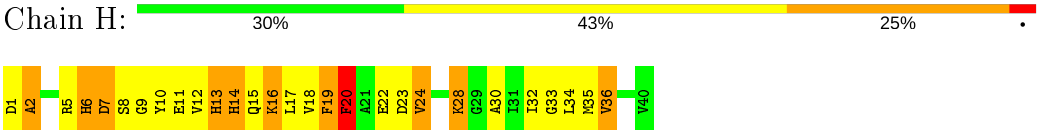
• Molecule 1: Amyloid-beta precursor protein

Chain G:



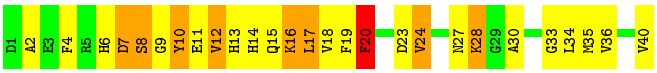
• Molecule 1: Amyloid-beta precursor protein

Chain H:



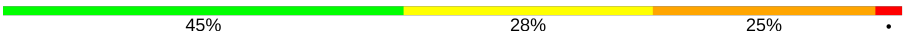
• Molecule 1: Amyloid-beta precursor protein

Chain I:



• Molecule 1: Amyloid-beta precursor protein

Chain J:



4.2.7 Score per residue for model 7

• Molecule 1: Amyloid-beta precursor protein

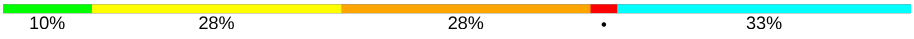
Chain A:

• Molecule 1: Amyloid-beta precursor protein

Chain B:

• Molecule 1: Amyloid-beta precursor protein

Chain C:



• Molecule 1: Amyloid-beta precursor protein

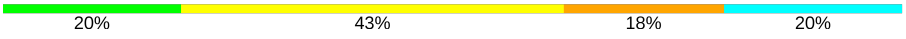
Chain D:

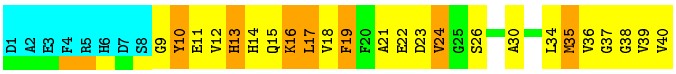
• Molecule 1: Amyloid-beta precursor protein

Chain E:

• Molecule 1: Amyloid-beta precursor protein

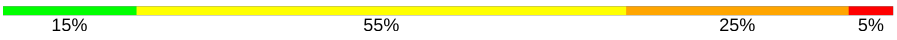
Chain F:





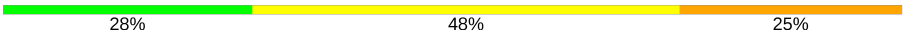
• Molecule 1: Amyloid-beta precursor protein

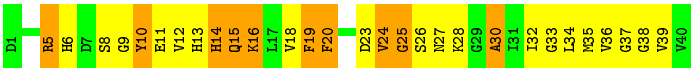
Chain G:



• Molecule 1: Amyloid-beta precursor protein

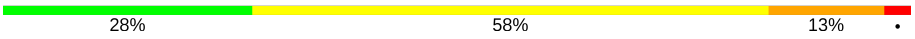
Chain H:





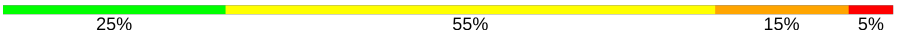
• Molecule 1: Amyloid-beta precursor protein

Chain I:



• Molecule 1: Amyloid-beta precursor protein

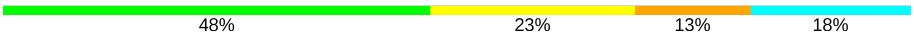
Chain J:



4.2.8 Score per residue for model 8

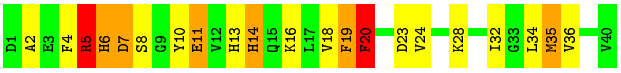
• Molecule 1: Amyloid-beta precursor protein

Chain A:



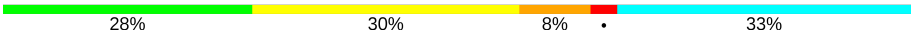
• Molecule 1: Amyloid-beta precursor protein

Chain B:



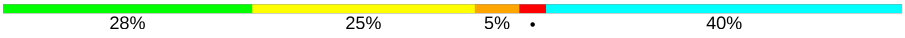
• Molecule 1: Amyloid-beta precursor protein

Chain C:



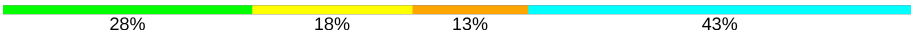
• Molecule 1: Amyloid-beta precursor protein

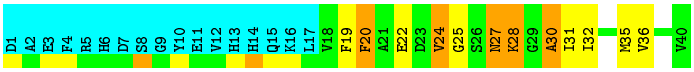
Chain D:



• Molecule 1: Amyloid-beta precursor protein

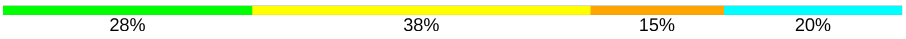
Chain E:





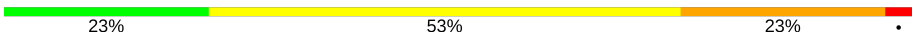
• Molecule 1: Amyloid-beta precursor protein

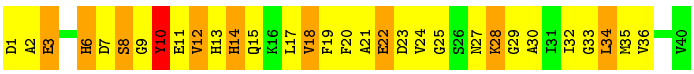
Chain F:



• Molecule 1: Amyloid-beta precursor protein

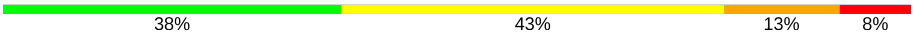
Chain G:





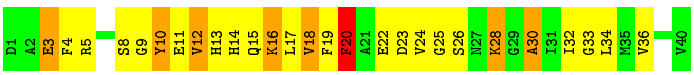
• Molecule 1: Amyloid-beta precursor protein

Chain H:



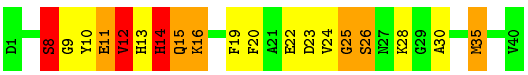
• Molecule 1: Amyloid-beta precursor protein

Chain I:



• Molecule 1: Amyloid-beta precursor protein

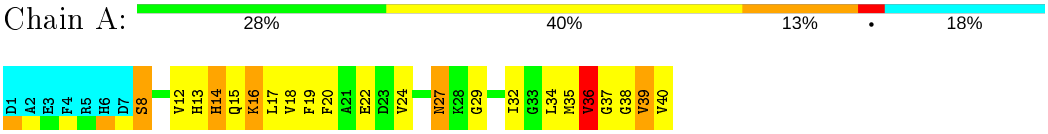
Chain J:



4.2.9 Score per residue for model 9

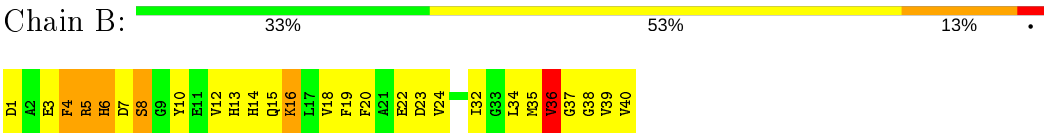
• Molecule 1: Amyloid-beta precursor protein

Chain A:



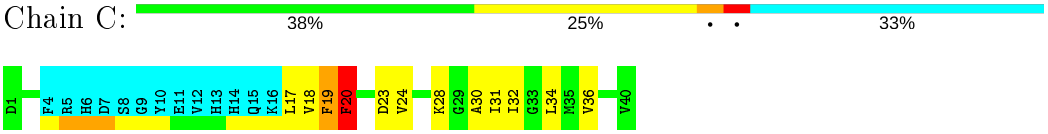
• Molecule 1: Amyloid-beta precursor protein

Chain B:



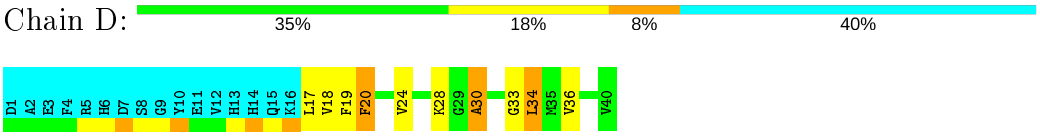
• Molecule 1: Amyloid-beta precursor protein

Chain C:



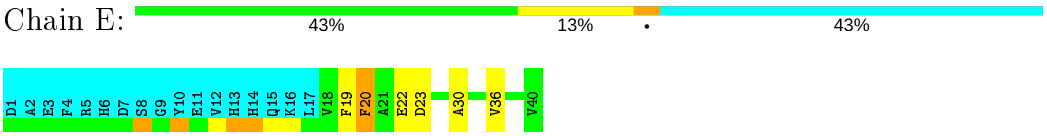
• Molecule 1: Amyloid-beta precursor protein

Chain D:



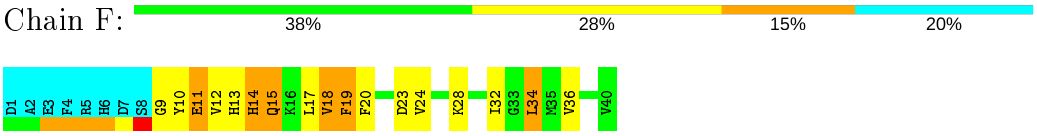
• Molecule 1: Amyloid-beta precursor protein

Chain E:



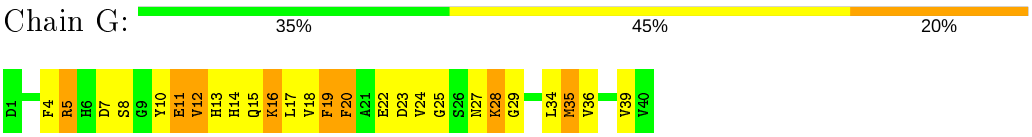
• Molecule 1: Amyloid-beta precursor protein

Chain F:



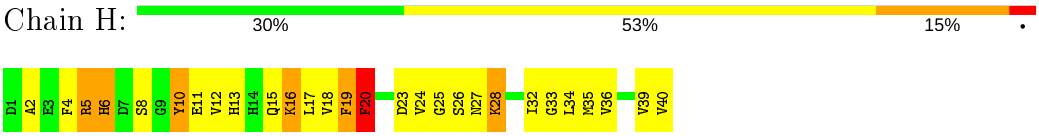
• Molecule 1: Amyloid-beta precursor protein

Chain G:



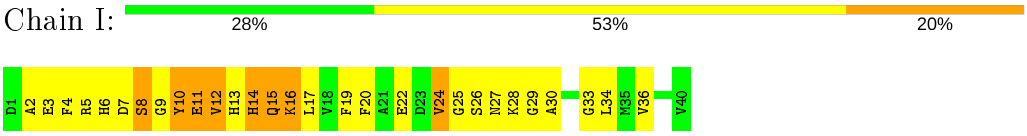
• Molecule 1: Amyloid-beta precursor protein

Chain H:



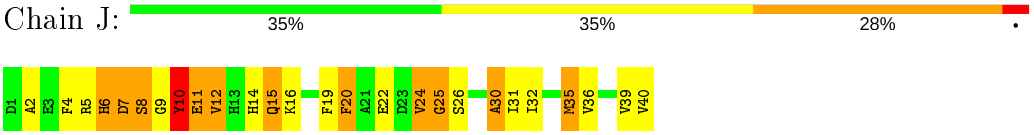
- Molecule 1: Amyloid-beta precursor protein

Chain I:



- Molecule 1: Amyloid-beta precursor protein

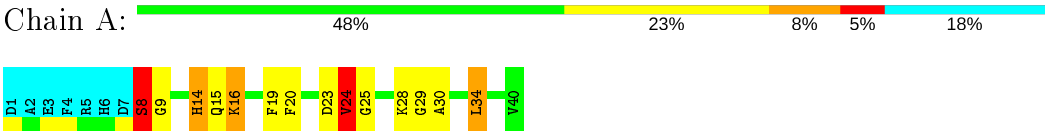
Chain J:



4.2.10 Score per residue for model 10 (medoid)

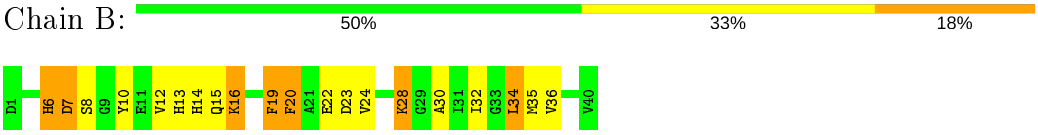
- Molecule 1: Amyloid-beta precursor protein

Chain A:



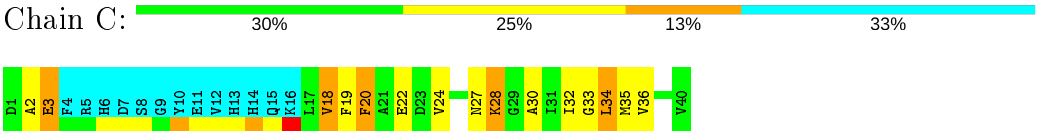
- Molecule 1: Amyloid-beta precursor protein

Chain B:



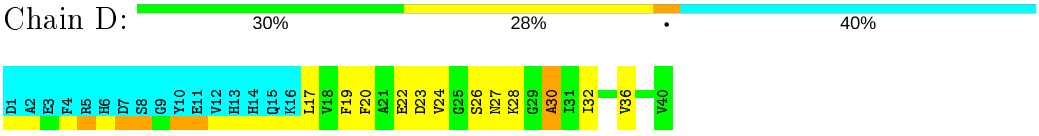
- Molecule 1: Amyloid-beta precursor protein

Chain C:



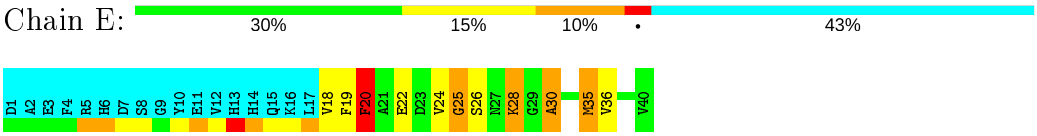
- Molecule 1: Amyloid-beta precursor protein

Chain D:



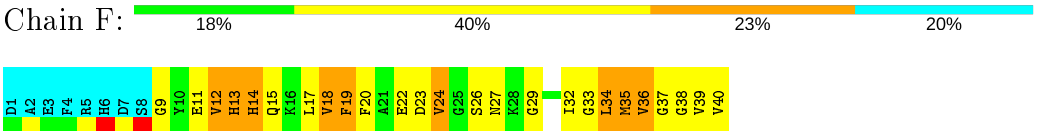
- Molecule 1: Amyloid-beta precursor protein

Chain E:



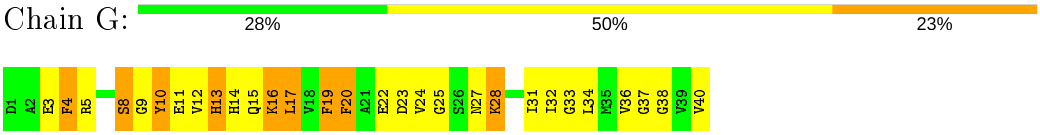
• Molecule 1: Amyloid-beta precursor protein

Chain F:



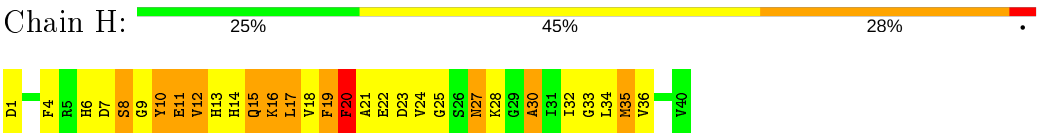
• Molecule 1: Amyloid-beta precursor protein

Chain G:



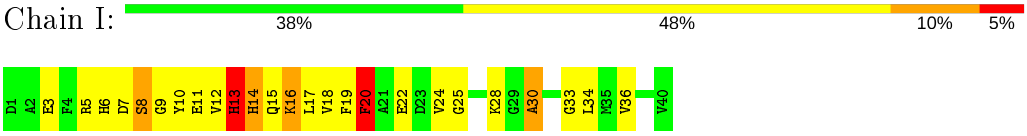
• Molecule 1: Amyloid-beta precursor protein

Chain H:



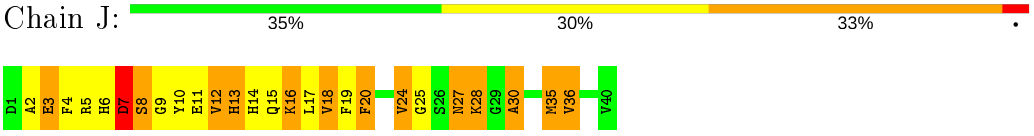
• Molecule 1: Amyloid-beta precursor protein

Chain I:



• Molecule 1: Amyloid-beta precursor protein

Chain J:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 40 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	
X-PLOR NIH	structure calculation	

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

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	123
Number of shifts mapped to atoms	123
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2PO

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	244	241	241	66±70
1	B	306	291	291	84±87
1	C	190	192	192	67±79
1	D	168	175	175	64±75
1	E	160	164	164	40±45
1	F	238	237	237	41±13
1	G	306	291	291	68±28
1	H	306	291	291	65±23
1	I	306	291	291	70±21
1	J	306	291	291	53±16
2	A	4	0	0	4±2
2	B	4	0	0	4±3
2	C	4	0	0	0±1
2	D	4	0	0	0±1
2	E	4	0	0	0±0
2	F	4	0	0	1±2
2	G	4	0	0	3±1
2	H	4	0	0	3±1
2	I	4	0	0	3±1
2	J	4	0	0	4±1
All	All	25700	24640	24633	4190

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 83.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:19:PHE:CD1	1:C:19:PHE:HB2	1.63	1.15	7	1
1:D:20:PHE:H	1:E:20:PHE:N	1.49	0.94	7	1
1:D:20:PHE:N	1:E:20:PHE:H	1.48	1.01	7	1
1:B:19:PHE:CG	1:C:19:PHE:HB2	1.43	1.48	7	1
1:A:17:LEU:O	1:B:17:LEU:CB	1.43	1.64	3	1
1:A:32:ILE:H	1:C:22:GLU:C	1.41	1.18	7	1
1:B:19:PHE:CD1	1:C:19:PHE:CB	1.37	2.04	7	1
1:B:31:ILE:O	1:B:32:ILE:HG23	1.33	1.19	3	1
1:D:19:PHE:O	1:D:20:PHE:CD1	1.32	1.82	7	1
1:A:35:MET:CA	1:B:35:MET:O	1.31	1.76	3	1
1:H:11:GLU:O	1:H:12:VAL:HG13	1.31	1.18	8	1
1:A:35:MET:HA	1:B:35:MET:O	1.31	1.13	3	1
1:I:38:GLY:N	1:J:37:GLY:O	1.30	1.61	3	1
1:G:9:GLY:O	1:H:10:TYR:N	1.29	1.64	8	1
1:A:32:ILE:N	1:C:22:GLU:C	1.28	1.87	7	1
1:A:32:ILE:CG2	1:A:33:GLY:H	1.28	1.40	3	1
1:A:31:ILE:CB	1:B:31:ILE:HB	1.27	1.57	3	1
1:A:31:ILE:HB	1:B:31:ILE:CB	1.26	1.57	3	1
1:F:35:MET:O	1:G:35:MET:HA	1.26	1.07	3	1
1:B:33:GLY:O	1:C:34:LEU:CG	1.25	1.85	7	1
1:F:37:GLY:O	1:G:37:GLY:O	1.24	1.55	7	1
1:C:20:PHE:HA	1:D:20:PHE:CD1	1.24	1.67	7	2
1:A:32:ILE:H	1:C:22:GLU:CA	1.23	1.46	7	1
1:D:32:ILE:O	1:E:32:ILE:O	1.23	1.56	5	2
1:D:19:PHE:CD1	1:E:18:VAL:O	1.22	1.90	7	1
1:D:28:LYS:N	1:E:31:ILE:H	1.21	1.33	3	1
1:A:32:ILE:HG13	1:C:22:GLU:O	1.20	1.31	7	1
1:G:8:SER:OG	2:G:101:2PO:P	1.20	2.00	3	10
1:J:8:SER:OG	2:J:101:2PO:P	1.20	2.00	10	10
1:B:8:SER:OG	2:B:101:2PO:P	1.20	2.00	10	10
1:A:8:SER:OG	2:A:101:2PO:P	1.20	2.00	5	10
1:I:8:SER:OG	2:I:101:2PO:P	1.20	2.00	4	10
1:H:8:SER:OG	2:H:101:2PO:P	1.20	2.00	2	10
1:A:32:ILE:N	1:C:22:GLU:N	1.20	1.90	7	1
1:D:30:ALA:N	1:E:31:ILE:HG21	1.20	1.39	3	1
1:B:33:GLY:O	1:C:34:LEU:HG	1.20	1.31	7	1
1:A:31:ILE:HA	1:C:23:ASP:N	1.19	1.51	7	1
1:A:17:LEU:O	1:B:17:LEU:HB2	1.19	1.12	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ILE:HA	1:B:32:ILE:O	1.18	1.33	7	1
1:D:19:PHE:HD1	1:E:18:VAL:N	1.18	1.35	7	1
1:C:33:GLY:O	1:D:34:LEU:HG	1.18	1.35	7	1
1:J:35:MET:O	1:J:36:VAL:HG22	1.18	1.34	3	2
1:D:34:LEU:HB2	1:E:34:LEU:O	1.18	1.34	1	1
1:F:35:MET:O	1:G:35:MET:CA	1.18	1.92	3	1
1:I:10:TYR:HA	1:J:10:TYR:N	1.17	1.53	9	2
1:D:30:ALA:O	1:E:30:ALA:O	1.17	1.62	5	2
1:H:11:GLU:HA	1:I:10:TYR:O	1.17	1.38	9	2
1:B:18:VAL:HB	1:C:18:VAL:CB	1.17	1.69	3	1
1:A:35:MET:HA	1:B:35:MET:C	1.17	1.60	3	1
1:B:18:VAL:CB	1:C:18:VAL:HB	1.17	1.69	3	1
1:F:9:GLY:O	1:G:9:GLY:O	1.16	1.63	10	1
1:I:39:VAL:O	1:J:39:VAL:HG12	1.15	1.38	3	1
1:C:31:ILE:O	1:D:31:ILE:O	1.15	1.60	5	1
1:H:37:GLY:O	1:I:37:GLY:O	1.15	1.59	7	1
1:C:34:LEU:HD22	1:C:34:LEU:N	1.15	1.57	3	1
1:D:19:PHE:HA	1:E:18:VAL:C	1.15	1.62	7	1
1:A:18:VAL:O	1:B:18:VAL:HG11	1.15	1.40	7	1
1:D:20:PHE:CA	1:E:21:ALA:HB2	1.15	1.70	3	1
1:D:19:PHE:O	1:D:20:PHE:CG	1.14	1.99	7	2
1:C:37:GLY:O	1:D:37:GLY:O	1.14	1.65	3	1
1:E:19:PHE:C	1:E:20:PHE:CD2	1.14	2.21	3	2
1:B:19:PHE:HD2	1:B:20:PHE:N	1.13	1.40	7	1
1:H:11:GLU:O	1:H:12:VAL:CG1	1.13	1.95	8	1
1:D:34:LEU:HD22	1:D:35:MET:N	1.13	1.56	3	1
1:G:35:MET:O	1:G:36:VAL:HG13	1.12	1.44	3	1
1:F:36:VAL:O	1:G:36:VAL:O	1.12	1.66	10	1
1:G:35:MET:O	1:H:35:MET:HB3	1.11	1.44	3	1
1:E:19:PHE:CG	1:E:19:PHE:O	1.11	2.00	7	1
1:D:29:GLY:C	1:E:31:ILE:HB	1.11	1.65	3	1
1:G:17:LEU:O	1:G:18:VAL:HG13	1.10	1.45	7	1
1:A:31:ILE:HG23	1:C:22:GLU:N	1.10	1.61	7	1
1:F:10:TYR:O	1:G:10:TYR:O	1.09	1.70	7	2
1:D:20:PHE:HA	1:E:21:ALA:CB	1.09	1.75	3	1
1:F:38:GLY:HA3	1:G:38:GLY:O	1.09	1.47	7	2
1:E:35:MET:O	1:E:36:VAL:HG13	1.09	1.44	3	5
1:A:32:ILE:HG22	1:A:33:GLY:N	1.09	1.54	3	1
1:C:31:ILE:O	1:D:31:ILE:HG23	1.09	1.45	3	1
1:D:30:ALA:N	1:E:31:ILE:CG2	1.09	2.15	3	1
1:B:31:ILE:O	1:B:32:ILE:CG2	1.09	1.99	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:19:PHE:CE1	1:E:18:VAL:O	1.09	2.05	7	1
1:C:19:PHE:CG	1:C:19:PHE:O	1.08	2.06	7	1
1:E:19:PHE:CD1	1:E:19:PHE:O	1.08	2.06	7	1
1:D:30:ALA:C	1:E:31:ILE:HG12	1.08	1.38	3	1
1:B:19:PHE:CE2	1:C:20:PHE:CE2	1.08	2.39	3	1
1:A:30:ALA:O	1:A:31:ILE:HD12	1.08	1.45	7	1
1:D:19:PHE:HA	1:E:18:VAL:CA	1.07	1.79	7	1
1:C:18:VAL:HG22	1:C:19:PHE:N	1.07	1.60	7	1
1:C:31:ILE:HG13	1:C:32:ILE:H	1.07	1.00	3	1
1:I:39:VAL:HG13	1:I:40:VAL:N	1.06	1.61	3	1
1:C:19:PHE:O	1:C:19:PHE:CD2	1.06	2.09	7	1
1:B:24:VAL:O	1:C:24:VAL:HG11	1.05	1.48	7	1
1:D:20:PHE:N	1:E:20:PHE:N	1.05	1.73	7	1
1:A:31:ILE:HA	1:C:23:ASP:H	1.05	0.90	7	1
1:H:38:GLY:O	1:I:38:GLY:CA	1.05	2.03	3	1
1:I:17:LEU:HA	1:J:17:LEU:O	1.05	1.51	3	2
1:D:19:PHE:CG	1:D:19:PHE:O	1.05	2.09	3	1
1:J:39:VAL:HG13	1:J:40:VAL:N	1.05	1.56	3	1
1:D:17:LEU:O	1:D:18:VAL:HG13	1.05	1.51	3	1
1:H:9:GLY:O	1:I:9:GLY:O	1.05	1.75	8	1
1:B:21:ALA:HA	1:C:20:PHE:CE1	1.05	1.86	3	1
1:H:39:VAL:O	1:I:39:VAL:HG12	1.04	1.51	3	1
1:D:19:PHE:CD1	1:E:18:VAL:C	1.04	2.31	7	1
1:J:18:VAL:HG22	1:J:19:PHE:H	1.04	1.07	10	1
1:C:38:GLY:HA2	1:D:38:GLY:O	1.04	1.52	3	4
1:F:17:LEU:O	1:F:18:VAL:HG13	1.04	1.51	4	2
1:D:19:PHE:HD2	1:E:20:PHE:HA	1.04	1.10	7	1
1:J:39:VAL:HG13	1:J:40:VAL:H	1.04	1.01	3	1
1:I:11:GLU:HA	1:J:10:TYR:O	1.03	1.52	8	3
1:C:18:VAL:HG22	1:D:20:PHE:CZ	1.03	1.88	3	1
1:F:38:GLY:CA	1:G:38:GLY:O	1.03	2.06	7	1
1:G:11:GLU:O	1:H:11:GLU:O	1.03	1.75	1	2
1:B:30:ALA:N	1:C:30:ALA:O	1.03	1.91	3	1
1:I:39:VAL:CG1	1:I:40:VAL:H	1.02	1.64	3	1
1:A:32:ILE:HG22	1:A:33:GLY:H	1.02	0.94	3	1
1:H:11:GLU:CA	1:I:10:TYR:O	1.02	2.05	9	2
1:F:38:GLY:O	1:G:38:GLY:HA3	1.02	1.54	3	1
1:C:18:VAL:CG1	1:C:19:PHE:N	1.02	2.23	3	2
1:A:17:LEU:C	1:B:17:LEU:HB2	1.02	1.74	3	1
1:A:35:MET:HB3	1:B:19:PHE:CD1	1.01	1.89	7	1
1:C:19:PHE:CE1	1:D:20:PHE:CD1	1.01	2.47	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:J:30:ALA:O	1:J:31:ILE:HG22	1.01	1.53	3	1
1:F:9:GLY:HA2	1:G:9:GLY:H	1.01	1.09	8	1
1:D:19:PHE:CD1	1:E:18:VAL:N	1.01	2.28	7	1
1:C:33:GLY:O	1:D:34:LEU:CG	1.01	2.07	7	1
1:C:19:PHE:CZ	1:E:20:PHE:CE1	1.01	2.49	3	1
1:G:36:VAL:CG2	1:H:36:VAL:H	1.01	1.68	3	1
1:D:20:PHE:CA	1:E:20:PHE:H	1.00	1.69	7	1
1:B:33:GLY:O	1:B:34:LEU:HD22	1.00	1.55	3	1
1:H:20:PHE:O	1:I:20:PHE:HB2	1.00	1.55	7	5
1:B:33:GLY:O	1:C:34:LEU:CD2	1.00	2.09	7	1
1:D:19:PHE:CE1	1:E:21:ALA:HB3	1.00	1.92	3	1
1:A:34:LEU:N	1:B:34:LEU:HB3	1.00	1.72	3	1
1:A:19:PHE:CE2	1:A:34:LEU:O	1.00	2.14	7	1
1:A:36:VAL:HG23	1:A:36:VAL:O	1.00	1.51	3	1
1:G:36:VAL:HG21	1:H:36:VAL:N	1.00	1.70	3	1
1:G:36:VAL:HB	1:H:36:VAL:O	1.00	1.54	3	1
1:B:19:PHE:O	1:B:20:PHE:CG	1.00	2.14	7	1
1:C:18:VAL:CG2	1:C:19:PHE:H	1.00	1.64	7	1
1:I:31:ILE:H	1:J:31:ILE:N	1.00	1.55	3	1
1:F:18:VAL:O	1:G:18:VAL:HG23	1.00	1.56	8	1
1:A:31:ILE:CA	1:C:23:ASP:N	0.99	2.24	7	1
1:B:19:PHE:CG	1:C:19:PHE:CB	0.99	2.34	7	1
1:A:32:ILE:HG23	1:C:23:ASP:HB2	0.99	1.05	7	1
1:B:35:MET:O	1:B:36:VAL:HG22	0.99	1.57	9	1
1:G:36:VAL:HG21	1:H:36:VAL:H	0.99	0.87	3	1
1:B:19:PHE:CE1	1:C:19:PHE:HB2	0.99	1.93	7	1
1:J:38:GLY:O	1:J:39:VAL:O	0.98	1.80	3	1
1:C:34:LEU:HB3	1:D:34:LEU:HD21	0.98	1.32	7	1
1:F:18:VAL:N	1:G:18:VAL:HG11	0.98	1.71	7	1
1:B:35:MET:HB2	1:C:35:MET:HA	0.98	1.33	3	1
1:H:30:ALA:HB3	1:I:30:ALA:O	0.98	1.59	7	1
1:J:36:VAL:O	1:J:36:VAL:HG23	0.98	1.58	3	1
1:A:36:VAL:CG2	1:A:36:VAL:O	0.98	2.12	3	1
1:G:20:PHE:O	1:H:20:PHE:HB2	0.98	1.59	7	5
1:B:14:HIS:NE2	1:B:18:VAL:HG23	0.98	1.72	7	1
1:D:30:ALA:CA	1:E:31:ILE:HG12	0.98	1.89	3	1
1:A:32:ILE:CG2	1:A:33:GLY:N	0.98	2.13	3	1
1:D:19:PHE:HA	1:E:19:PHE:N	0.98	1.72	7	1
1:I:10:TYR:O	1:J:10:TYR:O	0.97	1.81	10	5
1:D:19:PHE:CD2	1:E:19:PHE:O	0.97	2.17	7	2
1:B:21:ALA:HA	1:C:20:PHE:CZ	0.97	1.94	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:32:ILE:HD13	1:C:32:ILE:O	0.97	1.59	3	1
1:G:33:GLY:C	1:G:34:LEU:HD13	0.97	1.80	7	1
1:A:32:ILE:HG23	1:C:23:ASP:CB	0.97	1.86	7	1
1:A:36:VAL:CG1	1:B:36:VAL:HG23	0.97	1.90	9	1
1:C:18:VAL:CG1	1:C:19:PHE:H	0.97	1.71	3	1
1:A:35:MET:SD	1:B:18:VAL:O	0.97	2.22	7	1
1:D:20:PHE:CD2	1:D:34:LEU:HD21	0.97	1.93	3	1
1:A:16:LYS:HA	1:B:16:LYS:CB	0.97	1.88	3	1
1:C:21:ALA:HB3	1:D:21:ALA:O	0.97	1.59	3	1
1:A:32:ILE:O	1:B:21:ALA:HB1	0.97	1.60	7	1
1:F:18:VAL:HG22	1:F:19:PHE:H	0.96	1.13	8	4
1:C:31:ILE:H	1:D:31:ILE:CG2	0.96	1.73	3	1
1:F:10:TYR:O	1:G:10:TYR:C	0.96	2.02	7	2
1:D:19:PHE:HB3	1:E:20:PHE:CG	0.96	1.94	7	1
1:C:20:PHE:O	1:D:20:PHE:O	0.96	1.82	3	1
1:H:35:MET:O	1:I:35:MET:HA	0.96	1.60	3	1
1:C:17:LEU:HG	1:D:17:LEU:HB3	0.96	1.37	7	1
1:D:19:PHE:CD2	1:E:20:PHE:HA	0.96	1.95	7	1
1:B:19:PHE:CD2	1:B:20:PHE:N	0.95	2.25	7	2
1:B:32:ILE:CD1	1:C:32:ILE:O	0.95	2.15	3	1
1:B:12:VAL:O	1:B:13:HIS:O	0.95	1.83	7	1
1:D:18:VAL:HG23	1:D:19:PHE:N	0.95	1.72	7	1
1:F:20:PHE:O	1:G:20:PHE:HB2	0.95	1.60	9	8
1:I:39:VAL:HG13	1:I:40:VAL:H	0.95	0.78	3	1
1:H:17:LEU:O	1:H:18:VAL:HG13	0.95	1.60	8	1
1:B:19:PHE:CZ	1:B:34:LEU:O	0.94	2.19	7	1
1:C:17:LEU:HB2	1:D:17:LEU:N	0.94	1.76	7	1
1:I:10:TYR:CA	1:J:10:TYR:N	0.94	2.29	9	2
1:I:18:VAL:O	1:J:18:VAL:HG21	0.94	1.61	10	1
1:A:35:MET:O	1:A:36:VAL:HG13	0.94	1.62	9	2
1:A:31:ILE:HG13	1:C:22:GLU:HA	0.94	1.39	7	1
1:I:35:MET:O	1:I:36:VAL:HG13	0.94	1.60	3	1
1:C:20:PHE:CE1	1:C:21:ALA:O	0.94	2.20	3	1
1:F:10:TYR:C	1:G:10:TYR:O	0.94	2.04	7	2
1:J:35:MET:O	1:J:36:VAL:HG13	0.94	1.62	7	3
1:H:14:HIS:CG	1:H:15:GLN:H	0.94	1.80	6	1
1:A:32:ILE:CA	1:B:32:ILE:O	0.94	2.16	7	1
1:A:32:ILE:N	1:C:22:GLU:H	0.94	1.53	7	1
1:B:36:VAL:HB	1:C:36:VAL:O	0.94	1.63	9	1
1:B:34:LEU:HD12	1:B:35:MET:N	0.94	1.77	1	2
1:A:31:ILE:HG22	1:D:21:ALA:O	0.94	1.63	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:29:GLY:O	1:E:31:ILE:HD13	0.93	1.62	3	1
1:C:31:ILE:C	1:D:31:ILE:O	0.93	2.07	5	1
1:H:38:GLY:O	1:I:38:GLY:HA3	0.93	1.58	3	1
1:G:9:GLY:O	1:H:9:GLY:O	0.93	1.85	1	2
1:C:18:VAL:HG22	1:C:19:PHE:H	0.93	0.77	7	1
1:A:35:MET:N	1:A:35:MET:SD	0.93	2.42	3	1
1:G:8:SER:O	1:H:9:GLY:N	0.93	2.01	8	1
1:C:33:GLY:C	1:C:34:LEU:HD13	0.93	1.83	3	1
1:D:19:PHE:CE2	1:E:19:PHE:HA	0.93	1.98	3	1
1:F:34:LEU:HB3	1:G:34:LEU:O	0.93	1.63	3	1
1:G:9:GLY:O	1:G:10:TYR:HB2	0.93	1.64	8	1
1:C:18:VAL:HG13	1:C:19:PHE:N	0.93	1.79	3	1
1:C:36:VAL:HA	1:D:36:VAL:O	0.92	1.62	1	3
1:B:19:PHE:O	1:B:20:PHE:CD2	0.92	2.21	7	3
1:B:19:PHE:CD1	1:B:19:PHE:C	0.92	2.40	3	2
1:A:31:ILE:CG2	1:D:21:ALA:O	0.92	2.17	7	1
1:D:32:ILE:CG1	1:D:33:GLY:H	0.92	1.77	5	2
1:B:19:PHE:CE1	1:C:19:PHE:CG	0.92	2.58	7	1
1:A:31:ILE:CA	1:C:23:ASP:H	0.92	1.74	7	1
1:D:20:PHE:H	1:E:19:PHE:C	0.92	1.66	7	1
1:D:21:ALA:H	1:E:21:ALA:HA	0.92	1.22	3	1
1:G:12:VAL:O	1:H:12:VAL:HG23	0.92	1.63	8	1
1:D:20:PHE:O	1:E:20:PHE:N	0.92	2.03	7	1
1:C:19:PHE:O	1:C:19:PHE:CG	0.92	2.21	3	1
1:I:39:VAL:O	1:J:39:VAL:CG1	0.92	2.18	3	1
1:C:20:PHE:CA	1:D:20:PHE:CD1	0.92	2.53	7	1
1:D:29:GLY:C	1:E:31:ILE:CB	0.92	2.37	3	1
1:D:20:PHE:CE2	1:D:34:LEU:HD11	0.91	1.99	3	1
1:D:18:VAL:CG2	1:D:19:PHE:N	0.91	2.32	7	1
1:D:34:LEU:O	1:E:19:PHE:CD2	0.91	2.22	7	1
1:D:28:LYS:N	1:E:31:ILE:N	0.91	2.07	3	1
1:I:11:GLU:N	1:J:10:TYR:N	0.91	2.17	9	1
1:C:20:PHE:HA	1:D:20:PHE:CG	0.91	2.00	7	1
1:F:39:VAL:HA	1:G:39:VAL:H	0.91	1.22	3	1
1:F:9:GLY:N	1:G:8:SER:HA	0.91	1.80	8	1
1:G:32:ILE:HA	1:H:32:ILE:O	0.91	1.65	3	2
1:A:31:ILE:N	1:B:30:ALA:O	0.91	2.03	3	1
1:I:8:SER:CB	2:I:101:2PO:P	0.91	2.59	3	10
1:I:10:TYR:O	1:J:10:TYR:C	0.91	2.09	7	5
1:B:8:SER:CB	2:B:101:2PO:P	0.91	2.59	10	10
1:I:10:TYR:C	1:J:10:TYR:O	0.91	2.08	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:8:SER:CB	2:H:101:2PO:P	0.90	2.60	3	10
1:F:10:TYR:H	1:G:10:TYR:H	0.90	1.08	7	1
1:G:38:GLY:O	1:H:38:GLY:HA2	0.90	1.65	3	1
1:J:8:SER:CB	2:J:101:2PO:P	0.90	2.60	5	10
1:G:8:SER:CB	2:G:101:2PO:P	0.90	2.60	2	10
1:A:18:VAL:HB	1:B:18:VAL:HG13	0.90	1.40	3	1
1:G:18:VAL:HG22	1:G:19:PHE:H	0.90	1.24	8	1
1:B:35:MET:C	1:B:36:VAL:HG22	0.90	1.85	9	1
1:B:18:VAL:HA	1:C:18:VAL:H	0.90	1.25	3	1
1:A:8:SER:CB	2:A:101:2PO:P	0.90	2.59	6	10
1:A:18:VAL:O	1:B:18:VAL:CG1	0.90	2.19	7	1
1:B:32:ILE:CG1	1:C:32:ILE:O	0.90	2.19	3	1
1:C:19:PHE:HB3	1:D:18:VAL:CG1	0.90	1.97	3	1
1:I:11:GLU:N	1:J:10:TYR:H	0.89	1.64	9	1
1:B:19:PHE:CE1	1:B:34:LEU:O	0.89	2.24	7	1
1:D:19:PHE:HB3	1:E:20:PHE:CD2	0.89	2.02	7	1
1:C:31:ILE:HG13	1:C:32:ILE:N	0.89	1.82	3	1
1:D:18:VAL:CG2	1:D:19:PHE:H	0.89	1.78	7	1
1:C:34:LEU:CD2	1:C:34:LEU:N	0.89	2.33	3	1
1:I:33:GLY:C	1:I:34:LEU:HD23	0.89	1.87	3	2
1:C:21:ALA:CB	1:D:21:ALA:O	0.89	2.21	3	1
1:C:19:PHE:O	1:C:19:PHE:CD1	0.89	2.25	3	1
1:D:34:LEU:C	1:D:34:LEU:HD13	0.89	1.88	3	1
1:J:30:ALA:O	1:J:31:ILE:CG2	0.89	2.21	3	1
1:D:34:LEU:CB	1:E:34:LEU:O	0.89	2.20	1	1
1:B:20:PHE:O	1:C:20:PHE:HB2	0.89	1.67	4	6
1:I:30:ALA:HB1	1:J:30:ALA:O	0.89	1.68	5	7
1:I:11:GLU:CA	1:J:10:TYR:O	0.88	2.18	8	2
1:A:38:GLY:O	1:B:38:GLY:O	0.88	1.91	9	1
1:C:18:VAL:HG22	1:D:20:PHE:HZ	0.88	1.23	3	1
1:D:20:PHE:HA	1:E:21:ALA:HB2	0.88	0.91	3	1
1:F:38:GLY:HA3	1:G:38:GLY:H	0.88	1.28	10	1
1:A:31:ILE:HG23	1:C:22:GLU:H	0.88	1.24	7	1
1:D:19:PHE:HD1	1:E:18:VAL:H	0.88	1.07	7	1
1:G:35:MET:O	1:G:36:VAL:CG1	0.88	2.20	3	1
1:B:11:GLU:O	1:B:12:VAL:HG12	0.88	1.69	3	1
1:C:31:ILE:O	1:D:31:ILE:CG2	0.88	2.21	3	1
1:H:18:VAL:O	1:I:18:VAL:HG21	0.88	1.67	3	1
1:G:14:HIS:CG	1:G:15:GLN:H	0.88	1.87	8	1
1:C:31:ILE:O	1:D:31:ILE:C	0.88	2.12	5	1
1:H:30:ALA:CB	1:I:30:ALA:O	0.88	2.20	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:VAL:HA	1:B:36:VAL:O	0.88	1.68	9	1
1:J:35:MET:O	1:J:36:VAL:CG2	0.88	2.21	3	1
1:A:34:LEU:N	1:B:34:LEU:CB	0.88	2.36	3	1
1:B:24:VAL:HG12	1:B:25:GLY:H	0.87	1.29	5	1
1:G:36:VAL:HA	1:H:36:VAL:O	0.87	1.69	7	1
1:I:35:MET:HB3	1:J:35:MET:HB3	0.87	1.42	3	1
1:C:19:PHE:CE1	1:D:20:PHE:CG	0.87	2.62	3	1
1:A:12:VAL:HG21	1:B:12:VAL:CA	0.87	1.97	7	1
1:A:12:VAL:HG21	1:B:12:VAL:HA	0.87	1.43	7	1
1:D:30:ALA:H	1:E:31:ILE:HG21	0.87	1.29	3	1
1:H:30:ALA:HB1	1:I:30:ALA:O	0.87	1.69	8	7
1:C:30:ALA:HB1	1:D:30:ALA:O	0.87	1.70	2	6
1:I:14:HIS:NE2	1:I:17:LEU:N	0.87	2.21	10	2
1:B:30:ALA:H	1:C:31:ILE:HB	0.87	1.30	3	1
1:I:12:VAL:H	1:J:12:VAL:H	0.87	1.04	2	4
1:C:19:PHE:CD1	1:D:20:PHE:CD1	0.87	2.62	3	1
1:D:27:ASN:HB3	1:E:31:ILE:C	0.87	1.90	3	1
1:G:20:PHE:O	1:H:20:PHE:CB	0.87	2.23	7	7
1:D:19:PHE:CB	1:E:20:PHE:CD2	0.87	2.58	7	1
1:J:39:VAL:CG1	1:J:40:VAL:H	0.87	1.82	3	1
1:D:30:ALA:O	1:E:31:ILE:HA	0.86	1.69	1	1
1:I:37:GLY:H	1:J:37:GLY:HA2	0.86	1.30	7	1
1:B:34:LEU:N	1:B:34:LEU:HD23	0.86	1.86	10	3
1:B:19:PHE:CD2	1:C:20:PHE:CE2	0.86	2.62	3	1
1:I:38:GLY:O	1:J:38:GLY:HA3	0.86	1.70	3	1
1:A:12:VAL:O	1:B:12:VAL:HB	0.86	1.71	4	1
1:A:32:ILE:CG2	1:C:23:ASP:HB2	0.86	1.98	7	1
1:A:19:PHE:HB3	1:B:20:PHE:CD2	0.86	2.06	3	1
1:D:20:PHE:CZ	1:D:34:LEU:HD11	0.86	2.05	3	1
1:E:21:ALA:O	1:E:22:GLU:HB2	0.85	1.71	7	1
1:I:8:SER:O	1:J:8:SER:N	0.85	2.09	2	1
1:A:31:ILE:HB	1:B:31:ILE:HB	0.85	0.86	3	1
1:I:14:HIS:CG	1:I:15:GLN:N	0.85	2.37	10	5
1:A:34:LEU:HA	1:B:34:LEU:HG	0.85	1.47	7	2
1:B:16:LYS:O	1:B:17:LEU:HB2	0.85	1.72	7	1
1:A:18:VAL:HG21	1:B:35:MET:CE	0.85	2.00	3	1
1:B:35:MET:HE3	1:C:36:VAL:O	0.85	1.71	3	1
1:H:39:VAL:HG12	1:H:40:VAL:N	0.85	1.87	3	1
1:G:19:PHE:CD1	1:G:20:PHE:N	0.85	2.44	3	4
1:J:18:VAL:HG22	1:J:19:PHE:N	0.85	1.86	10	1
1:B:19:PHE:CE1	1:C:19:PHE:CB	0.85	2.58	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ILE:H	1:C:22:GLU:N	0.85	1.57	7	1
1:B:34:LEU:HD12	1:B:34:LEU:C	0.85	1.91	7	2
1:B:16:LYS:O	1:C:17:LEU:HB2	0.85	1.71	3	1
1:F:11:GLU:H	1:G:11:GLU:H	0.85	1.12	9	1
1:D:34:LEU:HD22	1:D:35:MET:H	0.85	1.24	3	1
1:G:18:VAL:H	1:H:18:VAL:HG12	0.85	1.32	8	1
1:J:39:VAL:CG1	1:J:40:VAL:N	0.85	2.32	3	1
1:G:18:VAL:HG22	1:G:19:PHE:N	0.85	1.84	8	1
1:B:19:PHE:CE2	1:C:20:PHE:CZ	0.85	2.64	3	1
1:C:34:LEU:H	1:C:34:LEU:HD22	0.85	1.06	3	1
1:G:12:VAL:HG12	1:G:12:VAL:O	0.85	1.70	8	1
1:I:18:VAL:O	1:J:18:VAL:HG11	0.85	1.71	10	1
1:B:35:MET:O	1:B:36:VAL:HG13	0.85	1.71	9	1
1:E:20:PHE:N	1:E:20:PHE:CD2	0.85	2.43	3	2
1:D:19:PHE:O	1:D:19:PHE:CD1	0.85	2.30	3	1
1:E:35:MET:O	1:E:36:VAL:CG1	0.84	2.25	3	4
1:B:39:VAL:N	1:C:38:GLY:O	0.84	2.10	7	1
1:F:36:VAL:O	1:G:36:VAL:HG23	0.84	1.72	10	1
1:I:14:HIS:CG	1:I:15:GLN:H	0.84	1.86	10	3
1:F:21:ALA:HB2	1:G:34:LEU:HD21	0.84	1.48	1	1
1:G:9:GLY:O	1:H:9:GLY:CA	0.84	2.24	8	1
1:F:33:GLY:O	1:F:34:LEU:HB2	0.84	1.70	10	2
1:C:17:LEU:CB	1:D:17:LEU:N	0.84	2.41	7	1
1:F:33:GLY:H	1:G:33:GLY:HA2	0.84	1.33	10	1
1:F:34:LEU:N	1:F:34:LEU:HD12	0.84	1.87	8	4
1:G:34:LEU:H	1:G:34:LEU:HD22	0.84	1.33	7	1
1:B:11:GLU:O	1:B:12:VAL:CG1	0.84	2.26	3	1
1:A:8:SER:OG	1:A:9:GLY:N	0.83	2.07	7	1
1:A:31:ILE:O	1:A:32:ILE:CG1	0.83	2.26	3	1
1:A:32:ILE:N	1:C:22:GLU:CA	0.83	2.22	7	1
1:C:18:VAL:HG12	1:C:19:PHE:H	0.83	1.31	3	1
1:A:39:VAL:HG22	1:A:39:VAL:O	0.83	1.71	9	1
1:B:36:VAL:CB	1:C:36:VAL:O	0.83	2.26	9	1
1:C:20:PHE:HA	1:D:20:PHE:O	0.83	1.73	3	1
1:H:38:GLY:O	1:I:38:GLY:HA2	0.83	1.74	3	1
1:I:35:MET:O	1:J:35:MET:HA	0.83	1.73	3	1
1:G:34:LEU:HD23	1:G:34:LEU:N	0.83	1.88	4	2
1:B:21:ALA:CB	1:C:21:ALA:O	0.83	2.26	7	1
1:A:31:ILE:HB	1:B:31:ILE:CA	0.83	2.02	3	1
1:D:31:ILE:HG23	1:E:30:ALA:O	0.83	1.73	1	1
1:E:20:PHE:C	1:G:39:VAL:HG11	0.83	1.92	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:19:PHE:O	1:H:20:PHE:CD2	0.83	2.32	8	1
1:D:35:MET:O	1:E:35:MET:HA	0.83	1.73	5	2
1:C:34:LEU:HB3	1:D:34:LEU:CD2	0.83	2.02	7	1
1:B:32:ILE:HG22	1:C:34:LEU:CD2	0.83	2.03	7	1
1:H:18:VAL:O	1:I:18:VAL:HG11	0.83	1.74	3	1
1:I:16:LYS:O	1:J:16:LYS:O	0.83	1.97	3	2
1:A:34:LEU:N	1:B:19:PHE:CE2	0.83	2.46	7	1
1:A:35:MET:N	1:B:35:MET:O	0.83	2.10	3	1
1:G:35:MET:C	1:G:36:VAL:HG22	0.83	1.94	3	1
1:G:9:GLY:O	1:H:9:GLY:C	0.83	2.17	8	1
1:D:30:ALA:HB1	1:E:30:ALA:O	0.83	1.74	4	5
1:B:33:GLY:O	1:C:34:LEU:N	0.83	2.12	7	1
1:B:21:ALA:HB3	1:C:21:ALA:O	0.82	1.73	7	1
1:I:18:VAL:O	1:J:18:VAL:CG2	0.82	2.27	10	1
1:I:30:ALA:N	1:J:30:ALA:HB1	0.82	1.89	3	1
1:F:9:GLY:H	1:G:8:SER:HA	0.82	1.29	8	1
1:G:17:LEU:O	1:G:18:VAL:CG1	0.82	2.27	7	1
1:A:18:VAL:HG22	1:A:19:PHE:H	0.82	1.33	4	2
1:A:18:VAL:HG22	1:A:36:VAL:HG12	0.82	1.52	3	1
1:J:11:GLU:HG3	1:J:12:VAL:H	0.82	1.32	6	2
1:C:35:MET:O	1:C:36:VAL:HB	0.82	1.73	3	1
1:A:34:LEU:HD12	1:A:34:LEU:N	0.82	1.90	6	2
1:A:19:PHE:O	1:A:20:PHE:CG	0.82	2.32	3	3
1:F:18:VAL:H	1:G:18:VAL:HG11	0.82	1.34	7	1
1:D:30:ALA:O	1:D:31:ILE:HG22	0.81	1.74	3	1
1:H:12:VAL:HB	1:I:13:HIS:H	0.81	1.35	10	1
1:A:20:PHE:CG	1:C:34:LEU:HD23	0.81	2.10	3	1
1:C:17:LEU:HB2	1:D:17:LEU:H	0.81	1.34	7	1
1:C:19:PHE:O	1:D:20:PHE:HD1	0.81	1.57	3	1
1:B:14:HIS:CG	1:B:15:GLN:H	0.81	1.93	1	3
1:F:10:TYR:N	1:G:10:TYR:O	0.81	2.13	7	1
1:D:29:GLY:O	1:E:31:ILE:HB	0.81	1.75	3	1
1:A:16:LYS:HA	1:B:16:LYS:HB3	0.81	1.52	3	1
1:A:35:MET:HB3	1:B:19:PHE:CG	0.81	2.10	7	1
1:I:10:TYR:C	1:J:10:TYR:H	0.81	1.77	9	2
1:D:34:LEU:HD23	1:D:34:LEU:N	0.81	1.89	9	1
1:C:35:MET:HG3	1:D:36:VAL:H	0.81	1.36	7	1
1:I:14:HIS:ND1	1:I:15:GLN:N	0.81	2.28	4	3
1:A:32:ILE:O	1:C:21:ALA:C	0.81	2.18	7	1
1:F:9:GLY:O	1:F:10:TYR:HB2	0.81	1.74	7	1
1:C:31:ILE:CG1	1:C:32:ILE:H	0.81	1.87	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:20:PHE:CD1	1:D:20:PHE:O	0.81	2.34	3	1
1:D:19:PHE:CA	1:E:19:PHE:N	0.80	2.44	7	1
1:G:10:TYR:OH	1:H:24:VAL:HG11	0.80	1.75	9	1
1:D:20:PHE:O	1:D:21:ALA:CB	0.80	2.30	3	2
1:G:35:MET:O	1:G:36:VAL:HG22	0.80	1.76	3	1
1:H:11:GLU:O	1:I:11:GLU:O	0.80	1.99	10	1
1:C:32:ILE:N	1:C:32:ILE:HD12	0.80	1.90	5	1
1:A:35:MET:CB	1:B:19:PHE:CD1	0.80	2.62	7	1
1:A:17:LEU:O	1:B:17:LEU:HB3	0.80	1.71	3	1
1:A:20:PHE:CD1	1:B:20:PHE:C	0.80	2.55	3	1
1:D:23:ASP:HA	1:E:22:GLU:CG	0.80	2.07	3	1
1:A:36:VAL:HG12	1:B:36:VAL:C	0.80	1.97	9	1
1:A:32:ILE:CG1	1:C:22:GLU:O	0.80	2.24	7	1
1:C:34:LEU:HD12	1:C:34:LEU:N	0.80	1.90	5	4
1:I:10:TYR:O	1:I:10:TYR:CD1	0.80	2.35	8	1
1:C:19:PHE:C	1:C:19:PHE:CD2	0.80	2.55	7	3
1:I:18:VAL:HG22	1:I:19:PHE:H	0.80	1.33	3	1
1:A:30:ALA:HB3	1:B:30:ALA:O	0.80	1.77	4	1
1:F:20:PHE:O	1:G:20:PHE:CB	0.80	2.29	9	8
1:B:19:PHE:H	1:C:18:VAL:HG12	0.80	1.37	3	1
1:C:19:PHE:HZ	1:E:20:PHE:CE1	0.79	1.92	3	1
1:A:34:LEU:HD23	1:A:34:LEU:N	0.79	1.92	9	2
1:A:19:PHE:O	1:B:20:PHE:HA	0.79	1.76	3	1
1:A:30:ALA:O	1:A:31:ILE:CD1	0.79	2.29	7	1
1:C:33:GLY:C	1:C:34:LEU:HD12	0.79	1.97	6	5
1:C:20:PHE:N	1:C:20:PHE:CD1	0.79	2.48	7	2
1:G:16:LYS:O	1:H:16:LYS:HB2	0.79	1.78	3	3
1:G:10:TYR:CZ	1:H:10:TYR:CD1	0.79	2.70	9	1
1:A:20:PHE:CD1	1:B:20:PHE:HA	0.79	2.11	3	1
1:D:28:LYS:O	1:D:29:GLY:O	0.79	1.99	3	3
1:B:18:VAL:O	1:B:19:PHE:HB2	0.79	1.77	7	1
1:A:8:SER:O	1:B:9:GLY:O	0.79	2.00	4	1
1:H:18:VAL:C	1:I:18:VAL:HG21	0.79	1.98	3	1
1:D:19:PHE:CE2	1:E:19:PHE:O	0.79	2.36	7	1
1:I:35:MET:C	1:I:36:VAL:HG22	0.79	1.98	3	1
1:G:30:ALA:HB1	1:H:30:ALA:O	0.78	1.77	6	4
1:A:32:ILE:O	1:B:21:ALA:CB	0.78	2.31	7	1
1:H:11:GLU:O	1:H:12:VAL:HG22	0.78	1.78	8	1
1:B:35:MET:O	1:C:36:VAL:N	0.78	2.17	7	1
1:B:18:VAL:HB	1:C:18:VAL:HB	0.78	0.84	3	1
1:G:36:VAL:CB	1:H:36:VAL:O	0.78	2.31	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:32:ILE:HG12	1:D:33:GLY:H	0.78	1.39	3	2
1:A:21:ALA:CB	1:B:21:ALA:O	0.78	2.32	7	1
1:C:31:ILE:O	1:D:32:ILE:CB	0.78	2.32	7	1
1:A:21:ALA:HB3	1:B:21:ALA:O	0.78	1.78	7	1
1:G:34:LEU:HD22	1:G:34:LEU:N	0.78	1.91	7	1
1:B:33:GLY:O	1:B:34:LEU:HD13	0.78	1.78	3	1
1:D:36:VAL:HA	1:E:36:VAL:O	0.78	1.79	3	2
1:C:21:ALA:O	1:C:22:GLU:CB	0.78	2.32	7	1
1:H:14:HIS:CG	1:H:15:GLN:N	0.78	2.50	6	2
1:H:24:VAL:CG1	1:H:25:GLY:N	0.78	2.47	8	1
1:H:9:GLY:HA2	1:I:9:GLY:H	0.78	1.37	6	1
1:C:19:PHE:O	1:D:20:PHE:CD1	0.78	2.35	3	1
1:I:35:MET:CG	1:I:36:VAL:N	0.78	2.47	3	1
1:G:19:PHE:CD2	1:G:19:PHE:C	0.78	2.57	7	2
1:C:17:LEU:CG	1:D:17:LEU:HB3	0.78	2.09	7	1
1:C:34:LEU:CB	1:D:34:LEU:HD11	0.78	2.08	7	1
1:H:33:GLY:C	1:H:34:LEU:HD12	0.77	2.00	7	7
1:B:35:MET:O	1:B:36:VAL:CG2	0.77	2.32	9	1
1:H:33:GLY:C	1:H:34:LEU:HD23	0.77	1.99	3	1
1:H:34:LEU:N	1:H:34:LEU:HD12	0.77	1.95	2	3
1:F:34:LEU:O	1:G:34:LEU:O	0.77	2.01	10	1
1:J:17:LEU:O	1:J:18:VAL:HB	0.77	1.77	10	1
1:G:12:VAL:HB	1:H:12:VAL:HA	0.77	1.55	1	2
1:B:11:GLU:O	1:B:12:VAL:CB	0.77	2.31	3	2
1:B:33:GLY:O	1:B:34:LEU:CD2	0.77	2.32	3	1
1:B:35:MET:CB	1:C:35:MET:HA	0.77	2.10	3	1
1:D:30:ALA:CA	1:E:31:ILE:CG1	0.77	2.62	3	1
1:C:34:LEU:N	1:C:34:LEU:HD23	0.77	1.93	10	3
1:H:10:TYR:H	1:I:10:TYR:HA	0.77	1.39	10	1
1:H:18:VAL:O	1:I:18:VAL:CG2	0.77	2.31	3	1
1:D:19:PHE:CA	1:E:18:VAL:CA	0.77	2.62	7	1
1:I:19:PHE:HA	1:J:19:PHE:O	0.77	1.79	1	6
1:E:22:GLU:H	1:G:39:VAL:HG21	0.77	1.40	7	1
1:D:23:ASP:HA	1:E:22:GLU:HG2	0.77	1.57	3	1
1:D:30:ALA:O	1:D:31:ILE:CG2	0.77	2.33	3	1
1:G:11:GLU:O	1:G:12:VAL:CB	0.77	2.32	8	2
1:G:12:VAL:O	1:H:12:VAL:CG2	0.77	2.33	8	1
1:D:34:LEU:HD12	1:E:34:LEU:O	0.77	1.80	5	1
1:I:10:TYR:CA	1:J:10:TYR:H	0.77	1.91	9	2
1:D:19:PHE:HA	1:E:19:PHE:O	0.77	1.79	4	4
1:A:31:ILE:H	1:B:31:ILE:HA	0.77	1.39	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:24:VAL:O	1:E:26:SER:N	0.77	2.18	6	4
1:D:27:ASN:HB2	1:E:31:ILE:N	0.77	1.94	3	1
1:A:35:MET:O	1:A:36:VAL:HG22	0.76	1.80	3	2
1:G:14:HIS:ND1	1:G:15:GLN:N	0.76	2.32	2	1
1:H:36:VAL:CG2	1:I:36:VAL:H	0.76	1.93	7	1
1:H:36:VAL:HG22	1:I:36:VAL:O	0.76	1.79	7	1
1:A:33:GLY:N	1:B:34:LEU:HD23	0.76	1.96	3	1
1:C:19:PHE:HB3	1:D:18:VAL:HG12	0.76	1.57	3	1
1:C:36:VAL:HG13	1:C:37:GLY:N	0.76	1.95	3	1
1:F:17:LEU:HD23	1:F:17:LEU:N	0.76	1.95	6	1
1:G:8:SER:O	1:H:9:GLY:CA	0.76	2.33	8	1
1:E:35:MET:C	1:E:36:VAL:HG22	0.76	2.01	3	3
1:C:18:VAL:CG2	1:C:19:PHE:N	0.76	2.36	7	1
1:E:19:PHE:C	1:E:19:PHE:CD1	0.76	2.59	7	1
1:I:33:GLY:C	1:I:34:LEU:HD12	0.76	2.00	8	6
1:C:38:GLY:CA	1:D:38:GLY:O	0.76	2.33	7	3
1:E:24:VAL:HG13	1:E:25:GLY:N	0.76	1.94	7	1
1:C:30:ALA:O	1:C:31:ILE:HB	0.76	1.79	3	1
1:F:12:VAL:HB	1:G:13:HIS:H	0.76	1.41	8	1
1:H:19:PHE:CD1	1:H:19:PHE:C	0.76	2.59	3	1
1:G:14:HIS:CG	1:G:15:GLN:N	0.76	2.53	8	1
1:A:19:PHE:CZ	1:A:34:LEU:O	0.76	2.38	7	1
1:G:18:VAL:CG2	1:G:19:PHE:H	0.76	1.94	8	1
1:A:20:PHE:HA	1:B:20:PHE:HB3	0.76	1.55	3	1
1:F:17:LEU:O	1:F:18:VAL:CG1	0.76	2.33	4	2
1:B:36:VAL:HG21	1:C:36:VAL:H	0.76	1.40	9	1
1:G:9:GLY:O	1:G:10:TYR:CD2	0.76	2.39	1	2
1:C:19:PHE:CB	1:D:18:VAL:HB	0.76	2.11	3	1
1:G:11:GLU:O	1:G:12:VAL:HG23	0.75	1.81	8	1
1:F:9:GLY:N	1:G:8:SER:CA	0.75	2.49	8	1
1:I:18:VAL:O	1:J:18:VAL:CG1	0.75	2.34	10	1
1:C:17:LEU:O	1:C:18:VAL:CB	0.75	2.34	7	1
1:A:17:LEU:O	1:B:17:LEU:CA	0.75	2.33	3	1
1:I:17:LEU:O	1:I:18:VAL:HB	0.75	1.80	3	1
1:J:36:VAL:O	1:J:36:VAL:CG2	0.75	2.30	3	1
1:B:19:PHE:CZ	1:B:34:LEU:HD12	0.75	2.16	10	1
1:D:34:LEU:HA	1:E:34:LEU:O	0.75	1.81	3	2
1:A:29:GLY:O	1:A:30:ALA:CB	0.75	2.34	7	1
1:F:9:GLY:HA2	1:G:9:GLY:N	0.75	1.91	8	1
1:B:31:ILE:HD13	1:D:23:ASP:CA	0.75	2.12	7	1
1:F:38:GLY:O	1:G:38:GLY:CA	0.75	2.34	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:VAL:O	1:A:19:PHE:HB2	0.75	1.80	7	1
1:G:34:LEU:HD13	1:G:34:LEU:N	0.75	1.96	7	1
1:H:36:VAL:HA	1:I:36:VAL:O	0.75	1.81	3	1
1:F:12:VAL:HB	1:G:12:VAL:H	0.75	1.42	1	1
1:F:18:VAL:HG22	1:F:19:PHE:N	0.75	1.94	8	4
1:A:34:LEU:CA	1:B:19:PHE:CZ	0.75	2.70	7	1
1:A:19:PHE:O	1:A:20:PHE:CD2	0.75	2.40	3	2
1:C:20:PHE:O	1:D:20:PHE:C	0.75	2.25	3	1
1:D:34:LEU:O	1:D:34:LEU:HD13	0.75	1.80	3	1
1:B:14:HIS:CE1	1:B:18:VAL:HG23	0.75	2.16	7	1
1:F:18:VAL:O	1:G:18:VAL:CB	0.75	2.35	7	1
1:B:32:ILE:HA	1:C:32:ILE:O	0.75	1.82	7	2
1:B:19:PHE:CE2	1:C:20:PHE:HE2	0.75	1.97	3	1
1:G:34:LEU:N	1:G:34:LEU:HD12	0.75	1.94	1	1
1:F:37:GLY:O	1:G:37:GLY:HA2	0.75	1.81	10	1
1:G:36:VAL:HG11	1:H:36:VAL:N	0.75	1.97	3	1
1:B:13:HIS:ND1	1:B:14:HIS:N	0.75	2.35	1	1
1:C:36:VAL:HG21	1:D:36:VAL:O	0.74	1.81	3	1
1:G:11:GLU:O	1:G:12:VAL:CG2	0.74	2.35	8	1
1:F:33:GLY:N	1:G:33:GLY:HA2	0.74	1.96	10	1
1:I:11:GLU:O	1:I:12:VAL:CB	0.74	2.34	9	2
1:D:21:ALA:O	1:D:22:GLU:HB2	0.74	1.81	7	1
1:C:19:PHE:HZ	1:E:20:PHE:CD1	0.74	2.00	3	1
1:C:21:ALA:O	1:C:22:GLU:CG	0.74	2.35	7	1
1:H:34:LEU:HD12	1:H:34:LEU:N	0.74	1.97	5	5
1:D:31:ILE:O	1:D:32:ILE:HD13	0.74	1.82	8	1
1:G:17:LEU:C	1:G:18:VAL:HG22	0.74	2.03	7	1
1:D:19:PHE:HB2	1:E:20:PHE:CE2	0.74	2.17	7	1
1:A:34:LEU:HD12	1:A:34:LEU:H	0.74	1.43	6	2
1:B:34:LEU:HD23	1:B:34:LEU:N	0.74	1.97	6	2
1:A:30:ALA:HB3	1:C:24:VAL:O	0.74	1.83	7	1
1:A:20:PHE:CD1	1:C:34:LEU:HD23	0.74	2.18	3	1
1:C:19:PHE:CD1	1:D:18:VAL:HA	0.74	2.17	3	1
1:E:30:ALA:C	1:E:31:ILE:HD12	0.74	2.03	3	1
1:J:24:VAL:O	1:J:26:SER:N	0.74	2.21	6	4
1:J:11:GLU:CG	1:J:12:VAL:H	0.74	1.95	9	2
1:B:33:GLY:O	1:C:34:LEU:HD23	0.74	1.81	7	1
1:D:19:PHE:HA	1:E:18:VAL:HA	0.74	1.56	7	1
1:D:34:LEU:C	1:E:19:PHE:CE2	0.74	2.61	7	1
1:H:11:GLU:O	1:H:12:VAL:CG2	0.73	2.36	8	1
1:A:20:PHE:O	1:B:20:PHE:HB2	0.73	1.81	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:I:14:HIS:CD2	1:I:15:GLN:H	0.73	2.01	1	2
1:A:18:VAL:C	1:B:18:VAL:HG21	0.73	2.03	7	1
1:A:17:LEU:H	1:B:17:LEU:H	0.73	1.23	3	1
1:I:10:TYR:O	1:J:10:TYR:CA	0.73	2.36	4	4
1:H:9:GLY:O	1:H:10:TYR:CD2	0.73	2.42	6	2
1:D:32:ILE:CG1	1:D:33:GLY:N	0.73	2.47	5	2
1:D:34:LEU:N	1:E:19:PHE:CZ	0.73	2.56	7	1
1:H:36:VAL:HG22	1:I:36:VAL:H	0.73	1.42	7	1
1:A:19:PHE:CB	1:B:20:PHE:CD2	0.73	2.71	3	1
1:G:16:LYS:O	1:H:16:LYS:CB	0.73	2.35	3	7
1:A:12:VAL:C	1:B:13:HIS:O	0.73	2.27	3	1
1:C:20:PHE:CA	1:D:20:PHE:O	0.73	2.36	3	1
1:C:33:GLY:N	1:D:32:ILE:HG13	0.73	1.99	3	1
1:F:38:GLY:N	1:G:37:GLY:O	0.73	2.21	3	1
1:H:18:VAL:O	1:I:18:VAL:CG1	0.73	2.35	3	1
1:F:30:ALA:HB1	1:G:30:ALA:O	0.73	1.83	7	2
1:A:30:ALA:CB	1:C:24:VAL:O	0.73	2.37	7	1
1:D:34:LEU:HA	1:E:34:LEU:HG	0.73	1.59	7	1
1:G:10:TYR:CB	1:H:10:TYR:C	0.73	2.57	8	1
1:I:10:TYR:O	1:J:10:TYR:CB	0.73	2.37	4	5
1:F:34:LEU:HD23	1:F:34:LEU:H	0.73	1.43	7	2
1:D:17:LEU:O	1:D:18:VAL:CG1	0.73	2.34	3	1
1:F:34:LEU:C	1:F:35:MET:HG3	0.73	2.02	7	1
1:I:12:VAL:O	1:J:12:VAL:HA	0.73	1.84	10	1
1:F:17:LEU:C	1:F:18:VAL:HG22	0.73	2.03	4	2
1:A:35:MET:C	1:A:36:VAL:HG22	0.73	2.04	9	1
1:G:12:VAL:O	1:H:12:VAL:HA	0.73	1.83	7	1
1:J:35:MET:C	1:J:36:VAL:HG22	0.73	2.04	7	2
1:A:21:ALA:HB2	1:B:34:LEU:HD23	0.73	1.58	1	1
1:A:12:VAL:HB	1:B:13:HIS:O	0.73	1.84	3	1
1:G:9:GLY:O	1:H:9:GLY:HA2	0.73	1.83	8	1
1:B:33:GLY:O	1:C:34:LEU:O	0.73	2.05	7	1
1:H:35:MET:O	1:I:35:MET:CA	0.73	2.36	3	1
1:H:11:GLU:C	1:H:12:VAL:HG13	0.72	2.04	8	1
1:H:33:GLY:O	1:H:34:LEU:HD23	0.72	1.83	6	2
1:A:23:ASP:OD2	1:A:27:ASN:N	0.72	2.22	7	1
1:A:16:LYS:O	1:A:17:LEU:HB2	0.72	1.83	3	2
1:A:20:PHE:CD1	1:B:20:PHE:CA	0.72	2.72	3	1
1:A:31:ILE:O	1:A:32:ILE:HG12	0.72	1.84	3	1
1:E:31:ILE:O	1:E:32:ILE:HD13	0.72	1.83	8	1
1:H:10:TYR:O	1:I:10:TYR:N	0.72	2.14	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:30:ALA:O	1:E:31:ILE:CA	0.72	2.37	1	1
1:G:9:GLY:C	1:G:10:TYR:CG	0.72	2.62	7	5
1:A:32:ILE:O	1:B:32:ILE:O	0.72	2.07	3	1
1:I:35:MET:C	1:J:35:MET:HA	0.72	2.03	3	1
1:H:24:VAL:HG12	1:H:25:GLY:N	0.72	1.98	8	1
1:A:35:MET:CG	1:B:19:PHE:CD1	0.72	2.73	7	1
1:I:14:HIS:NE2	1:I:17:LEU:C	0.72	2.43	10	1
1:B:19:PHE:N	1:C:18:VAL:HG12	0.72	1.99	3	1
1:H:24:VAL:HG22	1:H:25:GLY:H	0.72	1.45	5	2
1:B:19:PHE:CZ	1:C:19:PHE:CD2	0.72	2.78	7	1
1:C:35:MET:O	1:D:36:VAL:O	0.72	2.08	7	1
1:A:37:GLY:O	1:B:37:GLY:O	0.72	2.08	3	1
1:D:17:LEU:C	1:D:18:VAL:HG22	0.72	2.05	3	1
1:G:8:SER:H	1:H:9:GLY:H	0.72	1.27	1	1
1:D:33:GLY:O	1:E:33:GLY:CA	0.72	2.38	3	2
1:F:34:LEU:H	1:F:34:LEU:HD12	0.72	1.40	8	1
1:A:12:VAL:CB	1:B:13:HIS:O	0.72	2.38	3	1
1:B:35:MET:CE	1:C:36:VAL:O	0.72	2.38	3	1
1:G:14:HIS:CD2	1:G:15:GLN:H	0.71	2.03	8	1
1:H:11:GLU:O	1:H:12:VAL:CB	0.71	2.37	8	1
1:A:14:HIS:ND1	1:B:14:HIS:CE1	0.71	2.58	3	1
1:A:16:LYS:CA	1:B:16:LYS:CB	0.71	2.67	3	1
1:I:24:VAL:HG12	1:I:25:GLY:H	0.71	1.44	3	3
1:I:11:GLU:HA	1:J:11:GLU:HA	0.71	1.63	2	3
1:G:17:LEU:C	1:G:17:LEU:HD23	0.71	2.05	10	1
1:E:35:MET:SD	1:E:35:MET:O	0.71	2.49	3	4
1:G:30:ALA:C	1:G:31:ILE:HD12	0.71	2.05	2	1
1:A:35:MET:C	1:A:36:VAL:HG13	0.71	2.04	3	1
1:D:21:ALA:HB2	1:D:34:LEU:HG	0.71	1.59	3	1
1:F:18:VAL:O	1:G:18:VAL:HB	0.71	1.86	7	1
1:C:19:PHE:CZ	1:E:20:PHE:CD1	0.71	2.77	3	1
1:F:18:VAL:CG2	1:F:19:PHE:H	0.71	1.97	8	4
1:J:20:PHE:CD1	1:J:20:PHE:N	0.71	2.59	10	2
1:E:19:PHE:C	1:E:20:PHE:CG	0.71	2.64	3	7
1:D:19:PHE:CD2	1:E:20:PHE:CA	0.71	2.73	7	1
1:G:34:LEU:N	1:G:34:LEU:HD23	0.71	2.00	2	2
1:B:31:ILE:C	1:B:32:ILE:HG13	0.71	2.05	3	1
1:H:23:ASP:HA	1:I:23:ASP:O	0.71	1.86	7	1
1:A:20:PHE:CD1	1:C:34:LEU:CD2	0.71	2.73	3	1
1:G:24:VAL:HG12	1:G:25:GLY:H	0.71	1.43	5	2
1:B:29:GLY:H	1:C:27:ASN:HB3	0.71	1.46	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:31:ILE:O	1:C:32:ILE:CB	0.71	2.38	7	1
1:F:17:LEU:O	1:F:18:VAL:HB	0.71	1.85	8	4
1:B:14:HIS:ND1	1:B:15:GLN:N	0.71	2.39	1	2
1:D:30:ALA:N	1:E:27:ASN:OD1	0.71	2.23	7	1
1:I:35:MET:HB3	1:J:35:MET:CB	0.71	2.15	3	1
1:A:39:VAL:O	1:B:38:GLY:O	0.71	2.09	3	1
1:D:30:ALA:N	1:E:31:ILE:CB	0.71	2.54	3	1
1:A:12:VAL:CG2	1:B:13:HIS:N	0.70	2.53	7	1
1:G:12:VAL:HB	1:H:12:VAL:CA	0.70	2.16	1	1
1:A:37:GLY:O	1:B:37:GLY:CA	0.70	2.39	7	1
1:I:12:VAL:HG22	1:J:12:VAL:H	0.70	1.45	10	1
1:I:12:VAL:HG22	1:J:12:VAL:N	0.70	2.02	10	1
1:J:18:VAL:CG2	1:J:19:PHE:H	0.70	1.90	10	1
1:A:18:VAL:O	1:B:18:VAL:HG23	0.70	1.86	9	1
1:C:20:PHE:O	1:D:20:PHE:HB2	0.70	1.86	6	5
1:B:33:GLY:O	1:C:34:LEU:CA	0.70	2.39	7	1
1:C:35:MET:SD	1:D:36:VAL:O	0.70	2.49	7	1
1:H:8:SER:OG	1:H:10:TYR:CD1	0.70	2.45	7	1
1:C:33:GLY:N	1:D:32:ILE:CG1	0.70	2.54	3	1
1:J:38:GLY:O	1:J:39:VAL:C	0.70	2.29	3	1
1:B:31:ILE:C	1:B:32:ILE:HD12	0.70	2.06	1	1
1:D:24:VAL:O	1:D:26:SER:N	0.70	2.25	1	1
1:D:31:ILE:O	1:D:32:ILE:HB	0.70	1.86	5	2
1:I:11:GLU:O	1:I:12:VAL:CG2	0.70	2.40	9	2
1:D:19:PHE:CD2	1:E:19:PHE:C	0.70	2.64	7	1
1:J:11:GLU:O	1:J:12:VAL:HG12	0.70	1.86	8	2
1:F:35:MET:SD	1:G:35:MET:SD	0.70	2.90	7	1
1:B:39:VAL:HG22	1:C:40:VAL:H	0.70	1.47	3	1
1:D:27:ASN:O	1:E:29:GLY:HA3	0.70	1.86	3	1
1:H:39:VAL:C	1:I:39:VAL:HG12	0.70	2.07	3	1
1:I:10:TYR:O	1:J:10:TYR:N	0.70	2.25	3	4
1:F:32:ILE:HA	1:G:32:ILE:O	0.70	1.87	3	2
1:B:35:MET:C	1:B:36:VAL:CG2	0.70	2.58	9	1
1:D:18:VAL:HG23	1:E:20:PHE:CE1	0.70	2.21	7	1
1:I:28:LYS:H	1:I:28:LYS:CD	0.70	2.00	8	1
1:B:19:PHE:CD1	1:B:20:PHE:N	0.70	2.60	3	5
1:H:9:GLY:HA2	1:I:9:GLY:N	0.70	2.01	6	1
1:A:31:ILE:CG1	1:C:22:GLU:HA	0.70	2.14	7	1
1:D:20:PHE:CE2	1:D:36:VAL:HG12	0.70	2.22	3	1
1:D:26:SER:OG	1:E:29:GLY:N	0.70	2.25	3	1
1:I:11:GLU:O	1:I:12:VAL:HG23	0.70	1.86	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:20:PHE:CZ	1:C:20:PHE:CD2	0.70	2.80	9	1
1:D:35:MET:N	1:E:34:LEU:O	0.70	2.24	3	1
1:C:20:PHE:CE2	1:D:20:PHE:CD2	0.70	2.80	1	1
1:G:18:VAL:H	1:H:18:VAL:CG1	0.70	1.98	8	1
1:A:27:ASN:N	2:B:101:2PO:O3P	0.70	2.25	7	1
1:I:31:ILE:N	1:J:31:ILE:N	0.70	2.30	3	1
1:I:11:GLU:O	1:I:12:VAL:HB	0.69	1.87	6	2
1:B:29:GLY:N	1:C:27:ASN:CB	0.69	2.55	7	1
1:F:9:GLY:O	1:F:10:TYR:CB	0.69	2.39	7	1
1:E:18:VAL:O	1:E:19:PHE:CD1	0.69	2.45	3	1
1:I:35:MET:O	1:I:36:VAL:CG1	0.69	2.39	3	1
1:B:20:PHE:O	1:C:20:PHE:CB	0.69	2.39	4	7
1:A:33:GLY:CA	1:B:34:LEU:HD23	0.69	2.17	3	1
1:C:20:PHE:CG	1:C:21:ALA:N	0.69	2.58	3	1
1:F:19:PHE:CZ	1:F:36:VAL:HG13	0.69	2.22	9	4
1:C:31:ILE:O	1:D:32:ILE:HB	0.69	1.86	7	1
1:I:10:TYR:CD1	1:I:11:GLU:N	0.69	2.60	7	1
1:I:17:LEU:HD23	1:I:17:LEU:C	0.69	2.07	4	1
1:A:20:PHE:O	1:A:21:ALA:HB2	0.69	1.86	7	1
1:A:31:ILE:CG2	1:C:22:GLU:H	0.69	2.00	7	1
1:B:31:ILE:HG22	1:C:32:ILE:H	0.69	1.47	7	1
1:H:19:PHE:HB2	1:I:19:PHE:O	0.69	1.88	3	2
1:D:32:ILE:CD1	1:D:33:GLY:H	0.69	1.99	3	1
1:A:20:PHE:O	1:B:20:PHE:CB	0.69	2.40	2	6
1:C:19:PHE:CG	1:D:18:VAL:CB	0.69	2.64	3	1
1:C:31:ILE:H	1:D:31:ILE:HG23	0.69	1.48	3	1
1:A:32:ILE:HG22	1:B:32:ILE:N	0.69	2.03	7	1
1:B:34:LEU:HA	1:C:34:LEU:O	0.69	1.87	7	1
1:G:13:HIS:ND1	1:G:14:HIS:N	0.69	2.41	8	1
1:A:11:GLU:C	1:A:12:VAL:HG23	0.69	2.07	4	1
1:A:32:ILE:HG23	1:A:33:GLY:H	0.69	1.41	3	1
1:D:29:GLY:O	1:E:31:ILE:CD1	0.69	2.40	3	1
1:G:12:VAL:C	1:H:12:VAL:CG2	0.69	2.60	8	1
1:I:24:VAL:HG12	1:I:25:GLY:N	0.69	2.03	3	3
1:F:19:PHE:CE1	1:F:34:LEU:HD12	0.69	2.23	5	2
1:E:19:PHE:O	1:E:20:PHE:CG	0.69	2.46	3	2
1:I:8:SER:HB2	1:J:9:GLY:N	0.69	2.01	9	1
1:C:19:PHE:C	1:C:19:PHE:CD1	0.69	2.65	9	1
1:B:31:ILE:O	1:C:32:ILE:CA	0.69	2.41	7	1
1:A:23:ASP:HB2	1:B:23:ASP:O	0.69	1.88	7	1
1:D:34:LEU:HD23	1:E:34:LEU:HB2	0.69	1.64	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:VAL:HB	1:B:18:VAL:CG1	0.69	2.15	3	1
1:G:11:GLU:HA	1:H:11:GLU:HA	0.69	1.65	10	1
1:A:39:VAL:HG23	1:B:40:VAL:H	0.69	1.48	9	1
1:I:38:GLY:O	1:J:38:GLY:CA	0.69	2.41	3	1
1:A:30:ALA:HB1	1:B:30:ALA:O	0.69	1.88	1	3
1:B:19:PHE:CD2	1:C:20:PHE:HE2	0.69	2.01	3	1
1:D:32:ILE:HD13	1:D:33:GLY:N	0.69	2.02	3	1
1:D:34:LEU:HD23	1:E:34:LEU:CB	0.69	2.17	3	1
1:A:29:GLY:O	1:A:30:ALA:HB2	0.68	1.88	7	1
1:D:20:PHE:O	1:D:21:ALA:HB2	0.68	1.87	7	1
1:H:39:VAL:H	1:I:39:VAL:HA	0.68	1.48	7	1
1:A:39:VAL:N	1:B:38:GLY:O	0.68	2.26	3	2
1:C:19:PHE:CZ	1:D:20:PHE:HB3	0.68	2.24	3	1
1:A:34:LEU:C	1:B:35:MET:O	0.68	2.32	3	1
1:C:31:ILE:O	1:D:31:ILE:CG1	0.68	2.41	3	1
1:H:36:VAL:HG23	1:I:36:VAL:HG23	0.68	1.63	3	1
1:B:31:ILE:HG12	1:D:21:ALA:O	0.68	1.88	7	1
1:C:30:ALA:C	1:C:31:ILE:HD12	0.68	2.07	8	2
1:C:17:LEU:O	1:C:18:VAL:HB	0.68	1.88	7	1
1:I:35:MET:HG2	1:I:36:VAL:N	0.68	2.03	3	1
1:C:30:ALA:HB2	1:D:28:LYS:O	0.68	1.88	1	1
1:B:20:PHE:CZ	1:C:20:PHE:CE2	0.68	2.82	9	1
1:I:8:SER:OG	1:J:7:ASP:HA	0.68	1.88	9	1
1:A:23:ASP:OD1	1:A:25:GLY:N	0.68	2.27	7	1
1:A:32:ILE:N	1:C:23:ASP:N	0.68	2.42	7	1
1:B:19:PHE:C	1:B:19:PHE:CD1	0.68	2.66	4	1
1:C:20:PHE:CD1	1:C:21:ALA:N	0.68	2.62	3	1
1:H:36:VAL:CG2	1:I:36:VAL:HG23	0.68	2.18	3	1
1:F:9:GLY:H	1:G:8:SER:CA	0.68	2.00	8	1
1:B:35:MET:O	1:B:36:VAL:CG1	0.68	2.42	9	1
1:I:35:MET:O	1:I:36:VAL:HG22	0.68	1.89	3	2
1:A:11:GLU:O	1:A:12:VAL:HG23	0.68	1.89	4	1
1:A:19:PHE:CB	1:B:20:PHE:CE2	0.68	2.77	3	1
1:B:33:GLY:C	1:C:34:LEU:HG	0.68	2.09	7	1
1:D:19:PHE:CA	1:E:18:VAL:HA	0.68	2.16	7	1
1:I:37:GLY:H	1:J:37:GLY:CA	0.68	2.01	7	1
1:G:9:GLY:O	1:G:10:TYR:CG	0.68	2.47	1	2
1:H:8:SER:HB2	2:H:101:2PO:P	0.68	2.29	1	1
1:A:30:ALA:CB	1:B:30:ALA:O	0.68	2.42	7	2
1:B:31:ILE:O	1:C:32:ILE:O	0.68	2.12	7	1
1:E:20:PHE:CD1	1:E:20:PHE:N	0.68	2.61	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:34:LEU:HA	1:E:34:LEU:CG	0.68	2.19	7	1
1:I:12:VAL:N	1:J:12:VAL:H	0.68	1.84	2	3
1:G:10:TYR:HB3	1:H:10:TYR:C	0.67	2.09	8	1
1:C:36:VAL:HG22	1:C:37:GLY:H	0.67	1.49	3	1
1:H:12:VAL:HB	1:I:13:HIS:N	0.67	2.04	10	1
1:C:34:LEU:HB2	1:D:34:LEU:HD11	0.67	1.65	7	1
1:C:19:PHE:CB	1:D:18:VAL:CB	0.67	2.72	3	1
1:D:20:PHE:O	1:D:21:ALA:HB3	0.67	1.89	3	1
1:F:19:PHE:CD2	1:F:19:PHE:N	0.67	2.63	4	4
1:B:18:VAL:HG22	1:B:19:PHE:H	0.67	1.48	7	1
1:G:10:TYR:CD1	1:G:10:TYR:N	0.67	2.60	10	3
1:G:15:GLN:O	1:G:16:LYS:C	0.67	2.32	10	4
1:D:19:PHE:CD1	1:D:20:PHE:N	0.67	2.62	6	1
1:B:31:ILE:O	1:B:32:ILE:HG13	0.67	1.90	3	1
1:C:20:PHE:HA	1:D:20:PHE:CE1	0.67	2.24	3	1
1:B:11:GLU:C	1:B:12:VAL:HG23	0.67	2.09	1	1
1:F:34:LEU:N	1:F:34:LEU:HD23	0.67	2.05	5	2
1:B:31:ILE:HG12	1:D:22:GLU:C	0.67	2.10	7	1
1:G:35:MET:O	1:G:36:VAL:CG2	0.67	2.42	3	1
1:I:37:GLY:C	1:J:37:GLY:O	0.67	2.31	3	1
1:I:14:HIS:NE2	1:I:17:LEU:O	0.67	2.28	6	2
1:A:37:GLY:O	1:B:37:GLY:HA2	0.67	1.88	7	1
1:F:34:LEU:HD23	1:F:34:LEU:N	0.67	2.03	7	1
1:B:19:PHE:CZ	1:C:20:PHE:CE2	0.67	2.83	3	1
1:B:32:ILE:C	1:B:32:ILE:HD12	0.67	2.10	3	1
1:E:35:MET:SD	1:E:35:MET:N	0.67	2.68	1	2
1:F:11:GLU:HA	1:G:11:GLU:HA	0.67	1.66	8	1
1:G:11:GLU:O	1:G:12:VAL:HB	0.67	1.88	8	1
1:I:18:VAL:C	1:J:18:VAL:HG21	0.67	2.10	10	1
1:C:20:PHE:CA	1:D:20:PHE:CG	0.67	2.75	7	1
1:B:32:ILE:HG12	1:C:32:ILE:O	0.67	1.88	3	1
1:I:38:GLY:H	1:J:37:GLY:C	0.67	1.92	3	1
1:J:19:PHE:C	1:J:20:PHE:CG	0.67	2.66	7	5
1:A:23:ASP:C	1:A:23:ASP:OD1	0.67	2.33	7	2
1:A:32:ILE:N	1:C:22:GLU:O	0.67	2.28	7	1
1:A:34:LEU:N	1:B:19:PHE:CZ	0.67	2.63	7	1
1:H:10:TYR:OH	1:I:10:TYR:CD2	0.67	2.46	7	1
1:H:13:HIS:CD2	1:H:14:HIS:H	0.67	2.08	7	1
1:F:10:TYR:O	1:G:10:TYR:CA	0.67	2.43	1	1
1:A:34:LEU:C	1:B:19:PHE:CZ	0.67	2.69	7	1
1:B:31:ILE:O	1:B:32:ILE:CB	0.67	2.43	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:27:ASN:ND2	1:C:28:LYS:N	0.67	2.43	3	1
1:F:35:MET:O	1:G:35:MET:CB	0.67	2.43	3	1
1:G:18:VAL:O	1:H:18:VAL:HG12	0.66	1.89	8	1
1:H:20:PHE:O	1:I:20:PHE:CB	0.66	2.38	7	6
1:H:19:PHE:CD1	1:H:20:PHE:N	0.66	2.64	1	5
1:G:10:TYR:CD2	1:H:10:TYR:CD2	0.66	2.83	6	2
1:F:19:PHE:CD2	1:F:19:PHE:O	0.66	2.48	7	3
1:D:20:PHE:O	1:E:19:PHE:C	0.66	2.33	7	1
1:D:34:LEU:CD2	1:D:35:MET:N	0.66	2.48	3	1
1:I:39:VAL:CG1	1:I:40:VAL:N	0.66	2.36	3	1
1:A:19:PHE:O	1:A:19:PHE:CD1	0.66	2.48	8	2
1:I:15:GLN:O	1:I:16:LYS:C	0.66	2.33	8	5
1:H:12:VAL:CB	1:I:13:HIS:H	0.66	2.03	10	1
1:A:17:LEU:HD23	1:A:17:LEU:C	0.66	2.09	9	1
1:D:19:PHE:CD1	1:E:18:VAL:CA	0.66	2.78	7	1
1:A:31:ILE:O	1:A:32:ILE:CB	0.66	2.43	3	1
1:C:20:PHE:C	1:D:20:PHE:O	0.66	2.32	3	1
1:A:12:VAL:HG21	1:B:13:HIS:N	0.66	2.05	7	1
1:B:19:PHE:HZ	1:B:34:LEU:O	0.66	1.69	7	1
1:B:21:ALA:CA	1:C:20:PHE:CZ	0.66	2.75	3	1
1:F:39:VAL:HA	1:G:39:VAL:N	0.66	2.02	3	1
1:F:37:GLY:HA2	1:G:37:GLY:O	0.66	1.89	3	1
1:G:34:LEU:CB	1:H:34:LEU:O	0.66	2.43	3	1
1:C:32:ILE:HB	1:D:32:ILE:O	0.66	1.89	1	1
1:G:18:VAL:N	1:H:18:VAL:HG12	0.66	2.03	8	1
1:I:8:SER:HB2	2:I:101:2PO:P	0.66	2.29	6	4
1:D:24:VAL:HG13	1:D:24:VAL:O	0.66	1.91	5	1
1:B:31:ILE:O	1:C:32:ILE:N	0.66	2.28	7	1
1:A:20:PHE:HD1	1:B:20:PHE:C	0.66	1.92	3	1
1:B:19:PHE:CZ	1:C:20:PHE:CZ	0.66	2.82	3	1
1:F:9:GLY:CA	1:G:8:SER:N	0.66	2.58	8	1
1:G:12:VAL:O	1:G:12:VAL:CG1	0.66	2.44	8	1
1:B:14:HIS:CD2	1:B:15:GLN:H	0.66	2.09	6	2
1:G:13:HIS:O	1:G:14:HIS:CG	0.66	2.48	9	2
1:I:12:VAL:O	1:J:12:VAL:CA	0.66	2.44	10	2
1:J:13:HIS:O	1:J:14:HIS:CG	0.66	2.48	2	3
1:J:10:TYR:O	1:J:11:GLU:HB2	0.66	1.90	6	2
1:A:23:ASP:OD1	1:A:24:VAL:N	0.66	2.29	7	1
1:I:12:VAL:HB	1:J:12:VAL:H	0.66	1.50	7	2
1:A:34:LEU:C	1:B:34:LEU:HB3	0.66	2.11	3	1
1:H:20:PHE:CE1	1:I:20:PHE:CD1	0.66	2.84	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:G:10:TYR:CB	1:H:10:TYR:O	0.66	2.44	8	1
1:A:19:PHE:C	1:A:20:PHE:CG	0.66	2.67	7	2
1:C:17:LEU:CB	1:D:17:LEU:H	0.66	2.01	7	1
1:A:20:PHE:CA	1:B:20:PHE:HB3	0.66	2.21	3	1
1:D:33:GLY:O	1:D:34:LEU:HB3	0.66	1.90	1	1
1:H:8:SER:HB3	2:H:101:2PO:P	0.66	2.30	9	2
1:C:19:PHE:HB3	1:D:18:VAL:CB	0.66	2.20	3	1
1:B:35:MET:SD	1:C:36:VAL:O	0.66	2.53	3	1
1:H:12:VAL:HB	1:I:12:VAL:HA	0.66	1.66	10	1
1:I:12:VAL:H	1:J:12:VAL:N	0.66	1.89	7	3
1:D:27:ASN:CB	1:E:31:ILE:CA	0.66	2.74	3	1
1:D:31:ILE:HB	1:E:31:ILE:HG13	0.66	1.65	3	1
1:G:11:GLU:O	1:H:12:VAL:HA	0.66	1.90	1	1
1:J:17:LEU:O	1:J:18:VAL:CB	0.65	2.44	10	1
1:I:12:VAL:HG23	1:I:12:VAL:O	0.65	1.90	2	2
1:D:23:ASP:N	2:D:101:2PO:O2P	0.65	2.28	7	1
1:G:37:GLY:CA	1:H:37:GLY:O	0.65	2.43	3	1
1:I:19:PHE:CD2	1:I:20:PHE:N	0.65	2.65	10	6
1:A:18:VAL:HG22	1:A:19:PHE:N	0.65	2.07	7	3
1:A:27:ASN:HA	1:C:24:VAL:HB	0.65	1.65	7	1
1:B:24:VAL:O	1:B:26:SER:N	0.65	2.29	7	1
1:B:35:MET:O	1:C:36:VAL:CA	0.65	2.44	7	1
1:I:39:VAL:O	1:J:38:GLY:O	0.65	2.14	7	1
1:B:35:MET:HG3	1:B:36:VAL:N	0.65	2.04	3	1
1:J:35:MET:SD	1:J:35:MET:N	0.65	2.68	2	4
1:A:17:LEU:HD23	1:A:17:LEU:N	0.65	2.05	6	1
1:B:19:PHE:CG	1:C:19:PHE:CA	0.65	2.79	7	1
1:F:37:GLY:N	1:G:36:VAL:O	0.65	2.30	3	1
1:F:12:VAL:HB	1:G:12:VAL:N	0.65	2.05	1	1
1:B:30:ALA:HB1	1:C:30:ALA:O	0.65	1.90	10	2
1:G:22:GLU:O	1:H:23:ASP:O	0.65	2.15	10	4
1:A:20:PHE:O	1:A:21:ALA:CB	0.65	2.43	7	1
1:A:32:ILE:C	1:C:21:ALA:C	0.65	2.55	7	1
1:F:9:GLY:H	2:F:101:2PO:P	0.65	2.14	10	1
1:G:17:LEU:O	1:G:17:LEU:HD23	0.65	1.91	10	1
1:J:11:GLU:CG	1:J:12:VAL:N	0.65	2.59	9	2
1:G:19:PHE:C	1:G:19:PHE:CD1	0.65	2.68	9	1
1:F:38:GLY:HA3	1:G:38:GLY:N	0.65	2.06	10	1
1:D:20:PHE:CE1	1:E:20:PHE:CD2	0.65	2.84	9	2
1:D:33:GLY:O	1:E:34:LEU:HG	0.65	1.92	7	1
1:A:12:VAL:O	1:B:13:HIS:HB3	0.65	1.92	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:PHE:CE1	1:C:34:LEU:HG	0.65	2.26	3	1
1:E:30:ALA:O	1:E:31:ILE:HG13	0.65	1.91	3	1
1:D:36:VAL:HG23	1:E:36:VAL:HG23	0.65	1.67	3	1
1:G:10:TYR:HB3	1:H:10:TYR:O	0.65	1.91	8	1
1:J:35:MET:O	1:J:36:VAL:CG1	0.65	2.43	7	2
1:C:17:LEU:O	1:C:18:VAL:CG1	0.64	2.45	7	1
1:D:24:VAL:HG12	1:D:25:GLY:H	0.64	1.52	8	2
1:I:10:TYR:HA	1:J:10:TYR:CA	0.64	2.21	6	2
1:C:21:ALA:O	1:C:22:GLU:HB2	0.64	1.90	7	1
1:D:34:LEU:CB	1:E:34:LEU:HD21	0.64	2.20	7	1
1:E:21:ALA:O	1:E:22:GLU:CB	0.64	2.42	7	1
1:A:15:GLN:O	1:B:14:HIS:CE1	0.64	2.49	4	1
1:G:35:MET:O	1:H:35:MET:CB	0.64	2.36	3	1
1:G:34:LEU:H	1:G:34:LEU:HD12	0.64	1.53	1	1
1:H:10:TYR:N	1:I:10:TYR:HA	0.64	2.07	10	1
1:D:20:PHE:N	1:E:19:PHE:CA	0.64	2.60	7	1
1:A:11:GLU:O	1:A:12:VAL:CB	0.64	2.45	4	1
1:J:8:SER:HB2	2:J:101:2PO:P	0.64	2.30	9	1
1:F:38:GLY:HA2	1:G:38:GLY:O	0.64	1.90	7	1
1:I:10:TYR:CG	1:J:10:TYR:O	0.64	2.50	7	1
1:D:19:PHE:CE2	1:E:19:PHE:CA	0.64	2.80	3	1
1:B:24:VAL:HG13	1:B:25:GLY:N	0.64	2.08	1	1
1:F:34:LEU:HD12	1:F:34:LEU:H	0.64	1.50	9	3
1:C:17:LEU:O	1:C:18:VAL:HG12	0.64	1.93	7	1
1:H:34:LEU:HD12	1:H:34:LEU:H	0.64	1.52	2	1
1:A:18:VAL:CA	1:B:18:VAL:HG22	0.64	2.22	3	1
1:E:19:PHE:O	1:E:20:PHE:CD2	0.64	2.50	3	2
1:D:29:GLY:C	1:E:31:ILE:CG2	0.64	2.62	3	1
1:B:34:LEU:N	1:B:34:LEU:CD2	0.64	2.59	10	3
1:E:35:MET:O	1:E:36:VAL:HG22	0.64	1.93	3	2
1:A:39:VAL:CG2	1:A:39:VAL:O	0.64	2.45	9	1
1:A:34:LEU:N	1:B:19:PHE:HE2	0.64	1.90	7	1
1:B:18:VAL:HG22	1:B:19:PHE:N	0.64	2.07	7	1
1:B:31:ILE:CG1	1:D:21:ALA:O	0.64	2.46	7	1
1:A:18:VAL:HG21	1:B:35:MET:HE2	0.64	1.68	3	1
1:F:13:HIS:O	1:F:14:HIS:CG	0.64	2.50	9	3
1:B:31:ILE:CG2	1:D:21:ALA:HB1	0.64	2.22	7	1
1:E:20:PHE:O	1:E:21:ALA:HB2	0.64	1.91	7	1
1:A:31:ILE:CG2	1:B:31:ILE:HB	0.64	2.23	3	1
1:D:32:ILE:CD1	1:D:33:GLY:N	0.64	2.61	3	1
1:I:20:PHE:CD1	1:I:20:PHE:N	0.64	2.66	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ASP:HA	1:B:23:ASP:O	0.64	1.93	10	5
1:H:7:ASP:H	1:I:6:HIS:CG	0.64	2.10	6	1
1:B:35:MET:O	1:C:36:VAL:CB	0.64	2.46	7	1
1:A:32:ILE:CA	1:C:22:GLU:N	0.64	2.61	7	1
1:E:35:MET:SD	1:I:35:MET:SD	0.64	2.96	7	1
1:G:11:GLU:C	1:G:12:VAL:HG23	0.64	2.12	1	2
1:A:35:MET:HB3	1:B:19:PHE:CE1	0.64	2.28	7	1
1:B:19:PHE:O	1:B:20:PHE:CB	0.64	2.44	7	1
1:C:34:LEU:HA	1:D:34:LEU:O	0.64	1.93	7	2
1:A:21:ALA:C	1:B:21:ALA:O	0.64	2.36	3	2
1:G:8:SER:N	2:G:101:2PO:O2P	0.64	2.32	8	1
1:A:29:GLY:O	1:C:25:GLY:HA2	0.64	1.92	7	1
1:G:24:VAL:HG21	2:H:101:2PO:O1P	0.64	1.93	7	1
1:J:8:SER:N	2:J:101:2PO:O1P	0.64	2.31	7	1
1:J:8:SER:HB3	2:J:101:2PO:P	0.63	2.33	10	6
1:G:12:VAL:N	1:H:11:GLU:HB2	0.63	2.07	10	1
1:I:20:PHE:CE1	1:J:20:PHE:CD2	0.63	2.85	9	2
1:J:7:ASP:N	1:J:7:ASP:OD1	0.63	2.28	6	1
1:F:11:GLU:N	1:G:11:GLU:H	0.63	1.88	9	1
1:G:34:LEU:CD2	1:G:34:LEU:N	0.63	2.61	4	3
1:C:30:ALA:O	1:C:31:ILE:CB	0.63	2.46	3	1
1:C:31:ILE:H	1:D:31:ILE:HG21	0.63	1.51	3	1
1:F:17:LEU:HD23	1:F:17:LEU:H	0.63	1.53	6	1
1:C:17:LEU:C	1:C:18:VAL:HG12	0.63	2.13	7	1
1:C:20:PHE:O	1:C:21:ALA:HB2	0.63	1.94	3	2
1:G:14:HIS:HD1	1:G:15:GLN:N	0.63	1.88	2	1
1:B:11:GLU:O	1:B:12:VAL:HB	0.63	1.92	3	2
1:B:31:ILE:O	1:B:32:ILE:CG1	0.63	2.46	3	1
1:J:24:VAL:HG23	1:J:26:SER:H	0.63	1.52	3	1
1:F:14:HIS:N	1:G:15:GLN:NE2	0.63	2.46	1	1
1:D:30:ALA:O	1:D:31:ILE:HG13	0.63	1.93	5	1
1:A:35:MET:O	1:A:36:VAL:CG1	0.63	2.44	9	1
1:A:9:GLY:O	1:A:10:TYR:HB2	0.63	1.92	3	2
1:A:32:ILE:HD12	1:A:32:ILE:O	0.63	1.93	9	2
1:F:15:GLN:O	1:F:17:LEU:N	0.63	2.32	7	3
1:H:14:HIS:HB3	1:I:14:HIS:HD1	0.63	1.53	6	1
1:A:31:ILE:CG2	1:C:21:ALA:HB3	0.63	2.23	7	1
1:G:8:SER:H	1:H:9:GLY:N	0.63	1.91	1	1
1:H:11:GLU:C	1:H:12:VAL:HG22	0.63	2.12	8	1
1:H:15:GLN:OE1	1:I:14:HIS:ND1	0.63	2.32	8	1
1:G:8:SER:CA	2:G:101:2PO:P	0.63	2.86	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:20:PHE:HA	1:C:20:PHE:HE1	0.63	1.53	7	1
1:C:20:PHE:HA	1:D:20:PHE:HD1	0.63	1.48	7	1
1:C:19:PHE:CD1	1:C:19:PHE:C	0.63	2.69	3	1
1:G:14:HIS:NE2	1:G:17:LEU:N	0.63	2.47	8	1
1:B:19:PHE:CG	1:B:20:PHE:N	0.63	2.67	3	4
1:G:6:HIS:ND1	1:G:6:HIS:N	0.63	2.44	8	1
1:F:22:GLU:O	1:G:23:ASP:O	0.63	2.16	6	4
1:B:17:LEU:CD1	1:B:18:VAL:H	0.63	2.05	7	1
1:B:23:ASP:OD1	1:B:24:VAL:N	0.63	2.32	7	1
1:D:31:ILE:CB	1:E:31:ILE:HG13	0.63	2.24	3	1
1:A:20:PHE:H	1:B:20:PHE:HB3	0.63	1.52	5	5
1:F:37:GLY:O	1:G:38:GLY:N	0.63	2.32	10	1
1:F:35:MET:SD	1:F:36:VAL:N	0.63	2.71	6	2
1:D:27:ASN:HB2	1:E:31:ILE:CA	0.63	2.23	3	1
1:E:29:GLY:O	1:E:30:ALA:HB2	0.63	1.94	1	3
1:G:20:PHE:CD1	1:G:20:PHE:N	0.63	2.67	7	2
1:A:33:GLY:C	1:B:34:LEU:HD23	0.63	2.14	3	1
1:J:31:ILE:O	1:J:31:ILE:HG23	0.63	1.93	3	1
1:A:19:PHE:CE1	1:A:36:VAL:HG13	0.63	2.28	1	1
1:G:13:HIS:CG	1:G:14:HIS:N	0.62	2.67	8	4
1:F:10:TYR:CG	1:F:11:GLU:N	0.62	2.64	7	1
1:D:34:LEU:C	1:D:34:LEU:HD22	0.62	2.13	3	1
1:D:34:LEU:HD22	1:E:34:LEU:O	0.62	1.94	3	1
1:G:35:MET:C	1:G:36:VAL:CG2	0.62	2.67	3	1
1:H:24:VAL:CG1	1:H:25:GLY:H	0.62	2.07	8	1
1:H:15:GLN:CD	1:I:14:HIS:ND1	0.62	2.51	8	1
1:A:34:LEU:H	1:A:34:LEU:HD23	0.62	1.55	5	2
1:A:34:LEU:CD2	1:A:34:LEU:N	0.62	2.62	9	2
1:F:12:VAL:H	1:G:12:VAL:H	0.62	1.36	7	2
1:I:12:VAL:HB	1:J:12:VAL:N	0.62	2.09	7	2
1:G:10:TYR:CD1	1:G:10:TYR:C	0.62	2.72	6	2
1:H:11:GLU:HA	1:I:11:GLU:HA	0.62	1.70	6	2
1:A:10:TYR:HA	1:B:10:TYR:HA	0.62	1.71	4	1
1:D:20:PHE:CZ	1:E:20:PHE:CD1	0.62	2.87	4	1
1:D:23:ASP:OD1	1:D:23:ASP:N	0.62	2.32	3	1
1:H:24:VAL:HG22	1:H:25:GLY:N	0.62	2.09	10	4
1:A:14:HIS:N	1:B:14:HIS:ND1	0.62	2.47	5	1
1:G:24:VAL:HG12	1:G:25:GLY:N	0.62	2.10	5	1
1:H:4:PHE:CD2	1:H:5:ARG:N	0.62	2.68	9	2
1:J:8:SER:HB3	2:J:101:2PO:O1P	0.62	1.94	6	1
1:C:35:MET:O	1:D:36:VAL:N	0.62	2.32	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:GLY:O	1:A:10:TYR:CB	0.62	2.48	1	2
1:G:19:PHE:CE1	1:H:19:PHE:CE2	0.62	2.87	8	1
1:D:19:PHE:C	1:D:20:PHE:CG	0.62	2.72	1	4
1:F:19:PHE:N	1:F:19:PHE:CD1	0.62	2.66	6	1
1:B:18:VAL:O	1:B:20:PHE:CE2	0.62	2.53	3	1
1:A:34:LEU:N	1:A:34:LEU:CD1	0.62	2.57	8	2
2:G:101:2PO:P	1:H:24:VAL:HG21	0.62	2.33	5	1
1:J:35:MET:N	1:J:35:MET:SD	0.62	2.73	9	1
1:B:31:ILE:HG21	1:D:21:ALA:HB1	0.62	1.72	7	1
1:D:20:PHE:CE2	1:D:36:VAL:CG1	0.62	2.82	3	1
1:G:37:GLY:N	1:H:37:GLY:O	0.62	2.33	3	1
1:B:13:HIS:HD1	1:B:14:HIS:N	0.62	1.91	1	1
1:H:17:LEU:O	1:H:18:VAL:CG1	0.62	2.45	8	1
1:G:18:VAL:N	1:H:18:VAL:CG1	0.62	2.62	8	1
1:B:14:HIS:CG	1:B:18:VAL:HG21	0.62	2.29	5	2
1:H:13:HIS:ND1	1:I:13:HIS:CE1	0.62	2.68	9	1
1:D:19:PHE:O	1:D:20:PHE:CD2	0.62	2.53	1	1
1:C:32:ILE:N	1:C:32:ILE:CD1	0.62	2.61	5	1
1:A:15:GLN:H	1:B:14:HIS:CE1	0.62	2.11	7	2
1:A:19:PHE:CD2	1:A:20:PHE:N	0.62	2.62	7	2
1:G:10:TYR:N	1:G:10:TYR:CD1	0.62	2.67	2	1
1:J:30:ALA:C	1:J:31:ILE:HG22	0.62	2.15	3	1
1:A:34:LEU:HD23	1:A:34:LEU:H	0.62	1.54	1	1
1:F:21:ALA:CB	1:G:34:LEU:HD21	0.62	2.25	8	2
1:J:12:VAL:CG1	1:J:12:VAL:O	0.62	2.48	8	1
1:I:18:VAL:CG2	1:I:20:PHE:CE1	0.62	2.83	10	2
1:D:35:MET:SD	1:D:36:VAL:N	0.62	2.73	5	1
1:A:17:LEU:CA	1:B:17:LEU:HB2	0.62	2.24	3	1
1:A:34:LEU:N	1:A:34:LEU:HD23	0.61	2.09	5	1
1:A:27:ASN:N	2:B:101:2PO:P	0.61	2.74	7	1
1:A:13:HIS:O	1:A:14:HIS:ND1	0.61	2.33	3	1
1:B:35:MET:SD	1:B:35:MET:N	0.61	2.73	8	2
1:A:29:GLY:O	1:C:25:GLY:CA	0.61	2.47	7	1
1:B:29:GLY:O	1:C:28:LYS:C	0.61	2.38	7	1
1:F:13:HIS:ND1	1:F:13:HIS:N	0.61	2.46	7	1
1:I:37:GLY:N	1:J:37:GLY:O	0.61	2.32	3	1
1:H:39:VAL:O	1:I:39:VAL:N	0.61	2.34	3	1
1:G:19:PHE:CZ	1:G:21:ALA:HB2	0.61	2.30	8	1
1:I:13:HIS:CD2	1:I:14:HIS:H	0.61	2.13	1	2
1:H:20:PHE:N	1:H:20:PHE:CD1	0.61	2.65	9	2
1:B:20:PHE:CD1	1:B:20:PHE:N	0.61	2.66	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:J:6:HIS:ND1	1:J:7:ASP:N	0.61	2.48	5	1
1:A:27:ASN:ND2	1:B:8:SER:O	0.61	2.33	7	1
1:F:12:VAL:O	1:G:13:HIS:O	0.61	2.18	8	1
1:H:10:TYR:OH	1:H:22:GLU:C	0.61	2.39	10	1
1:I:14:HIS:CE1	1:I:17:LEU:N	0.61	2.68	10	1
1:G:18:VAL:HG12	1:G:36:VAL:HG21	0.61	1.70	7	1
1:H:8:SER:OG	1:H:10:TYR:CE1	0.61	2.53	7	1
1:A:11:GLU:O	1:A:12:VAL:CG2	0.61	2.48	4	1
1:J:8:SER:CA	2:J:101:2PO:P	0.61	2.88	4	2
1:J:27:ASN:ND2	1:J:28:LYS:H	0.61	1.92	2	1
1:D:23:ASP:N	2:D:101:2PO:O3P	0.61	2.34	5	1
1:J:11:GLU:HG3	1:J:12:VAL:N	0.61	2.08	6	2
1:C:19:PHE:CG	1:D:18:VAL:HB	0.61	2.28	3	1
1:H:15:GLN:O	1:I:14:HIS:NE2	0.61	2.34	1	1
1:A:17:LEU:HD12	1:A:17:LEU:O	0.61	1.96	4	4
1:J:24:VAL:HG22	1:J:25:GLY:N	0.61	2.10	10	2
1:B:24:VAL:HG12	1:B:25:GLY:N	0.61	2.07	5	1
1:F:19:PHE:O	1:F:19:PHE:CD1	0.61	2.53	6	1
1:D:34:LEU:CD2	1:D:34:LEU:N	0.61	2.63	9	1
1:B:14:HIS:O	1:B:15:GLN:O	0.61	2.18	3	1
1:B:33:GLY:O	1:B:34:LEU:CD1	0.61	2.48	3	1
1:A:34:LEU:H	1:B:34:LEU:HB3	0.61	1.47	3	1
1:D:21:ALA:HB2	1:D:34:LEU:CG	0.61	2.25	3	1
1:C:36:VAL:HG11	1:D:36:VAL:O	0.61	1.96	3	1
1:D:32:ILE:HG12	1:D:33:GLY:N	0.61	2.10	3	2
1:E:20:PHE:CD2	1:F:38:GLY:HA2	0.61	2.31	7	1
1:F:12:VAL:H	1:G:12:VAL:N	0.61	1.94	7	2
1:D:19:PHE:HE2	1:E:19:PHE:HA	0.61	1.52	3	1
1:G:10:TYR:HB2	1:H:10:TYR:N	0.61	2.11	8	1
1:D:19:PHE:CD2	1:D:20:PHE:N	0.61	2.69	9	4
1:I:9:GLY:O	1:I:10:TYR:CD2	0.61	2.54	2	4
1:A:30:ALA:HB1	1:C:23:ASP:HB3	0.61	1.72	7	1
1:A:20:PHE:HA	1:B:20:PHE:CB	0.61	2.26	3	1
1:E:35:MET:HB2	1:J:36:VAL:HG11	0.61	1.72	3	1
1:J:8:SER:N	2:J:101:2PO:P	0.61	2.74	1	1
1:A:19:PHE:CZ	1:A:36:VAL:HG13	0.61	2.31	4	2
1:I:34:LEU:HD12	1:I:34:LEU:N	0.61	2.09	10	1
1:D:34:LEU:O	1:E:19:PHE:CE2	0.61	2.53	7	1
1:D:34:LEU:C	1:D:34:LEU:CD1	0.61	2.62	3	1
1:H:14:HIS:N	1:H:14:HIS:ND1	0.61	2.48	3	1
1:J:16:LYS:N	1:J:16:LYS:CD	0.61	2.63	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:30:ALA:CB	1:D:28:LYS:O	0.61	2.48	1	2
1:C:18:VAL:HG12	1:D:18:VAL:HG22	0.61	1.72	9	1
1:H:15:GLN:O	1:H:17:LEU:N	0.61	2.34	4	3
1:B:15:GLN:O	1:B:16:LYS:C	0.61	2.39	4	4
1:B:31:ILE:HG22	1:C:32:ILE:O	0.61	1.96	7	1
1:C:34:LEU:HA	1:D:34:LEU:HG	0.61	1.73	7	1
1:C:33:GLY:HA3	1:E:19:PHE:CD1	0.61	2.29	7	1
1:D:27:ASN:CB	1:E:31:ILE:C	0.61	2.67	3	1
1:H:27:ASN:H	1:H:28:LYS:NZ	0.61	1.93	3	1
1:F:11:GLU:H	1:G:11:GLU:N	0.60	1.90	9	1
1:F:19:PHE:H	1:F:19:PHE:HD2	0.60	1.38	4	2
1:B:36:VAL:HA	1:C:36:VAL:O	0.60	1.95	7	1
1:D:17:LEU:HD12	1:E:18:VAL:HG22	0.60	1.71	7	1
1:D:18:VAL:CG2	1:E:20:PHE:CE1	0.60	2.84	7	1
1:F:10:TYR:N	1:G:10:TYR:H	0.60	1.88	7	1
1:I:28:LYS:O	1:I:30:ALA:N	0.60	2.34	9	1
1:A:27:ASN:H	2:B:101:2PO:P	0.60	2.19	7	1
1:A:31:ILE:C	1:C:23:ASP:N	0.60	2.54	7	1
1:A:14:HIS:CG	1:A:15:GLN:N	0.60	2.66	9	4
1:J:7:ASP:O	1:J:8:SER:C	0.60	2.39	6	4
1:C:20:PHE:N	1:C:20:PHE:CD2	0.60	2.67	4	1
1:C:31:ILE:N	1:D:31:ILE:CG2	0.60	2.58	3	1
1:C:36:VAL:HG12	1:D:36:VAL:HG22	0.60	1.73	2	4
1:J:12:VAL:O	1:J:13:HIS:CG	0.60	2.54	6	3
1:B:14:HIS:CD2	1:B:18:VAL:HG21	0.60	2.32	9	2
1:B:34:LEU:N	1:C:19:PHE:CZ	0.60	2.69	7	1
1:H:23:ASP:CA	1:I:23:ASP:O	0.60	2.49	7	1
1:A:18:VAL:CG2	1:A:19:PHE:N	0.60	2.64	3	4
1:C:20:PHE:CD2	1:C:20:PHE:N	0.60	2.69	3	1
1:D:28:LYS:CA	1:E:31:ILE:H	0.60	2.07	3	1
1:H:5:ARG:HE	1:H:5:ARG:N	0.60	1.93	3	1
1:G:13:HIS:CE1	1:G:14:HIS:ND1	0.60	2.69	1	1
1:H:13:HIS:CB	1:I:13:HIS:O	0.60	2.49	8	1
1:A:8:SER:CA	2:A:101:2PO:P	0.60	2.90	9	3
1:H:17:LEU:C	1:H:17:LEU:HD12	0.60	2.16	10	1
1:I:12:VAL:O	1:J:12:VAL:N	0.60	2.35	10	1
1:J:7:ASP:O	1:J:8:SER:O	0.60	2.20	10	3
1:I:8:SER:OG	1:J:7:ASP:CA	0.60	2.49	9	1
1:B:21:ALA:O	1:B:22:GLU:HB2	0.60	1.97	7	1
1:D:19:PHE:CA	1:E:18:VAL:C	0.60	2.56	7	1
1:G:14:HIS:ND1	1:G:15:GLN:O	0.60	2.35	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:G:39:VAL:C	1:G:40:VAL:HG23	0.60	2.16	3	1
1:G:19:PHE:CE2	1:G:36:VAL:HG13	0.60	2.31	1	1
1:F:23:ASP:CB	1:G:23:ASP:O	0.60	2.49	1	1
1:E:20:PHE:CE2	1:F:38:GLY:HA2	0.60	2.31	7	1
1:B:30:ALA:N	1:C:31:ILE:HB	0.60	2.07	3	1
1:J:29:GLY:O	1:J:30:ALA:C	0.60	2.39	3	1
1:C:32:ILE:HB	1:D:32:ILE:HB	0.60	1.73	1	1
1:F:34:LEU:CD1	1:F:34:LEU:N	0.60	2.55	8	2
1:F:34:LEU:N	1:F:34:LEU:CD2	0.60	2.65	5	3
1:A:19:PHE:CE1	1:A:36:VAL:CG2	0.60	2.84	9	1
1:H:27:ASN:ND2	1:I:26:SER:CB	0.60	2.65	9	1
1:A:19:PHE:CE2	1:A:20:PHE:O	0.60	2.55	7	1
1:E:20:PHE:CD1	1:F:39:VAL:HG13	0.60	2.31	7	1
1:H:14:HIS:H	1:I:15:GLN:NE2	0.60	1.95	2	1
1:A:15:GLN:O	1:A:17:LEU:N	0.60	2.34	1	1
1:J:27:ASN:ND2	1:J:27:ASN:N	0.60	2.48	10	2
1:B:21:ALA:O	1:B:22:GLU:CB	0.60	2.49	7	1
1:D:19:PHE:CZ	1:E:19:PHE:CD2	0.60	2.90	7	1
1:H:36:VAL:CG1	1:H:37:GLY:N	0.60	2.65	7	1
1:E:31:ILE:HD11	1:I:39:VAL:HG22	0.60	1.74	1	1
1:E:20:PHE:N	1:E:20:PHE:HD1	0.60	1.93	8	1
1:H:19:PHE:CD2	1:H:19:PHE:C	0.60	2.75	10	1
1:A:8:SER:N	2:A:101:2PO:O2P	0.60	2.35	4	2
1:D:19:PHE:HB2	1:E:20:PHE:CD2	0.60	2.30	7	1
1:E:34:LEU:HD12	1:E:35:MET:N	0.60	2.12	7	1
1:G:34:LEU:CD1	1:G:34:LEU:N	0.60	2.60	1	2
1:B:32:ILE:CG1	1:C:31:ILE:CG1	0.60	2.80	3	1
1:G:24:VAL:N	1:H:24:VAL:HG11	0.60	2.12	3	1
1:I:17:LEU:CA	1:J:17:LEU:O	0.60	2.49	1	1
1:A:13:HIS:ND1	1:A:13:HIS:N	0.60	2.50	6	1
1:I:12:VAL:HG22	1:J:11:GLU:CB	0.60	2.27	4	1
1:A:18:VAL:CB	1:B:18:VAL:HG22	0.60	2.26	3	1
1:C:24:VAL:HG22	1:C:25:GLY:N	0.59	2.12	5	2
1:D:31:ILE:O	1:D:32:ILE:CB	0.59	2.50	5	2
1:I:8:SER:HB3	2:I:101:2PO:P	0.59	2.35	9	1
1:C:34:LEU:HB3	1:D:34:LEU:CG	0.59	2.25	7	1
1:G:18:VAL:HG12	1:G:36:VAL:CG2	0.59	2.27	7	1
1:C:18:VAL:CG2	1:D:20:PHE:HZ	0.59	2.04	3	1
1:J:35:MET:C	1:J:36:VAL:HG13	0.59	2.17	3	1
1:F:20:PHE:O	1:G:20:PHE:CG	0.59	2.55	6	4
1:B:11:GLU:HB3	1:B:20:PHE:CD1	0.59	2.32	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:VAL:O	1:B:12:VAL:CB	0.59	2.49	4	1
1:D:27:ASN:O	1:D:28:LYS:O	0.59	2.20	5	1
1:D:34:LEU:HB2	1:E:34:LEU:HD21	0.59	1.73	7	1
1:D:20:PHE:HB3	1:E:20:PHE:CD1	0.59	2.31	3	1
1:B:29:GLY:O	1:C:28:LYS:O	0.59	2.19	7	1
1:F:16:LYS:O	1:G:16:LYS:CB	0.59	2.51	5	6
1:A:10:TYR:CE2	1:B:10:TYR:CE1	0.59	2.91	7	1
1:D:18:VAL:HG23	1:D:19:PHE:H	0.59	1.36	7	1
1:D:19:PHE:HD2	1:E:20:PHE:CA	0.59	1.98	7	1
1:F:19:PHE:HD2	1:F:19:PHE:N	0.59	1.93	4	2
1:B:32:ILE:CD1	1:B:33:GLY:N	0.59	2.64	3	1
1:G:10:TYR:CE1	1:G:24:VAL:HG11	0.59	2.33	3	1
1:I:6:HIS:CG	1:I:7:ASP:H	0.59	2.16	10	1
1:G:14:HIS:CE1	1:G:18:VAL:HG11	0.59	2.32	5	1
1:J:31:ILE:C	1:J:32:ILE:HD12	0.59	2.18	9	1
1:E:20:PHE:HB3	1:G:39:VAL:CG1	0.59	2.27	7	1
1:A:19:PHE:O	1:A:19:PHE:CD2	0.59	2.54	2	1
1:C:28:LYS:CD	1:C:28:LYS:N	0.59	2.65	2	1
1:D:30:ALA:C	1:D:31:ILE:HG22	0.59	2.18	3	1
1:E:30:ALA:O	1:E:31:ILE:CG1	0.59	2.51	3	1
1:I:18:VAL:HG22	1:I:19:PHE:N	0.59	2.12	3	1
1:D:22:GLU:N	1:E:21:ALA:O	0.59	2.36	7	1
1:G:16:LYS:NZ	1:H:15:GLN:HE21	0.59	1.95	7	1
1:J:12:VAL:HG12	1:J:13:HIS:N	0.59	2.11	2	1
1:A:34:LEU:H	1:G:40:VAL:C	0.59	2.00	3	1
1:A:34:LEU:CA	1:B:34:LEU:HB3	0.59	2.27	3	1
1:C:24:VAL:HG21	2:D:101:2PO:O1P	0.59	1.97	1	1
1:I:19:PHE:CD2	1:I:19:PHE:C	0.59	2.75	1	4
1:C:23:ASP:OD1	1:D:26:SER:OG	0.59	2.20	5	1
1:A:15:GLN:NE2	1:A:16:LYS:NZ	0.59	2.51	6	1
1:A:39:VAL:HB	1:B:40:VAL:H	0.59	1.58	7	1
1:C:34:LEU:CA	1:D:34:LEU:HG	0.59	2.27	7	1
1:E:24:VAL:CG1	1:E:25:GLY:N	0.59	2.66	7	1
1:A:14:HIS:ND1	1:B:14:HIS:NE2	0.59	2.50	3	1
1:E:19:PHE:N	1:E:20:PHE:CE2	0.59	2.70	3	1
1:I:39:VAL:HA	1:J:39:VAL:HB	0.59	1.75	3	1
1:D:34:LEU:HB3	1:E:34:LEU:H	0.59	1.56	1	1
1:I:14:HIS:CD2	1:I:15:GLN:N	0.59	2.71	1	1
2:F:101:2PO:O3P	1:G:25:GLY:CA	0.59	2.51	8	1
1:F:19:PHE:O	1:F:19:PHE:CD2	0.59	2.55	5	4
1:F:34:LEU:N	1:F:34:LEU:CD1	0.59	2.58	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:34:LEU:C	1:E:34:LEU:HD12	0.59	2.18	7	1
1:B:19:PHE:HD1	1:B:19:PHE:C	0.59	1.94	3	1
1:I:37:GLY:CA	1:J:37:GLY:O	0.59	2.51	3	1
1:C:19:PHE:C	1:C:20:PHE:CG	0.59	2.76	4	6
1:J:11:GLU:OE1	1:J:12:VAL:N	0.59	2.36	9	1
1:I:8:SER:O	1:J:7:ASP:C	0.59	2.41	2	1
1:E:18:VAL:O	1:E:19:PHE:CG	0.59	2.56	3	1
1:C:34:LEU:N	1:C:34:LEU:CD2	0.58	2.66	10	2
1:A:35:MET:SD	1:A:36:VAL:N	0.58	2.75	5	1
1:G:6:HIS:CG	1:G:7:ASP:N	0.58	2.69	5	2
1:J:9:GLY:O	1:J:10:TYR:CD1	0.58	2.56	9	3
1:A:12:VAL:CG2	1:B:11:GLU:O	0.58	2.51	7	1
1:B:31:ILE:O	1:C:32:ILE:HG13	0.58	1.97	7	1
1:A:28:LYS:C	1:C:25:GLY:N	0.58	2.56	7	1
1:B:31:ILE:C	1:C:32:ILE:O	0.58	2.42	7	1
1:F:12:VAL:N	1:G:12:VAL:H	0.58	1.96	7	2
1:J:20:PHE:N	1:J:20:PHE:CD2	0.58	2.65	2	1
1:A:15:GLN:O	1:B:15:GLN:CB	0.58	2.51	3	1
1:A:9:GLY:O	1:A:10:TYR:CD1	0.58	2.56	1	1
1:A:10:TYR:O	1:B:10:TYR:N	0.58	2.35	1	1
1:H:24:VAL:HG13	2:I:101:2PO:O3P	0.58	1.98	9	1
1:A:31:ILE:HA	1:C:22:GLU:C	0.58	2.17	7	1
1:E:40:VAL:HG22	1:E:40:VAL:O	0.58	1.98	7	1
1:I:4:PHE:CD2	1:I:5:ARG:N	0.58	2.72	7	1
1:H:15:GLN:N	1:I:14:HIS:NE2	0.58	2.51	4	1
1:I:20:PHE:CD1	1:I:22:GLU:OE2	0.58	2.57	4	1
1:I:18:VAL:HG13	1:I:19:PHE:N	0.58	2.12	3	1
1:A:32:ILE:HG22	1:B:32:ILE:H	0.58	1.59	7	1
1:A:20:PHE:CD1	1:C:34:LEU:HG	0.58	2.33	3	1
1:F:12:VAL:CB	1:G:12:VAL:H	0.58	2.10	1	1
1:I:35:MET:SD	1:I:35:MET:N	0.58	2.77	1	1
1:A:32:ILE:O	1:C:22:GLU:N	0.58	2.36	7	1
1:B:19:PHE:HB2	1:C:18:VAL:HG13	0.58	1.74	7	1
1:D:19:PHE:CD1	1:D:19:PHE:C	0.58	2.77	3	1
1:F:24:VAL:CG2	1:F:25:GLY:N	0.58	2.66	8	1
1:C:19:PHE:CD2	1:C:20:PHE:N	0.58	2.71	1	2
1:D:37:GLY:O	1:E:37:GLY:HA3	0.58	1.99	5	1
1:D:33:GLY:O	1:E:33:GLY:HA2	0.58	1.97	3	2
1:J:12:VAL:O	1:J:13:HIS:CB	0.58	2.50	4	2
1:B:33:GLY:C	1:C:34:LEU:O	0.58	2.42	7	1
1:H:23:ASP:CB	1:I:23:ASP:O	0.58	2.52	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:HB3	1:B:20:PHE:CE2	0.58	2.34	3	1
1:A:31:ILE:N	1:B:31:ILE:HA	0.58	2.12	3	1
1:G:35:MET:SD	1:G:35:MET:O	0.58	2.61	3	1
1:H:10:TYR:HA	1:I:10:TYR:HA	0.58	1.74	8	1
1:J:13:HIS:O	1:J:14:HIS:CB	0.58	2.52	7	5
1:A:16:LYS:O	1:A:17:LEU:CB	0.58	2.51	7	2
1:B:22:GLU:OE1	1:C:22:GLU:CG	0.58	2.52	7	1
1:G:8:SER:O	1:H:9:GLY:HA2	0.58	1.98	8	1
1:I:13:HIS:O	1:I:14:HIS:CG	0.58	2.57	8	1
1:F:33:GLY:O	1:F:34:LEU:CB	0.58	2.48	3	2
1:B:19:PHE:CB	1:C:18:VAL:HG13	0.58	2.28	7	1
1:J:27:ASN:HD22	1:J:28:LYS:H	0.58	1.41	2	1
1:C:34:LEU:H	1:C:34:LEU:CD2	0.58	1.97	3	1
1:H:17:LEU:C	1:H:18:VAL:HG22	0.58	2.18	8	1
1:D:24:VAL:HG12	1:D:25:GLY:N	0.58	2.13	6	2
1:A:8:SER:HB2	2:A:101:2PO:P	0.58	2.37	2	2
1:F:23:ASP:HA	1:G:23:ASP:O	0.58	1.99	4	4
1:D:29:GLY:O	1:D:30:ALA:C	0.58	2.40	5	2
1:C:20:PHE:HA	1:D:20:PHE:CB	0.58	2.28	7	1
1:H:19:PHE:CE2	1:H:36:VAL:HG21	0.58	2.34	7	1
1:A:35:MET:HG2	1:A:36:VAL:HG13	0.58	1.74	3	1
1:I:9:GLY:C	1:I:10:TYR:CD1	0.58	2.77	3	1
1:B:14:HIS:CG	1:B:15:GLN:N	0.58	2.70	10	4
1:H:13:HIS:C	1:H:14:HIS:CG	0.58	2.78	2	3
1:A:13:HIS:O	1:A:14:HIS:CG	0.58	2.57	6	2
1:F:19:PHE:CZ	1:F:36:VAL:CG1	0.58	2.87	1	3
1:A:13:HIS:CA	1:B:14:HIS:HA	0.58	2.29	3	1
1:B:31:ILE:O	1:C:31:ILE:HG21	0.58	1.98	3	1
1:F:36:VAL:CG1	1:G:36:VAL:HG22	0.58	2.29	8	1
1:F:20:PHE:H	1:G:20:PHE:HB3	0.58	1.58	2	7
1:H:18:VAL:CG2	1:H:20:PHE:CE2	0.58	2.87	6	3
1:C:31:ILE:O	1:D:31:ILE:CA	0.58	2.51	5	1
1:G:15:GLN:O	1:G:17:LEU:N	0.58	2.37	9	2
1:J:16:LYS:CD	1:J:16:LYS:N	0.58	2.67	9	1
1:D:20:PHE:C	1:E:20:PHE:N	0.58	2.57	7	1
1:H:23:ASP:O	1:H:24:VAL:O	0.58	2.22	7	1
1:J:12:VAL:C	1:J:13:HIS:CG	0.58	2.76	4	1
1:B:14:HIS:ND1	1:B:14:HIS:N	0.57	2.51	8	1
2:F:101:2PO:P	1:G:24:VAL:HG13	0.57	2.39	8	1
1:H:15:GLN:CG	1:I:14:HIS:ND1	0.57	2.67	8	1
1:B:8:SER:CA	2:B:101:2PO:P	0.57	2.92	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:CD2	1:A:19:PHE:O	0.57	2.56	4	2
1:A:30:ALA:CA	1:B:30:ALA:O	0.57	2.52	7	1
1:F:19:PHE:O	1:F:20:PHE:CD1	0.57	2.57	2	3
1:A:23:ASP:CB	1:B:23:ASP:O	0.57	2.51	7	1
1:A:39:VAL:HB	1:B:39:VAL:HA	0.57	1.75	7	1
1:A:13:HIS:N	1:A:13:HIS:ND1	0.57	2.49	2	1
1:G:35:MET:O	1:G:36:VAL:CB	0.57	2.50	3	1
1:I:11:GLU:CB	1:J:11:GLU:O	0.57	2.52	3	1
1:G:8:SER:N	2:G:101:2PO:P	0.57	2.77	8	1
1:A:14:HIS:CG	1:A:15:GLN:H	0.57	2.17	2	4
1:B:6:HIS:O	1:B:7:ASP:O	0.57	2.22	7	3
1:F:24:VAL:CG1	1:G:25:GLY:H	0.57	2.11	10	2
1:G:22:GLU:OE1	1:G:22:GLU:N	0.57	2.38	10	1
1:H:15:GLN:O	1:H:16:LYS:C	0.57	2.41	5	6
1:C:17:LEU:HB3	1:D:17:LEU:CA	0.57	2.29	7	1
1:A:30:ALA:HB3	1:C:24:VAL:C	0.57	2.19	7	1
1:F:10:TYR:O	1:G:10:TYR:CB	0.57	2.53	1	1
1:A:35:MET:SD	1:B:34:LEU:CD1	0.57	2.92	3	1
1:B:7:ASP:O	1:B:9:GLY:N	0.57	2.38	1	1
1:B:32:ILE:CA	1:C:32:ILE:O	0.57	2.52	7	1
1:C:31:ILE:O	1:D:31:ILE:HG13	0.57	1.98	3	1
1:H:38:GLY:N	1:I:37:GLY:O	0.57	2.36	3	1
1:J:11:GLU:O	1:J:12:VAL:CG1	0.57	2.51	8	2
1:F:37:GLY:O	1:G:37:GLY:CA	0.57	2.53	10	1
1:C:24:VAL:CG2	1:C:25:GLY:N	0.57	2.67	5	2
1:F:24:VAL:CG2	1:G:25:GLY:H	0.57	2.12	6	1
1:A:12:VAL:HG21	1:B:12:VAL:C	0.57	2.20	7	1
1:B:33:GLY:H	1:C:34:LEU:HD23	0.57	1.60	7	1
1:I:12:VAL:O	1:J:12:VAL:HB	0.57	1.99	4	2
1:G:9:GLY:C	1:H:10:TYR:H	0.57	1.96	8	1
1:C:39:VAL:H	1:D:39:VAL:HA	0.57	1.58	7	2
1:I:35:MET:C	1:I:36:VAL:CG2	0.57	2.70	3	2
1:F:38:GLY:CA	1:G:38:GLY:H	0.57	2.09	10	1
1:D:31:ILE:CG2	1:D:32:ILE:N	0.57	2.67	5	1
1:D:21:ALA:O	1:D:22:GLU:CB	0.57	2.53	7	2
1:D:22:GLU:N	1:D:22:GLU:CD	0.57	2.57	7	1
1:B:11:GLU:O	1:B:12:VAL:HG23	0.57	1.99	1	1
1:F:27:ASN:HD22	1:F:27:ASN:H	0.57	1.43	6	1
1:I:12:VAL:CB	1:J:12:VAL:H	0.57	2.12	7	2
1:I:10:TYR:OH	1:I:12:VAL:HG22	0.57	1.99	7	1
1:G:19:PHE:CE2	1:G:36:VAL:CG1	0.57	2.88	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:C	1:B:20:PHE:CD2	0.57	2.79	3	1
1:B:32:ILE:HD11	1:C:31:ILE:CG1	0.57	2.30	3	1
1:I:11:GLU:HA	1:J:11:GLU:O	0.57	1.99	3	1
1:I:19:PHE:CD1	1:J:19:PHE:O	0.57	2.58	10	2
1:F:17:LEU:O	1:F:17:LEU:HD12	0.57	2.00	5	1
1:A:17:LEU:HD23	1:A:17:LEU:H	0.57	1.58	6	1
1:B:15:GLN:OE1	1:B:15:GLN:N	0.57	2.38	9	1
1:I:14:HIS:O	1:I:14:HIS:ND1	0.57	2.38	9	1
1:A:39:VAL:HG22	1:B:17:LEU:HD23	0.57	1.77	7	1
1:B:34:LEU:CA	1:C:34:LEU:HG	0.57	2.30	7	1
1:B:31:ILE:HD13	1:D:23:ASP:C	0.57	2.19	7	1
1:C:33:GLY:C	1:D:34:LEU:HG	0.57	2.19	7	1
1:F:18:VAL:H	1:G:18:VAL:CG1	0.57	2.10	7	1
1:A:19:PHE:HB3	1:B:20:PHE:CG	0.57	2.35	3	1
1:I:14:HIS:CE1	1:I:17:LEU:CA	0.56	2.88	10	1
1:A:29:GLY:CA	1:D:25:GLY:H	0.56	2.13	7	1
1:E:20:PHE:CD2	1:G:38:GLY:O	0.56	2.59	7	1
1:G:8:SER:HB3	2:G:101:2PO:P	0.56	2.40	1	2
1:J:15:GLN:O	1:J:16:LYS:C	0.56	2.42	4	2
1:B:29:GLY:C	1:C:30:ALA:O	0.56	2.43	3	1
1:H:31:ILE:O	1:I:32:ILE:HG23	0.56	1.99	3	1
1:D:24:VAL:HG22	1:D:25:GLY:N	0.56	2.13	1	1
1:G:10:TYR:HB2	1:H:10:TYR:C	0.56	2.20	8	1
1:H:20:PHE:H	1:I:20:PHE:HB3	0.56	1.60	7	4
1:I:10:TYR:C	1:J:10:TYR:N	0.56	2.50	9	1
1:C:33:GLY:O	1:C:34:LEU:HG	0.56	2.00	1	3
1:D:28:LYS:CD	1:D:28:LYS:N	0.56	2.67	2	1
1:I:10:TYR:O	1:J:10:TYR:CD2	0.56	2.58	2	1
1:I:19:PHE:CG	1:I:20:PHE:N	0.56	2.72	3	5
1:F:17:LEU:CD2	1:F:17:LEU:N	0.56	2.66	6	1
1:F:17:LEU:O	1:F:18:VAL:HG22	0.56	2.00	4	2
1:H:24:VAL:O	1:H:26:SER:N	0.56	2.38	7	1
1:A:19:PHE:O	1:A:20:PHE:CB	0.56	2.53	7	1
1:H:10:TYR:CZ	1:I:10:TYR:CD2	0.56	2.94	7	1
1:A:31:ILE:CG1	1:B:31:ILE:HB	0.56	2.29	3	1
1:C:19:PHE:CD1	1:D:20:PHE:CE1	0.56	2.92	3	1
1:F:38:GLY:O	1:G:39:VAL:N	0.56	2.38	3	1
1:A:34:LEU:O	1:B:35:MET:O	0.56	2.23	3	1
1:J:29:GLY:O	1:J:32:ILE:HB	0.56	2.00	3	1
1:B:9:GLY:C	1:B:10:TYR:CD2	0.56	2.79	1	1
1:H:9:GLY:O	1:H:10:TYR:CD1	0.56	2.57	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:18:VAL:CG2	1:D:20:PHE:CE1	0.56	2.88	8	1
1:J:11:GLU:O	1:J:12:VAL:CB	0.56	2.54	8	3
1:I:24:VAL:CG2	1:I:25:GLY:N	0.56	2.67	10	1
1:B:34:LEU:CB	1:C:34:LEU:CD1	0.56	2.84	7	1
1:G:17:LEU:O	1:G:18:VAL:HG22	0.56	2.00	7	1
1:G:26:SER:O	1:H:25:GLY:O	0.56	2.23	7	1
1:I:38:GLY:O	1:I:39:VAL:C	0.56	2.43	3	1
1:H:34:LEU:CD1	1:H:34:LEU:N	0.56	2.67	8	2
1:B:20:PHE:CE1	1:C:20:PHE:CD2	0.56	2.94	10	2
1:G:5:ARG:CD	1:G:5:ARG:N	0.56	2.69	6	1
1:F:17:LEU:C	1:F:18:VAL:CG2	0.56	2.74	4	2
1:G:35:MET:SD	1:G:35:MET:N	0.56	2.79	9	2
1:F:10:TYR:CA	1:G:10:TYR:O	0.56	2.54	7	1
1:F:9:GLY:HA3	1:G:9:GLY:N	0.56	2.16	7	1
1:D:20:PHE:HA	1:E:21:ALA:CA	0.56	2.31	3	1
1:I:22:GLU:N	1:I:22:GLU:CD	0.56	2.59	10	1
1:E:24:VAL:HG23	1:E:25:GLY:N	0.56	2.15	5	1
1:F:19:PHE:H	1:F:19:PHE:HD1	0.56	1.42	6	1
1:C:20:PHE:HB3	1:D:20:PHE:CG	0.56	2.36	7	1
1:H:35:MET:O	1:H:36:VAL:HG23	0.56	2.00	7	1
1:I:20:PHE:CD1	1:I:20:PHE:C	0.56	2.78	7	1
1:A:11:GLU:H	1:B:11:GLU:H	0.56	1.40	4	1
1:E:20:PHE:HA	1:E:34:LEU:HD22	0.56	1.77	3	1
1:I:13:HIS:O	1:I:14:HIS:CD2	0.56	2.59	8	1
1:A:28:LYS:O	1:A:30:ALA:N	0.56	2.38	10	2
1:D:30:ALA:C	1:E:30:ALA:O	0.56	2.41	5	1
1:B:31:ILE:O	1:C:32:ILE:CG1	0.56	2.53	7	1
1:D:37:GLY:O	1:E:37:GLY:CA	0.56	2.53	7	1
1:F:10:TYR:H	1:G:10:TYR:N	0.56	1.90	7	1
1:A:18:VAL:HG23	1:A:19:PHE:N	0.56	2.16	3	1
1:B:32:ILE:CD1	1:B:32:ILE:C	0.56	2.74	3	1
1:I:38:GLY:O	1:I:39:VAL:O	0.56	2.24	3	1
1:D:36:VAL:HG12	1:E:36:VAL:O	0.56	2.01	1	1
1:A:23:ASP:O	2:A:101:2PO:O1P	0.56	2.23	7	1
1:A:32:ILE:O	1:C:22:GLU:O	0.56	2.24	7	1
1:B:34:LEU:HB3	1:C:34:LEU:HD11	0.56	1.78	7	1
1:B:19:PHE:HE1	1:B:34:LEU:O	0.56	1.80	7	1
1:E:27:ASN:OD1	1:E:30:ALA:O	0.56	2.24	7	1
1:G:20:PHE:O	1:H:20:PHE:CG	0.56	2.58	7	1
1:H:24:VAL:HG11	1:I:25:GLY:C	0.56	2.21	7	1
1:I:12:VAL:O	1:I:13:HIS:O	0.56	2.23	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:13:HIS:ND1	1:I:13:HIS:ND1	0.56	2.48	2	1
1:B:31:ILE:O	1:B:31:ILE:HD13	0.56	2.00	3	1
1:D:19:PHE:CD2	1:E:36:VAL:HG21	0.56	2.36	8	1
1:B:8:SER:HB2	2:B:101:2PO:P	0.56	2.37	5	1
1:D:30:ALA:O	1:E:30:ALA:C	0.56	2.41	5	1
1:G:13:HIS:C	1:G:14:HIS:CG	0.56	2.78	9	2
1:B:23:ASP:CB	1:C:23:ASP:O	0.56	2.54	9	1
1:G:14:HIS:CB	1:G:18:VAL:HG21	0.56	2.31	9	1
1:A:17:LEU:HD21	1:A:38:GLY:O	0.56	2.01	7	1
1:A:19:PHE:CG	1:A:20:PHE:N	0.56	2.74	7	1
1:C:29:GLY:O	1:D:28:LYS:NZ	0.56	2.38	7	1
1:D:18:VAL:HG23	1:E:20:PHE:CZ	0.56	2.36	7	1
1:H:10:TYR:CE1	1:I:10:TYR:CG	0.56	2.94	7	1
1:I:8:SER:H	1:J:9:GLY:N	0.56	1.99	4	1
1:J:27:ASN:N	1:J:27:ASN:HD22	0.56	1.98	4	1
1:B:35:MET:CG	1:B:36:VAL:N	0.56	2.68	3	1
1:A:20:PHE:CD1	1:C:34:LEU:CG	0.56	2.89	3	1
1:D:31:ILE:HG23	1:D:31:ILE:O	0.56	2.00	3	1
1:E:22:GLU:CD	1:E:23:ASP:O	0.56	2.45	3	1
1:D:24:VAL:HG11	1:E:25:GLY:C	0.56	2.21	1	1
1:F:19:PHE:CE1	1:G:34:LEU:HD22	0.56	2.36	10	1
1:E:18:VAL:CG2	1:E:20:PHE:CE2	0.56	2.88	5	2
1:D:20:PHE:O	1:E:20:PHE:CB	0.56	2.54	6	5
1:G:12:VAL:HG23	1:G:12:VAL:O	0.56	1.99	5	1
1:B:36:VAL:HG11	1:C:36:VAL:N	0.56	2.15	9	1
1:H:18:VAL:CG1	1:H:20:PHE:CE2	0.56	2.89	9	2
1:A:30:ALA:HB3	1:C:24:VAL:N	0.56	2.16	7	1
1:D:21:ALA:HB3	1:E:21:ALA:CA	0.56	2.31	7	1
1:D:37:GLY:H	1:E:37:GLY:HA2	0.56	1.61	3	1
1:H:35:MET:SD	1:H:35:MET:N	0.55	2.79	10	1
1:A:24:VAL:O	1:B:24:VAL:HG13	0.55	2.01	5	1
1:D:33:GLY:O	1:E:33:GLY:HA3	0.55	2.01	5	1
1:H:13:HIS:O	1:H:14:HIS:CD2	0.55	2.59	5	1
1:A:26:SER:O	1:B:25:GLY:CA	0.55	2.54	7	1
1:A:14:HIS:CB	1:B:14:HIS:NE2	0.55	2.69	7	1
1:B:29:GLY:N	1:C:27:ASN:HB2	0.55	2.16	7	1
1:B:29:GLY:N	1:C:27:ASN:HB3	0.55	2.13	7	1
1:B:35:MET:O	1:C:36:VAL:O	0.55	2.24	7	1
1:J:22:GLU:N	1:J:22:GLU:OE1	0.55	2.39	7	1
1:J:39:VAL:O	1:J:39:VAL:HG23	0.55	2.02	7	1
1:H:14:HIS:N	1:I:15:GLN:NE2	0.55	2.54	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:34:LEU:N	1:H:34:LEU:CD1	0.55	2.61	2	1
1:E:35:MET:CB	1:J:36:VAL:HG11	0.55	2.31	3	1
1:G:22:GLU:N	1:G:22:GLU:OE1	0.55	2.39	3	1
1:I:34:LEU:HA	1:J:34:LEU:CB	0.55	2.31	3	1
1:A:12:VAL:HB	1:B:12:VAL:H	0.55	1.61	1	1
2:F:101:2PO:O1P	1:H:25:GLY:N	0.55	2.39	8	1
1:E:35:MET:C	1:E:36:VAL:CG2	0.55	2.75	5	3
1:C:20:PHE:CD1	1:C:20:PHE:N	0.55	2.69	6	2
1:D:19:PHE:C	1:E:19:PHE:N	0.55	2.60	7	1
1:C:24:VAL:HG12	1:C:25:GLY:H	0.55	1.60	8	1
1:A:16:LYS:O	1:B:16:LYS:CB	0.55	2.55	6	6
1:C:19:PHE:CG	1:C:20:PHE:N	0.55	2.73	4	6
1:B:7:ASP:O	1:B:8:SER:CB	0.55	2.54	9	1
1:F:13:HIS:ND1	1:F:13:HIS:O	0.55	2.39	9	1
1:G:10:TYR:CE1	1:H:10:TYR:CD1	0.55	2.95	9	1
1:D:31:ILE:O	1:E:32:ILE:HG13	0.55	2.02	7	1
1:I:34:LEU:HD23	1:I:34:LEU:N	0.55	2.17	7	2
1:D:22:GLU:H	1:E:32:ILE:CG2	0.55	2.14	3	1
1:G:15:GLN:CG	1:G:16:LYS:N	0.55	2.69	1	1
1:I:28:LYS:N	1:I:28:LYS:CD	0.55	2.70	8	4
1:J:14:HIS:O	1:J:15:GLN:CB	0.55	2.54	8	1
1:H:16:LYS:O	1:I:16:LYS:CB	0.55	2.54	4	6
1:A:30:ALA:HA	1:B:30:ALA:O	0.55	2.00	7	2
1:H:11:GLU:OE1	1:H:13:HIS:ND1	0.55	2.39	4	1
1:F:10:TYR:O	1:G:10:TYR:HB2	0.55	2.01	1	1
1:G:13:HIS:C	1:H:13:HIS:O	0.55	2.45	1	1
1:B:34:LEU:CD2	1:B:34:LEU:N	0.55	2.68	8	2
1:I:10:TYR:HA	1:J:9:GLY:C	0.55	2.17	9	1
1:B:14:HIS:CE1	1:B:18:VAL:CG2	0.55	2.89	7	1
1:A:35:MET:SD	1:B:34:LEU:HD12	0.55	2.41	3	1
1:A:37:GLY:H	1:B:37:GLY:H	0.55	1.43	3	1
1:B:32:ILE:HG21	1:D:32:ILE:HG13	0.55	1.78	3	1
1:C:35:MET:SD	1:C:35:MET:N	0.55	2.79	8	1
1:A:16:LYS:O	1:B:16:LYS:HB2	0.55	2.02	9	4
1:H:19:PHE:C	1:H:19:PHE:CD2	0.55	2.79	9	1
1:A:13:HIS:CG	1:A:14:HIS:H	0.55	2.20	7	1
1:B:19:PHE:C	1:B:20:PHE:CD2	0.55	2.80	7	1
1:C:33:GLY:O	1:D:34:LEU:N	0.55	2.40	7	1
1:C:31:ILE:O	1:D:32:ILE:CG1	0.55	2.55	7	1
1:G:10:TYR:HA	1:H:10:TYR:HA	0.55	1.79	7	1
1:A:19:PHE:CA	1:B:20:PHE:CD2	0.55	2.89	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:37:GLY:CA	1:G:37:GLY:O	0.55	2.54	3	1
1:I:30:ALA:N	1:J:30:ALA:CB	0.55	2.67	3	1
1:I:18:VAL:CG2	1:I:20:PHE:CE2	0.55	2.89	6	1
1:B:10:TYR:OH	1:B:12:VAL:HG12	0.55	2.02	9	1
1:A:31:ILE:CG2	1:C:22:GLU:N	0.55	2.53	7	1
1:B:21:ALA:HB2	1:C:34:LEU:HD21	0.55	1.77	3	1
1:E:19:PHE:CA	1:E:20:PHE:CD2	0.55	2.89	3	1
1:I:20:PHE:CD2	1:I:20:PHE:N	0.55	2.73	1	1
1:I:10:TYR:C	1:I:10:TYR:CD1	0.55	2.80	8	1
1:F:19:PHE:CB	1:G:19:PHE:O	0.55	2.55	6	2
1:G:23:ASP:OD2	1:H:27:ASN:ND2	0.55	2.40	9	2
1:C:34:LEU:CB	1:D:34:LEU:CD1	0.55	2.82	7	1
1:A:16:LYS:CA	1:B:16:LYS:HB3	0.55	2.27	3	1
1:D:35:MET:SD	1:I:36:VAL:O	0.55	2.65	1	1
1:H:10:TYR:O	1:H:11:GLU:CB	0.55	2.54	10	1
1:F:34:LEU:H	1:F:34:LEU:HD23	0.55	1.58	5	1
1:G:12:VAL:O	1:H:13:HIS:ND1	0.55	2.40	5	1
1:H:19:PHE:CG	1:H:20:PHE:N	0.55	2.75	3	6
1:A:37:GLY:H	1:B:37:GLY:HA2	0.55	1.62	9	1
1:A:31:ILE:O	1:B:32:ILE:N	0.55	2.38	7	1
1:A:30:ALA:CB	1:C:23:ASP:HB3	0.55	2.31	7	1
1:I:6:HIS:N	1:I:6:HIS:CD2	0.55	2.74	7	1
1:G:34:LEU:N	1:G:34:LEU:CD2	0.55	2.70	2	1
1:I:14:HIS:O	1:I:15:GLN:CB	0.55	2.55	2	1
1:B:12:VAL:O	1:B:12:VAL:HG22	0.55	2.02	3	1
1:B:13:HIS:C	1:B:13:HIS:ND1	0.55	2.61	1	1
1:C:33:GLY:O	1:D:33:GLY:HA2	0.55	2.02	1	1
1:H:12:VAL:O	1:H:13:HIS:CB	0.55	2.54	8	1
1:E:22:GLU:OE1	1:E:22:GLU:N	0.55	2.39	10	1
1:F:13:HIS:CD2	1:G:13:HIS:CG	0.55	2.94	9	1
1:J:24:VAL:C	1:J:26:SER:H	0.55	2.06	7	3
1:J:14:HIS:O	1:J:15:GLN:O	0.55	2.25	2	2
1:D:20:PHE:CD1	1:D:20:PHE:N	0.55	2.75	3	1
1:H:5:ARG:N	1:H:5:ARG:NE	0.55	2.54	3	1
1:B:34:LEU:CD1	1:B:34:LEU:C	0.55	2.73	1	1
1:I:14:HIS:ND1	1:I:14:HIS:C	0.54	2.61	10	1
1:D:29:GLY:O	1:D:30:ALA:O	0.54	2.24	5	1
1:I:13:HIS:CD2	1:J:13:HIS:O	0.54	2.60	5	1
1:G:16:LYS:O	1:H:16:LYS:HB3	0.54	2.02	6	4
1:B:16:LYS:O	1:B:17:LEU:CB	0.54	2.51	7	1
1:E:27:ASN:C	1:E:27:ASN:HD22	0.54	2.06	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:27:ASN:OD1	1:B:28:LYS:N	0.54	2.40	1	1
1:F:27:ASN:ND2	1:F:28:LYS:H	0.54	2.00	1	1
1:I:23:ASP:OD2	1:I:27:ASN:ND2	0.54	2.41	6	3
1:G:19:PHE:O	1:G:20:PHE:HB3	0.54	2.01	9	3
1:C:31:ILE:HG22	1:D:32:ILE:O	0.54	2.01	7	1
1:D:17:LEU:CG	1:D:17:LEU:O	0.54	2.56	7	1
1:J:34:LEU:O	1:J:35:MET:HB3	0.54	2.03	3	1
1:H:13:HIS:ND1	1:H:14:HIS:N	0.54	2.54	1	1
1:A:12:VAL:O	1:B:13:HIS:O	0.54	2.26	3	2
1:A:34:LEU:O	1:A:34:LEU:HD12	0.54	2.03	2	2
1:C:28:LYS:O	1:C:30:ALA:N	0.54	2.40	5	2
1:A:38:GLY:O	1:A:40:VAL:N	0.54	2.36	9	1
1:A:10:TYR:CD2	1:B:10:TYR:CE1	0.54	2.96	7	1
1:D:29:GLY:O	1:E:30:ALA:HB3	0.54	2.02	7	1
1:D:19:PHE:CB	1:E:20:PHE:CG	0.54	2.80	7	1
1:I:19:PHE:CE1	1:I:20:PHE:O	0.54	2.60	3	1
1:J:34:LEU:O	1:J:35:MET:SD	0.54	2.66	3	1
1:F:18:VAL:C	1:G:18:VAL:HG23	0.54	2.22	8	1
1:I:13:HIS:ND1	1:I:14:HIS:N	0.54	2.56	5	1
1:J:5:ARG:O	1:J:6:HIS:CG	0.54	2.61	6	1
1:G:19:PHE:O	1:G:19:PHE:CD1	0.54	2.60	9	1
1:B:19:PHE:CE2	1:B:20:PHE:O	0.54	2.60	7	1
1:D:27:ASN:ND2	1:D:28:LYS:O	0.54	2.41	7	1
1:B:32:ILE:HB	1:C:33:GLY:CA	0.54	2.33	3	1
1:D:20:PHE:CD2	1:D:20:PHE:N	0.54	2.72	8	1
1:I:6:HIS:CD2	1:I:7:ASP:H	0.54	2.20	10	1
1:H:24:VAL:CG2	1:H:25:GLY:N	0.54	2.70	9	4
1:C:34:LEU:N	1:C:34:LEU:CD1	0.54	2.60	5	1
1:A:16:LYS:O	1:A:17:LEU:HD23	0.54	2.02	7	1
1:B:28:LYS:CD	1:B:28:LYS:N	0.54	2.67	7	1
1:A:35:MET:C	1:A:36:VAL:CG1	0.54	2.75	3	1
1:C:33:GLY:O	1:C:34:LEU:HD13	0.54	2.01	3	1
1:G:32:ILE:CA	1:H:32:ILE:O	0.54	2.50	3	1
1:G:35:MET:CE	1:H:35:MET:SD	0.54	2.95	3	1
1:I:13:HIS:CD2	1:I:14:HIS:N	0.54	2.75	8	1
1:I:20:PHE:O	1:J:20:PHE:CB	0.54	2.56	2	6
1:I:14:HIS:NE2	1:I:17:LEU:CA	0.54	2.70	10	1
1:F:19:PHE:HD1	1:F:19:PHE:N	0.54	1.99	6	1
1:B:14:HIS:CE1	1:B:18:VAL:HG21	0.54	2.38	9	1
1:A:28:LYS:O	1:C:24:VAL:HA	0.54	2.03	7	1
1:B:15:GLN:O	1:B:17:LEU:N	0.54	2.41	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:22:GLU:OE1	1:C:22:GLU:CB	0.54	2.55	7	1
1:I:37:GLY:N	1:J:37:GLY:CA	0.54	2.70	7	1
1:I:12:VAL:O	1:J:12:VAL:CB	0.54	2.55	4	1
1:A:34:LEU:O	1:B:34:LEU:HB3	0.54	2.03	3	1
1:A:18:VAL:HG23	1:B:18:VAL:CG2	0.54	2.32	3	1
1:C:20:PHE:HD2	1:C:20:PHE:H	0.54	1.45	3	1
1:D:17:LEU:C	1:D:18:VAL:CG2	0.54	2.76	3	1
1:D:19:PHE:CE1	1:E:21:ALA:CB	0.54	2.82	3	1
1:F:31:ILE:O	1:G:31:ILE:HA	0.54	2.03	3	1
1:H:31:ILE:HB	1:I:31:ILE:HG23	0.54	1.79	3	1
1:C:32:ILE:CB	1:D:32:ILE:O	0.54	2.55	1	1
1:J:6:HIS:ND1	1:J:6:HIS:N	0.54	2.52	1	1
1:C:20:PHE:O	1:D:20:PHE:CB	0.54	2.56	8	7
1:H:14:HIS:O	1:H:15:GLN:CB	0.54	2.56	8	1
1:G:17:LEU:CD2	1:G:17:LEU:C	0.54	2.73	10	1
1:J:7:ASP:OD2	1:J:23:ASP:O	0.54	2.25	6	1
1:I:15:GLN:O	1:I:17:LEU:N	0.54	2.40	9	1
1:J:19:PHE:O	1:J:20:PHE:CG	0.54	2.61	7	1
1:C:19:PHE:CB	1:D:18:VAL:CG1	0.54	2.82	3	1
1:C:22:GLU:N	1:D:22:GLU:OE1	0.54	2.39	3	1
1:E:18:VAL:O	1:E:19:PHE:CB	0.54	2.56	3	1
1:J:8:SER:N	2:J:101:2PO:O2P	0.54	2.41	4	3
1:F:11:GLU:N	1:F:11:GLU:OE1	0.54	2.40	6	1
1:A:31:ILE:HB	1:B:31:ILE:HA	0.54	1.76	3	1
1:H:31:ILE:O	1:I:32:ILE:CG2	0.54	2.56	3	1
1:J:4:PHE:CG	1:J:4:PHE:O	0.54	2.61	1	1
1:J:11:GLU:CD	1:J:11:GLU:N	0.54	2.61	7	2
2:I:101:2PO:O1P	1:J:7:ASP:N	0.54	2.40	6	1
1:A:32:ILE:C	1:C:22:GLU:N	0.54	2.62	7	1
1:I:34:LEU:HA	1:J:34:LEU:O	0.54	2.03	7	1
1:A:8:SER:HB3	2:A:101:2PO:P	0.54	2.42	1	3
1:A:17:LEU:O	1:B:18:VAL:N	0.54	2.41	3	1
1:C:18:VAL:CG2	1:D:20:PHE:CZ	0.54	2.80	3	1
1:H:15:GLN:O	1:I:14:HIS:CE1	0.54	2.60	6	1
1:B:35:MET:O	1:B:36:VAL:CB	0.54	2.55	9	1
1:A:31:ILE:CA	1:C:22:GLU:CA	0.54	2.85	7	1
1:D:19:PHE:N	1:E:18:VAL:HA	0.54	2.18	7	1
1:E:20:PHE:O	1:E:21:ALA:CB	0.54	2.55	7	1
1:F:17:LEU:HD12	1:F:17:LEU:O	0.54	2.03	7	1
1:G:19:PHE:CE2	1:G:34:LEU:CB	0.54	2.90	7	1
1:F:23:ASP:OD2	1:G:27:ASN:N	0.54	2.41	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:12:VAL:C	1:H:13:HIS:CG	0.53	2.78	8	2
1:G:9:GLY:C	1:G:10:TYR:CD1	0.53	2.82	1	5
1:I:11:GLU:C	1:I:12:VAL:HG23	0.53	2.24	9	2
1:G:34:LEU:H	1:G:34:LEU:HD23	0.53	1.61	2	1
1:C:36:VAL:CG2	1:D:36:VAL:O	0.53	2.54	3	1
1:I:39:VAL:C	1:J:39:VAL:HG12	0.53	2.20	3	1
1:C:22:GLU:N	1:C:22:GLU:OE2	0.53	2.41	1	1
1:H:13:HIS:O	1:H:14:HIS:CG	0.53	2.61	10	1
1:H:24:VAL:H	1:I:24:VAL:HG13	0.53	1.63	6	2
1:A:35:MET:C	1:A:36:VAL:CG2	0.53	2.75	9	1
1:G:19:PHE:HB2	1:H:19:PHE:CD2	0.53	2.39	7	1
1:I:19:PHE:O	1:I:20:PHE:HB3	0.53	2.03	7	1
1:F:19:PHE:N	1:F:19:PHE:CD2	0.53	2.76	2	1
1:A:10:TYR:H	1:B:10:TYR:H	0.53	1.46	1	1
1:I:4:PHE:O	1:I:6:HIS:N	0.53	2.41	1	1
1:H:15:GLN:OE1	1:I:14:HIS:CE1	0.53	2.61	8	1
1:H:4:PHE:CG	1:H:5:ARG:N	0.53	2.76	9	2
1:J:8:SER:O	1:J:8:SER:OG	0.53	2.27	6	2
1:C:19:PHE:CG	1:D:36:VAL:HG21	0.53	2.39	9	1
1:A:13:HIS:CB	1:B:13:HIS:O	0.53	2.57	1	2
1:B:30:ALA:O	1:B:31:ILE:HD12	0.53	2.03	7	1
1:E:23:ASP:OD1	1:E:24:VAL:N	0.53	2.40	7	1
1:G:19:PHE:HB2	1:H:19:PHE:O	0.53	2.03	7	1
1:I:20:PHE:HD1	1:I:20:PHE:C	0.53	2.06	7	1
1:A:18:VAL:HA	1:B:18:VAL:HG22	0.53	1.79	3	1
1:C:19:PHE:HB3	1:D:18:VAL:HB	0.53	1.78	3	1
1:C:19:PHE:CE1	1:E:20:PHE:CE1	0.53	2.95	3	1
1:D:28:LYS:C	1:E:31:ILE:HB	0.53	2.23	3	1
1:H:39:VAL:CG1	1:H:40:VAL:N	0.53	2.60	3	1
1:J:29:GLY:O	1:J:30:ALA:O	0.53	2.26	3	1
1:I:13:HIS:C	1:I:14:HIS:CG	0.53	2.81	5	2
1:B:28:LYS:N	1:B:28:LYS:CD	0.53	2.72	10	2
1:A:31:ILE:HA	1:C:22:GLU:CA	0.53	2.33	7	1
1:C:17:LEU:CB	1:D:17:LEU:CA	0.53	2.86	7	1
1:C:35:MET:O	1:D:36:VAL:CA	0.53	2.56	7	1
1:G:13:HIS:O	1:H:13:HIS:O	0.53	2.27	7	1
1:B:27:ASN:ND2	1:B:28:LYS:O	0.53	2.42	4	1
1:F:14:HIS:CE1	1:F:20:PHE:CD1	0.53	2.96	4	1
1:G:19:PHE:CE2	1:G:36:VAL:HG11	0.53	2.38	2	1
1:D:20:PHE:HD1	1:D:20:PHE:H	0.53	1.44	3	1
1:I:13:HIS:C	1:I:14:HIS:CD2	0.53	2.82	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:36:VAL:HG12	1:I:36:VAL:H	0.53	1.63	8	1
1:E:24:VAL:HG22	1:E:25:GLY:N	0.53	2.19	6	2
1:B:23:ASP:HA	1:C:23:ASP:O	0.53	2.03	9	1
1:A:8:SER:H	1:B:7:ASP:C	0.53	2.06	7	1
1:B:24:VAL:C	1:B:26:SER:N	0.53	2.62	7	1
1:B:17:LEU:CB	1:C:17:LEU:HA	0.53	2.34	7	1
1:D:19:PHE:CG	1:E:19:PHE:C	0.53	2.82	7	1
1:G:10:TYR:C	1:G:10:TYR:CD1	0.53	2.80	4	1
1:A:36:VAL:HG12	1:B:36:VAL:HG22	0.53	1.79	2	4
1:F:36:VAL:C	1:G:36:VAL:O	0.53	2.43	10	1
1:F:11:GLU:HA	1:G:11:GLU:H	0.53	1.64	4	2
1:H:13:HIS:ND1	1:H:13:HIS:N	0.53	2.56	5	1
1:H:16:LYS:O	1:I:16:LYS:HB2	0.53	2.03	4	3
1:A:36:VAL:HG11	1:B:36:VAL:HG23	0.53	1.75	9	1
1:A:23:ASP:CA	1:B:23:ASP:O	0.53	2.57	7	1
1:G:14:HIS:O	1:G:15:GLN:CB	0.53	2.55	7	1
1:H:19:PHE:CE2	1:H:36:VAL:CG2	0.53	2.91	7	1
1:B:21:ALA:CB	1:C:34:LEU:HD21	0.53	2.33	3	1
1:A:39:VAL:O	1:B:39:VAL:CB	0.53	2.56	3	1
1:H:10:TYR:O	1:H:11:GLU:HB3	0.53	2.04	10	1
1:D:24:VAL:O	1:D:24:VAL:CG1	0.53	2.57	5	1
1:F:16:LYS:O	1:G:16:LYS:HB3	0.53	2.04	5	3
1:C:33:GLY:O	1:D:34:LEU:O	0.53	2.27	7	1
1:D:31:ILE:O	1:E:32:ILE:CG1	0.53	2.57	7	1
1:G:19:PHE:C	1:G:20:PHE:CG	0.53	2.79	3	3
1:A:35:MET:HA	1:B:35:MET:CA	0.53	2.30	3	1
1:G:15:GLN:O	1:H:14:HIS:NE2	0.53	2.42	6	1
1:A:27:ASN:O	2:B:101:2PO:O3P	0.53	2.27	7	1
1:D:19:PHE:CG	1:E:18:VAL:C	0.53	2.81	7	1
1:D:22:GLU:HA	1:E:22:GLU:CB	0.53	2.34	7	1
1:H:15:GLN:H	1:I:14:HIS:CE1	0.53	2.21	4	1
1:I:20:PHE:O	1:J:20:PHE:HB2	0.53	2.04	2	1
1:A:38:GLY:HA2	1:F:34:LEU:HD22	0.53	1.79	3	1
1:E:21:ALA:N	1:E:34:LEU:HD13	0.53	2.18	3	1
1:I:5:ARG:O	1:I:6:HIS:ND1	0.53	2.41	3	1
1:I:12:VAL:O	1:I:12:VAL:HG23	0.53	2.03	4	2
1:F:10:TYR:HA	1:G:10:TYR:HA	0.53	1.79	9	1
1:G:28:LYS:CD	1:G:28:LYS:H	0.53	2.14	9	1
1:E:19:PHE:CD2	1:E:19:PHE:O	0.53	2.59	7	1
1:F:13:HIS:CB	1:G:14:HIS:O	0.53	2.57	7	1
1:C:33:GLY:H	1:D:32:ILE:CG1	0.53	2.17	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:19:PHE:O	1:D:19:PHE:CD2	0.53	2.61	3	1
1:G:36:VAL:CG2	1:H:36:VAL:O	0.53	2.57	3	1
1:I:24:VAL:O	1:J:25:GLY:N	0.53	2.42	8	1
1:B:36:VAL:HG12	1:C:36:VAL:HG22	0.53	1.80	4	4
1:H:11:GLU:HB3	1:I:10:TYR:O	0.53	2.04	6	1
1:G:13:HIS:C	1:G:14:HIS:ND1	0.53	2.62	9	1
1:F:13:HIS:O	1:F:14:HIS:ND1	0.53	2.42	4	2
1:H:19:PHE:O	1:H:20:PHE:HB3	0.53	2.03	7	1
1:A:16:LYS:CA	1:B:16:LYS:HB2	0.53	2.33	3	1
1:D:20:PHE:CE2	1:D:34:LEU:CD1	0.53	2.87	3	1
1:G:13:HIS:ND1	1:H:14:HIS:O	0.52	2.41	10	1
1:H:15:GLN:NE2	1:H:15:GLN:C	0.52	2.63	10	1
1:B:18:VAL:C	1:C:18:VAL:CG1	0.52	2.77	7	1
1:B:21:ALA:CB	1:C:22:GLU:HB2	0.52	2.33	7	1
1:H:14:HIS:CD2	1:H:15:GLN:N	0.52	2.77	7	1
1:E:20:PHE:CE2	1:E:22:GLU:OE2	0.52	2.62	4	1
1:C:28:LYS:CD	1:C:28:LYS:H	0.52	2.18	2	1
1:D:34:LEU:CD2	1:E:34:LEU:O	0.52	2.57	3	1
1:D:28:LYS:O	1:E:31:ILE:HB	0.52	2.05	3	1
1:D:27:ASN:CB	1:E:31:ILE:N	0.52	2.71	3	1
1:G:18:VAL:CG2	1:G:19:PHE:N	0.52	2.55	8	1
1:H:16:LYS:O	1:I:16:LYS:HB3	0.52	2.04	10	2
1:D:32:ILE:HG23	1:I:39:VAL:CG2	0.52	2.35	5	1
1:A:19:PHE:CZ	1:A:36:VAL:CG1	0.52	2.92	4	2
1:G:13:HIS:CD2	1:G:13:HIS:O	0.52	2.62	6	1
1:B:31:ILE:CG1	1:D:22:GLU:O	0.52	2.57	7	1
1:H:8:SER:HA	2:H:101:2PO:P	0.52	2.44	7	1
1:A:23:ASP:OD2	1:B:26:SER:CB	0.52	2.58	3	1
1:B:18:VAL:CA	1:C:18:VAL:HB	0.52	2.31	3	1
1:I:35:MET:HG3	1:I:36:VAL:H	0.52	1.64	3	1
1:J:12:VAL:O	1:J:12:VAL:HG23	0.52	2.03	3	1
1:B:23:ASP:OD2	1:B:26:SER:O	0.52	2.27	1	2
1:J:17:LEU:HD13	1:J:18:VAL:H	0.52	1.63	5	1
1:A:36:VAL:HG12	1:B:37:GLY:N	0.52	2.18	9	1
1:H:27:ASN:OD1	1:H:28:LYS:N	0.52	2.41	9	1
1:A:31:ILE:O	1:B:31:ILE:HA	0.52	2.05	7	1
1:C:35:MET:HG3	1:D:36:VAL:N	0.52	2.13	7	1
1:D:19:PHE:CB	1:E:20:PHE:CE2	0.52	2.88	7	1
1:I:4:PHE:CG	1:I:5:ARG:N	0.52	2.77	7	1
1:A:19:PHE:C	1:A:19:PHE:CD2	0.52	2.83	4	2
1:F:28:LYS:O	1:F:30:ALA:N	0.52	2.42	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:31:ILE:CG1	1:C:32:ILE:N	0.52	2.56	3	1
1:A:8:SER:O	2:A:101:2PO:P	0.52	2.67	1	1
1:B:20:PHE:H	1:C:20:PHE:HB3	0.52	1.65	4	4
1:F:35:MET:C	1:F:35:MET:SD	0.52	2.88	10	1
1:I:12:VAL:CG2	1:J:12:VAL:H	0.52	2.17	10	1
1:H:27:ASN:CG	1:H:28:LYS:N	0.52	2.63	9	2
1:I:3:GLU:OE1	1:I:3:GLU:N	0.52	2.42	9	1
1:A:18:VAL:O	1:A:19:PHE:CB	0.52	2.56	7	1
1:A:31:ILE:O	1:A:32:ILE:CG2	0.52	2.58	7	1
1:D:24:VAL:HG12	1:D:27:ASN:N	0.52	2.19	7	1
1:F:22:GLU:CG	1:F:23:ASP:N	0.52	2.72	7	1
1:H:8:SER:CA	2:H:101:2PO:P	0.52	2.97	7	1
1:A:39:VAL:CG1	1:A:40:VAL:N	0.52	2.72	3	1
1:F:12:VAL:O	1:G:13:HIS:C	0.52	2.48	8	1
1:J:7:ASP:O	1:J:8:SER:OG	0.52	2.27	10	2
1:H:14:HIS:CB	1:H:18:VAL:HG21	0.52	2.35	5	2
1:B:12:VAL:HG11	1:B:20:PHE:CZ	0.52	2.39	9	1
1:F:11:GLU:N	1:G:11:GLU:O	0.52	2.43	9	1
1:F:13:HIS:CD2	1:G:13:HIS:ND1	0.52	2.78	9	1
1:A:32:ILE:CG2	1:C:23:ASP:CB	0.52	2.75	7	1
1:I:14:HIS:CD2	1:J:18:VAL:CG1	0.52	2.92	7	1
1:D:29:GLY:O	1:E:31:ILE:CB	0.52	2.54	3	1
1:E:31:ILE:HG22	1:E:32:ILE:N	0.52	2.20	3	1
1:I:11:GLU:CA	1:J:11:GLU:O	0.52	2.58	3	1
1:F:36:VAL:O	1:G:36:VAL:C	0.52	2.44	10	1
1:F:12:VAL:N	1:G:11:GLU:O	0.52	2.34	10	3
1:I:14:HIS:CE1	1:I:17:LEU:C	0.52	2.83	10	1
1:F:19:PHE:HB2	1:G:19:PHE:O	0.52	2.04	6	2
1:B:9:GLY:C	1:B:10:TYR:CG	0.52	2.83	6	3
1:E:22:GLU:OE2	1:E:22:GLU:N	0.52	2.42	9	1
1:A:31:ILE:CG2	1:C:21:ALA:CB	0.52	2.87	7	1
1:D:19:PHE:HB3	1:E:20:PHE:CA	0.52	2.34	7	1
1:H:24:VAL:C	1:H:26:SER:N	0.52	2.63	7	1
1:J:15:GLN:O	1:J:16:LYS:O	0.52	2.27	4	1
1:E:35:MET:O	1:E:36:VAL:CB	0.52	2.58	3	1
1:G:28:LYS:N	1:G:28:LYS:CD	0.52	2.72	10	2
1:I:24:VAL:O	1:J:25:GLY:CA	0.52	2.58	7	2
1:A:34:LEU:N	1:A:34:LEU:CD2	0.52	2.72	5	1
1:C:23:ASP:OD2	1:D:27:ASN:N	0.52	2.42	5	1
1:H:10:TYR:CE2	1:I:10:TYR:CD2	0.52	2.97	5	1
1:B:31:ILE:CG2	1:C:32:ILE:O	0.52	2.57	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:G:37:GLY:H	1:H:37:GLY:HA2	0.52	1.64	7	1
1:A:20:PHE:CE1	1:C:34:LEU:CG	0.52	2.92	3	1
1:A:22:GLU:O	1:A:24:VAL:N	0.52	2.43	3	1
1:C:31:ILE:N	1:D:31:ILE:HG23	0.52	2.20	3	1
1:D:34:LEU:C	1:D:35:MET:SD	0.52	2.88	3	1
1:D:22:GLU:HA	1:E:32:ILE:HB	0.52	1.81	3	1
1:H:4:PHE:CD1	1:H:4:PHE:O	0.52	2.63	3	1
1:I:23:ASP:OD1	1:J:27:ASN:ND2	0.52	2.43	1	1
1:G:9:GLY:O	1:G:10:TYR:CB	0.52	2.46	8	1
1:B:19:PHE:C	1:B:20:PHE:CG	0.52	2.81	5	4
1:F:39:VAL:O	1:G:38:GLY:O	0.52	2.28	6	1
1:D:18:VAL:O	1:D:19:PHE:CD1	0.52	2.63	7	1
1:I:10:TYR:H	1:J:10:TYR:H	0.52	1.46	3	1
1:D:33:GLY:O	1:D:34:LEU:CB	0.52	2.57	1	1
1:F:14:HIS:CG	1:F:15:GLN:H	0.52	2.21	2	4
1:A:12:VAL:CG1	1:B:11:GLU:O	0.52	2.57	7	1
1:A:31:ILE:C	1:C:22:GLU:H	0.52	2.03	7	1
1:D:18:VAL:HA	1:F:35:MET:HE2	0.52	1.82	7	1
1:I:6:HIS:ND1	1:I:6:HIS:N	0.52	2.57	4	1
1:I:12:VAL:HG23	1:J:13:HIS:H	0.52	1.65	2	1
1:A:15:GLN:O	1:A:16:LYS:C	0.52	2.48	3	1
1:G:37:GLY:HA2	1:H:37:GLY:O	0.52	2.05	3	1
1:B:11:GLU:O	1:B:12:VAL:CG2	0.52	2.58	1	1
1:G:3:GLU:O	1:G:6:HIS:CE1	0.52	2.63	8	1
1:H:23:ASP:OD1	1:I:26:SER:N	0.52	2.43	9	1
1:A:31:ILE:CB	1:B:31:ILE:CB	0.52	2.45	3	1
1:I:19:PHE:CA	1:J:19:PHE:O	0.52	2.56	1	1
1:C:20:PHE:CE2	1:D:20:PHE:CD1	0.51	2.97	8	1
1:D:20:PHE:CZ	1:E:20:PHE:CD2	0.51	2.98	10	1
1:A:32:ILE:C	1:A:32:ILE:HD12	0.51	2.25	9	1
1:B:14:HIS:CE1	1:B:17:LEU:O	0.51	2.63	7	1
1:B:19:PHE:CZ	1:C:19:PHE:CG	0.51	2.98	7	1
1:B:22:GLU:OE1	1:C:22:GLU:OE2	0.51	2.28	7	1
1:H:24:VAL:C	1:H:26:SER:H	0.51	2.08	7	1
1:H:36:VAL:CG2	1:I:36:VAL:N	0.51	2.69	7	1
1:I:10:TYR:HB3	1:J:10:TYR:H	0.51	1.65	1	3
1:H:12:VAL:O	1:H:13:HIS:CG	0.51	2.64	8	1
1:F:29:GLY:O	1:G:28:LYS:O	0.51	2.27	10	1
1:D:35:MET:O	1:D:36:VAL:HG13	0.51	2.04	5	1
1:C:29:GLY:O	1:D:27:ASN:ND2	0.51	2.42	7	1
1:I:7:ASP:OD2	1:J:10:TYR:CE1	0.51	2.63	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:I:14:HIS:O	1:I:15:GLN:CG	0.51	2.59	2	1
1:A:31:ILE:HG22	1:A:32:ILE:N	0.51	2.19	3	1
1:C:19:PHE:HE1	1:D:20:PHE:CG	0.51	2.19	3	1
1:D:20:PHE:CA	1:E:21:ALA:CB	0.51	2.61	3	1
1:D:23:ASP:HA	1:E:22:GLU:CB	0.51	2.35	3	1
1:F:10:TYR:O	1:G:10:TYR:N	0.51	2.44	1	1
1:E:24:VAL:CG2	1:E:25:GLY:N	0.51	2.74	10	3
1:B:34:LEU:HB2	1:C:34:LEU:O	0.51	2.05	9	1
1:A:12:VAL:HG22	1:B:11:GLU:O	0.51	2.06	7	1
1:G:10:TYR:CE2	1:H:10:TYR:CG	0.51	2.99	4	1
1:J:8:SER:N	2:J:101:2PO:O3P	0.51	2.43	8	2
1:I:19:PHE:CD2	1:J:36:VAL:HG21	0.51	2.40	10	2
1:H:28:LYS:NZ	1:I:28:LYS:O	0.51	2.40	6	1
1:C:18:VAL:CG2	1:C:20:PHE:CE2	0.51	2.94	2	2
1:B:33:GLY:O	1:C:34:LEU:C	0.51	2.48	7	1
1:C:20:PHE:CB	1:D:20:PHE:CG	0.51	2.93	7	1
1:D:17:LEU:HG	1:D:17:LEU:O	0.51	2.04	7	1
1:C:19:PHE:CZ	1:D:19:PHE:C	0.51	2.73	3	1
1:D:26:SER:HG	1:E:27:ASN:HB2	0.51	1.64	3	1
1:D:24:VAL:CG2	1:D:25:GLY:N	0.51	2.73	1	1
1:F:18:VAL:O	1:G:18:VAL:CG2	0.51	2.59	7	1
1:I:19:PHE:O	1:I:20:PHE:CB	0.51	2.58	7	1
1:B:23:ASP:OD2	1:C:27:ASN:N	0.51	2.41	4	1
1:E:30:ALA:O	1:E:31:ILE:CD1	0.51	2.59	3	1
1:C:22:GLU:N	1:C:22:GLU:CD	0.51	2.63	1	1
1:E:33:GLY:O	1:E:34:LEU:CB	0.51	2.58	1	1
1:H:10:TYR:O	1:H:11:GLU:OE1	0.51	2.29	10	1
1:B:34:LEU:CA	1:C:34:LEU:O	0.51	2.58	7	1
1:B:19:PHE:CD1	1:B:20:PHE:CG	0.51	2.98	3	1
1:J:24:VAL:CG2	1:J:25:GLY:N	0.51	2.73	7	2
1:J:12:VAL:O	1:J:13:HIS:CD2	0.51	2.63	5	2
1:H:20:PHE:CD1	1:H:20:PHE:N	0.51	2.78	2	2
1:B:34:LEU:CB	1:C:34:LEU:O	0.51	2.59	9	2
1:A:16:LYS:O	1:A:17:LEU:CD2	0.51	2.59	7	1
1:D:18:VAL:CG2	1:E:20:PHE:CZ	0.51	2.94	7	1
1:H:36:VAL:HG22	1:I:36:VAL:N	0.51	2.18	7	1
1:I:10:TYR:CD2	1:J:10:TYR:O	0.51	2.64	7	2
1:A:16:LYS:C	1:B:14:HIS:NE2	0.51	2.64	1	2
1:I:39:VAL:C	1:J:39:VAL:CG1	0.51	2.78	3	1
1:H:19:PHE:CZ	1:H:34:LEU:HD23	0.51	2.40	1	1
1:I:12:VAL:CA	1:J:12:VAL:H	0.51	2.18	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:I:7:ASP:OD1	1:I:7:ASP:N	0.51	2.42	9	1
1:J:14:HIS:CD2	1:J:15:GLN:H	0.51	2.22	9	1
1:C:31:ILE:HD11	1:D:23:ASP:HB2	0.51	1.83	7	1
1:H:5:ARG:O	1:H:6:HIS:CG	0.51	2.64	7	1
1:B:33:GLY:O	1:B:34:LEU:CG	0.51	2.59	3	1
1:E:31:ILE:CG2	1:E:32:ILE:N	0.51	2.74	3	1
1:J:32:ILE:CG2	1:J:33:GLY:N	0.51	2.73	3	1
1:H:33:GLY:O	1:H:34:LEU:HG	0.51	2.06	10	2
1:I:20:PHE:CZ	1:J:20:PHE:CD2	0.51	2.99	9	1
1:A:28:LYS:O	2:C:101:2PO:O3P	0.51	2.28	7	1
1:B:27:ASN:OD1	1:C:23:ASP:OD1	0.51	2.27	7	1
1:F:30:ALA:CB	1:G:27:ASN:ND2	0.51	2.74	2	1
1:H:11:GLU:OE2	1:I:13:HIS:NE2	0.51	2.44	2	1
1:C:24:VAL:O	1:D:25:GLY:CA	0.51	2.59	1	1
1:C:27:ASN:ND2	1:C:28:LYS:O	0.51	2.43	8	1
1:D:36:VAL:HG12	1:E:36:VAL:HG22	0.51	1.82	10	4
1:F:19:PHE:CE1	1:F:36:VAL:HG22	0.51	2.41	6	1
1:B:17:LEU:CD1	1:B:18:VAL:N	0.51	2.74	7	1
1:B:31:ILE:CG1	1:D:22:GLU:C	0.51	2.78	7	1
1:H:12:VAL:HG11	1:H:20:PHE:CZ	0.51	2.41	7	1
1:G:39:VAL:O	1:H:38:GLY:O	0.51	2.29	7	1
1:B:23:ASP:OD2	1:C:27:ASN:CB	0.51	2.59	4	1
1:I:17:LEU:C	1:I:17:LEU:CD2	0.51	2.76	4	1
1:B:14:HIS:CG	1:B:18:VAL:CG2	0.51	2.94	2	2
1:A:12:VAL:CG2	1:B:13:HIS:O	0.51	2.58	3	1
1:D:39:VAL:O	1:E:38:GLY:O	0.51	2.29	3	1
1:J:18:VAL:O	1:J:19:PHE:CD2	0.51	2.64	3	1
1:I:3:GLU:O	1:I:4:PHE:CG	0.50	2.64	8	1
1:A:34:LEU:C	1:B:19:PHE:CE2	0.50	2.85	7	1
1:B:19:PHE:CD2	1:B:20:PHE:O	0.50	2.65	7	1
1:C:40:VAL:HG22	1:C:40:VAL:O	0.50	2.06	2	1
1:E:20:PHE:CE1	1:E:22:GLU:OE2	0.50	2.65	10	1
1:B:34:LEU:HD23	1:B:34:LEU:H	0.50	1.65	6	2
1:E:22:GLU:N	1:E:22:GLU:OE1	0.50	2.43	6	1
1:B:24:VAL:CG2	1:B:25:GLY:N	0.50	2.75	7	1
1:F:18:VAL:N	1:G:18:VAL:CG1	0.50	2.61	7	1
1:I:30:ALA:HB3	1:J:30:ALA:HB1	0.50	1.82	3	1
1:F:9:GLY:CA	1:G:9:GLY:H	0.50	2.00	8	1
1:I:13:HIS:C	1:I:13:HIS:ND1	0.50	2.63	5	1
1:C:36:VAL:HG12	1:D:36:VAL:O	0.50	2.06	6	1
1:H:33:GLY:O	1:H:34:LEU:CD2	0.50	2.57	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ASP:OD1	1:B:24:VAL:HG23	0.50	2.06	7	1
1:F:34:LEU:HD12	1:F:34:LEU:O	0.50	2.07	4	1
1:J:11:GLU:N	1:J:11:GLU:CD	0.50	2.63	4	1
1:I:12:VAL:N	1:J:11:GLU:HA	0.50	2.21	1	2
1:C:19:PHE:CB	1:D:18:VAL:HG12	0.50	2.32	3	1
1:C:20:PHE:CA	1:D:20:PHE:CE1	0.50	2.95	3	1
1:D:19:PHE:CD1	1:E:21:ALA:HB3	0.50	2.40	3	1
1:I:24:VAL:CG1	1:I:25:GLY:H	0.50	2.18	3	1
1:E:19:PHE:O	1:E:20:PHE:CB	0.50	2.59	1	1
1:H:4:PHE:O	1:H:6:HIS:N	0.50	2.44	1	1
1:F:36:VAL:HG12	1:G:36:VAL:HG22	0.50	1.83	8	2
1:J:11:GLU:OE1	1:J:11:GLU:O	0.50	2.30	8	1
1:J:24:VAL:C	1:J:26:SER:N	0.50	2.65	7	4
1:I:36:VAL:HG12	1:J:36:VAL:HG22	0.50	1.82	9	1
1:A:33:GLY:CA	1:B:21:ALA:HB2	0.50	2.37	7	1
1:B:23:ASP:OD1	1:B:23:ASP:C	0.50	2.48	3	2
1:F:22:GLU:H	1:G:22:GLU:HB3	0.50	1.67	8	1
1:H:15:GLN:NE2	1:H:18:VAL:HG22	0.50	2.22	8	1
1:H:19:PHE:O	1:H:20:PHE:CB	0.50	2.59	10	4
1:D:36:VAL:CA	1:E:36:VAL:O	0.50	2.59	5	1
1:C:27:ASN:ND2	1:C:28:LYS:H	0.50	2.03	3	2
1:H:11:GLU:CB	1:I:10:TYR:O	0.50	2.59	6	2
1:G:19:PHE:O	1:G:20:PHE:CB	0.50	2.60	9	5
1:C:18:VAL:CG1	1:D:18:VAL:HG22	0.50	2.35	9	1
1:G:7:ASP:OD2	1:H:5:ARG:NE	0.50	2.44	9	1
1:B:26:SER:O	1:C:26:SER:CB	0.50	2.60	4	1
1:F:15:GLN:O	1:G:14:HIS:CE1	0.50	2.65	4	2
1:A:39:VAL:O	1:B:39:VAL:HA	0.50	2.07	3	1
1:B:29:GLY:HA3	1:C:31:ILE:HD13	0.50	1.83	3	1
1:G:38:GLY:O	1:H:38:GLY:CA	0.50	2.52	3	1
1:H:4:PHE:CE2	1:H:5:ARG:NH1	0.50	2.80	3	1
1:I:13:HIS:O	1:I:14:HIS:CB	0.50	2.60	3	1
1:H:34:LEU:HA	1:I:34:LEU:O	0.50	2.06	3	1
1:G:10:TYR:CD2	1:H:24:VAL:HG23	0.50	2.42	8	1
2:F:101:2PO:P	1:H:25:GLY:N	0.50	2.85	8	1
1:I:5:ARG:O	1:I:6:HIS:CD2	0.50	2.65	5	1
1:A:27:ASN:N	2:B:101:2PO:O1P	0.50	2.41	7	1
1:J:35:MET:C	1:J:36:VAL:CG2	0.50	2.75	7	1
1:C:24:VAL:CG1	1:D:25:GLY:N	0.50	2.74	4	1
1:C:34:LEU:CD1	1:C:34:LEU:N	0.50	2.70	4	2
1:I:7:ASP:OD2	1:J:10:TYR:CD1	0.50	2.64	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:28:LYS:CD	1:B:28:LYS:H	0.50	2.19	3	1
1:D:20:PHE:CD2	1:D:34:LEU:CD2	0.50	2.85	3	1
1:G:23:ASP:N	1:G:23:ASP:OD1	0.50	2.44	3	1
1:H:39:VAL:O	1:I:39:VAL:CG1	0.50	2.43	3	1
1:H:23:ASP:OD2	1:I:27:ASN:ND2	0.50	2.45	1	1
1:I:24:VAL:HG22	1:I:25:GLY:N	0.50	2.22	10	1
1:J:28:LYS:H	1:J:28:LYS:CD	0.50	2.18	5	1
1:J:6:HIS:CD2	1:J:7:ASP:OD1	0.50	2.64	9	1
1:E:21:ALA:CB	1:H:39:VAL:HG13	0.50	2.37	7	1
1:G:19:PHE:HB2	1:H:19:PHE:CE2	0.50	2.42	7	1
1:A:9:GLY:HA2	1:B:9:GLY:HA3	0.50	1.84	1	1
1:H:10:TYR:C	1:H:10:TYR:CD1	0.50	2.84	5	1
1:H:14:HIS:CG	1:H:18:VAL:HG21	0.50	2.41	5	3
1:F:19:PHE:CE2	1:F:34:LEU:CB	0.50	2.95	6	1
1:I:18:VAL:HG12	1:J:18:VAL:HG12	0.50	1.84	6	1
1:B:14:HIS:NE2	1:B:18:VAL:HG21	0.50	2.22	9	1
1:A:18:VAL:CA	1:B:18:VAL:HG21	0.50	2.36	7	1
1:A:31:ILE:CA	1:C:22:GLU:HA	0.50	2.37	7	1
1:E:35:MET:O	1:E:36:VAL:CG2	0.50	2.58	3	1
1:E:33:GLY:O	1:E:34:LEU:HB3	0.50	2.06	1	1
1:G:20:PHE:CE2	1:H:20:PHE:CD2	0.50	3.00	5	1
1:H:7:ASP:N	1:I:6:HIS:CG	0.50	2.79	6	1
1:A:12:VAL:HG23	1:B:13:HIS:N	0.50	2.22	7	1
1:B:34:LEU:CB	1:C:34:LEU:HD11	0.50	2.37	7	1
1:C:27:ASN:O	1:C:28:LYS:O	0.50	2.30	7	1
1:C:31:ILE:O	1:D:31:ILE:CB	0.50	2.60	3	1
1:D:31:ILE:CA	1:E:31:ILE:HG13	0.50	2.31	3	1
1:D:34:LEU:CD1	1:E:34:LEU:O	0.50	2.60	1	1
1:G:36:VAL:CG1	1:H:36:VAL:HG22	0.49	2.36	8	1
1:G:35:MET:C	1:G:35:MET:SD	0.49	2.90	3	2
1:A:24:VAL:CG2	1:A:25:GLY:N	0.49	2.75	10	1
1:F:24:VAL:CG1	1:G:25:GLY:N	0.49	2.75	10	2
1:I:12:VAL:CG2	1:I:12:VAL:O	0.49	2.59	10	2
1:B:11:GLU:C	1:B:12:VAL:HG12	0.49	2.26	3	1
1:E:29:GLY:O	1:E:30:ALA:CB	0.49	2.60	1	1
1:I:12:VAL:HG21	1:I:20:PHE:CZ	0.49	2.42	8	1
1:C:27:ASN:OD1	1:C:28:LYS:N	0.49	2.45	10	1
1:I:6:HIS:CG	1:I:7:ASP:N	0.49	2.80	10	1
1:H:13:HIS:N	1:H:13:HIS:ND1	0.49	2.58	6	2
1:B:22:GLU:OE2	1:C:22:GLU:OE2	0.49	2.30	7	1
1:H:36:VAL:HG13	1:H:37:GLY:N	0.49	2.22	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:PHE:CD2	1:B:35:MET:HB3	0.49	2.42	3	1
1:C:34:LEU:HD13	1:C:34:LEU:N	0.49	2.20	3	1
1:C:35:MET:O	1:D:35:MET:CG	0.49	2.60	3	1
1:G:11:GLU:HA	1:H:11:GLU:CA	0.49	2.37	10	1
1:J:18:VAL:HG13	1:J:19:PHE:N	0.49	2.22	10	1
1:A:8:SER:H	1:B:8:SER:CB	0.49	2.20	9	1
1:J:14:HIS:CG	1:J:15:GLN:N	0.49	2.81	9	1
1:D:20:PHE:N	1:E:19:PHE:N	0.49	2.60	7	1
1:H:10:TYR:OH	1:I:10:TYR:CE2	0.49	2.55	7	1
1:J:8:SER:O	2:J:101:2PO:P	0.49	2.70	7	1
1:A:11:GLU:O	1:A:12:VAL:HB	0.49	2.05	4	1
1:I:10:TYR:HB2	1:J:10:TYR:O	0.49	2.08	2	1
1:I:26:SER:O	1:J:25:GLY:O	0.49	2.30	8	2
1:C:18:VAL:CG1	1:C:20:PHE:CE2	0.49	2.95	6	1
1:F:27:ASN:HD22	1:F:27:ASN:N	0.49	2.05	6	1
1:H:14:HIS:CE1	1:H:17:LEU:O	0.49	2.65	6	1
1:I:10:TYR:CA	1:J:10:TYR:CA	0.49	2.86	6	1
1:I:11:GLU:O	1:J:10:TYR:C	0.49	2.51	9	2
1:H:11:GLU:CD	1:H:11:GLU:N	0.49	2.66	9	1
1:A:21:ALA:O	1:B:21:ALA:O	0.49	2.29	7	1
1:G:19:PHE:CE1	1:H:34:LEU:HD22	0.49	2.43	7	1
1:H:35:MET:O	1:H:35:MET:SD	0.49	2.70	2	1
1:A:24:VAL:HG13	1:A:24:VAL:O	0.49	2.07	3	1
1:A:39:VAL:O	1:B:39:VAL:CA	0.49	2.60	3	1
1:A:15:GLN:O	1:B:15:GLN:CA	0.49	2.60	3	1
1:A:20:PHE:HZ	1:C:18:VAL:HG21	0.49	1.67	3	1
1:A:20:PHE:CZ	1:C:34:LEU:HB2	0.49	2.43	3	1
1:G:32:ILE:HG23	1:H:32:ILE:O	0.49	2.07	3	1
1:G:36:VAL:CG1	1:H:36:VAL:N	0.49	2.72	3	1
1:I:35:MET:O	1:I:36:VAL:CG2	0.49	2.59	3	1
1:D:34:LEU:HD13	1:E:34:LEU:O	0.49	2.07	1	1
1:A:19:PHE:CE2	1:A:36:VAL:CG1	0.49	2.95	5	1
1:H:13:HIS:C	1:H:14:HIS:CD2	0.49	2.86	5	1
1:A:19:PHE:CE1	1:A:36:VAL:HG22	0.49	2.43	9	1
1:G:19:PHE:CE1	1:G:36:VAL:HB	0.49	2.43	9	1
1:A:31:ILE:HA	1:C:22:GLU:HA	0.49	1.83	7	1
1:C:24:VAL:HG23	1:C:25:GLY:N	0.49	2.23	7	1
1:A:14:HIS:CE1	1:B:14:HIS:CE1	0.49	3.00	3	1
1:C:20:PHE:CD1	1:C:21:ALA:O	0.49	2.65	3	1
1:G:39:VAL:O	1:G:40:VAL:CB	0.49	2.60	3	1
1:D:24:VAL:HG11	1:E:25:GLY:O	0.49	2.07	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:G:13:HIS:C	1:G:13:HIS:ND1	0.49	2.66	8	1
1:F:19:PHE:C	1:F:19:PHE:CD2	0.49	2.86	5	3
1:B:17:LEU:HD13	1:B:18:VAL:N	0.49	2.23	7	1
1:B:31:ILE:O	1:C:32:ILE:C	0.49	2.51	7	1
1:A:29:GLY:O	1:C:24:VAL:C	0.49	2.51	7	1
1:E:22:GLU:CA	1:F:39:VAL:HG23	0.49	2.36	7	1
1:A:20:PHE:CE2	1:B:35:MET:HB3	0.49	2.43	3	1
1:A:16:LYS:N	1:B:16:LYS:HB2	0.49	2.22	3	1
1:D:34:LEU:CA	1:E:34:LEU:O	0.49	2.60	3	1
1:H:19:PHE:CD1	1:H:36:VAL:HB	0.49	2.42	3	1
1:I:30:ALA:CA	1:J:30:ALA:HB1	0.49	2.37	3	1
1:B:2:ALA:O	1:B:3:GLU:O	0.49	2.31	1	1
1:G:18:VAL:O	1:H:18:VAL:HG23	0.49	2.08	1	1
1:C:31:ILE:HD12	1:C:31:ILE:N	0.49	2.23	8	1
1:J:13:HIS:CD2	1:J:13:HIS:O	0.49	2.66	8	1
1:F:19:PHE:CE1	1:F:34:LEU:CB	0.49	2.96	9	2
1:F:14:HIS:CG	1:F:15:GLN:N	0.49	2.81	10	3
1:D:19:PHE:C	1:D:19:PHE:CD1	0.49	2.86	6	1
1:B:14:HIS:ND1	1:B:17:LEU:O	0.49	2.46	7	1
1:C:18:VAL:O	1:C:19:PHE:HB3	0.49	2.07	7	1
1:B:35:MET:HB3	1:C:19:PHE:CD1	0.49	2.43	7	1
1:B:31:ILE:CB	1:D:22:GLU:O	0.49	2.61	7	1
1:D:33:GLY:CA	1:E:19:PHE:CE1	0.49	2.96	7	1
1:H:14:HIS:HE2	1:H:16:LYS:C	0.49	2.11	7	1
1:I:1:ASP:OD1	1:I:1:ASP:N	0.49	2.44	3	1
1:D:23:ASP:CG	1:D:27:ASN:ND2	0.49	2.66	10	1
1:H:19:PHE:C	1:H:20:PHE:CG	0.49	2.85	9	6
1:G:39:VAL:HG12	1:G:40:VAL:N	0.49	2.21	5	1
1:H:36:VAL:HG12	1:I:36:VAL:HG22	0.49	1.85	5	2
1:E:35:MET:SD	1:E:35:MET:C	0.49	2.91	7	2
1:F:13:HIS:O	1:F:14:HIS:CB	0.49	2.61	9	1
1:F:28:LYS:CB	1:G:27:ASN:O	0.49	2.60	2	2
1:C:34:LEU:CB	1:D:34:LEU:CG	0.49	2.90	7	1
1:G:12:VAL:HG13	1:G:20:PHE:CE1	0.49	2.43	7	1
1:F:14:HIS:N	1:G:14:HIS:CD2	0.49	2.80	2	1
1:I:19:PHE:C	1:I:20:PHE:CG	0.49	2.85	1	3
1:G:19:PHE:CG	1:G:20:PHE:N	0.49	2.77	3	4
1:G:10:TYR:CE1	1:H:10:TYR:CG	0.49	3.01	9	1
1:I:3:GLU:H	1:I:3:GLU:CD	0.49	2.10	9	1
1:I:10:TYR:CB	1:J:10:TYR:O	0.49	2.61	7	2
1:J:20:PHE:CD2	1:J:22:GLU:OE2	0.49	2.66	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:GLY:HA3	1:B:38:GLY:HA2	0.49	1.84	3	1
1:C:40:VAL:O	1:D:40:VAL:OXT	0.49	2.30	3	1
1:J:32:ILE:HG23	1:J:33:GLY:N	0.49	2.23	3	1
1:C:32:ILE:HG22	1:D:31:ILE:O	0.49	2.08	1	1
1:B:20:PHE:CE1	1:C:20:PHE:CD1	0.49	3.00	8	1
1:G:12:VAL:HB	1:H:12:VAL:H	0.49	1.68	10	1
1:I:14:HIS:CE1	1:I:15:GLN:O	0.49	2.66	10	1
1:I:20:PHE:N	1:I:20:PHE:CD2	0.49	2.78	10	1
1:I:9:GLY:C	1:I:10:TYR:CG	0.49	2.86	9	2
1:A:19:PHE:CD1	1:A:36:VAL:CG2	0.49	2.96	9	1
1:B:1:ASP:OD2	1:B:4:PHE:CE2	0.49	2.66	9	1
1:F:19:PHE:CD2	1:F:19:PHE:C	0.49	2.83	7	2
1:B:12:VAL:O	1:B:13:HIS:C	0.49	2.51	7	1
1:C:31:ILE:O	1:D:32:ILE:CA	0.49	2.60	7	1
1:D:38:GLY:CA	1:E:38:GLY:O	0.49	2.60	7	1
1:D:37:GLY:O	1:E:37:GLY:HA2	0.49	2.08	1	2
1:A:23:ASP:O	1:A:23:ASP:OD1	0.49	2.30	3	2
1:A:24:VAL:O	1:A:24:VAL:CG1	0.49	2.61	3	1
1:B:36:VAL:HG21	1:G:35:MET:HG3	0.49	1.84	3	1
1:J:23:ASP:OD2	1:J:27:ASN:CB	0.49	2.61	3	1
1:J:17:LEU:CD2	1:J:17:LEU:N	0.49	2.76	1	1
1:D:24:VAL:O	1:E:24:VAL:HG23	0.48	2.07	8	1
1:D:24:VAL:O	1:E:25:GLY:CA	0.48	2.61	10	1
1:D:19:PHE:CD1	1:E:36:VAL:HG21	0.48	2.43	10	1
1:H:6:HIS:CG	1:H:7:ASP:H	0.48	2.26	5	1
1:J:12:VAL:CG2	1:J:13:HIS:N	0.48	2.76	5	1
1:B:33:GLY:O	1:C:34:LEU:CB	0.48	2.57	7	1
1:C:39:VAL:N	1:D:39:VAL:HA	0.48	2.23	7	1
1:E:39:VAL:HG11	1:H:33:GLY:O	0.48	2.08	7	1
1:E:40:VAL:O	1:E:40:VAL:CG2	0.48	2.61	7	1
1:H:5:ARG:NH1	1:I:4:PHE:CE2	0.48	2.81	7	1
1:H:15:GLN:CD	1:H:18:VAL:CG2	0.48	2.81	8	1
1:F:19:PHE:CZ	1:F:34:LEU:HB2	0.48	2.43	6	3
1:F:26:SER:OG	1:F:27:ASN:N	0.48	2.45	10	1
1:I:14:HIS:CD2	1:I:17:LEU:C	0.48	2.86	6	1
1:I:11:GLU:OE2	1:I:22:GLU:OE1	0.48	2.30	9	1
1:A:12:VAL:CG2	1:B:13:HIS:H	0.48	2.21	7	1
1:A:22:GLU:N	1:A:22:GLU:OE1	0.48	2.43	7	1
1:A:33:GLY:HA2	1:B:21:ALA:CB	0.48	2.39	7	1
1:J:6:HIS:ND1	1:J:6:HIS:O	0.48	2.46	4	1
1:D:22:GLU:CG	1:D:23:ASP:N	0.48	2.76	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:I:34:LEU:HA	1:J:34:LEU:HB3	0.48	1.84	3	1
1:G:14:HIS:CD2	1:G:15:GLN:N	0.48	2.78	8	1
1:B:6:HIS:N	1:B:6:HIS:ND1	0.48	2.61	10	1
1:E:20:PHE:N	1:E:20:PHE:CD1	0.48	2.77	5	1
1:J:8:SER:OG	1:J:8:SER:O	0.48	2.31	5	1
1:F:19:PHE:CE1	1:F:36:VAL:CG2	0.48	2.96	6	1
1:B:35:MET:SD	1:B:36:VAL:N	0.48	2.86	9	1
1:A:35:MET:SD	1:B:19:PHE:CD1	0.48	3.07	7	1
1:B:20:PHE:O	1:B:21:ALA:HB2	0.48	2.08	7	1
1:B:33:GLY:C	1:C:19:PHE:CZ	0.48	2.86	7	1
1:D:31:ILE:HG22	1:E:32:ILE:O	0.48	2.09	7	1
1:D:29:GLY:O	1:E:30:ALA:CB	0.48	2.62	7	1
1:F:23:ASP:OD2	1:F:26:SER:O	0.48	2.30	7	1
1:J:34:LEU:HD13	1:J:35:MET:H	0.48	1.68	3	2
1:F:19:PHE:CG	1:F:36:VAL:HG11	0.48	2.44	8	1
1:G:8:SER:O	1:H:8:SER:OG	0.48	2.31	8	2
1:I:23:ASP:OD1	1:J:23:ASP:O	0.48	2.32	8	1
1:C:33:GLY:C	1:C:34:LEU:HD23	0.48	2.28	10	1
1:J:9:GLY:O	1:J:10:TYR:CB	0.48	2.59	9	2
1:G:7:ASP:OD2	1:H:5:ARG:CZ	0.48	2.61	9	1
1:B:32:ILE:HG22	1:C:34:LEU:HD22	0.48	1.84	7	1
1:C:35:MET:O	1:D:36:VAL:CB	0.48	2.62	7	1
1:D:19:PHE:CZ	1:E:19:PHE:CE2	0.48	3.01	7	1
1:F:10:TYR:O	1:G:10:TYR:HA	0.48	2.07	4	1
1:I:30:ALA:CB	1:J:30:ALA:HB1	0.48	2.38	3	1
1:I:31:ILE:O	1:J:32:ILE:N	0.48	2.45	3	1
1:I:30:ALA:CB	1:J:30:ALA:O	0.48	2.57	8	1
1:C:40:VAL:O	1:D:40:VAL:N	0.48	2.46	5	1
1:A:32:ILE:O	1:C:21:ALA:O	0.48	2.31	7	1
1:C:31:ILE:HG12	1:D:23:ASP:HA	0.48	1.85	7	1
1:D:27:ASN:ND2	1:D:28:LYS:HD2	0.48	2.23	7	1
1:H:23:ASP:CG	1:I:27:ASN:ND2	0.48	2.67	7	1
1:F:32:ILE:CA	1:G:32:ILE:O	0.48	2.60	3	1
1:I:18:VAL:CG1	1:I:20:PHE:CZ	0.48	2.96	3	1
1:D:26:SER:OG	1:D:26:SER:O	0.48	2.29	1	1
1:H:15:GLN:NE2	1:H:18:VAL:CG2	0.48	2.77	8	1
1:B:28:LYS:N	1:B:28:LYS:HD2	0.48	2.22	10	1
1:G:4:PHE:CG	1:G:5:ARG:N	0.48	2.81	10	1
1:C:24:VAL:O	1:D:25:GLY:O	0.48	2.31	5	1
1:F:35:MET:O	1:G:36:VAL:HB	0.48	2.07	6	1
1:A:12:VAL:O	1:A:13:HIS:O	0.48	2.32	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ASN:O	2:B:101:2PO:P	0.48	2.71	7	1
1:A:31:ILE:HG21	1:D:21:ALA:O	0.48	2.03	7	1
1:H:19:PHE:CD1	1:I:34:LEU:HD12	0.48	2.44	7	1
1:C:24:VAL:HG12	1:C:25:GLY:N	0.48	2.23	8	1
1:H:12:VAL:HG23	1:H:13:HIS:N	0.48	2.24	8	1
1:I:10:TYR:CE1	1:J:8:SER:CB	0.48	2.97	8	1
1:H:10:TYR:OH	1:H:23:ASP:N	0.48	2.46	10	1
1:D:24:VAL:CG1	1:E:25:GLY:O	0.48	2.62	5	1
1:J:5:ARG:NE	1:J:5:ARG:N	0.48	2.62	6	1
1:A:19:PHE:CE1	1:A:34:LEU:HD12	0.48	2.44	9	1
1:F:36:VAL:HG12	1:G:36:VAL:HG12	0.48	1.84	9	1
1:A:33:GLY:HA2	1:B:21:ALA:HB2	0.48	1.84	7	1
1:B:18:VAL:O	1:C:18:VAL:CG1	0.48	2.62	7	1
1:B:21:ALA:HB3	1:C:22:GLU:HB2	0.48	1.86	7	1
1:B:33:GLY:C	1:C:34:LEU:CD2	0.48	2.82	7	1
1:I:23:ASP:OD2	1:J:27:ASN:ND2	0.48	2.47	7	1
1:B:23:ASP:OD1	1:B:26:SER:O	0.48	2.30	4	2
1:B:19:PHE:CE1	1:B:20:PHE:HB2	0.48	2.43	3	1
1:H:27:ASN:H	1:H:28:LYS:HZ3	0.48	1.51	3	1
1:I:19:PHE:CD1	1:I:20:PHE:N	0.48	2.82	3	1
1:B:1:ASP:OD1	1:B:2:ALA:N	0.48	2.44	1	1
1:D:26:SER:O	1:E:25:GLY:O	0.48	2.32	10	1
1:G:12:VAL:H	1:H:12:VAL:H	0.48	1.50	10	1
1:G:40:VAL:O	1:G:40:VAL:HG12	0.48	2.09	6	1
1:H:33:GLY:C	1:H:34:LEU:HG	0.48	2.28	6	1
1:A:17:LEU:CD2	1:A:17:LEU:C	0.48	2.79	9	1
1:I:12:VAL:N	1:J:11:GLU:HB3	0.48	2.24	9	1
1:A:23:ASP:OD2	2:B:101:2PO:O1P	0.48	2.31	7	1
1:C:33:GLY:O	1:D:34:LEU:CB	0.48	2.61	7	1
1:D:20:PHE:CA	1:E:20:PHE:N	0.48	2.50	7	1
1:J:11:GLU:O	1:J:12:VAL:HB	0.48	2.09	7	1
1:C:28:LYS:H	1:C:28:LYS:HD3	0.48	1.68	2	1
1:I:12:VAL:O	1:I:12:VAL:CG2	0.48	2.59	2	1
1:I:35:MET:N	1:I:35:MET:SD	0.48	2.86	2	1
1:F:11:GLU:CD	1:F:11:GLU:N	0.48	2.67	8	1
1:A:23:ASP:O	1:A:24:VAL:O	0.48	2.31	10	1
1:D:32:ILE:HG13	1:D:33:GLY:H	0.48	1.63	5	1
1:J:12:VAL:HG22	1:J:13:HIS:N	0.48	2.23	5	1
1:G:10:TYR:CE1	1:H:10:TYR:HB2	0.48	2.43	9	1
1:C:20:PHE:CA	1:D:20:PHE:CB	0.48	2.91	7	1
1:A:35:MET:C	1:B:35:MET:O	0.48	2.48	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:30:ALA:HA	1:E:31:ILE:CG1	0.48	2.36	3	1
1:D:31:ILE:O	1:D:32:ILE:CD1	0.48	2.60	8	1
1:F:20:PHE:HB2	1:G:20:PHE:CE2	0.48	2.44	8	1
1:I:24:VAL:CG1	1:I:25:GLY:N	0.48	2.73	3	2
1:G:28:LYS:CD	1:G:28:LYS:N	0.48	2.76	4	3
1:A:8:SER:HB3	2:A:101:2PO:O3P	0.48	2.08	7	1
1:A:32:ILE:CB	1:B:32:ILE:O	0.48	2.62	7	1
1:G:17:LEU:O	1:G:18:VAL:CB	0.48	2.62	7	1
1:A:18:VAL:CG2	1:A:19:PHE:H	0.48	2.15	4	1
1:B:32:ILE:CB	1:C:32:ILE:O	0.48	2.62	3	1
1:B:32:ILE:CG1	1:C:31:ILE:CG2	0.48	2.92	3	1
1:B:32:ILE:HD11	1:C:31:ILE:HG12	0.48	1.85	3	1
1:D:21:ALA:H	1:E:21:ALA:CA	0.48	2.09	3	1
1:J:12:VAL:HG21	1:J:20:PHE:CE1	0.48	2.44	3	1
1:I:38:GLY:C	1:J:38:GLY:HA3	0.48	2.29	3	1
1:H:11:GLU:C	1:H:12:VAL:CG2	0.47	2.79	8	1
1:H:9:GLY:C	1:I:9:GLY:O	0.47	2.50	8	1
1:G:13:HIS:ND1	1:G:13:HIS:C	0.47	2.67	10	1
1:I:17:LEU:HD23	1:I:18:VAL:H	0.47	1.69	5	1
1:B:36:VAL:CG1	1:C:36:VAL:O	0.47	2.62	6	2
1:F:38:GLY:H	1:G:37:GLY:HA2	0.47	1.69	6	1
1:B:35:MET:HG2	1:C:36:VAL:O	0.47	2.09	7	1
1:A:29:GLY:O	1:D:24:VAL:HG22	0.47	2.09	7	1
1:E:20:PHE:C	1:E:34:LEU:HD13	0.47	2.29	3	1
1:J:35:MET:HG2	1:J:36:VAL:HG13	0.47	1.86	3	1
1:B:18:VAL:CG2	1:B:20:PHE:CE1	0.47	2.96	1	1
1:F:15:GLN:CD	1:G:15:GLN:NE2	0.47	2.68	8	1
1:B:12:VAL:C	1:B:13:HIS:O	0.47	2.48	7	1
1:D:33:GLY:O	1:E:34:LEU:CG	0.47	2.60	7	1
1:A:15:GLN:N	1:B:14:HIS:CE1	0.47	2.81	4	1
1:H:11:GLU:OE1	1:H:13:HIS:CE1	0.47	2.68	4	1
1:A:35:MET:CA	1:B:35:MET:N	0.47	2.78	3	1
1:D:21:ALA:N	1:E:21:ALA:HA	0.47	2.07	3	1
1:A:36:VAL:HG12	1:B:36:VAL:H	0.47	1.69	1	1
1:C:24:VAL:HG22	1:D:23:ASP:O	0.47	2.09	1	1
1:G:19:PHE:CD1	1:H:36:VAL:CG2	0.47	2.97	1	1
1:C:20:PHE:CE2	1:C:22:GLU:OE2	0.47	2.68	8	1
1:H:15:GLN:OE1	1:H:18:VAL:HG23	0.47	2.09	8	1
1:D:20:PHE:CD1	1:D:22:GLU:OE2	0.47	2.67	10	1
1:J:13:HIS:C	1:J:16:LYS:NZ	0.47	2.67	10	1
1:H:19:PHE:CD2	1:H:36:VAL:HG11	0.47	2.44	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:MET:HG2	1:B:19:PHE:CD1	0.47	2.42	7	1
1:B:1:ASP:O	1:B:2:ALA:HB2	0.47	2.09	7	1
1:C:31:ILE:O	1:D:32:ILE:HG13	0.47	2.10	7	1
1:A:22:GLU:O	1:B:22:GLU:CG	0.47	2.63	4	1
1:C:19:PHE:O	1:C:20:PHE:CG	0.47	2.68	4	1
1:A:39:VAL:HG12	1:A:40:VAL:N	0.47	2.24	3	1
1:E:30:ALA:C	1:E:31:ILE:CD1	0.47	2.80	3	1
1:F:19:PHE:CE2	1:F:36:VAL:CG1	0.47	2.97	1	1
1:I:23:ASP:OD1	1:I:24:VAL:N	0.47	2.48	8	1
1:I:12:VAL:H	1:J:11:GLU:HA	0.47	1.69	8	1
1:E:24:VAL:C	1:E:26:SER:N	0.47	2.66	10	1
1:I:11:GLU:C	1:J:11:GLU:CB	0.47	2.83	9	1
1:A:28:LYS:O	1:A:29:GLY:C	0.47	2.51	7	1
1:F:18:VAL:O	1:G:18:VAL:HG21	0.47	2.10	7	1
1:G:14:HIS:N	1:H:15:GLN:OE1	0.47	2.44	4	1
1:F:19:PHE:CZ	1:F:36:VAL:HG11	0.47	2.45	2	1
1:A:15:GLN:N	1:B:15:GLN:HA	0.47	2.24	3	1
1:B:27:ASN:OD1	1:C:32:ILE:HD11	0.47	2.10	3	1
1:G:10:TYR:CD1	1:G:24:VAL:HG11	0.47	2.45	3	1
1:F:13:HIS:CB	1:G:13:HIS:O	0.47	2.61	6	1
1:I:12:VAL:O	1:J:11:GLU:HB3	0.47	2.09	6	2
1:B:23:ASP:HB3	1:C:24:VAL:HG12	0.47	1.86	7	1
1:G:13:HIS:O	1:G:15:GLN:OE1	0.47	2.33	7	1
1:F:30:ALA:CB	1:G:30:ALA:O	0.47	2.61	7	1
1:C:20:PHE:O	1:C:21:ALA:CB	0.47	2.60	3	2
1:H:9:GLY:C	1:H:10:TYR:CG	0.47	2.87	4	1
1:I:8:SER:CB	1:J:8:SER:O	0.47	2.62	4	1
1:A:39:VAL:HG13	1:A:39:VAL:O	0.47	2.10	2	1
1:A:16:LYS:HA	1:B:16:LYS:CA	0.47	2.37	3	1
1:C:32:ILE:HA	1:D:31:ILE:O	0.47	2.09	3	1
1:I:28:LYS:HB2	1:J:30:ALA:HB3	0.47	1.86	3	1
1:J:34:LEU:C	1:J:35:MET:SD	0.47	2.92	3	1
1:J:34:LEU:O	1:J:35:MET:CB	0.47	2.61	3	1
1:H:17:LEU:CD1	1:H:17:LEU:C	0.47	2.82	10	1
1:C:23:ASP:OD2	1:D:27:ASN:ND2	0.47	2.48	6	1
1:J:23:ASP:O	1:J:24:VAL:C	0.47	2.52	6	1
1:H:8:SER:OG	1:I:8:SER:N	0.47	2.46	9	1
1:B:18:VAL:CG2	1:B:19:PHE:H	0.47	2.22	7	1
1:B:31:ILE:HD13	1:D:23:ASP:HA	0.47	1.85	7	1
1:B:18:VAL:C	1:C:18:VAL:HG11	0.47	2.29	7	1
1:C:35:MET:C	1:D:36:VAL:O	0.47	2.53	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:23:ASP:OD1	1:D:24:VAL:N	0.47	2.47	7	1
1:G:8:SER:O	1:H:9:GLY:O	0.47	2.31	7	1
1:B:8:SER:HB3	2:B:101:2PO:P	0.47	2.47	3	1
1:C:19:PHE:C	1:D:20:PHE:CE1	0.47	2.88	3	1
1:B:9:GLY:O	1:B:10:TYR:CD2	0.47	2.67	1	1
1:F:19:PHE:CE1	1:F:36:VAL:HG13	0.47	2.44	8	1
1:C:39:VAL:O	1:C:39:VAL:HG23	0.47	2.08	8	1
1:H:24:VAL:HG13	1:H:25:GLY:H	0.47	1.69	8	1
1:C:23:ASP:OD2	1:D:26:SER:CB	0.47	2.63	5	1
1:B:22:GLU:O	1:C:23:ASP:O	0.47	2.33	5	1
1:E:29:GLY:C	1:E:31:ILE:H	0.47	2.11	6	1
1:I:10:TYR:CB	1:J:10:TYR:C	0.47	2.82	6	2
1:H:10:TYR:CE2	1:I:11:GLU:HB3	0.47	2.45	9	1
1:I:24:VAL:HG11	1:J:25:GLY:N	0.47	2.24	9	1
1:D:19:PHE:C	1:E:19:PHE:H	0.47	2.13	7	1
1:D:19:PHE:HB3	1:E:20:PHE:N	0.47	2.24	7	1
1:E:34:LEU:C	1:E:34:LEU:CD1	0.47	2.83	7	1
1:A:26:SER:N	1:B:3:GLU:OE1	0.47	2.48	7	1
1:B:19:PHE:CG	1:C:19:PHE:HA	0.47	2.43	7	1
1:A:22:GLU:C	1:B:22:GLU:O	0.47	2.53	7	1
1:B:31:ILE:HG12	1:D:22:GLU:CA	0.47	2.39	7	1
1:B:31:ILE:HG22	1:C:32:ILE:N	0.47	2.20	7	1
1:G:33:GLY:CA	1:G:34:LEU:HD13	0.47	2.40	7	1
1:F:39:VAL:HG22	1:G:39:VAL:HB	0.47	1.85	7	1
1:C:19:PHE:O	1:C:20:PHE:CB	0.47	2.62	4	1
1:G:31:ILE:HD12	1:G:31:ILE:N	0.47	2.25	2	1
1:H:27:ASN:CG	1:H:28:LYS:H	0.47	2.13	2	1
1:H:37:GLY:CA	1:I:37:GLY:O	0.47	2.62	3	1
1:J:34:LEU:CD1	1:J:35:MET:H	0.47	2.23	3	1
1:G:18:VAL:O	1:H:18:VAL:CG2	0.47	2.63	1	1
2:F:101:2PO:O2P	1:H:25:GLY:N	0.47	2.48	8	1
1:I:14:HIS:CD2	1:I:17:LEU:N	0.47	2.83	6	1
1:F:39:VAL:H	1:G:39:VAL:HB	0.47	1.70	7	1
1:A:23:ASP:CB	1:B:27:ASN:H	0.47	2.23	3	1
1:C:18:VAL:HG22	1:D:20:PHE:CE1	0.47	2.43	3	1
1:B:22:GLU:O	1:C:22:GLU:HB2	0.47	2.10	1	1
1:I:22:GLU:O	1:J:22:GLU:OE1	0.47	2.33	8	1
1:A:17:LEU:N	1:A:17:LEU:CD2	0.47	2.75	6	1
1:H:35:MET:C	1:H:36:VAL:CG1	0.47	2.83	6	1
1:A:15:GLN:CD	1:A:16:LYS:H	0.47	2.13	7	1
1:B:18:VAL:O	1:B:19:PHE:CB	0.47	2.56	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:17:LEU:C	1:C:18:VAL:CG1	0.47	2.79	7	1
1:A:17:LEU:O	1:A:18:VAL:HB	0.47	2.10	4	1
1:I:17:LEU:HD23	1:I:17:LEU:O	0.47	2.10	4	1
1:B:5:ARG:O	1:B:6:HIS:CD2	0.47	2.68	2	1
1:A:8:SER:N	1:B:8:SER:O	0.47	2.36	8	1
1:H:8:SER:OG	1:H:9:GLY:N	0.47	2.48	8	1
1:G:27:ASN:OD1	1:G:28:LYS:N	0.47	2.48	10	2
1:C:34:LEU:C	1:C:35:MET:SD	0.47	2.94	5	1
1:F:27:ASN:O	1:F:27:ASN:ND2	0.47	2.47	6	1
1:H:34:LEU:C	1:H:35:MET:SD	0.47	2.94	6	1
1:J:5:ARG:NE	1:J:5:ARG:CA	0.47	2.78	6	1
1:E:20:PHE:C	1:G:39:VAL:CG1	0.47	2.78	7	1
1:C:24:VAL:HG13	1:D:25:GLY:O	0.47	2.09	4	1
1:B:39:VAL:O	1:B:40:VAL:O	0.47	2.33	2	1
1:H:14:HIS:ND1	1:I:15:GLN:NE2	0.47	2.62	2	1
1:A:15:GLN:O	1:B:15:GLN:HA	0.47	2.10	3	1
1:A:35:MET:CG	1:B:34:LEU:HD12	0.47	2.39	3	1
1:B:19:PHE:CD1	1:B:20:PHE:CD1	0.47	3.02	3	1
1:C:19:PHE:CZ	1:D:20:PHE:CB	0.47	2.96	3	1
1:I:39:VAL:O	1:J:39:VAL:CB	0.47	2.62	3	1
1:C:23:ASP:OD1	1:D:26:SER:N	0.47	2.46	1	1
1:H:5:ARG:O	1:H:6:HIS:ND1	0.47	2.48	1	1
1:J:4:PHE:CD2	1:J:4:PHE:O	0.47	2.68	1	1
1:H:36:VAL:CG1	1:I:36:VAL:HG22	0.46	2.40	5	2
1:G:15:GLN:NE2	1:G:20:PHE:CE2	0.46	2.83	7	1
1:E:24:VAL:HG12	1:E:25:GLY:H	0.46	1.70	2	1
1:F:19:PHE:CB	1:G:19:PHE:CE2	0.46	2.98	1	2
1:B:32:ILE:CG1	1:C:31:ILE:HG12	0.46	2.41	3	1
1:H:19:PHE:CB	1:I:19:PHE:O	0.46	2.62	3	1
1:H:13:HIS:CD2	1:H:13:HIS:N	0.46	2.81	8	1
1:E:26:SER:O	1:E:26:SER:OG	0.46	2.31	10	1
1:F:12:VAL:O	1:G:14:HIS:CE1	0.46	2.68	10	1
1:I:13:HIS:O	1:I:13:HIS:CG	0.46	2.66	10	1
1:D:19:PHE:O	1:D:20:PHE:CB	0.46	2.55	7	2
1:G:14:HIS:O	1:G:15:GLN:HB3	0.46	2.10	7	1
1:A:23:ASP:OD1	1:A:24:VAL:O	0.46	2.33	4	1
1:A:19:PHE:H	1:B:18:VAL:CG2	0.46	2.22	3	1
1:F:13:HIS:C	1:F:13:HIS:ND1	0.46	2.68	3	1
1:G:24:VAL:O	1:H:24:VAL:CG1	0.46	2.64	3	1
1:G:33:GLY:O	1:H:33:GLY:CA	0.46	2.63	3	1
1:B:34:LEU:H	1:B:34:LEU:HD23	0.46	1.64	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:12:VAL:HG13	1:G:20:PHE:CG	0.46	2.45	8	1
1:B:35:MET:SD	1:B:35:MET:C	0.46	2.93	10	2
1:I:8:SER:HB3	1:J:9:GLY:N	0.46	2.25	10	1
1:J:11:GLU:OE2	1:J:11:GLU:N	0.46	2.49	4	2
1:G:12:VAL:O	1:G:12:VAL:CG2	0.46	2.63	5	1
1:J:5:ARG:C	1:J:6:HIS:CG	0.46	2.89	6	1
1:B:35:MET:O	1:C:36:VAL:HB	0.46	2.11	7	1
1:C:31:ILE:O	1:D:32:ILE:O	0.46	2.34	7	1
1:C:33:GLY:O	1:D:34:LEU:CA	0.46	2.63	7	1
1:D:33:GLY:HA3	1:E:19:PHE:CE1	0.46	2.44	7	1
1:B:35:MET:HB2	1:C:35:MET:CA	0.46	2.24	3	1
1:G:40:VAL:C	1:H:40:VAL:CG2	0.46	2.83	3	1
1:A:9:GLY:O	1:A:10:TYR:CG	0.46	2.68	1	1
1:B:32:ILE:N	1:B:32:ILE:HD12	0.46	2.25	1	1
1:D:32:ILE:HG22	1:D:32:ILE:O	0.46	2.10	1	1
1:I:39:VAL:O	1:I:39:VAL:HG13	0.46	2.11	1	1
1:J:17:LEU:HD22	1:J:17:LEU:N	0.46	2.24	1	1
1:H:13:HIS:O	1:H:14:HIS:CB	0.46	2.63	8	1
1:E:20:PHE:CD1	1:E:22:GLU:OE1	0.46	2.69	10	1
1:J:16:LYS:N	1:J:16:LYS:HD3	0.46	2.25	10	1
1:D:40:VAL:HG12	1:D:40:VAL:O	0.46	2.10	6	2
1:D:26:SER:OG	1:E:28:LYS:N	0.46	2.47	3	1
1:F:21:ALA:HB2	1:G:34:LEU:HD11	0.46	1.88	8	1
1:H:35:MET:SD	1:H:35:MET:C	0.46	2.94	2	2
1:F:18:VAL:HG12	1:G:18:VAL:HG22	0.46	1.86	5	1
1:B:14:HIS:CD2	1:B:15:GLN:N	0.46	2.80	6	1
1:D:20:PHE:O	1:E:20:PHE:HB3	0.46	2.10	6	1
1:F:33:GLY:C	1:F:34:LEU:HG	0.46	2.31	6	1
1:H:6:HIS:O	1:H:7:ASP:O	0.46	2.33	6	1
1:I:17:LEU:HD23	1:J:17:LEU:O	0.46	2.10	6	1
1:J:9:GLY:O	1:J:10:TYR:CG	0.46	2.69	9	2
1:A:27:ASN:N	1:A:27:ASN:ND2	0.46	2.61	9	1
1:G:10:TYR:O	1:H:10:TYR:CD1	0.46	2.68	2	1
1:A:20:PHE:HA	1:B:20:PHE:CA	0.46	2.41	3	1
1:G:12:VAL:CG2	1:H:10:TYR:OH	0.46	2.63	3	1
1:G:10:TYR:OH	1:I:22:GLU:C	0.46	2.54	8	1
1:H:10:TYR:HB2	1:I:10:TYR:HB3	0.46	1.88	10	1
1:A:19:PHE:C	1:A:19:PHE:CD1	0.46	2.86	5	1
1:I:8:SER:O	1:J:9:GLY:CA	0.46	2.64	9	1
1:A:28:LYS:C	2:C:101:2PO:O3P	0.46	2.53	7	1
1:A:13:HIS:HA	1:B:14:HIS:HA	0.46	1.87	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:32:ILE:HG13	1:C:31:ILE:HG21	0.46	1.87	3	1
1:G:33:GLY:O	1:H:33:GLY:HA2	0.46	2.11	3	1
1:A:21:ALA:HB3	1:A:34:LEU:HB3	0.46	1.88	1	1
1:F:26:SER:O	1:G:27:ASN:O	0.46	2.34	8	1
1:A:19:PHE:HB2	1:B:19:PHE:CD2	0.46	2.46	10	1
1:A:23:ASP:O	1:A:24:VAL:C	0.46	2.54	10	1
1:C:19:PHE:CD2	1:C:36:VAL:HG11	0.46	2.46	10	1
1:G:31:ILE:C	1:G:32:ILE:CG1	0.46	2.84	10	1
1:J:13:HIS:O	1:J:14:HIS:ND1	0.46	2.48	10	2
1:H:18:VAL:CG1	1:H:20:PHE:CZ	0.46	2.98	9	1
1:A:34:LEU:CA	1:B:34:LEU:HG	0.46	2.30	7	2
1:F:36:VAL:HG12	1:G:36:VAL:CG2	0.46	2.41	7	1
1:H:13:HIS:CD2	1:H:14:HIS:N	0.46	2.81	7	1
1:F:23:ASP:N	1:F:23:ASP:OD1	0.46	2.48	2	1
1:C:32:ILE:HA	1:D:32:ILE:HB	0.46	1.87	3	1
1:E:39:VAL:O	1:E:40:VAL:O	0.46	2.34	3	2
1:H:10:TYR:OH	1:H:23:ASP:CA	0.46	2.64	10	1
1:F:19:PHE:N	1:F:19:PHE:HD2	0.46	2.08	9	1
1:H:13:HIS:HA	1:I:13:HIS:HB2	0.46	1.88	9	1
1:F:9:GLY:HA3	1:G:9:GLY:H	0.46	1.70	7	1
1:A:11:GLU:O	1:B:11:GLU:O	0.46	2.34	4	1
1:B:29:GLY:HA3	1:C:31:ILE:HB	0.46	1.86	3	1
1:D:27:ASN:O	1:D:28:LYS:HG3	0.46	2.10	3	1
1:H:12:VAL:HG12	1:I:13:HIS:C	0.46	2.31	10	1
1:G:39:VAL:CG1	1:G:40:VAL:N	0.46	2.78	5	1
1:A:16:LYS:O	1:B:14:HIS:CD2	0.46	2.69	4	1
1:H:35:MET:C	1:H:36:VAL:HG12	0.46	2.32	4	1
1:I:14:HIS:O	1:I:15:GLN:HG2	0.46	2.09	2	1
1:J:35:MET:C	1:J:35:MET:SD	0.46	2.94	1	1
1:C:36:VAL:CG1	1:D:36:VAL:HG22	0.46	2.40	2	4
1:A:36:VAL:CG1	1:B:36:VAL:HG22	0.46	2.41	1	4
1:I:20:PHE:CD2	1:I:22:GLU:OE2	0.46	2.68	10	1
1:H:12:VAL:H	1:I:11:GLU:HA	0.46	1.71	9	1
1:A:37:GLY:O	1:B:37:GLY:HA3	0.46	2.08	7	1
1:B:35:MET:CG	1:C:36:VAL:O	0.46	2.64	7	1
1:C:17:LEU:HB3	1:D:17:LEU:HA	0.46	1.86	7	1
1:I:6:HIS:ND1	1:I:6:HIS:O	0.46	2.49	2	1
1:J:27:ASN:HD22	1:J:28:LYS:N	0.46	2.09	2	1
1:A:35:MET:HB3	1:B:35:MET:N	0.46	2.26	3	1
1:B:22:GLU:OE1	1:B:22:GLU:O	0.46	2.34	3	1
1:H:15:GLN:OE1	1:H:18:VAL:CG2	0.45	2.64	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:22:GLU:CD	1:H:22:GLU:N	0.45	2.69	8	1
1:F:17:LEU:O	1:F:18:VAL:CB	0.45	2.65	4	3
1:H:12:VAL:HB	1:I:12:VAL:CA	0.45	2.40	10	1
1:G:36:VAL:HG12	1:H:36:VAL:HG22	0.45	1.87	5	2
1:A:16:LYS:HB2	1:B:16:LYS:N	0.45	2.26	7	1
1:B:39:VAL:H	1:C:39:VAL:HA	0.45	1.72	7	1
1:C:36:VAL:CA	1:D:36:VAL:O	0.45	2.62	7	1
1:E:24:VAL:O	1:E:25:GLY:C	0.45	2.55	7	1
1:B:19:PHE:CZ	1:C:20:PHE:HZ	0.45	2.27	3	1
1:C:23:ASP:O	1:C:24:VAL:C	0.45	2.54	3	1
1:I:20:PHE:CD1	1:J:19:PHE:O	0.45	2.69	3	1
1:D:34:LEU:CB	1:E:34:LEU:H	0.45	2.21	1	1
1:G:10:TYR:CE2	1:H:24:VAL:HG23	0.45	2.46	8	1
1:E:26:SER:OG	1:E:27:ASN:N	0.45	2.48	5	1
1:I:9:GLY:C	1:I:10:TYR:CD2	0.45	2.89	5	1
1:H:24:VAL:N	1:I:24:VAL:HG13	0.45	2.26	6	1
1:H:39:VAL:O	1:H:40:VAL:O	0.45	2.34	9	1
1:A:29:GLY:O	1:C:24:VAL:O	0.45	2.33	7	1
1:C:31:ILE:HD12	1:D:31:ILE:HG13	0.45	1.87	7	1
1:G:19:PHE:CD2	1:G:19:PHE:O	0.45	2.69	7	1
1:H:9:GLY:C	1:H:10:TYR:CD2	0.45	2.90	4	1
1:H:18:VAL:HG13	1:I:18:VAL:HG23	0.45	1.87	4	1
1:J:33:GLY:O	1:J:34:LEU:HD22	0.45	2.10	3	1
1:H:33:GLY:C	1:H:34:LEU:CD1	0.45	2.83	10	5
1:F:19:PHE:CE2	1:F:35:MET:N	0.45	2.84	6	1
1:I:17:LEU:CD2	1:J:17:LEU:O	0.45	2.64	6	1
1:J:19:PHE:O	1:J:20:PHE:CD2	0.45	2.69	7	1
1:C:35:MET:CB	1:H:40:VAL:OXT	0.45	2.64	3	1
1:A:21:ALA:HB2	1:B:34:LEU:CD2	0.45	2.38	1	1
1:C:39:VAL:O	1:C:40:VAL:O	0.45	2.35	8	3
1:H:17:LEU:HA	1:I:17:LEU:O	0.45	2.12	8	1
1:H:28:LYS:C	1:H:28:LYS:CD	0.45	2.85	8	1
1:B:18:VAL:CG1	1:B:20:PHE:CE2	0.45	3.00	5	3
1:B:7:ASP:OD1	1:B:7:ASP:N	0.45	2.47	9	1
1:A:22:GLU:O	1:B:22:GLU:CB	0.45	2.64	4	2
1:C:39:VAL:CG1	1:C:40:VAL:N	0.45	2.79	7	1
1:A:18:VAL:HG12	1:B:14:HIS:CE1	0.45	2.46	4	1
1:I:22:GLU:CD	1:I:22:GLU:N	0.45	2.70	4	1
1:G:39:VAL:O	1:G:40:VAL:OXT	0.45	2.35	2	1
1:B:18:VAL:HA	1:C:18:VAL:N	0.45	2.09	3	1
1:F:10:TYR:CD2	1:F:22:GLU:OE2	0.45	2.69	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:G:18:VAL:CG1	1:G:20:PHE:CE2	0.45	2.99	1	1
1:G:33:GLY:O	1:G:34:LEU:HG	0.45	2.11	10	1
1:G:6:HIS:CG	1:G:7:ASP:H	0.45	2.27	5	1
1:J:35:MET:SD	1:J:35:MET:C	0.45	2.95	5	1
1:B:5:ARG:O	1:B:6:HIS:O	0.45	2.34	9	3
1:A:19:PHE:CZ	1:A:36:VAL:CG2	0.45	3.00	9	1
1:G:8:SER:HA	2:G:101:2PO:P	0.45	2.52	9	1
1:G:11:GLU:C	1:G:11:GLU:OE1	0.45	2.54	9	1
1:H:27:ASN:OD1	1:H:28:LYS:O	0.45	2.35	9	1
1:A:26:SER:C	2:B:101:2PO:O3P	0.45	2.54	7	1
1:C:20:PHE:CB	1:D:20:PHE:CD1	0.45	2.98	7	1
1:J:12:VAL:CG2	1:J:20:PHE:CZ	0.45	3.00	7	1
1:D:20:PHE:HD2	1:D:34:LEU:HD21	0.45	1.62	3	1
1:F:33:GLY:O	1:G:33:GLY:CA	0.45	2.65	3	1
1:B:23:ASP:OD2	1:B:24:VAL:O	0.45	2.34	1	1
1:G:8:SER:N	2:G:101:2PO:O1P	0.45	2.49	5	1
1:A:8:SER:H	1:B:8:SER:HB3	0.45	1.71	9	1
1:A:23:ASP:OD1	1:B:24:VAL:CG2	0.45	2.65	7	1
1:D:31:ILE:O	1:E:32:ILE:CB	0.45	2.64	7	1
1:B:32:ILE:CD1	1:C:31:ILE:CG1	0.45	2.95	3	1
1:C:19:PHE:CE1	1:D:18:VAL:HA	0.45	2.44	3	1
1:B:34:LEU:HD12	1:B:35:MET:CA	0.45	2.40	1	1
1:I:19:PHE:C	1:I:19:PHE:CD2	0.45	2.90	6	1
1:A:31:ILE:C	1:A:32:ILE:HG23	0.45	2.31	7	1
1:B:34:LEU:HA	1:C:34:LEU:HG	0.45	1.87	7	1
1:D:18:VAL:O	1:D:19:PHE:CB	0.45	2.62	7	1
1:B:35:MET:SD	1:E:18:VAL:HG11	0.45	2.52	7	1
1:C:19:PHE:HA	1:D:19:PHE:O	0.45	2.12	4	1
1:A:12:VAL:HG23	1:B:13:HIS:O	0.45	2.11	3	1
1:C:36:VAL:CG1	1:D:36:VAL:O	0.45	2.65	3	1
1:G:39:VAL:C	1:G:40:VAL:CG2	0.45	2.85	3	1
1:B:2:ALA:O	1:B:4:PHE:CE1	0.45	2.70	8	1
1:F:28:LYS:CD	1:F:28:LYS:N	0.45	2.80	8	1
2:F:101:2PO:O3P	1:G:25:GLY:N	0.45	2.50	8	1
1:D:34:LEU:HD12	1:D:35:MET:N	0.45	2.27	1	2
1:G:8:SER:OG	1:G:10:TYR:CD1	0.45	2.70	9	1
1:B:31:ILE:HG12	1:D:22:GLU:O	0.45	2.10	7	1
1:B:34:LEU:C	1:B:34:LEU:CD1	0.45	2.63	7	1
1:G:34:LEU:O	1:G:35:MET:HG2	0.45	2.12	7	1
1:A:17:LEU:CA	1:B:14:HIS:NE2	0.45	2.80	4	1
1:A:35:MET:O	1:A:36:VAL:CG2	0.45	2.59	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:29:GLY:CA	1:C:30:ALA:O	0.45	2.64	3	1
1:D:19:PHE:O	1:E:19:PHE:O	0.45	2.35	3	1
1:D:31:ILE:CG2	1:E:30:ALA:O	0.45	2.57	1	1
1:G:19:PHE:CG	1:H:36:VAL:HG21	0.45	2.47	1	1
1:H:3:GLU:O	1:H:4:PHE:O	0.45	2.35	1	1
1:A:19:PHE:CD1	1:A:19:PHE:C	0.45	2.89	8	1
1:B:8:SER:HA	2:B:101:2PO:P	0.45	2.52	8	1
1:G:17:LEU:O	1:G:18:VAL:HB	0.45	2.11	8	1
1:I:13:HIS:CD2	1:I:14:HIS:O	0.45	2.70	10	1
1:G:20:PHE:H	1:H:20:PHE:HB3	0.45	1.70	6	1
1:B:13:HIS:ND1	1:B:13:HIS:N	0.45	2.64	7	1
1:D:35:MET:HG2	1:E:36:VAL:H	0.45	1.72	7	1
1:G:17:LEU:O	1:G:18:VAL:CG2	0.45	2.65	7	1
1:J:39:VAL:O	1:J:39:VAL:CG2	0.45	2.64	7	1
1:B:24:VAL:HG21	2:C:101:2PO:O2P	0.45	2.12	3	2
1:A:34:LEU:N	1:B:34:LEU:CG	0.45	2.80	3	1
1:A:33:GLY:HA3	1:B:34:LEU:HB2	0.45	1.88	3	1
1:C:19:PHE:CE1	1:D:36:VAL:HG11	0.45	2.47	1	1
1:G:24:VAL:HG11	1:H:10:TYR:CZ	0.45	2.47	1	1
1:I:33:GLY:C	1:I:34:LEU:CD1	0.45	2.84	10	2
1:D:39:VAL:O	1:D:40:VAL:OXT	0.45	2.35	6	1
1:E:29:GLY:C	1:E:31:ILE:N	0.45	2.71	6	1
1:F:23:ASP:CA	1:G:23:ASP:O	0.45	2.65	9	2
1:F:24:VAL:CG2	1:G:23:ASP:O	0.45	2.65	7	1
1:H:38:GLY:HA2	1:I:38:GLY:O	0.45	2.12	7	1
1:C:17:LEU:O	1:C:18:VAL:HG23	0.45	2.12	4	1
1:A:33:GLY:C	1:B:34:LEU:CB	0.45	2.85	3	1
1:D:22:GLU:O	1:E:22:GLU:HG2	0.45	2.12	3	1
1:F:27:ASN:CG	1:F:28:LYS:N	0.45	2.71	1	1
1:G:14:HIS:CG	1:G:18:VAL:HG21	0.44	2.47	5	1
1:J:5:ARG:HE	1:J:5:ARG:N	0.44	2.10	6	1
1:H:15:GLN:OE1	1:I:15:GLN:NE2	0.44	2.50	9	1
1:A:19:PHE:CD2	1:A:20:PHE:O	0.44	2.70	7	1
1:G:17:LEU:C	1:G:18:VAL:CG2	0.44	2.75	7	1
1:C:27:ASN:ND2	1:D:31:ILE:HD13	0.44	2.26	3	1
1:D:34:LEU:O	1:D:35:MET:HG3	0.44	2.12	3	1
1:E:30:ALA:CB	1:E:31:ILE:HD12	0.44	2.42	3	1
1:I:16:LYS:O	1:J:17:LEU:HB2	0.44	2.12	3	1
1:B:22:GLU:O	1:C:22:GLU:CB	0.44	2.65	1	1
1:G:7:ASP:O	1:G:8:SER:C	0.44	2.54	8	1
1:C:35:MET:C	1:C:35:MET:SD	0.44	2.96	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:34:LEU:C	1:G:34:LEU:O	0.44	2.56	10	1
1:G:13:HIS:CG	1:H:14:HIS:O	0.44	2.71	10	1
1:H:10:TYR:CD2	1:I:10:TYR:CD2	0.44	3.05	5	1
1:C:33:GLY:O	1:D:34:LEU:CD2	0.44	2.63	7	1
1:F:24:VAL:CG2	1:G:25:GLY:N	0.44	2.80	3	1
1:H:5:ARG:CA	1:H:5:ARG:NE	0.44	2.80	3	1
1:G:19:PHE:CD1	1:H:19:PHE:CD2	0.44	3.05	8	1
1:G:1:ASP:O	1:G:6:HIS:NE2	0.44	2.50	8	1
1:F:15:GLN:CB	1:G:15:GLN:HE21	0.44	2.25	10	1
1:H:15:GLN:CG	1:H:16:LYS:N	0.44	2.80	10	1
1:I:14:HIS:CE1	1:I:15:GLN:C	0.44	2.91	10	1
1:G:19:PHE:CD2	1:G:36:VAL:HG11	0.44	2.47	5	1
1:I:39:VAL:O	1:I:40:VAL:OXT	0.44	2.35	5	1
1:G:22:GLU:OE1	1:G:22:GLU:C	0.44	2.56	6	1
1:A:36:VAL:HG13	1:B:36:VAL:HG23	0.44	1.83	9	1
1:G:14:HIS:O	1:G:15:GLN:OE1	0.44	2.36	9	1
1:A:31:ILE:C	1:A:32:ILE:CG2	0.44	2.85	7	1
1:B:10:TYR:O	1:B:22:GLU:OE2	0.44	2.36	7	1
1:B:36:VAL:CA	1:C:36:VAL:O	0.44	2.65	7	1
1:B:31:ILE:C	1:B:32:ILE:CG1	0.44	2.75	3	2
1:E:22:GLU:OE2	1:E:23:ASP:O	0.44	2.35	3	1
1:G:24:VAL:H	1:H:24:VAL:HG11	0.44	1.70	3	1
1:H:14:HIS:NE2	1:H:18:VAL:HG11	0.44	2.28	3	1
1:H:4:PHE:CD2	1:H:5:ARG:NH1	0.44	2.84	3	1
1:C:32:ILE:CA	1:D:32:ILE:O	0.44	2.65	1	1
1:H:7:ASP:O	1:H:8:SER:O	0.44	2.35	1	1
1:I:22:GLU:O	1:J:23:ASP:O	0.44	2.35	1	1
1:F:12:VAL:N	1:G:11:GLU:HG2	0.44	2.28	8	1
1:G:33:GLY:C	1:G:34:LEU:HD23	0.44	2.32	8	1
1:H:14:HIS:O	1:H:15:GLN:HB3	0.44	2.12	8	1
1:H:9:GLY:O	1:I:9:GLY:C	0.44	2.53	8	1
1:I:16:LYS:O	1:J:16:LYS:CB	0.44	2.65	4	4
1:I:15:GLN:O	1:I:16:LYS:O	0.44	2.36	10	2
1:F:14:HIS:O	1:F:15:GLN:HB2	0.44	2.11	9	1
1:J:32:ILE:HD12	1:J:32:ILE:N	0.44	2.27	9	1
1:D:18:VAL:HG22	1:D:19:PHE:H	0.44	1.61	7	1
1:I:34:LEU:C	1:I:35:MET:SD	0.44	2.95	2	1
1:A:15:GLN:O	1:A:16:LYS:O	0.44	2.35	3	1
1:B:32:ILE:CG1	1:C:31:ILE:HG13	0.44	2.42	3	1
1:B:36:VAL:CG1	1:C:36:VAL:HG22	0.44	2.42	8	3
1:H:17:LEU:HD23	1:H:18:VAL:H	0.44	1.73	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:CD1	1:A:36:VAL:HG21	0.44	2.47	9	1
1:H:5:ARG:O	1:H:6:HIS:O	0.44	2.34	9	1
1:I:7:ASP:O	1:J:6:HIS:O	0.44	2.35	9	1
1:A:13:HIS:CG	1:A:14:HIS:N	0.44	2.85	7	1
1:D:22:GLU:HA	1:E:22:GLU:HB2	0.44	1.87	7	1
1:I:23:ASP:CG	1:J:27:ASN:HD21	0.44	2.15	7	1
1:A:20:PHE:HB2	1:B:34:LEU:HA	0.44	1.88	3	1
1:C:21:ALA:HB3	1:D:22:GLU:OE1	0.44	2.11	3	1
1:D:22:GLU:HG3	1:D:23:ASP:N	0.44	2.28	3	1
1:F:35:MET:O	1:G:35:MET:HB2	0.44	2.10	3	1
1:A:8:SER:N	2:A:101:2PO:O3P	0.44	2.50	1	1
1:B:11:GLU:C	1:B:12:VAL:CG2	0.44	2.78	1	1
1:F:12:VAL:O	1:G:13:HIS:HB3	0.44	2.12	8	1
1:H:12:VAL:O	1:I:13:HIS:O	0.44	2.35	10	1
1:G:23:ASP:OD1	1:H:27:ASN:ND2	0.44	2.50	10	1
1:F:28:LYS:N	1:F:28:LYS:CD	0.44	2.80	5	2
1:D:36:VAL:HG12	1:E:36:VAL:CG2	0.44	2.43	9	1
1:B:20:PHE:HA	1:C:20:PHE:CE1	0.44	2.43	7	1
1:B:31:ILE:O	1:C:32:ILE:HB	0.44	2.11	7	1
1:C:19:PHE:CZ	1:C:34:LEU:O	0.44	2.70	7	1
1:B:34:LEU:HB2	1:C:34:LEU:CD1	0.44	2.42	7	1
1:G:34:LEU:C	1:G:35:MET:CG	0.44	2.86	7	1
1:A:17:LEU:C	1:A:18:VAL:HG12	0.44	2.32	3	1
1:A:32:ILE:HG21	1:F:40:VAL:C	0.44	2.33	3	1
1:G:7:ASP:O	1:G:8:SER:OG	0.44	2.36	3	1
1:I:35:MET:CB	1:J:35:MET:CB	0.44	2.93	3	1
1:J:10:TYR:C	1:J:11:GLU:CD	0.44	2.75	1	1
1:C:22:GLU:OE1	1:D:22:GLU:OE2	0.44	2.35	10	1
1:G:8:SER:O	1:H:8:SER:CB	0.44	2.66	10	1
1:H:10:TYR:HB2	1:I:11:GLU:N	0.44	2.28	10	1
1:B:23:ASP:CA	1:C:23:ASP:O	0.44	2.66	9	1
1:H:27:ASN:HD22	1:I:26:SER:CB	0.44	2.26	9	1
1:H:26:SER:N	1:I:3:GLU:OE2	0.44	2.51	9	1
1:A:8:SER:C	2:A:101:2PO:P	0.44	2.96	7	1
1:A:31:ILE:C	1:C:23:ASP:HB2	0.44	2.33	7	1
1:B:11:GLU:CB	1:B:20:PHE:CD1	0.44	3.00	7	1
1:D:33:GLY:C	1:E:19:PHE:CZ	0.44	2.91	7	1
1:H:23:ASP:O	1:H:24:VAL:C	0.44	2.54	7	1
1:H:14:HIS:C	1:I:15:GLN:NE2	0.44	2.71	2	1
1:J:13:HIS:O	1:J:14:HIS:CD2	0.44	2.70	2	1
1:A:17:LEU:H	1:B:17:LEU:N	0.44	2.02	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:32:ILE:HG12	1:C:32:ILE:C	0.44	2.33	3	1
1:A:28:LYS:CB	1:A:28:LYS:NZ	0.44	2.80	1	1
1:C:20:PHE:CE2	1:D:20:PHE:CE2	0.44	3.04	1	1
1:J:35:MET:O	1:J:35:MET:SD	0.44	2.76	1	1
1:J:24:VAL:HG22	1:J:25:GLY:H	0.44	1.69	10	1
1:F:19:PHE:CE1	1:F:36:VAL:CG1	0.44	3.01	5	1
1:G:13:HIS:CE1	1:G:14:HIS:O	0.44	2.71	9	1
1:B:24:VAL:C	1:B:26:SER:H	0.44	2.17	7	1
1:H:15:GLN:O	1:I:15:GLN:OE1	0.44	2.36	2	1
1:A:23:ASP:N	1:B:27:ASN:HB3	0.44	2.28	3	1
1:A:33:GLY:C	1:B:34:LEU:CG	0.44	2.86	3	1
1:H:26:SER:O	1:H:26:SER:OG	0.44	2.35	3	1
1:B:12:VAL:O	1:B:13:HIS:CB	0.44	2.65	1	1
1:A:14:HIS:ND1	1:A:18:VAL:CG2	0.44	2.81	8	1
1:I:10:TYR:CD1	1:J:9:GLY:N	0.44	2.86	8	1
1:I:16:LYS:O	1:J:16:LYS:HB3	0.44	2.12	4	3
1:B:10:TYR:C	1:B:10:TYR:CD1	0.44	2.90	10	1
1:B:13:HIS:N	1:B:13:HIS:CD2	0.44	2.86	10	1
1:C:40:VAL:O	1:D:40:VAL:O	0.44	2.36	5	1
1:G:35:MET:SD	1:G:35:MET:C	0.44	2.96	6	1
1:H:20:PHE:CE1	1:I:20:PHE:CD2	0.44	3.06	6	1
1:A:17:LEU:CD2	1:A:38:GLY:O	0.44	2.65	7	1
1:C:29:GLY:C	1:D:27:ASN:HD22	0.44	2.16	7	1
1:E:27:ASN:ND2	1:E:30:ALA:O	0.44	2.51	7	1
1:I:7:ASP:CG	1:J:10:TYR:CD1	0.44	2.92	4	1
1:A:14:HIS:N	1:B:14:HIS:HA	0.44	2.27	3	1
1:D:29:GLY:CA	1:E:31:ILE:HB	0.44	2.40	3	1
1:A:14:HIS:ND1	1:A:15:GLN:N	0.43	2.65	10	1
1:H:6:HIS:CG	1:H:7:ASP:N	0.43	2.86	5	1
1:F:24:VAL:O	1:G:24:VAL:CG1	0.43	2.65	9	1
1:A:39:VAL:CG2	1:B:17:LEU:HD23	0.43	2.42	7	1
1:B:14:HIS:CE1	1:B:18:VAL:CB	0.43	3.01	7	1
1:B:18:VAL:CG2	1:B:19:PHE:N	0.43	2.77	7	1
1:B:31:ILE:CD1	1:D:23:ASP:C	0.43	2.86	7	1
1:J:12:VAL:O	1:J:13:HIS:HB3	0.43	2.12	4	1
1:I:8:SER:H	1:J:8:SER:C	0.43	2.17	4	1
1:A:17:LEU:N	1:B:17:LEU:H	0.43	2.02	3	1
1:B:27:ASN:OD1	1:C:32:ILE:CD1	0.43	2.66	3	1
1:C:19:PHE:CZ	1:D:20:PHE:N	0.43	2.86	3	1
1:A:10:TYR:O	1:B:10:TYR:CD1	0.43	2.71	1	1
1:I:13:HIS:CB	1:J:13:HIS:H	0.43	2.26	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:24:VAL:CG1	1:B:25:GLY:N	0.43	2.76	5	2
1:B:10:TYR:N	1:B:10:TYR:CD1	0.43	2.86	6	1
1:J:11:GLU:CD	1:J:12:VAL:H	0.43	2.15	9	1
1:B:23:ASP:OD2	1:B:27:ASN:CG	0.43	2.56	7	1
1:J:27:ASN:ND2	1:J:28:LYS:N	0.43	2.65	2	1
1:A:19:PHE:H	1:B:18:VAL:HG22	0.43	1.73	3	1
1:A:12:VAL:O	1:B:13:HIS:C	0.43	2.55	3	1
1:H:10:TYR:CE2	1:H:12:VAL:CG1	0.43	3.02	3	1
1:B:8:SER:CB	2:B:101:2PO:O3P	0.43	2.67	8	1
1:E:31:ILE:O	1:E:32:ILE:CD1	0.43	2.62	8	1
1:I:10:TYR:CZ	1:J:11:GLU:CG	0.43	3.01	8	1
1:C:19:PHE:CZ	1:D:34:LEU:HD12	0.43	2.48	9	1
1:B:24:VAL:HG22	1:B:25:GLY:N	0.43	2.28	7	1
1:A:21:ALA:HB2	1:B:34:LEU:HD21	0.43	1.89	4	1
1:H:22:GLU:N	1:H:22:GLU:CD	0.43	2.71	2	1
1:I:10:TYR:O	1:J:10:TYR:CG	0.43	2.71	2	1
1:D:20:PHE:CD2	1:D:36:VAL:HB	0.43	2.48	3	1
1:F:40:VAL:O	1:F:40:VAL:HG23	0.43	2.13	3	1
1:C:19:PHE:CD2	1:D:36:VAL:HG21	0.43	2.48	5	1
1:D:24:VAL:HG13	1:E:25:GLY:O	0.43	2.13	5	1
1:I:14:HIS:N	1:I:14:HIS:ND1	0.43	2.62	5	1
1:I:9:GLY:C	1:J:9:GLY:HA3	0.43	2.32	9	1
1:A:8:SER:CB	2:A:101:2PO:O3P	0.43	2.65	7	1
1:F:36:VAL:HG12	1:G:36:VAL:HG23	0.43	1.90	7	1
1:F:16:LYS:O	1:G:16:LYS:HB2	0.43	2.12	2	1
1:A:15:GLN:O	1:B:15:GLN:HB3	0.43	2.13	3	1
1:A:24:VAL:CG1	1:B:23:ASP:O	0.43	2.67	3	1
1:C:39:VAL:O	1:C:40:VAL:C	0.43	2.56	3	1
1:E:20:PHE:HD2	1:E:20:PHE:N	0.43	2.00	3	1
1:H:39:VAL:HG12	1:H:40:VAL:H	0.43	1.65	3	1
1:H:4:PHE:CD2	1:H:4:PHE:N	0.43	2.86	3	1
1:C:20:PHE:CZ	1:D:20:PHE:CD2	0.43	3.05	1	1
1:C:27:ASN:CG	1:C:28:LYS:N	0.43	2.72	8	1
1:D:28:LYS:NZ	1:E:28:LYS:O	0.43	2.40	8	1
1:C:2:ALA:O	1:C:3:GLU:O	0.43	2.37	10	1
1:H:14:HIS:HB3	1:H:18:VAL:HG21	0.43	1.91	5	1
1:H:7:ASP:O	1:H:8:SER:OG	0.43	2.36	5	1
1:F:38:GLY:H	1:G:37:GLY:CA	0.43	2.27	6	1
1:I:4:PHE:N	1:I:4:PHE:CD1	0.43	2.86	6	1
1:A:21:ALA:HB3	1:B:21:ALA:CA	0.43	2.43	7	1
1:A:27:ASN:CA	1:C:24:VAL:HB	0.43	2.40	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:23:ASP:OD2	1:H:26:SER:O	0.43	2.36	7	1
1:F:17:LEU:HA	1:G:17:LEU:O	0.43	2.14	4	1
1:A:9:GLY:HA2	1:B:9:GLY:O	0.43	2.13	3	1
1:C:35:MET:SD	1:C:35:MET:C	0.43	2.96	3	1
1:G:36:VAL:CG2	1:H:36:VAL:N	0.43	2.53	3	1
1:C:20:PHE:H	1:D:20:PHE:HB3	0.43	1.73	8	2
1:B:19:PHE:CD2	1:B:36:VAL:HG11	0.43	2.47	10	1
1:J:18:VAL:CG2	1:J:19:PHE:N	0.43	2.58	10	1
1:D:28:LYS:O	1:D:29:GLY:C	0.43	2.57	5	1
1:B:5:ARG:HE	1:B:6:HIS:H	0.43	1.57	6	1
1:A:39:VAL:HG23	1:B:40:VAL:N	0.43	2.24	9	1
1:E:22:GLU:O	1:E:23:ASP:OD1	0.43	2.36	9	1
1:G:36:VAL:HG23	1:H:36:VAL:HG23	0.43	1.90	9	1
1:J:39:VAL:O	1:J:40:VAL:OXT	0.43	2.37	9	1
1:A:12:VAL:HG13	1:B:11:GLU:O	0.43	2.13	7	1
1:B:19:PHE:CD2	1:C:19:PHE:HA	0.43	2.48	7	1
1:D:39:VAL:O	1:E:40:VAL:N	0.43	2.52	7	1
1:G:5:ARG:C	1:G:6:HIS:CG	0.43	2.92	7	1
1:B:4:PHE:CD2	1:B:4:PHE:N	0.43	2.86	4	1
1:A:31:ILE:H	1:B:31:ILE:CA	0.43	2.21	3	1
1:A:8:SER:CB	1:B:24:VAL:HG22	0.43	2.44	1	1
1:A:8:SER:OG	1:B:3:GLU:CG	0.43	2.67	1	1
1:D:20:PHE:O	1:E:20:PHE:HB2	0.43	2.14	1	1
1:I:10:TYR:CD2	1:I:11:GLU:N	0.43	2.86	1	1
1:E:27:ASN:N	1:E:27:ASN:ND2	0.43	2.67	8	1
1:G:14:HIS:CG	1:G:18:VAL:HG12	0.43	2.48	8	1
1:H:12:VAL:HG22	1:I:12:VAL:HG12	0.43	1.91	5	1
1:H:7:ASP:N	1:I:6:HIS:CB	0.43	2.82	6	1
1:G:10:TYR:CE1	1:H:10:TYR:CB	0.43	3.01	9	1
1:H:5:ARG:NH1	1:I:4:PHE:CD2	0.43	2.87	7	1
1:F:17:LEU:O	1:F:18:VAL:CG2	0.43	2.66	4	1
1:G:34:LEU:HD23	1:G:34:LEU:H	0.43	1.67	4	1
1:A:8:SER:CA	2:A:101:2PO:O1P	0.43	2.67	3	1
1:B:32:ILE:HD13	1:B:33:GLY:N	0.43	2.27	3	1
1:A:37:GLY:HA3	1:B:36:VAL:HG12	0.43	1.91	3	1
1:E:19:PHE:CB	1:E:20:PHE:CD2	0.43	3.02	3	1
1:G:40:VAL:OXT	1:H:40:VAL:CG2	0.43	2.66	3	1
1:B:6:HIS:HD1	1:B:6:HIS:C	0.43	2.17	8	1
1:F:12:VAL:O	1:G:13:HIS:CB	0.43	2.67	8	1
1:G:14:HIS:O	1:H:14:HIS:O	0.43	2.36	8	1
1:G:30:ALA:CB	1:H:30:ALA:O	0.43	2.65	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:11:GLU:OE1	1:I:12:VAL:CG2	0.43	2.67	8	1
1:G:4:PHE:CD2	1:G:5:ARG:N	0.43	2.87	10	1
1:F:19:PHE:C	1:F:19:PHE:CD1	0.43	2.88	6	1
1:I:24:VAL:O	1:J:25:GLY:O	0.43	2.36	6	1
1:I:40:VAL:O	1:J:40:VAL:OXT	0.43	2.36	6	1
1:J:5:ARG:O	1:J:24:VAL:CG1	0.43	2.66	6	1
1:F:10:TYR:CD2	1:F:10:TYR:N	0.43	2.87	9	1
1:J:14:HIS:CG	1:J:15:GLN:H	0.43	2.32	9	1
1:A:19:PHE:CE1	1:A:36:VAL:CG1	0.43	3.01	4	1
1:C:36:VAL:HG22	1:C:37:GLY:N	0.43	2.24	3	1
1:H:36:VAL:HG23	1:I:36:VAL:CG2	0.43	2.41	3	1
1:J:17:LEU:HD13	1:J:18:VAL:N	0.43	2.28	5	1
1:B:36:VAL:CG2	1:C:36:VAL:H	0.43	2.19	9	1
1:F:11:GLU:CA	1:F:11:GLU:OE1	0.43	2.66	9	1
1:F:24:VAL:H	1:G:24:VAL:HG13	0.43	1.73	9	1
1:G:39:VAL:CG1	1:H:39:VAL:HG13	0.43	2.44	9	1
1:I:36:VAL:HG12	1:J:36:VAL:CG2	0.43	2.43	9	1
1:A:33:GLY:N	1:C:21:ALA:HA	0.43	2.28	7	1
1:I:7:ASP:O	1:I:8:SER:O	0.43	2.36	7	2
1:F:14:HIS:C	1:G:14:HIS:NE2	0.43	2.72	2	1
1:I:10:TYR:H	1:J:10:TYR:HB3	0.43	1.74	2	1
1:A:29:GLY:O	1:B:29:GLY:N	0.43	2.50	3	1
1:B:32:ILE:HG12	1:C:31:ILE:HG13	0.43	1.91	3	1
1:B:32:ILE:HG13	1:C:31:ILE:CG2	0.43	2.44	3	1
1:D:34:LEU:HA	1:E:34:LEU:H	0.43	1.74	3	1
1:G:36:VAL:CB	1:H:36:VAL:H	0.43	2.23	3	1
1:I:10:TYR:H	1:J:9:GLY:HA2	0.43	1.73	3	1
1:J:3:GLU:O	1:J:4:PHE:O	0.43	2.36	5	1
1:F:11:GLU:N	1:F:11:GLU:CD	0.43	2.73	6	1
1:F:10:TYR:CE1	1:F:24:VAL:HG11	0.43	2.49	6	1
1:A:12:VAL:HG22	1:B:10:TYR:OH	0.43	2.14	9	1
1:G:17:LEU:O	1:G:18:VAL:HG23	0.43	2.13	9	1
1:H:10:TYR:O	1:I:10:TYR:CD1	0.43	2.72	7	1
1:H:11:GLU:OE2	1:I:13:HIS:CD2	0.43	2.72	7	1
1:I:23:ASP:OD2	1:I:27:ASN:OD1	0.43	2.37	7	1
1:A:39:VAL:CG2	1:B:39:VAL:HG23	0.43	2.44	4	1
1:C:19:PHE:CD1	1:C:20:PHE:N	0.43	2.87	4	1
1:H:14:HIS:CE1	1:H:18:VAL:HG11	0.43	2.48	3	1
1:I:10:TYR:H	1:J:10:TYR:N	0.43	2.11	3	1
1:B:11:GLU:O	1:B:11:GLU:OE2	0.42	2.36	8	1
1:B:4:PHE:O	1:B:5:ARG:O	0.42	2.37	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:G:10:TYR:HB3	1:H:11:GLU:HA	0.42	1.91	8	1
1:B:23:ASP:C	1:B:23:ASP:OD1	0.42	2.57	10	1
1:C:31:ILE:O	1:D:31:ILE:N	0.42	2.52	5	1
1:A:14:HIS:CB	1:A:18:VAL:HG21	0.42	2.44	6	1
1:F:12:VAL:HG23	1:G:14:HIS:CE1	0.42	2.49	6	1
1:H:15:GLN:HE22	1:I:15:GLN:HE21	0.42	1.56	9	1
1:I:12:VAL:C	1:J:11:GLU:HB3	0.42	2.34	9	1
1:A:18:VAL:C	1:B:18:VAL:HG11	0.42	2.24	7	1
1:A:35:MET:CB	1:B:19:PHE:CG	0.42	2.93	7	1
1:B:8:SER:HB3	2:B:101:2PO:O1P	0.42	2.14	7	1
1:D:34:LEU:HG	1:D:34:LEU:O	0.42	2.14	7	1
1:F:24:VAL:O	1:G:25:GLY:O	0.42	2.36	7	1
1:F:19:PHE:CE1	1:F:34:LEU:HB2	0.42	2.49	7	1
1:H:19:PHE:CD2	1:H:36:VAL:HG21	0.42	2.48	7	1
1:A:28:LYS:O	1:B:27:ASN:O	0.42	2.35	4	1
1:A:39:VAL:HG23	1:B:39:VAL:HG23	0.42	1.91	4	1
1:H:11:GLU:C	1:H:11:GLU:OE1	0.42	2.57	4	1
1:I:12:VAL:HG13	1:J:11:GLU:HB3	0.42	1.90	2	1
1:D:17:LEU:O	1:D:18:VAL:HG22	0.42	2.14	3	1
1:C:31:ILE:N	1:D:31:ILE:HG21	0.42	2.25	3	1
1:G:12:VAL:CG1	1:H:10:TYR:OH	0.42	2.67	3	1
1:I:13:HIS:O	1:I:15:GLN:OE1	0.42	2.37	3	1
1:H:7:ASP:N	1:H:7:ASP:OD1	0.42	2.51	1	1
1:I:39:VAL:O	1:I:39:VAL:CG1	0.42	2.67	1	1
2:F:101:2PO:O3P	1:G:24:VAL:C	0.42	2.58	8	1
1:B:19:PHE:CE2	1:B:36:VAL:CG1	0.42	3.02	10	1
1:A:28:LYS:CA	1:C:25:GLY:H	0.42	2.27	7	1
1:B:22:GLU:H	1:C:22:GLU:HB2	0.42	1.74	7	1
1:B:35:MET:CB	1:C:19:PHE:CD1	0.42	3.02	7	1
1:B:27:ASN:O	1:C:27:ASN:OD1	0.42	2.37	7	1
1:D:21:ALA:HB3	1:E:21:ALA:HA	0.42	1.90	7	1
1:E:22:GLU:OE1	1:F:40:VAL:OXT	0.42	2.37	7	1
1:I:36:VAL:HA	1:J:36:VAL:O	0.42	2.14	7	1
1:E:24:VAL:HG12	1:E:25:GLY:N	0.42	2.29	2	1
1:A:29:GLY:O	1:B:29:GLY:C	0.42	2.57	3	1
1:A:8:SER:O	2:A:101:2PO:O3P	0.42	2.36	1	1
1:G:19:PHE:HA	1:H:19:PHE:O	0.42	2.14	1	1
1:A:8:SER:HB2	2:A:101:2PO:O2P	0.42	2.15	8	1
1:D:19:PHE:CG	1:E:36:VAL:HG21	0.42	2.50	8	1
1:J:12:VAL:O	1:J:12:VAL:HG13	0.42	2.14	8	1
1:E:35:MET:C	1:E:35:MET:SD	0.42	2.97	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:G:22:GLU:OE1	1:H:21:ALA:O	0.42	2.38	10	1
1:G:24:VAL:CG1	1:G:25:GLY:N	0.42	2.80	5	1
1:G:2:ALA:O	1:G:4:PHE:CE1	0.42	2.72	6	1
1:G:13:HIS:O	1:G:14:HIS:CD2	0.42	2.72	9	1
1:I:13:HIS:CD2	1:I:14:HIS:ND1	0.42	2.87	9	1
1:G:28:LYS:HD2	1:G:28:LYS:N	0.42	2.29	4	2
1:G:12:VAL:HB	1:H:12:VAL:CB	0.42	2.43	7	1
1:H:36:VAL:HG23	1:H:37:GLY:N	0.42	2.29	4	1
1:B:24:VAL:O	1:C:25:GLY:O	0.42	2.37	1	2
1:B:29:GLY:HA3	1:C:31:ILE:CD1	0.42	2.44	3	1
1:I:33:GLY:O	1:I:34:LEU:HD23	0.42	2.13	3	1
1:D:24:VAL:HG11	1:E:26:SER:CA	0.42	2.44	1	1
1:G:23:ASP:OD1	1:G:27:ASN:OD1	0.42	2.36	8	1
1:H:14:HIS:C	1:H:15:GLN:CG	0.42	2.87	8	1
1:H:8:SER:C	2:H:101:2PO:P	0.42	2.97	8	1
1:I:11:GLU:HA	1:J:11:GLU:CA	0.42	2.44	8	2
1:F:40:VAL:OXT	1:G:40:VAL:O	0.42	2.38	10	1
1:H:1:ASP:O	1:H:1:ASP:OD1	0.42	2.37	10	1
1:H:9:GLY:HA2	1:I:9:GLY:O	0.42	2.15	10	1
1:F:39:VAL:O	1:F:39:VAL:HG13	0.42	2.14	6	1
1:B:30:ALA:CA	1:D:24:VAL:HG23	0.42	2.44	7	1
1:C:1:ASP:CG	1:C:2:ALA:N	0.42	2.73	4	1
1:H:6:HIS:C	1:H:8:SER:H	0.42	2.18	2	1
1:A:37:GLY:O	1:B:37:GLY:C	0.42	2.58	3	1
1:G:34:LEU:CA	1:H:34:LEU:O	0.42	2.67	3	1
1:B:28:LYS:CG	1:C:26:SER:OG	0.42	2.67	1	1
1:G:8:SER:N	1:H:8:SER:HA	0.42	2.29	1	1
1:I:14:HIS:O	1:J:15:GLN:CG	0.42	2.67	1	1
1:C:23:ASP:O	1:C:23:ASP:OD1	0.42	2.37	5	1
1:G:14:HIS:CD2	1:G:18:VAL:HG21	0.42	2.49	5	1
1:H:2:ALA:C	1:H:4:PHE:N	0.42	2.72	5	1
1:I:6:HIS:N	1:I:6:HIS:ND1	0.42	2.63	9	1
1:A:38:GLY:C	1:B:17:LEU:HD21	0.42	2.35	7	1
1:B:17:LEU:HB3	1:C:17:LEU:HA	0.42	1.91	7	1
1:F:23:ASP:OD2	1:G:27:ASN:OD1	0.42	2.37	7	1
1:I:2:ALA:O	1:I:3:GLU:O	0.42	2.38	4	2
1:J:1:ASP:CG	1:J:2:ALA:N	0.42	2.71	4	1
1:E:23:ASP:CG	1:E:26:SER:O	0.42	2.58	3	1
1:I:35:MET:O	1:I:36:VAL:CB	0.42	2.65	3	1
1:B:8:SER:HB3	2:B:101:2PO:O3P	0.42	2.14	8	1
1:G:33:GLY:C	1:G:34:LEU:HD12	0.42	2.35	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:24:VAL:CG2	1:H:25:GLY:H	0.42	2.23	5	2
1:D:23:ASP:HA	1:E:23:ASP:O	0.42	2.14	5	1
1:D:23:ASP:OD2	1:E:27:ASN:OD1	0.42	2.38	5	1
1:G:13:HIS:O	1:G:13:HIS:CG	0.42	2.73	6	1
1:J:11:GLU:O	1:J:12:VAL:C	0.42	2.58	9	1
1:B:8:SER:HA	2:B:101:2PO:O2P	0.42	2.14	7	1
1:H:13:HIS:N	1:H:13:HIS:HD1	0.42	2.13	4	1
1:I:40:VAL:O	1:J:40:VAL:O	0.42	2.38	2	1
1:I:12:VAL:CG2	1:J:13:HIS:H	0.42	2.27	2	1
1:A:19:PHE:CD1	1:A:36:VAL:CG1	0.42	3.02	1	1
1:F:19:PHE:O	1:F:20:PHE:CG	0.42	2.73	1	1
1:G:7:ASP:O	1:H:8:SER:OG	0.42	2.38	8	1
1:I:10:TYR:CD1	1:J:8:SER:HA	0.42	2.49	8	1
1:A:8:SER:HA	2:A:101:2PO:P	0.42	2.55	9	2
1:D:23:ASP:OD2	1:D:27:ASN:ND2	0.42	2.53	10	1
1:F:9:GLY:N	2:F:101:2PO:P	0.42	2.91	10	1
1:I:33:GLY:O	1:I:34:LEU:HG	0.42	2.15	10	2
1:I:6:HIS:O	1:I:7:ASP:O	0.42	2.37	5	1
1:A:19:PHE:CZ	1:A:36:VAL:HG23	0.42	2.49	9	1
1:B:23:ASP:OD1	1:B:23:ASP:O	0.42	2.37	9	1
1:A:12:VAL:CG2	1:B:12:VAL:C	0.42	2.88	7	1
1:B:31:ILE:CG2	1:D:21:ALA:C	0.42	2.88	7	1
1:B:22:GLU:CD	1:C:22:GLU:OE2	0.42	2.57	7	1
1:D:27:ASN:ND2	1:D:28:LYS:N	0.42	2.67	7	1
1:G:23:ASP:CG	1:H:27:ASN:HD22	0.42	2.17	7	1
1:D:28:LYS:N	1:D:28:LYS:CD	0.42	2.82	4	1
1:I:8:SER:H	1:J:9:GLY:CA	0.42	2.26	4	1
1:D:19:PHE:CG	1:D:20:PHE:N	0.42	2.88	2	1
1:H:6:HIS:O	1:I:8:SER:OG	0.42	2.38	2	1
1:I:38:GLY:H	1:J:38:GLY:HA3	0.42	1.75	3	1
1:C:36:VAL:HG23	1:D:36:VAL:O	0.42	2.14	1	1
1:A:19:PHE:HA	1:B:19:PHE:O	0.42	2.15	8	1
1:B:19:PHE:CE1	1:B:34:LEU:HD12	0.42	2.48	10	1
1:F:19:PHE:HA	1:G:19:PHE:O	0.42	2.14	10	1
1:D:23:ASP:CA	2:D:101:2PO:O3P	0.42	2.68	5	1
1:G:35:MET:O	1:G:36:VAL:HG23	0.42	2.15	6	1
1:G:34:LEU:HA	1:H:34:LEU:O	0.42	2.14	7	1
1:H:8:SER:CB	2:H:101:2PO:O3P	0.42	2.67	7	1
1:D:30:ALA:CA	1:E:31:ILE:CB	0.42	2.96	3	1
1:E:23:ASP:N	1:E:23:ASP:OD1	0.42	2.46	3	1
1:J:18:VAL:C	1:J:19:PHE:CG	0.42	2.92	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:1:ASP:O	1:C:2:ALA:O	0.42	2.37	1	1
1:D:19:PHE:CD1	1:E:19:PHE:O	0.42	2.73	8	1
1:G:19:PHE:CD2	1:H:36:VAL:HG21	0.42	2.50	10	1
1:F:33:GLY:O	1:G:34:LEU:HD12	0.42	2.14	6	1
1:I:24:VAL:O	1:J:25:GLY:C	0.42	2.58	6	1
1:A:15:GLN:CG	1:A:16:LYS:N	0.42	2.82	7	1
1:D:34:LEU:HA	1:E:34:LEU:CD1	0.42	2.44	7	1
1:A:23:ASP:OD1	1:A:27:ASN:OD1	0.42	2.37	2	1
1:A:18:VAL:HA	1:B:18:VAL:O	0.42	2.14	3	1
1:D:26:SER:OG	1:E:28:LYS:C	0.42	2.58	3	1
1:I:10:TYR:N	1:I:10:TYR:CD1	0.42	2.88	3	1
1:G:24:VAL:O	1:H:25:GLY:O	0.42	2.38	1	1
1:G:25:GLY:CA	1:H:3:GLU:OE2	0.42	2.68	5	1
1:I:17:LEU:HD23	1:I:18:VAL:N	0.42	2.29	5	1
1:A:30:ALA:HA	1:B:31:ILE:HD12	0.42	1.91	7	1
1:A:13:HIS:N	1:A:13:HIS:CD2	0.42	2.88	3	1
1:B:32:ILE:HB	1:C:33:GLY:HA3	0.42	1.92	3	1
1:C:19:PHE:O	1:D:20:PHE:N	0.42	2.41	3	1
1:C:20:PHE:N	1:D:20:PHE:CE1	0.42	2.88	3	1
1:B:13:HIS:C	1:B:14:HIS:CD2	0.41	2.93	9	1
1:I:2:ALA:O	1:I:4:PHE:CE1	0.41	2.73	9	1
1:I:11:GLU:C	1:J:11:GLU:HB3	0.41	2.36	9	1
1:G:19:PHE:CB	1:H:19:PHE:CE2	0.41	3.03	7	1
1:A:40:VAL:O	1:B:40:VAL:OXT	0.41	2.37	4	1
1:C:18:VAL:CG1	1:C:20:PHE:CE1	0.41	3.03	4	1
1:C:33:GLY:C	1:C:34:LEU:CD1	0.41	2.84	2	2
1:H:14:HIS:N	1:I:15:GLN:HE22	0.41	2.10	2	1
1:J:18:VAL:CG1	1:J:20:PHE:CE1	0.41	3.02	2	1
1:I:10:TYR:CD1	1:J:8:SER:CA	0.41	3.03	8	1
1:I:14:HIS:CE1	1:I:18:VAL:HG12	0.41	2.50	10	1
1:D:35:MET:O	1:D:36:VAL:CG1	0.41	2.67	5	1
1:D:20:PHE:H	1:E:20:PHE:HB3	0.41	1.75	6	1
1:H:10:TYR:OH	1:H:12:VAL:HG23	0.41	2.15	9	1
1:A:12:VAL:O	1:A:13:HIS:C	0.41	2.59	7	1
1:A:17:LEU:HB3	1:B:18:VAL:HB	0.41	1.90	7	1
1:B:22:GLU:OE1	1:B:22:GLU:N	0.41	2.53	7	1
1:G:31:ILE:O	1:H:32:ILE:N	0.41	2.52	7	1
1:A:23:ASP:OD2	1:B:23:ASP:O	0.41	2.37	4	1
1:G:18:VAL:HG12	1:H:18:VAL:HG22	0.41	1.92	2	1
1:B:19:PHE:HD1	1:B:20:PHE:CD1	0.41	2.33	3	1
1:C:27:ASN:HD22	1:C:28:LYS:N	0.41	2.12	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:33:GLY:O	1:E:34:LEU:HD23	0.41	2.14	1	1
1:H:22:GLU:OE1	1:I:10:TYR:OH	0.41	2.35	1	1
1:D:35:MET:SD	1:D:35:MET:C	0.41	2.99	8	1
1:H:27:ASN:ND2	1:H:28:LYS:O	0.41	2.52	8	1
1:I:14:HIS:CD2	1:I:18:VAL:HG11	0.41	2.51	8	1
1:G:24:VAL:CG2	1:H:25:GLY:H	0.41	2.28	10	1
1:G:11:GLU:HG2	1:G:12:VAL:N	0.41	2.30	9	1
1:C:20:PHE:HB3	1:D:20:PHE:CD2	0.41	2.49	7	1
1:D:34:LEU:C	1:E:19:PHE:CD2	0.41	2.89	7	1
1:I:15:GLN:O	1:J:15:GLN:CB	0.41	2.68	4	1
1:I:17:LEU:HD12	1:J:17:LEU:O	0.41	2.15	2	1
1:J:11:GLU:CD	1:J:11:GLU:O	0.41	2.58	2	1
1:F:32:ILE:HG22	1:G:32:ILE:HB	0.41	1.91	3	1
1:D:24:VAL:O	1:E:24:VAL:CG2	0.41	2.67	8	1
1:F:19:PHE:CD2	1:F:36:VAL:HG11	0.41	2.50	8	1
1:F:33:GLY:CA	1:G:33:GLY:HA2	0.41	2.45	10	1
1:D:28:LYS:C	1:D:29:GLY:O	0.41	2.58	1	2
1:I:2:ALA:O	1:I:4:PHE:CZ	0.41	2.73	9	1
1:B:19:PHE:HB3	1:C:19:PHE:N	0.41	2.30	7	1
1:B:28:LYS:O	1:C:23:ASP:OD2	0.41	2.37	7	1
1:D:21:ALA:C	1:D:22:GLU:CD	0.41	2.78	7	1
1:E:21:ALA:HB3	1:G:39:VAL:HG21	0.41	1.93	7	1
1:J:3:GLU:O	1:J:5:ARG:N	0.41	2.53	7	1
1:H:6:HIS:N	1:H:6:HIS:ND1	0.41	2.68	4	1
1:C:40:VAL:CG2	1:C:40:VAL:O	0.41	2.68	2	1
1:A:34:LEU:HD21	1:F:35:MET:CE	0.41	2.45	3	1
1:E:27:ASN:CG	1:E:28:LYS:H	0.41	2.18	1	1
1:J:15:GLN:CD	1:J:16:LYS:H	0.41	2.17	1	1
1:G:13:HIS:HB2	1:H:12:VAL:HG21	0.41	1.92	8	1
1:J:13:HIS:CG	1:J:14:HIS:N	0.41	2.89	10	1
1:C:35:MET:C	1:C:36:VAL:CG1	0.41	2.88	5	1
1:G:5:ARG:C	1:G:7:ASP:N	0.41	2.74	9	1
1:H:23:ASP:OD1	1:I:25:GLY:C	0.41	2.58	9	1
1:A:15:GLN:O	1:B:17:LEU:O	0.41	2.38	7	1
1:B:28:LYS:N	1:B:28:LYS:HD3	0.41	2.29	7	1
1:A:19:PHE:O	1:A:20:PHE:CD1	0.41	2.73	2	1
1:J:20:PHE:CE2	1:J:22:GLU:OE2	0.41	2.73	2	1
1:A:19:PHE:O	1:B:20:PHE:HD2	0.41	1.99	3	1
1:C:19:PHE:CE1	1:D:20:PHE:CB	0.41	3.03	3	1
1:B:32:ILE:HG12	1:C:31:ILE:HG23	0.41	1.91	3	1
1:D:26:SER:O	1:D:27:ASN:OD1	0.41	2.39	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:31:ILE:C	1:D:31:ILE:HG23	0.41	2.27	3	1
1:D:20:PHE:N	1:E:21:ALA:HB2	0.41	2.22	3	1
1:F:34:LEU:HD12	1:G:35:MET:CB	0.41	2.45	3	1
1:H:36:VAL:CG2	1:I:36:VAL:O	0.41	2.68	3	1
1:F:19:PHE:CE2	1:F:36:VAL:HG22	0.41	2.50	8	1
1:E:28:LYS:HD2	1:E:28:LYS:H	0.41	1.76	10	1
1:G:3:GLU:CG	1:H:1:ASP:H2	0.41	2.28	10	1
1:C:34:LEU:N	1:C:34:LEU:HD12	0.41	2.30	6	1
1:G:20:PHE:O	1:H:20:PHE:HB3	0.41	2.14	6	1
1:H:19:PHE:CD2	1:I:36:VAL:HG21	0.41	2.50	6	1
1:H:19:PHE:CG	1:I:36:VAL:HG21	0.41	2.51	9	1
1:E:19:PHE:CE1	1:E:19:PHE:O	0.41	2.69	7	1
1:H:20:PHE:H	1:I:20:PHE:CB	0.41	2.27	7	1
1:I:40:VAL:HA	1:J:40:VAL:H	0.41	1.74	7	1
1:F:24:VAL:HG12	1:G:25:GLY:N	0.41	2.30	4	1
1:A:16:LYS:HA	1:B:16:LYS:N	0.41	2.31	3	1
1:A:20:PHE:CE1	1:C:34:LEU:HB2	0.41	2.50	3	1
1:D:19:PHE:O	1:E:21:ALA:HB2	0.41	2.16	3	1
1:D:36:VAL:HG12	1:E:36:VAL:H	0.41	1.74	1	1
1:H:15:GLN:O	1:H:16:LYS:O	0.41	2.39	10	1
1:E:34:LEU:C	1:E:35:MET:SD	0.41	2.99	5	1
1:G:24:VAL:CG1	1:G:25:GLY:H	0.41	2.22	5	1
1:G:10:TYR:CE2	1:H:10:TYR:CB	0.41	3.04	5	1
1:H:1:ASP:O	1:H:2:ALA:O	0.41	2.39	6	1
1:B:36:VAL:CG2	1:C:36:VAL:O	0.41	2.69	9	1
1:G:18:VAL:CG1	1:G:19:PHE:N	0.41	2.83	9	1
1:H:35:MET:C	1:H:36:VAL:HG13	0.41	2.36	9	1
1:I:27:ASN:N	1:I:27:ASN:OD1	0.41	2.54	9	1
1:B:31:ILE:HG12	1:D:21:ALA:C	0.41	2.35	7	1
1:B:35:MET:C	1:C:36:VAL:O	0.41	2.59	7	1
1:G:12:VAL:CG2	1:H:12:VAL:HG12	0.41	2.46	4	1
1:I:11:GLU:N	1:J:10:TYR:O	0.41	2.53	4	1
1:G:18:VAL:CG2	1:G:20:PHE:CE2	0.41	3.04	2	1
1:B:35:MET:CE	1:B:36:VAL:C	0.41	2.89	3	1
1:C:19:PHE:C	1:D:20:PHE:CD1	0.41	2.93	3	1
1:D:30:ALA:C	1:E:31:ILE:CG1	0.41	2.27	3	1
1:E:23:ASP:OD1	1:E:26:SER:O	0.41	2.39	3	1
1:D:19:PHE:HD2	1:D:20:PHE:N	0.41	2.11	1	1
1:D:24:VAL:HG21	1:E:25:GLY:O	0.41	2.15	1	1
1:A:23:ASP:OD2	1:A:26:SER:O	0.41	2.39	5	1
1:A:12:VAL:HG23	1:A:12:VAL:O	0.41	2.14	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:VAL:H	1:B:18:VAL:HG11	0.41	1.74	7	1
1:A:34:LEU:HB3	1:B:34:LEU:CD2	0.41	2.46	7	1
1:D:19:PHE:CB	1:E:20:PHE:N	0.41	2.84	7	1
1:H:19:PHE:CD2	1:I:36:VAL:CG2	0.41	3.04	4	1
1:J:6:HIS:CD2	1:J:6:HIS:H	0.41	2.34	2	1
1:D:39:VAL:CG2	1:D:40:VAL:N	0.41	2.84	3	1
1:I:40:VAL:C	1:J:39:VAL:CG1	0.41	2.89	3	1
1:H:24:VAL:O	1:I:24:VAL:HG23	0.41	2.15	10	1
1:I:8:SER:N	1:J:9:GLY:HA2	0.41	2.31	10	1
1:J:7:ASP:C	1:J:8:SER:OG	0.41	2.59	10	1
1:A:19:PHE:HB2	1:B:19:PHE:CE2	0.41	2.51	10	1
1:B:20:PHE:CD1	1:B:22:GLU:OE2	0.41	2.73	10	1
1:I:8:SER:CB	1:J:9:GLY:N	0.41	2.84	10	2
1:D:24:VAL:CG1	1:D:25:GLY:N	0.41	2.83	6	1
1:I:18:VAL:CG1	1:J:18:VAL:HG12	0.41	2.45	6	1
1:D:33:GLY:C	1:D:34:LEU:HD23	0.41	2.35	9	1
1:G:8:SER:HB2	2:G:101:2PO:O1P	0.41	2.15	9	1
1:A:8:SER:C	2:A:101:2PO:O2P	0.41	2.58	7	1
1:A:31:ILE:C	1:C:22:GLU:C	0.41	2.66	7	1
1:D:19:PHE:C	1:E:20:PHE:CD1	0.41	2.94	7	1
1:A:21:ALA:HB3	1:B:21:ALA:C	0.41	2.35	7	1
1:C:23:ASP:C	1:C:24:VAL:HG12	0.41	2.36	7	1
1:C:34:LEU:CA	1:D:34:LEU:CG	0.41	2.99	7	1
1:E:27:ASN:CG	1:E:30:ALA:O	0.41	2.59	7	1
1:D:39:VAL:HG11	1:H:33:GLY:HA3	0.41	1.93	7	1
1:J:19:PHE:O	1:J:20:PHE:CB	0.41	2.69	7	1
1:A:8:SER:O	1:B:9:GLY:N	0.41	2.51	4	1
1:F:15:GLN:H	1:G:14:HIS:CD2	0.41	2.34	4	1
1:I:7:ASP:CG	1:J:10:TYR:CE1	0.41	2.94	4	1
1:H:14:HIS:C	1:H:15:GLN:CD	0.41	2.79	4	1
1:B:40:VAL:OXT	1:B:40:VAL:HG12	0.41	2.14	2	1
1:G:20:PHE:CE1	1:H:20:PHE:CD2	0.41	3.09	2	1
1:A:39:VAL:CG1	1:A:39:VAL:O	0.41	2.68	2	1
1:B:14:HIS:CG	1:B:18:VAL:HG23	0.41	2.51	2	1
1:B:32:ILE:CD1	1:C:31:ILE:HG12	0.41	2.45	3	1
1:D:27:ASN:HB3	1:E:32:ILE:N	0.41	2.30	3	1
1:H:36:VAL:CG2	1:I:36:VAL:C	0.41	2.89	3	1
1:I:10:TYR:N	1:J:9:GLY:HA2	0.41	2.31	3	1
1:A:8:SER:N	2:A:101:2PO:O1P	0.41	2.54	3	1
1:C:17:LEU:CD1	1:C:17:LEU:C	0.41	2.89	3	1
1:B:23:ASP:CG	1:B:26:SER:O	0.41	2.59	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:3:GLU:OE1	1:I:25:GLY:O	0.41	2.39	1	1
1:G:1:ASP:O	1:G:6:HIS:CE1	0.41	2.74	8	1
1:H:12:VAL:O	1:H:13:HIS:HB3	0.41	2.15	8	1
1:C:33:GLY:C	1:C:34:LEU:HG	0.41	2.36	5	1
1:G:5:ARG:O	1:G:6:HIS:O	0.41	2.38	5	1
1:G:8:SER:CB	2:G:101:2PO:O1P	0.41	2.69	9	1
1:I:22:GLU:OE1	1:J:22:GLU:OE2	0.41	2.38	9	1
1:A:28:LYS:C	1:C:25:GLY:H	0.41	2.18	7	1
1:A:34:LEU:HA	1:B:19:PHE:CZ	0.41	2.48	7	1
1:B:24:VAL:O	1:B:25:GLY:C	0.41	2.59	7	1
1:G:13:HIS:O	1:H:13:HIS:C	0.41	2.59	7	1
1:E:28:LYS:CD	1:E:28:LYS:N	0.41	2.84	2	1
1:G:36:VAL:HG12	1:H:36:VAL:H	0.41	1.76	2	1
1:A:33:GLY:C	1:B:34:LEU:CD2	0.41	2.86	3	1
1:B:32:ILE:HG23	1:C:32:ILE:HG12	0.41	1.93	1	1
1:G:18:VAL:HB	1:H:14:HIS:NE2	0.41	2.31	1	1
1:I:17:LEU:CB	1:J:17:LEU:O	0.41	2.69	1	1
2:F:101:2PO:P	1:H:25:GLY:H	0.40	2.39	8	1
1:J:2:ALA:O	1:J:3:GLU:O	0.40	2.39	10	1
1:I:3:GLU:O	1:I:4:PHE:O	0.40	2.39	5	1
1:H:14:HIS:CG	1:H:18:VAL:HB	0.40	2.51	6	1
1:A:35:MET:SD	1:B:19:PHE:HD1	0.40	2.39	7	1
1:A:34:LEU:CB	1:B:34:LEU:HD21	0.40	2.46	7	1
1:D:39:VAL:O	1:D:39:VAL:CG2	0.40	2.68	7	1
1:G:33:GLY:O	1:H:34:LEU:N	0.40	2.54	7	1
1:G:12:VAL:HB	1:H:12:VAL:HG12	0.40	1.92	7	1
1:H:5:ARG:NH2	1:I:1:ASP:OD2	0.40	2.54	7	1
1:A:15:GLN:O	1:B:14:HIS:NE2	0.40	2.53	4	1
1:B:14:HIS:ND1	1:B:18:VAL:HG21	0.40	2.31	4	1
1:B:21:ALA:HB2	1:C:34:LEU:CD2	0.40	2.46	3	1
1:B:31:ILE:C	1:B:32:ILE:HG23	0.40	2.17	3	1
1:H:23:ASP:C	1:H:24:VAL:HG22	0.40	2.35	3	1
1:I:30:ALA:C	1:I:31:ILE:HG13	0.40	2.37	3	1
1:J:13:HIS:CD2	1:J:13:HIS:N	0.40	2.88	3	1
1:C:39:VAL:O	1:C:39:VAL:CG2	0.40	2.69	8	1
1:H:6:HIS:ND1	1:H:6:HIS:N	0.40	2.69	10	1
1:I:34:LEU:CD1	1:I:34:LEU:N	0.40	2.80	10	1
1:A:21:ALA:HB2	1:B:34:LEU:HD13	0.40	1.93	5	1
1:D:40:VAL:O	1:D:40:VAL:CG1	0.40	2.70	6	1
1:I:7:ASP:O	1:I:8:SER:C	0.40	2.59	6	1
1:F:13:HIS:CG	1:G:13:HIS:ND1	0.40	2.89	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:H:27:ASN:C	1:H:28:LYS:CD	0.40	2.89	9	1
1:A:31:ILE:O	1:A:32:ILE:HG22	0.40	2.16	7	1
1:B:17:LEU:HD12	1:B:18:VAL:H	0.40	1.74	7	1
1:F:21:ALA:HA	1:G:21:ALA:O	0.40	2.17	7	1
1:H:10:TYR:CD1	1:H:10:TYR:N	0.40	2.89	7	1
1:B:35:MET:HE3	1:B:36:VAL:C	0.40	2.37	3	1
1:C:20:PHE:C	1:D:21:ALA:HB3	0.40	2.36	3	1
1:C:23:ASP:N	1:D:22:GLU:OE2	0.40	2.53	3	1
1:F:18:VAL:CG2	1:F:19:PHE:N	0.40	2.71	3	1
1:F:13:HIS:N	1:F:13:HIS:ND1	0.40	2.69	10	1
1:J:7:ASP:OD2	2:J:101:2PO:O1P	0.40	2.40	6	1
1:A:13:HIS:ND1	1:A:13:HIS:C	0.40	2.75	9	1
1:F:14:HIS:O	1:F:15:GLN:CB	0.40	2.69	9	1
1:A:32:ILE:C	1:C:21:ALA:CA	0.40	2.89	7	1
1:A:33:GLY:O	1:B:34:LEU:N	0.40	2.55	7	1
1:D:19:PHE:CD2	1:E:20:PHE:N	0.40	2.89	7	1
1:F:18:VAL:O	1:G:18:VAL:CG1	0.40	2.68	7	1
1:I:10:TYR:OH	1:I:12:VAL:CG2	0.40	2.69	7	1
1:A:34:LEU:HD12	1:A:34:LEU:O	0.40	2.16	4	1
1:G:10:TYR:CE2	1:H:10:TYR:CD2	0.40	3.10	4	1
1:I:35:MET:CG	1:I:36:VAL:H	0.40	2.14	3	1
1:I:38:GLY:N	1:J:38:GLY:HA3	0.40	2.31	3	1
1:C:32:ILE:HB	1:D:32:ILE:CB	0.40	2.44	1	1
1:I:15:GLN:O	1:J:15:GLN:OE1	0.40	2.39	1	1
1:J:13:HIS:CG	1:J:13:HIS:O	0.40	2.74	8	1
1:A:16:LYS:O	1:B:16:LYS:HB3	0.40	2.17	10	1
1:F:34:LEU:CG	1:F:35:MET:H	0.40	2.30	10	1
1:J:28:LYS:N	1:J:28:LYS:CD	0.40	2.83	10	1
1:E:20:PHE:HB3	1:F:39:VAL:HG22	0.40	1.93	7	1
2:I:101:2PO:O3P	1:J:7:ASP:O	0.40	2.39	7	1
2:I:101:2PO:P	1:J:7:ASP:O	0.40	2.79	7	1
1:A:17:LEU:CD1	1:A:17:LEU:O	0.40	2.70	2	1
1:H:36:VAL:CG1	1:I:36:VAL:O	0.40	2.69	2	1
1:B:19:PHE:HD1	1:B:20:PHE:CG	0.40	2.35	3	1
1:D:36:VAL:HG22	1:D:37:GLY:H	0.40	1.76	3	1
1:D:30:ALA:HA	1:E:31:ILE:HG12	0.40	1.77	3	1
1:J:35:MET:O	1:J:36:VAL:CB	0.40	2.69	3	1
1:I:9:GLY:HA2	1:J:9:GLY:CA	0.40	2.46	8	1
1:C:22:GLU:CD	1:C:22:GLU:N	0.40	2.75	10	1
1:B:7:ASP:O	1:B:8:SER:OG	0.40	2.40	6	1
1:A:31:ILE:HG23	1:C:21:ALA:CB	0.40	2.47	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:101:2PO:P	1:E:22:GLU:OE2	0.40	2.80	7	1
1:E:27:ASN:C	1:E:27:ASN:ND2	0.40	2.74	7	1
1:A:12:VAL:HG12	1:A:12:VAL:O	0.40	2.16	4	1
1:C:36:VAL:HG21	1:D:36:VAL:C	0.40	2.35	3	1
1:D:30:ALA:C	1:D:31:ILE:CG2	0.40	2.84	3	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	32/40 (80%)	22±3 (68±11%)	6±1 (20±4%)	4±3 (12±9%)	1	6
1	B	38/40 (95%)	24±4 (64±10%)	8±2 (22±6%)	5±4 (14±10%)	1	5
1	C	25/40 (62%)	19±3 (75±14%)	4±2 (16±7%)	2±2 (10±8%)	1	10
1	D	23/40 (58%)	17±4 (73±17%)	3±2 (14±10%)	3±3 (13±11%)	1	6
1	E	22/40 (55%)	17±2 (77±11%)	3±2 (13±8%)	2±2 (10±7%)	1	9
1	F	31/40 (78%)	23±1 (74±5%)	6±2 (18±6%)	3±1 (8±3%)	2	14
1	G	38/40 (95%)	26±3 (67±7%)	8±2 (20±4%)	5±2 (13±4%)	1	6
1	H	38/40 (95%)	25±2 (65±6%)	8±3 (22±7%)	5±1 (13±4%)	1	5
1	I	38/40 (95%)	24±2 (64±4%)	9±2 (23±5%)	5±2 (13±4%)	1	6
1	J	38/40 (95%)	23±4 (61±10%)	7±2 (19±6%)	8±3 (21±9%)	0	2
All	All	3230/4000 (81%)	2190 (68%)	619 (19%)	421 (13%)	1	6

All 168 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	H	16	LYS	9
1	J	30	ALA	9
1	J	12	VAL	7
1	G	20	PHE	7
1	E	30	ALA	6

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Mol	Chain	Res	Type	Models (Total)
1	I	8	SER	6
1	I	16	LYS	6
1	B	20	PHE	6
1	H	20	PHE	6
1	A	29	GLY	6
1	A	16	LYS	6
1	G	16	LYS	6
1	F	14	HIS	6
1	F	18	VAL	6
1	B	16	LYS	6
1	G	4	PHE	5
1	B	6	HIS	5
1	B	5	ARG	5
1	I	5	ARG	5
1	H	5	ARG	5
1	J	8	SER	5
1	I	20	PHE	5
1	E	20	PHE	5
1	C	20	PHE	5
1	J	5	ARG	5
1	H	2	ALA	5
1	J	15	GLN	5
1	D	30	ALA	5
1	B	7	ASP	5
1	I	3	GLU	4
1	J	13	HIS	4
1	G	6	HIS	4
1	D	20	PHE	4
1	J	16	LYS	4
1	J	24	VAL	4
1	J	25	GLY	4
1	A	8	SER	4
1	J	14	HIS	4
1	D	29	GLY	4
1	J	7	ASP	4
1	J	6	HIS	4
1	F	16	LYS	4
1	J	4	PHE	4
1	A	14	HIS	4
1	I	7	ASP	3
1	B	14	HIS	3
1	H	4	PHE	3

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Mol	Chain	Res	Type	Models (Total)
1	H	30	ALA	3
1	E	25	GLY	3
1	G	29	GLY	3
1	F	29	GLY	3
1	B	8	SER	3
1	G	5	ARG	3
1	I	2	ALA	3
1	I	30	ALA	3
1	G	2	ALA	3
1	C	29	GLY	3
1	D	32	ILE	3
1	G	12	VAL	3
1	J	36	VAL	2
1	G	7	ASP	2
1	E	36	VAL	2
1	B	3	GLU	2
1	B	2	ALA	2
1	D	28	LYS	2
1	C	22	GLU	2
1	J	3	GLU	2
1	F	15	GLN	2
1	A	10	TYR	2
1	C	2	ALA	2
1	H	7	ASP	2
1	J	11	GLU	2
1	H	13	HIS	2
1	H	15	GLN	2
1	H	24	VAL	2
1	H	8	SER	2
1	C	18	VAL	2
1	C	21	ALA	2
1	F	34	LEU	2
1	H	12	VAL	2
1	J	20	PHE	2
1	D	18	VAL	2
1	H	6	HIS	2
1	I	12	VAL	2
1	G	18	VAL	2
1	B	13	HIS	2
1	D	21	ALA	2
1	A	17	LEU	2
1	J	10	TYR	2

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Mol	Chain	Res	Type	Models (Total)
1	B	4	PHE	2
1	I	13	HIS	2
1	A	36	VAL	2
1	I	15	GLN	2
1	A	21	ALA	2
1	I	14	HIS	2
1	G	14	HIS	2
1	E	21	ALA	2
1	B	12	VAL	2
1	D	27	ASN	1
1	G	36	VAL	1
1	I	18	VAL	1
1	A	24	VAL	1
1	B	36	VAL	1
1	E	22	GLU	1
1	I	39	VAL	1
1	J	39	VAL	1
1	D	34	LEU	1
1	H	14	HIS	1
1	B	17	LEU	1
1	I	29	GLY	1
1	A	13	HIS	1
1	I	24	VAL	1
1	C	31	ILE	1
1	B	21	ALA	1
1	A	39	VAL	1
1	F	10	TYR	1
1	B	30	ALA	1
1	G	10	TYR	1
1	B	25	GLY	1
1	C	27	ASN	1
1	D	19	PHE	1
1	E	34	LEU	1
1	D	36	VAL	1
1	H	39	VAL	1
1	J	18	VAL	1
1	J	35	MET	1
1	E	24	VAL	1
1	H	25	GLY	1
1	B	19	PHE	1
1	G	22	GLU	1
1	D	22	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	G	30	ALA	1
1	C	30	ALA	1
1	C	24	VAL	1
1	F	39	VAL	1
1	E	19	PHE	1
1	G	15	GLN	1
1	C	3	GLU	1
1	E	29	GLY	1
1	A	18	VAL	1
1	D	24	VAL	1
1	A	19	PHE	1
1	G	8	SER	1
1	I	36	VAL	1
1	A	20	PHE	1
1	H	11	GLU	1
1	H	18	VAL	1
1	D	25	GLY	1
1	G	3	GLU	1
1	B	23	ASP	1
1	C	17	LEU	1
1	B	15	GLN	1
1	B	22	GLU	1
1	H	29	GLY	1
1	A	25	GLY	1
1	A	12	VAL	1
1	J	27	ASN	1
1	B	18	VAL	1
1	A	23	ASP	1
1	A	22	GLU	1
1	A	32	ILE	1
1	C	28	LYS	1
1	I	4	PHE	1
1	J	2	ALA	1
1	A	30	ALA	1
1	G	25	GLY	1
1	B	32	ILE	1
1	C	36	VAL	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	25/31 (81%)	20±2 (80±8%)	5±2 (20±8%)	3	33
1	B	31/31 (100%)	24±3 (78±9%)	7±3 (22±9%)	3	29
1	C	19/31 (61%)	13±1 (69±8%)	6±1 (31±8%)	1	15
1	D	17/31 (55%)	12±3 (73±19%)	5±3 (27±19%)	2	21
1	E	16/31 (52%)	12±3 (75±17%)	4±3 (25±17%)	2	25
1	F	24/31 (77%)	19±2 (80±7%)	5±2 (20±7%)	4	34
1	G	31/31 (100%)	24±2 (76±8%)	7±2 (24±8%)	2	27
1	H	31/31 (100%)	23±2 (74±6%)	8±2 (26±6%)	2	23
1	I	31/31 (100%)	25±1 (81±2%)	6±1 (19±2%)	4	36
1	J	31/31 (100%)	25±2 (79±6%)	7±2 (21±6%)	3	32
All	All	2560/3100 (83%)	1970 (77%)	590 (23%)	3	28

All 192 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	G	28	LYS	10
1	J	35	MET	9
1	I	28	LYS	9
1	H	28	LYS	9
1	H	19	PHE	9
1	G	19	PHE	9
1	F	19	PHE	8
1	D	28	LYS	8
1	B	19	PHE	8
1	H	20	PHE	8
1	E	20	PHE	8
1	C	20	PHE	7
1	J	20	PHE	7
1	C	32	ILE	7
1	A	17	LEU	7
1	C	19	PHE	7
1	H	32	ILE	7
1	I	20	PHE	7
1	C	28	LYS	7
1	B	24	VAL	6
1	A	24	VAL	6

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Mol	Chain	Res	Type	Models (Total)
1	H	14	HIS	6
1	A	34	LEU	6
1	J	8	SER	6
1	F	34	LEU	6
1	C	24	VAL	6
1	A	19	PHE	6
1	E	35	MET	6
1	J	28	LYS	6
1	D	20	PHE	6
1	B	28	LYS	6
1	D	34	LEU	5
1	B	20	PHE	5
1	A	8	SER	5
1	G	20	PHE	5
1	I	36	VAL	5
1	H	36	VAL	5
1	G	34	LEU	5
1	G	10	TYR	5
1	B	34	LEU	5
1	J	36	VAL	4
1	D	17	LEU	4
1	B	36	VAL	4
1	E	28	LYS	4
1	E	36	VAL	4
1	I	10	TYR	4
1	D	36	VAL	4
1	F	24	VAL	4
1	H	13	HIS	4
1	H	15	GLN	4
1	E	27	ASN	4
1	H	34	LEU	4
1	F	17	LEU	4
1	G	22	GLU	4
1	H	10	TYR	4
1	C	34	LEU	4
1	G	17	LEU	4
1	J	10	TYR	4
1	I	32	ILE	4
1	C	17	LEU	4
1	B	35	MET	4
1	I	14	HIS	4
1	C	36	VAL	4

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Mol	Chain	Res	Type	Models (Total)
1	G	36	VAL	3
1	I	17	LEU	3
1	A	13	HIS	3
1	F	18	VAL	3
1	J	12	VAL	3
1	F	13	HIS	3
1	G	6	HIS	3
1	J	11	GLU	3
1	E	24	VAL	3
1	H	24	VAL	3
1	G	13	HIS	3
1	I	35	MET	3
1	B	8	SER	3
1	D	24	VAL	3
1	G	8	SER	3
1	H	18	VAL	3
1	H	35	MET	3
1	A	35	MET	3
1	F	35	MET	3
1	D	32	ILE	3
1	J	27	ASN	3
1	B	18	VAL	3
1	G	14	HIS	3
1	G	35	MET	3
1	F	36	VAL	3
1	E	22	GLU	2
1	D	27	ASN	2
1	H	27	ASN	2
1	D	19	PHE	2
1	G	18	VAL	2
1	I	8	SER	2
1	B	17	LEU	2
1	F	32	ILE	2
1	D	23	ASP	2
1	F	28	LYS	2
1	I	24	VAL	2
1	B	6	HIS	2
1	G	32	ILE	2
1	G	26	SER	2
1	F	10	TYR	2
1	A	10	TYR	2
1	B	31	ILE	2

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Mol	Chain	Res	Type	Models (Total)
1	E	18	VAL	2
1	C	27	ASN	2
1	B	14	HIS	2
1	B	10	TYR	2
1	E	34	LEU	2
1	A	36	VAL	2
1	H	7	ASP	2
1	A	28	LYS	2
1	C	18	VAL	2
1	C	23	ASP	2
1	C	35	MET	2
1	J	24	VAL	2
1	J	23	ASP	2
1	E	19	PHE	2
1	I	39	VAL	2
1	I	13	HIS	2
1	J	15	GLN	2
1	C	22	GLU	2
1	B	7	ASP	2
1	E	32	ILE	2
1	B	22	GLU	2
1	F	11	GLU	2
1	F	14	HIS	2
1	D	22	GLU	2
1	J	34	LEU	2
1	J	26	SER	2
1	I	11	GLU	2
1	A	32	ILE	2
1	B	1	ASP	2
1	A	27	ASN	2
1	I	18	VAL	2
1	I	34	LEU	2
1	B	32	ILE	2
1	H	17	LEU	2
1	C	1	ASP	1
1	I	12	VAL	1
1	D	26	SER	1
1	J	39	VAL	1
1	C	39	VAL	1
1	B	39	VAL	1
1	D	31	ILE	1
1	J	6	HIS	1

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Mol	Chain	Res	Type	Models (Total)
1	J	13	HIS	1
1	H	16	LYS	1
1	I	1	ASP	1
1	B	5	ARG	1
1	B	11	GLU	1
1	G	11	GLU	1
1	J	22	GLU	1
1	F	12	VAL	1
1	J	18	VAL	1
1	G	1	ASP	1
1	H	5	ARG	1
1	A	14	HIS	1
1	J	16	LYS	1
1	H	22	GLU	1
1	A	20	PHE	1
1	G	23	ASP	1
1	D	18	VAL	1
1	D	35	MET	1
1	H	6	HIS	1
1	F	23	ASP	1
1	F	39	VAL	1
1	B	13	HIS	1
1	B	27	ASN	1
1	D	39	VAL	1
1	F	27	ASN	1
1	G	15	GLN	1
1	J	14	HIS	1
1	J	32	ILE	1
1	A	18	VAL	1
1	I	19	PHE	1
1	E	39	VAL	1
1	G	5	ARG	1
1	J	17	LEU	1
1	H	11	GLU	1
1	G	39	VAL	1
1	I	26	SER	1
1	B	23	ASP	1
1	G	16	LYS	1
1	J	7	ASP	1
1	B	26	SER	1
1	A	12	VAL	1
1	G	12	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	22	GLU	1
1	C	26	SER	1
1	I	15	GLN	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	2PO	F	101	-	0,3,3	0.00±0.00	-
2	2PO	H	101	-	0,3,3	0.00±0.00	-
2	2PO	C	101	-	0,3,3	0.00±0.00	-
2	2PO	E	101	-	0,3,3	0.00±0.00	-
2	2PO	B	101	-	0,3,3	0.00±0.00	-
2	2PO	J	101	-	0,3,3	0.00±0.00	-
2	2PO	G	101	-	0,3,3	0.00±0.00	-
2	2PO	A	101	-	0,3,3	0.00±0.00	-
2	2PO	D	101	-	0,3,3	0.00±0.00	-
2	2PO	I	101	-	0,3,3	0.00±0.00	-

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	2PO	F	101	-	0,3,3	0.00±0.00	-
2	2PO	H	101	-	0,3,3	0.00±0.00	-
2	2PO	C	101	-	0,3,3	0.00±0.00	-
2	2PO	E	101	-	0,3,3	0.00±0.00	-
2	2PO	B	101	-	0,3,3	0.00±0.00	-
2	2PO	J	101	-	0,3,3	0.00±0.00	-
2	2PO	G	101	-	0,3,3	0.00±0.00	-
2	2PO	A	101	-	0,3,3	0.00±0.00	-
2	2PO	D	101	-	0,3,3	0.00±0.00	-
2	2PO	I	101	-	0,3,3	0.00±0.00	-

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 3% for the well-defined parts and 3% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *NMR-STAR_3.1_for_pABeta_fibrils_new1.txt*

7.1.1 Bookkeeping

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

Total number of shifts	123
Number of shifts mapped to atoms	123
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	32	1.12 ± 0.31	Should be applied
$^{13}C_{\beta}$	26	0.28 ± 0.44	None needed (< 0.5 ppm)
$^{13}C'$	32	1.72 ± 0.30	Should be applied
^{15}N	0	—	None (insufficient data)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 3%, i.e. 108 atoms were assigned a chemical shift out of a possible 3831. 2 out of 76 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	56/1695 (3%)	0/678 (0%)	56/678 (8%)	0/339 (0%)
Sidechain	52/1722 (3%)	0/983 (0%)	52/690 (8%)	0/49 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/414 (0%)	0/229 (0%)	0/166 (0%)	0/19 (0%)
Overall	108/3831 (3%)	0/1890 (0%)	108/1534 (7%)	0/407 (0%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 123 atoms were assigned a chemical shift out of a possible 4630. 2 out of 80 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	64/2000 (3%)	0/800 (0%)	64/800 (8%)	0/400 (0%)
Sidechain	59/2070 (3%)	0/1190 (0%)	59/810 (7%)	0/70 (0%)
Aromatic	0/560 (0%)	0/310 (0%)	0/220 (0%)	0/30 (0%)
Overall	123/4630 (3%)	0/2300 (0%)	123/1830 (7%)	0/500 (0%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots

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

Random coil index (RCI) for chain A: