Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 03:43 PM EDT

PDB ID	:	2JZ3
Title	:	SOCS box elonginBC ternary complex
Authors	:	Babon, J.J.; Sabo, J.; Soetopo, A.; Yao, S.; Bailey, M.F.; Zhang, J.; Nicola, N.A.; Norton, R.S.
Deposited on	:	2007-12-27

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

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

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

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

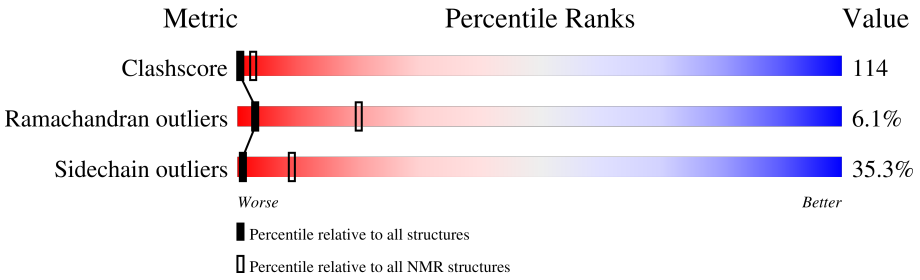
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	40	. 30% 5% 62%
2	B	118	8% 51% 15% . 25%
3	C	96	5% 53% 21% 21%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:1-A:15, B:1-B:80, B:86-B:93, C:17-C:46, C:58-C:83, C:93-C:112 (179)	1.24	6

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 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3578 atoms, of which 1781 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Suppressor of cytokine signaling 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	15	239	71	123	25	19	1	0

- Molecule 2 is a protein called Transcription elongation factor B polypeptide 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	118	1829	575	908	156	185	5	0

- Molecule 3 is a protein called Transcription elongation factor B polypeptide 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
3	C	96	1510	487	750	122	145	6	0

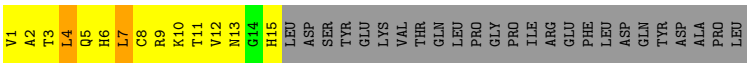
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

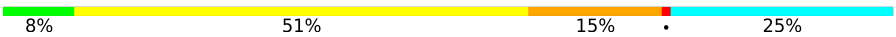
• Molecule 1: Suppressor of cytokine signaling 3

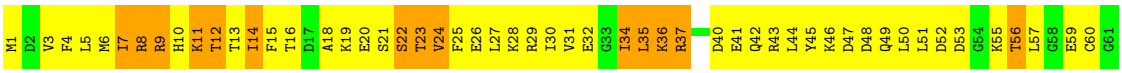
Chain A:



• Molecule 2: Transcription elongation factor B polypeptide 2

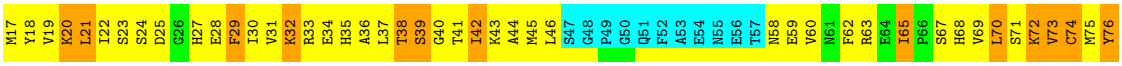
Chain B:





• Molecule 3: Transcription elongation factor B polypeptide 1

Chain C:



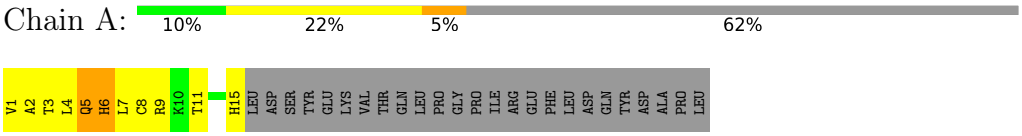
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

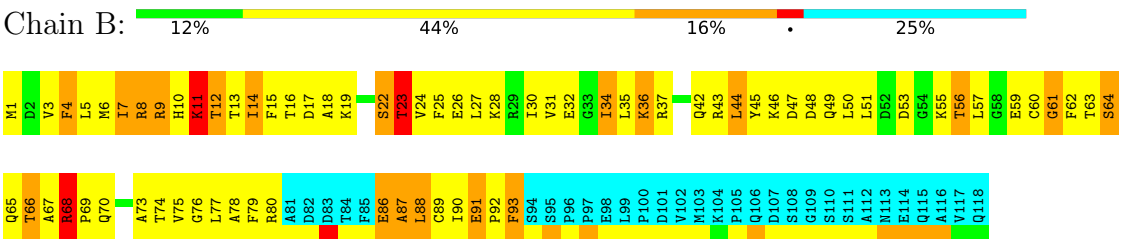
• Molecule 1: Suppressor of cytokine signaling 3

Chain A:



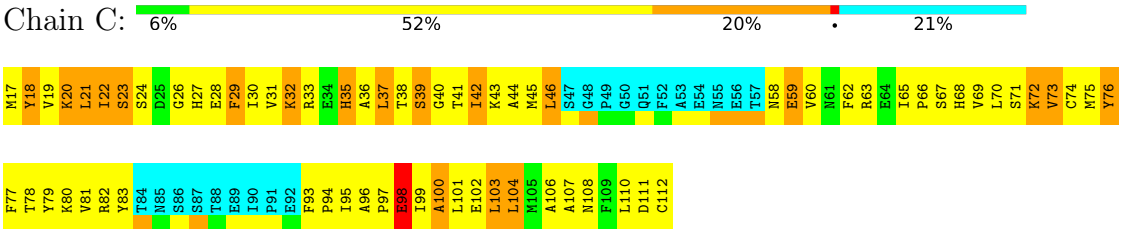
• Molecule 2: Transcription elongation factor B polypeptide 2

Chain B:



• Molecule 3: Transcription elongation factor B polypeptide 1

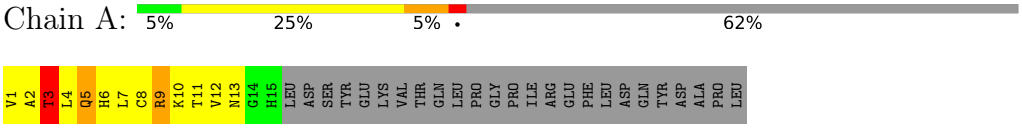
Chain C:



4.2.2 Score per residue for model 2

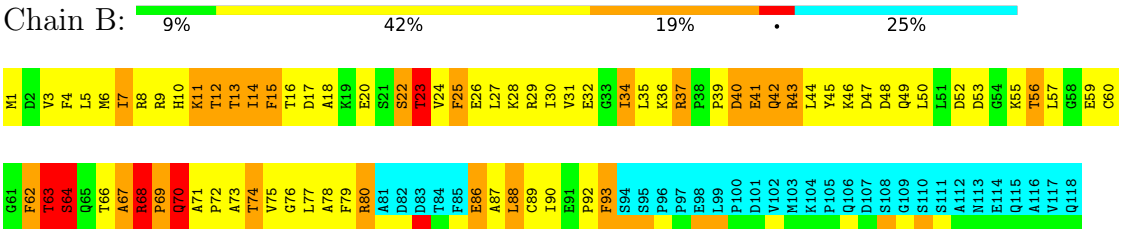
• Molecule 1: Suppressor of cytokine signaling 3

Chain A:



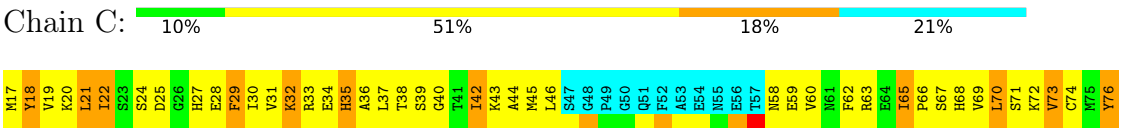
• Molecule 2: Transcription elongation factor B polypeptide 2

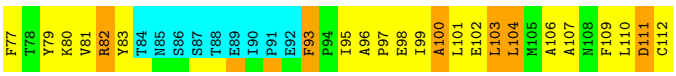
Chain B:



• Molecule 3: Transcription elongation factor B polypeptide 1

Chain C:





4.2.3 Score per residue for model 3

• Molecule 1: Suppressor of cytokine signaling 3

Chain A: 5% 18% 15% 62%

• Molecule 2: Transcription elongation factor B polypeptide 2

Chain B: 11% 37% 25% 25%

• Molecule 3: Transcription elongation factor B polypeptide 1

Chain C: 8% 44% 26% 21%

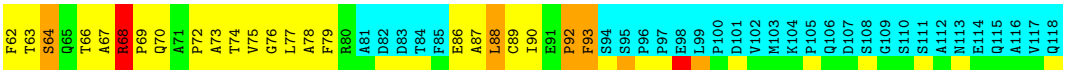
4.2.4 Score per residue for model 4

• Molecule 1: Suppressor of cytokine signaling 3

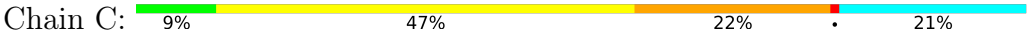
Chain A: 8% 18% 12% 62%

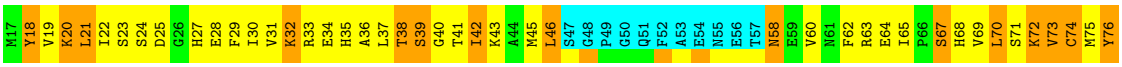
• Molecule 2: Transcription elongation factor B polypeptide 2

Chain B: 13% 39% 22% 25%



• Molecule 3: Transcription elongation factor B polypeptide 1

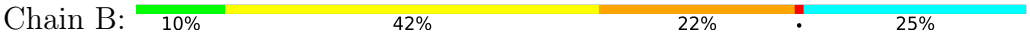


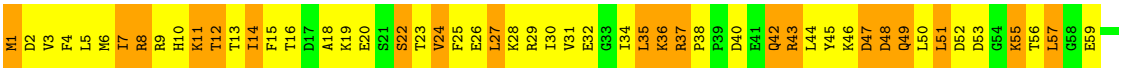


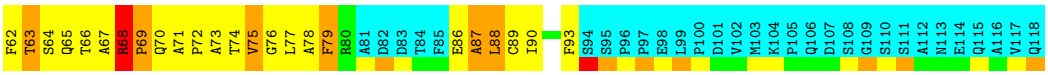
4.2.5 Score per residue for model 5

• Molecule 1: Suppressor of cytokine signaling 3

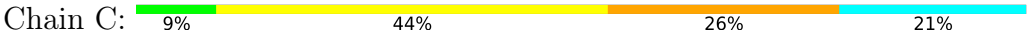
• Molecule 2: Transcription elongation factor B polypeptide 2

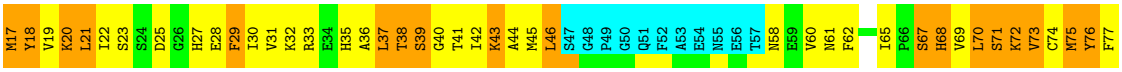






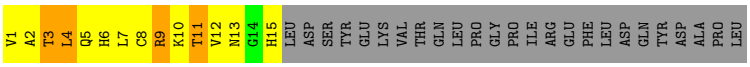
• Molecule 3: Transcription elongation factor B polypeptide 1





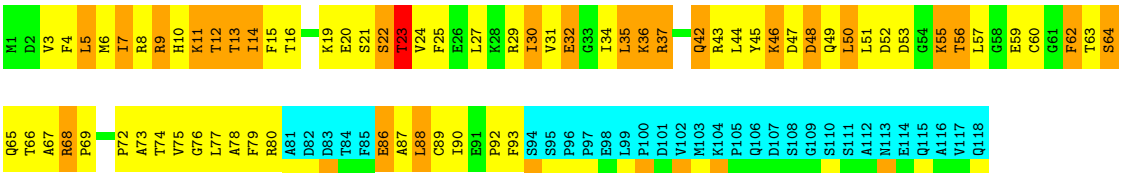
4.2.6 Score per residue for model 6 (medoid)

• Molecule 1: Suppressor of cytokine signaling 3



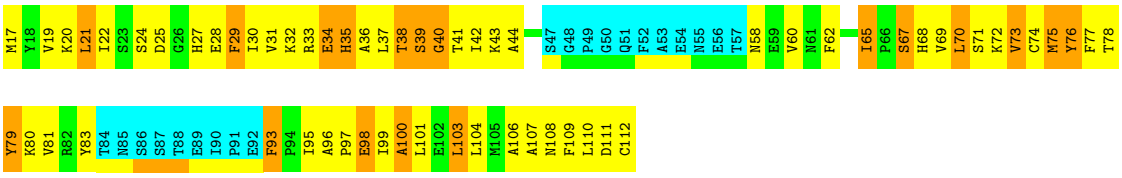
• Molecule 2: Transcription elongation factor B polypeptide 2

Chain B:



• Molecule 3: Transcription elongation factor B polypeptide 1

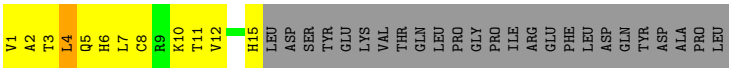
Chain C:



4.2.7 Score per residue for model 7

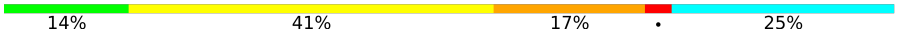
• Molecule 1: Suppressor of cytokine signaling 3

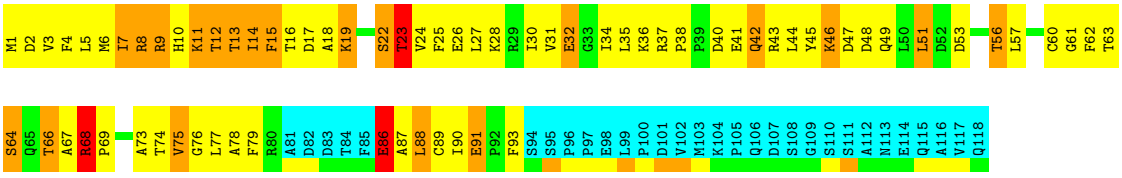
Chain A:



• Molecule 2: Transcription elongation factor B polypeptide 2

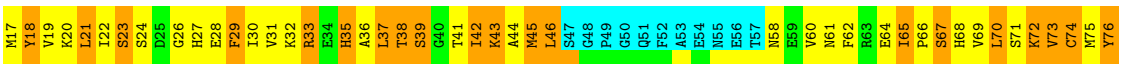
Chain B:





• Molecule 3: Transcription elongation factor B polypeptide 1

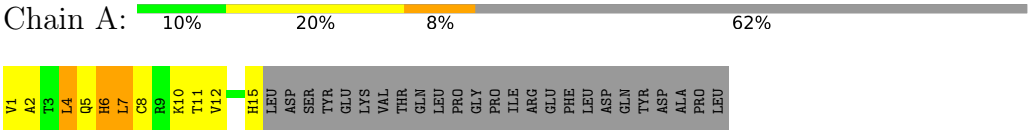
Chain C:



4.2.8 Score per residue for model 8

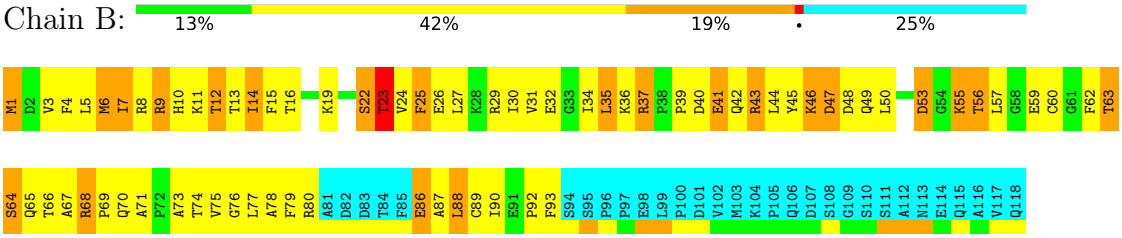
• Molecule 1: Suppressor of cytokine signaling 3

Chain A:



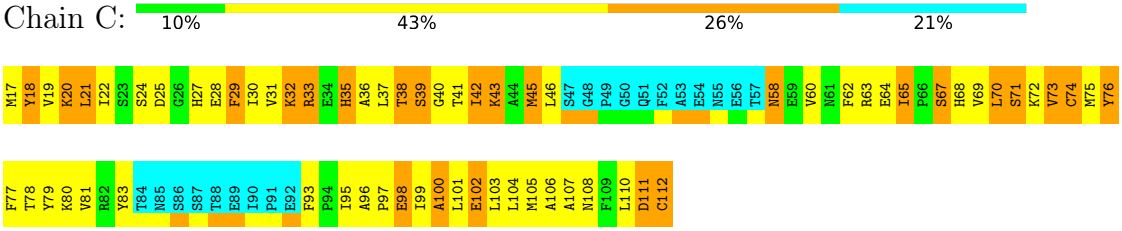
• Molecule 2: Transcription elongation factor B polypeptide 2

Chain B:



• Molecule 3: Transcription elongation factor B polypeptide 1

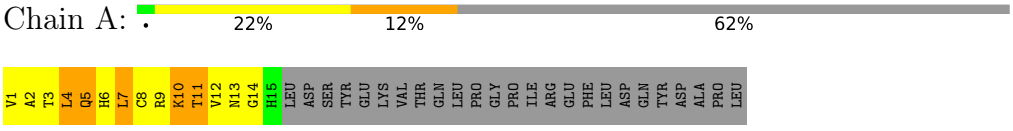
Chain C:



4.2.9 Score per residue for model 9

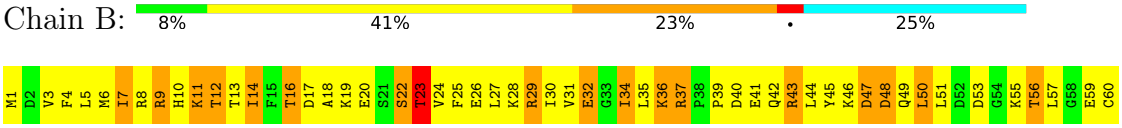
• Molecule 1: Suppressor of cytokine signaling 3

Chain A:



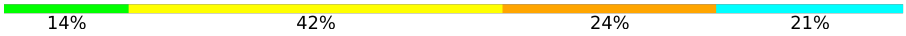
• Molecule 2: Transcription elongation factor B polypeptide 2

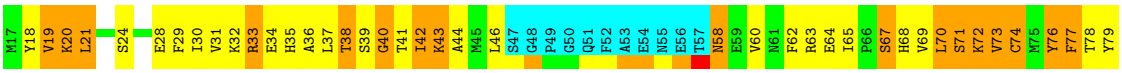
Chain B:



• Molecule 3: Transcription elongation factor B polypeptide 1

Chain C:

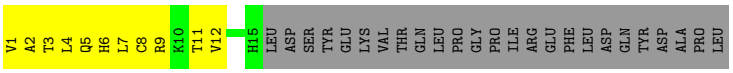




4.2.10 Score per residue for model 10

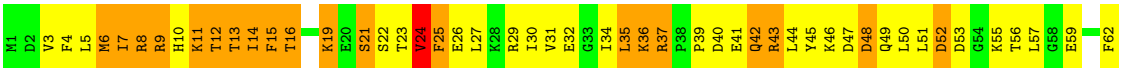
• Molecule 1: Suppressor of cytokine signaling 3

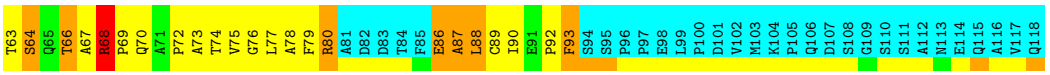
Chain A:



• Molecule 2: Transcription elongation factor B polypeptide 2

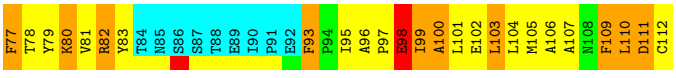
Chain B:





• Molecule 3: Transcription elongation factor B polypeptide 1

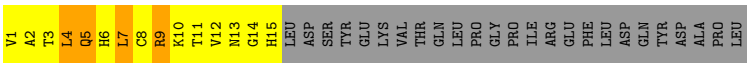
Chain C:



4.2.11 Score per residue for model 11

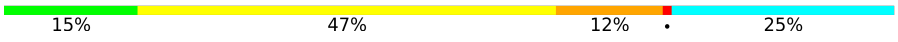
• Molecule 1: Suppressor of cytokine signaling 3

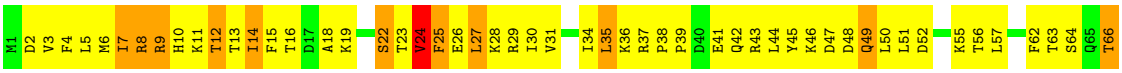
Chain A:

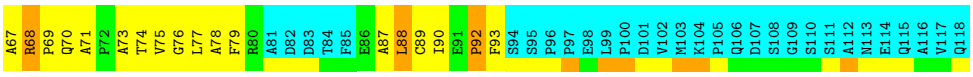


• Molecule 2: Transcription elongation factor B polypeptide 2

Chain B:







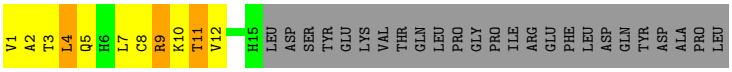
• Molecule 3: Transcription elongation factor B polypeptide 1

Chain C:

4.2.12 Score per residue for model 12

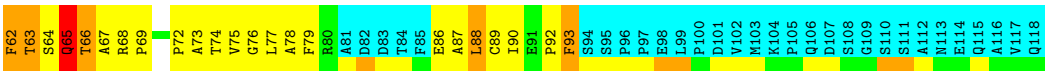
• Molecule 1: Suppressor of cytokine signaling 3

Chain A:



• Molecule 2: Transcription elongation factor B polypeptide 2

Chain B:



• Molecule 3: Transcription elongation factor B polypeptide 1

Chain C:

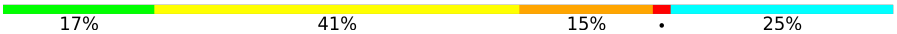
4.2.13 Score per residue for model 13

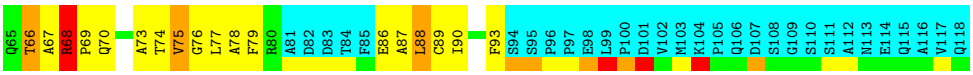
• Molecule 1: Suppressor of cytokine signaling 3

Chain A:

• Molecule 2: Transcription elongation factor B polypeptide 2

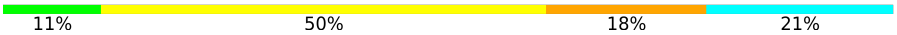
Chain B:





• Molecule 3: Transcription elongation factor B polypeptide 1

Chain C:



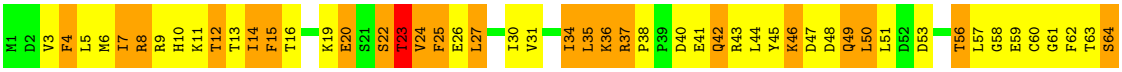
4.2.14 Score per residue for model 14

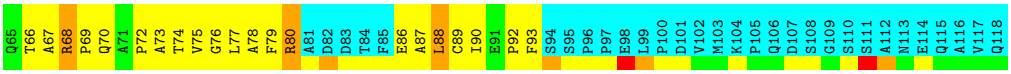
• Molecule 1: Suppressor of cytokine signaling 3

Chain A:

• Molecule 2: Transcription elongation factor B polypeptide 2

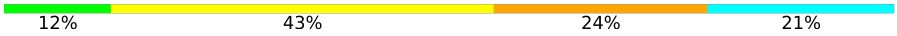
Chain B:

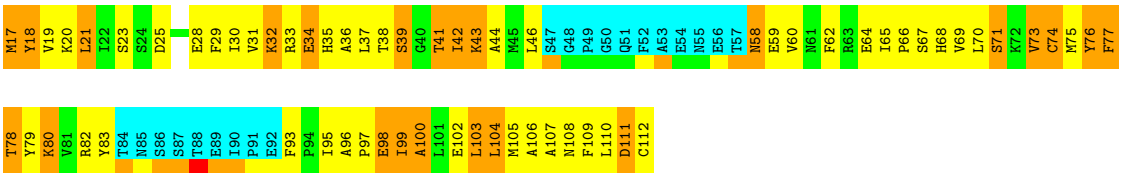




• Molecule 3: Transcription elongation factor B polypeptide 1

Chain C:

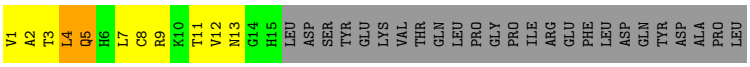




4.2.15 Score per residue for model 15

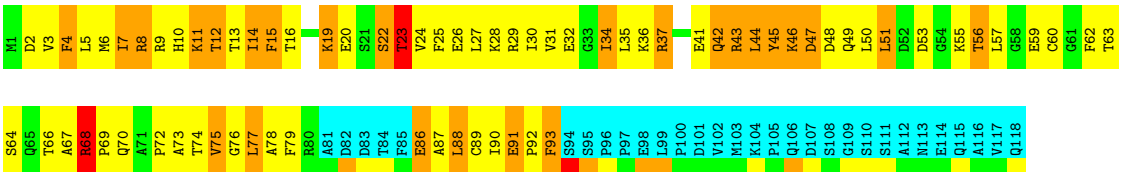
• Molecule 1: Suppressor of cytokine signaling 3

Chain A:



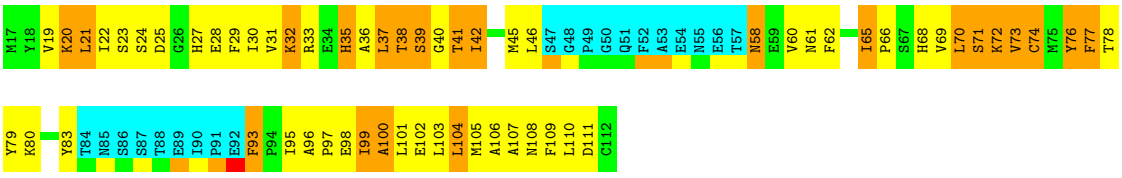
• Molecule 2: Transcription elongation factor B polypeptide 2

Chain B:



• Molecule 3: Transcription elongation factor B polypeptide 1

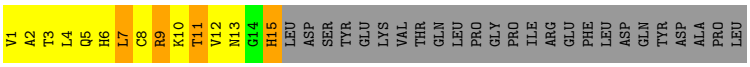
Chain C:



4.2.16 Score per residue for model 16

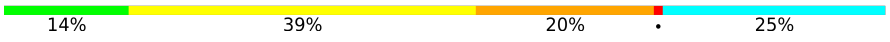
• Molecule 1: Suppressor of cytokine signaling 3

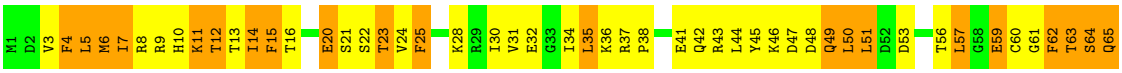
Chain A:



• Molecule 2: Transcription elongation factor B polypeptide 2

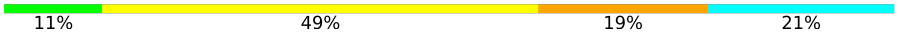
Chain B:

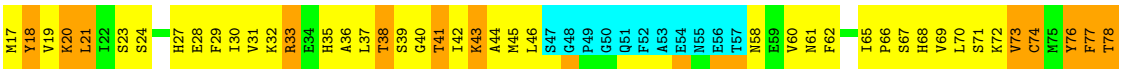




• Molecule 3: Transcription elongation factor B polypeptide 1

Chain C:

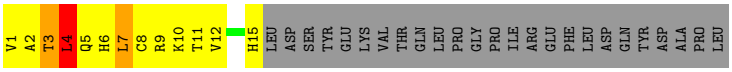




4.2.17 Score per residue for model 17

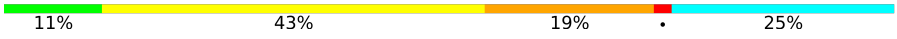
• Molecule 1: Suppressor of cytokine signaling 3

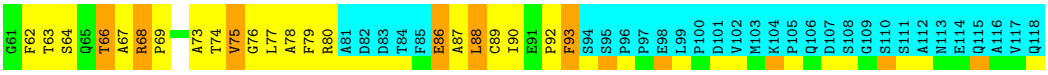
Chain A:



• Molecule 2: Transcription elongation factor B polypeptide 2

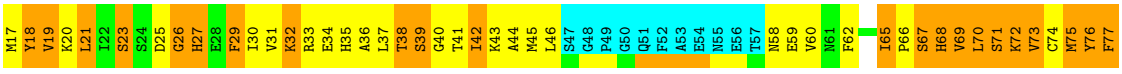
Chain B:

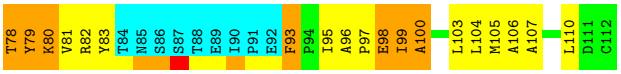




• Molecule 3: Transcription elongation factor B polypeptide 1

Chain C:

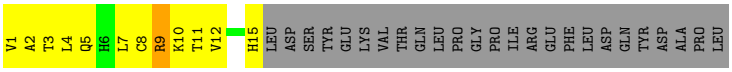




4.2.18 Score per residue for model 18

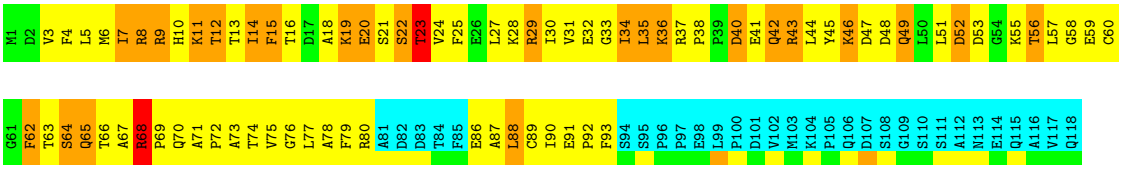
• Molecule 1: Suppressor of cytokine signaling 3

Chain A:



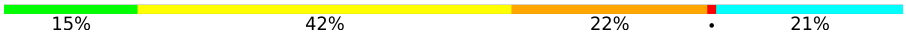
• Molecule 2: Transcription elongation factor B polypeptide 2

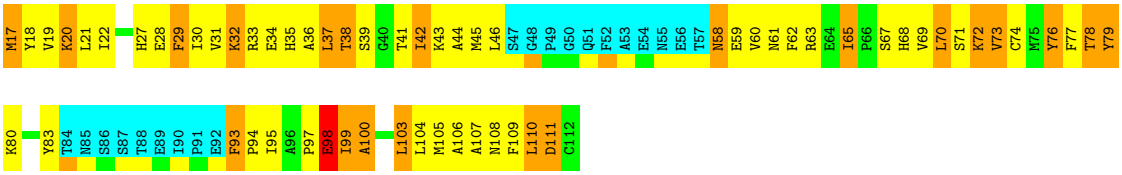
Chain B:



• Molecule 3: Transcription elongation factor B polypeptide 1

Chain C:

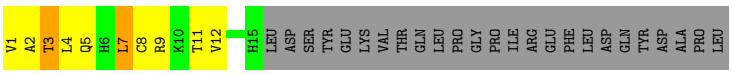




4.2.19 Score per residue for model 19

• Molecule 1: Suppressor of cytokine signaling 3

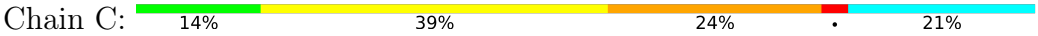
Chain A:

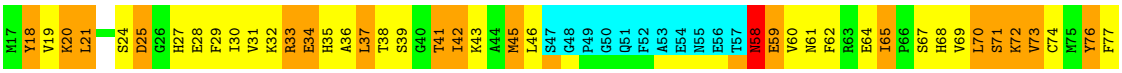


• Molecule 2: Transcription elongation factor B polypeptide 2

Chain B:

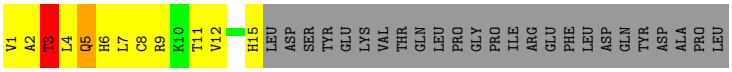
• Molecule 3: Transcription elongation factor B polypeptide 1





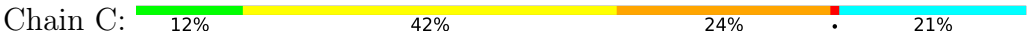
4.2.20 Score per residue for model 20

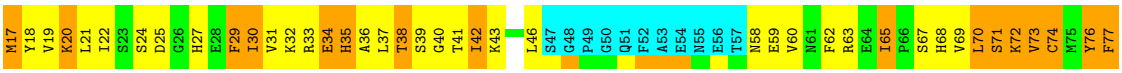
• Molecule 1: Suppressor of cytokine signaling 3



• Molecule 2: Transcription elongation factor B polypeptide 2

• Molecule 3: Transcription elongation factor B polypeptide 1





5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
TALOS	structure solution	
TALOS	refinement	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	116	123	123	42±7
2	B	701	712	712	160±12
3	C	614	625	624	175±12
All	All	28620	29200	29180	6579

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 114.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:70:LEU:HD13	3:C:71:SER:N	1.16	1.55	4	14
3:C:70:LEU:HD12	3:C:71:SER:N	1.16	1.54	3	6
2:B:10:HIS:O	2:B:12:THR:N	1.15	1.79	1	20
3:C:36:ALA:HB1	3:C:42:ILE:HG21	1.10	1.18	14	20
1:A:4:LEU:HD13	3:C:103:LEU:HD22	1.09	1.09	16	2
3:C:65:ILE:HG23	3:C:69:VAL:HG12	1.06	1.21	14	13
2:B:23:THR:HG21	2:B:57:LEU:HB2	1.06	1.28	19	4
2:B:62:PHE:CZ	2:B:73:ALA:HB1	1.04	1.87	12	1
1:A:3:THR:HG21	3:C:38:THR:O	1.04	1.52	9	2
1:A:4:LEU:HD11	3:C:103:LEU:HD13	1.03	1.26	9	1
2:B:77:LEU:O	2:B:87:ALA:HB3	1.01	1.55	20	5
2:B:5:LEU:HD11	2:B:57:LEU:HD21	1.01	1.13	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:34:ILE:HD13	2:B:35:LEU:N	1.01	1.70	18	4
2:B:7:ILE:CD1	2:B:77:LEU:HD21	1.01	1.84	2	10
3:C:19:VAL:HG11	3:C:36:ALA:HB2	1.01	1.33	18	6
3:C:36:ALA:CB	3:C:42:ILE:HG21	1.01	1.83	3	11
2:B:3:VAL:HG21	2:B:57:LEU:HD23	1.01	1.23	19	1
2:B:22:SER:O	2:B:23:THR:HG23	1.00	1.57	7	3
3:C:70:LEU:HD22	3:C:70:LEU:O	1.00	1.56	8	14
1:A:12:VAL:CG2	3:C:104:LEU:HD22	1.00	1.87	5	3
2:B:4:PHE:O	2:B:67:ALA:HB1	0.99	1.57	3	15
2:B:5:LEU:HD21	2:B:57:LEU:HD22	0.99	1.30	12	2
3:C:69:VAL:HG13	3:C:103:LEU:CD1	0.99	1.87	1	12
1:A:7:LEU:HD13	3:C:93:PHE:CZ	0.98	1.93	8	4
1:A:12:VAL:HG21	3:C:104:LEU:CD2	0.98	1.87	5	5
2:B:8:ARG:CG	2:B:90:ILE:HG21	0.98	1.87	12	5
1:A:12:VAL:HG21	3:C:104:LEU:HD22	0.98	0.99	5	4
2:B:5:LEU:HD21	2:B:57:LEU:CD2	0.98	1.88	12	3
1:A:12:VAL:HG21	3:C:104:LEU:CD1	0.98	1.87	4	4
1:A:7:LEU:HD13	3:C:93:PHE:CE2	0.98	1.94	13	4
3:C:69:VAL:HG22	3:C:103:LEU:CD1	0.98	1.88	7	10
2:B:78:ALA:HB2	2:B:88:LEU:HD23	0.97	1.35	5	2
2:B:3:VAL:HG11	2:B:57:LEU:HD22	0.97	1.35	4	3
1:A:4:LEU:HD11	3:C:103:LEU:HD22	0.96	1.35	6	2
3:C:19:VAL:HG12	3:C:31:VAL:O	0.96	1.59	19	16
3:C:35:HIS:CD2	3:C:78:THR:HG22	0.96	1.94	3	6
3:C:35:HIS:ND1	3:C:78:THR:HG22	0.96	1.75	1	3
1:A:4:LEU:HD12	3:C:73:VAL:HB	0.96	1.37	17	8
2:B:5:LEU:HD11	2:B:62:PHE:CZ	0.95	1.96	2	1
2:B:7:ILE:HD13	2:B:77:LEU:HD22	0.95	1.38	15	2
2:B:34:ILE:CG1	2:B:35:LEU:HD12	0.94	1.91	20	8
2:B:16:THR:OG1	2:B:30:ILE:HD13	0.94	1.61	13	7
1:A:7:LEU:HD12	3:C:76:TYR:CE2	0.94	1.98	8	2
3:C:19:VAL:HG21	3:C:46:LEU:HD13	0.94	1.36	17	1
2:B:23:THR:HG23	2:B:24:VAL:HG13	0.94	1.37	16	1
2:B:23:THR:CB	2:B:57:LEU:HD12	0.94	1.92	16	1
2:B:3:VAL:HG22	2:B:67:ALA:HB3	0.94	1.37	6	8
3:C:35:HIS:CE1	3:C:78:THR:HG22	0.93	1.97	9	5
1:A:11:THR:OG1	3:C:95:ILE:HG21	0.93	1.62	7	14
2:B:64:SER:O	2:B:66:THR:HG22	0.93	1.63	2	1
2:B:22:SER:O	2:B:24:VAL:HG22	0.93	1.62	19	1
1:A:4:LEU:HD12	3:C:73:VAL:CA	0.93	1.93	2	12
2:B:5:LEU:CD1	2:B:57:LEU:HD21	0.93	1.91	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:8:ARG:HG3	2:B:90:ILE:HG21	0.93	1.41	12	3
2:B:27:LEU:O	2:B:27:LEU:HD22	0.93	1.63	5	3
3:C:38:THR:HG22	3:C:80:LYS:CD	0.93	1.93	19	5
2:B:14:ILE:CG1	3:C:30:ILE:HD12	0.93	1.94	5	1
2:B:31:VAL:HG22	2:B:77:LEU:CD1	0.92	1.93	3	2
3:C:65:ILE:HG23	3:C:69:VAL:CG1	0.92	1.95	16	17
3:C:36:ALA:HB1	3:C:42:ILE:CG2	0.91	1.94	13	14
2:B:44:LEU:O	2:B:50:LEU:HD12	0.91	1.65	5	7
2:B:78:ALA:CB	2:B:88:LEU:HD23	0.91	1.94	5	5
2:B:21:SER:O	2:B:56:THR:HG21	0.91	1.65	12	3
2:B:23:THR:HG21	2:B:57:LEU:HD22	0.91	1.41	12	1
2:B:77:LEU:HD23	2:B:77:LEU:N	0.91	1.80	15	2
2:B:31:VAL:HG22	2:B:77:LEU:HD11	0.91	1.40	3	1
2:B:7:ILE:CG2	2:B:77:LEU:HD11	0.91	1.96	19	5
1:A:12:VAL:HG21	3:C:104:LEU:HD23	0.90	1.38	7	5
2:B:3:VAL:CG2	2:B:67:ALA:HB3	0.90	1.97	3	12
2:B:14:ILE:HG12	3:C:30:ILE:HD13	0.90	1.42	11	15
3:C:78:THR:O	3:C:81:VAL:HG22	0.90	1.65	16	1
2:B:57:LEU:HD23	2:B:63:THR:OG1	0.90	1.67	12	1
2:B:44:LEU:HD12	2:B:51:LEU:HB3	0.89	1.44	11	1
2:B:7:ILE:HG23	2:B:77:LEU:HD11	0.89	1.43	2	3
3:C:37:LEU:HD13	3:C:37:LEU:O	0.89	1.66	14	3
2:B:23:THR:CA	2:B:57:LEU:HD12	0.89	1.97	16	1
3:C:31:VAL:HG23	3:C:36:ALA:HB2	0.88	1.43	1	10
2:B:5:LEU:HD13	2:B:73:ALA:HB3	0.88	1.41	4	4
2:B:23:THR:HB	2:B:57:LEU:HD13	0.88	1.43	19	3
1:A:12:VAL:HG21	3:C:104:LEU:HD12	0.88	1.43	4	1
2:B:78:ALA:HB2	2:B:88:LEU:CD2	0.88	1.97	5	5
3:C:72:LYS:HB3	3:C:103:LEU:HD21	0.88	1.43	17	5
3:C:69:VAL:HG21	3:C:102:GLU:CB	0.88	1.98	14	14
3:C:94:PRO:O	3:C:95:ILE:HD13	0.88	1.68	16	3
1:A:3:THR:HG21	3:C:111:ASP:O	0.88	1.68	16	1
3:C:38:THR:HG21	3:C:77:PHE:O	0.87	1.68	13	7
2:B:5:LEU:HD11	2:B:57:LEU:CD2	0.87	1.99	10	1
2:B:7:ILE:HD13	2:B:77:LEU:HD21	0.87	1.46	17	9
1:A:4:LEU:HD11	3:C:103:LEU:CG	0.87	2.00	8	6
2:B:8:ARG:HB3	2:B:90:ILE:HD12	0.87	1.46	8	9
3:C:96:ALA:HB1	3:C:97:PRO:HD2	0.87	1.46	10	19
3:C:37:LEU:HD23	3:C:37:LEU:O	0.87	1.69	10	2
2:B:44:LEU:HD13	2:B:45:TYR:N	0.87	1.85	11	1
3:C:68:HIS:CD2	3:C:69:VAL:HG23	0.87	2.05	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:38:THR:HG22	3:C:80:LYS:HD3	0.87	1.47	6	6
1:A:7:LEU:HD22	3:C:93:PHE:CB	0.87	1.99	9	3
2:B:8:ARG:O	2:B:77:LEU:HD13	0.86	1.69	6	1
2:B:10:HIS:C	2:B:12:THR:H	0.86	1.74	1	20
1:A:4:LEU:HD21	3:C:103:LEU:HD23	0.86	1.46	3	7
1:A:4:LEU:HD12	3:C:73:VAL:CB	0.86	1.99	6	7
2:B:31:VAL:HG11	2:B:42:GLN:OE1	0.86	1.71	18	2
2:B:5:LEU:HD11	2:B:62:PHE:CD1	0.86	2.06	18	6
2:B:51:LEU:HD12	2:B:62:PHE:CE2	0.86	2.06	9	1
2:B:6:MET:O	2:B:75:VAL:HG13	0.86	1.71	8	20
3:C:73:VAL:HG21	3:C:110:LEU:HD12	0.86	1.46	13	2
3:C:21:LEU:HD11	3:C:31:VAL:CG2	0.86	1.99	12	3
3:C:68:HIS:CE1	3:C:69:VAL:HG23	0.85	2.06	12	2
2:B:76:GLY:C	2:B:77:LEU:HD22	0.85	1.91	17	3
2:B:19:LYS:O	2:B:57:LEU:HD12	0.85	1.70	13	3
2:B:5:LEU:HD13	2:B:57:LEU:CD2	0.85	2.01	1	1
2:B:3:VAL:HG11	2:B:57:LEU:HD23	0.85	1.44	14	2
2:B:3:VAL:HG23	2:B:67:ALA:HB3	0.85	1.49	11	11
1:A:1:VAL:HG11	3:C:80:LYS:HA	0.84	1.48	19	10
2:B:4:PHE:C	2:B:5:LEU:HD22	0.84	1.92	9	8
3:C:69:VAL:HG22	3:C:103:LEU:HD13	0.84	1.48	7	6
2:B:57:LEU:HD23	2:B:62:PHE:CB	0.84	2.02	20	4
3:C:19:VAL:HG11	3:C:36:ALA:CB	0.84	2.03	18	9
3:C:22:ILE:HD11	3:C:28:GLU:OE2	0.84	1.72	8	1
1:A:4:LEU:HD11	3:C:103:LEU:HG	0.84	1.48	17	6
3:C:99:ILE:O	3:C:100:ALA:CB	0.84	2.26	13	20
2:B:78:ALA:HB2	2:B:87:ALA:O	0.84	1.72	20	4
1:A:7:LEU:HB3	3:C:95:ILE:HD11	0.84	1.46	18	1
3:C:35:HIS:CD2	3:C:78:THR:HG23	0.83	2.07	4	6
2:B:78:ALA:HB2	2:B:88:LEU:HD22	0.83	1.50	11	14
3:C:70:LEU:HD13	3:C:70:LEU:C	0.83	1.94	12	14
2:B:24:VAL:HG12	2:B:53:ASP:HA	0.83	1.50	5	1
2:B:14:ILE:HG13	2:B:34:ILE:HG21	0.83	1.49	7	5
3:C:100:ALA:HA	3:C:103:LEU:HD12	0.83	1.51	16	3
2:B:57:LEU:HD22	2:B:62:PHE:CB	0.83	2.03	11	2
1:A:4:LEU:HD12	3:C:73:VAL:HA	0.83	1.50	2	10
1:A:4:LEU:HD23	1:A:4:LEU:O	0.83	1.74	1	10
2:B:8:ARG:O	2:B:77:LEU:HD12	0.83	1.73	2	1
2:B:7:ILE:HD11	2:B:77:LEU:HD13	0.83	1.51	1	1
2:B:3:VAL:HG13	2:B:67:ALA:HB1	0.83	1.49	4	2
2:B:9:ARG:HB2	2:B:77:LEU:HD12	0.83	1.48	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:43:ARG:CD	2:B:50:LEU:HD21	0.82	2.03	12	1
2:B:63:THR:O	2:B:66:THR:HG22	0.82	1.74	18	2
3:C:35:HIS:NE2	3:C:78:THR:HG22	0.82	1.88	6	4
2:B:46:LYS:HB2	2:B:51:LEU:HD22	0.82	1.48	16	1
3:C:95:ILE:HG23	3:C:100:ALA:CB	0.82	2.05	11	19
2:B:13:THR:O	3:C:30:ILE:HD12	0.82	1.75	11	17
2:B:15:PHE:CZ	3:C:78:THR:HG21	0.82	2.08	11	2
2:B:66:THR:O	2:B:73:ALA:HB2	0.82	1.75	12	16
2:B:44:LEU:HB3	2:B:51:LEU:HD21	0.82	1.52	10	1
2:B:3:VAL:HG22	2:B:67:ALA:CB	0.81	2.05	16	11
2:B:7:ILE:CD1	2:B:77:LEU:HD11	0.81	2.05	9	8
2:B:87:ALA:C	2:B:88:LEU:HD22	0.81	1.96	3	2
3:C:77:PHE:O	3:C:81:VAL:HG23	0.81	1.75	2	4
3:C:65:ILE:CG2	3:C:69:VAL:HG12	0.81	2.06	16	12
1:A:12:VAL:HG21	3:C:104:LEU:HD13	0.81	1.51	12	6
2:B:78:ALA:CB	2:B:88:LEU:HD22	0.81	2.04	11	9
2:B:8:ARG:CB	2:B:90:ILE:HD12	0.81	2.05	9	3
2:B:76:GLY:C	2:B:77:LEU:HD23	0.81	1.96	16	2
3:C:72:LYS:HG2	3:C:99:ILE:HD12	0.81	1.53	18	1
1:A:7:LEU:HD13	3:C:93:PHE:CB	0.80	2.06	6	3
3:C:42:ILE:HG23	3:C:46:LEU:HD12	0.80	1.52	17	1
2:B:9:ARG:HD2	2:B:35:LEU:HD21	0.80	1.53	7	1
2:B:78:ALA:HB1	2:B:86:GLU:HG2	0.80	1.51	19	2
1:A:1:VAL:HG13	3:C:80:LYS:CD	0.80	2.06	11	1
2:B:78:ALA:HB1	2:B:86:GLU:CG	0.80	2.06	19	1
3:C:70:LEU:HD22	3:C:70:LEU:C	0.80	1.97	10	14
3:C:69:VAL:HG22	3:C:103:LEU:CD2	0.80	2.05	9	2
2:B:24:VAL:HG21	2:B:55:LYS:O	0.80	1.77	11	6
2:B:24:VAL:HG11	2:B:55:LYS:O	0.80	1.76	19	3
2:B:78:ALA:HA	2:B:87:ALA:HB3	0.80	1.54	16	6
1:A:1:VAL:HG23	3:C:76:TYR:CE1	0.80	2.11	8	7
2:B:57:LEU:HD22	2:B:62:PHE:CG	0.80	2.12	11	1
2:B:14:ILE:CD1	3:C:30:ILE:HD11	0.80	2.07	18	2
2:B:14:ILE:HD13	3:C:30:ILE:HD11	0.79	1.52	18	1
3:C:103:LEU:HA	3:C:106:ALA:HB3	0.79	1.52	6	9
2:B:44:LEU:HD12	2:B:51:LEU:CB	0.79	2.08	11	1
2:B:51:LEU:O	2:B:51:LEU:HD23	0.79	1.78	9	2
1:A:7:LEU:HD22	3:C:93:PHE:HB3	0.79	1.54	5	2
2:B:44:LEU:HD13	2:B:44:LEU:C	0.79	1.97	11	1
2:B:43:ARG:HB3	2:B:78:ALA:HB3	0.78	1.54	15	1
3:C:46:LEU:HD12	3:C:46:LEU:O	0.78	1.77	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:VAL:HG11	3:C:104:LEU:HD13	0.78	1.53	3	2
2:B:22:SER:O	2:B:23:THR:HG22	0.78	1.77	16	1
2:B:5:LEU:HD12	2:B:73:ALA:HB3	0.78	1.56	11	8
2:B:44:LEU:O	2:B:50:LEU:HD23	0.78	1.77	3	5
2:B:3:VAL:HG22	2:B:63:THR:C	0.78	1.98	5	1
2:B:18:ALA:HB1	2:B:22:SER:O	0.78	1.77	5	3
2:B:51:LEU:HD21	2:B:62:PHE:CE2	0.78	2.14	16	1
2:B:7:ILE:HD12	2:B:77:LEU:HD21	0.78	1.55	2	1
2:B:31:VAL:HG12	2:B:37:ARG:HB2	0.78	1.56	17	3
2:B:3:VAL:HG22	2:B:63:THR:CA	0.77	2.09	5	1
3:C:39:SER:OG	3:C:42:ILE:HD12	0.77	1.79	2	9
3:C:66:PRO:HD2	3:C:69:VAL:HG21	0.77	1.55	17	1
2:B:27:LEU:C	2:B:27:LEU:HD13	0.77	2.00	11	3
3:C:69:VAL:HG22	3:C:103:LEU:HD11	0.77	1.57	13	8
2:B:42:GLN:OE1	2:B:77:LEU:HD11	0.77	1.79	1	1
3:C:46:LEU:HD22	3:C:58:ASN:HA	0.77	1.55	16	3
1:A:4:LEU:CD1	3:C:103:LEU:HD22	0.77	2.02	16	4
1:A:12:VAL:HG21	3:C:104:LEU:HG	0.77	1.57	17	1
2:B:78:ALA:HB2	2:B:88:LEU:N	0.76	1.94	2	1
3:C:65:ILE:HD11	3:C:106:ALA:HB1	0.76	1.54	5	11
2:B:14:ILE:CD1	2:B:34:ILE:HG21	0.76	2.11	6	3
3:C:72:LYS:HG3	3:C:103:LEU:HD11	0.76	1.56	9	1
1:A:4:LEU:HD11	3:C:72:LYS:HG3	0.76	1.55	2	2
1:A:7:LEU:HD13	3:C:93:PHE:CG	0.76	2.15	6	2
3:C:30:ILE:O	3:C:30:ILE:HD12	0.76	1.80	18	1
2:B:3:VAL:CG2	2:B:57:LEU:HD23	0.76	2.09	19	2
1:A:4:LEU:HD13	3:C:103:LEU:CD2	0.76	2.01	16	1
3:C:39:SER:CB	3:C:42:ILE:HD12	0.76	2.11	19	12
3:C:38:THR:HG21	3:C:80:LYS:CB	0.76	2.11	3	4
2:B:7:ILE:HB	2:B:14:ILE:HG22	0.75	1.56	20	20
2:B:14:ILE:HG13	2:B:34:ILE:HD12	0.75	1.57	18	7
2:B:51:LEU:HD21	2:B:62:PHE:CZ	0.75	2.15	16	1
2:B:7:ILE:HD13	2:B:77:LEU:CD2	0.75	2.12	17	12
3:C:65:ILE:HD11	3:C:106:ALA:CB	0.75	2.10	20	8
2:B:14:ILE:HG12	3:C:30:ILE:HD12	0.75	1.57	5	1
2:B:5:LEU:HD22	2:B:27:LEU:CD2	0.75	2.11	18	1
3:C:42:ILE:HD13	3:C:77:PHE:CZ	0.75	2.17	20	12
2:B:8:ARG:HG3	2:B:74:THR:HG23	0.75	1.57	9	1
3:C:68:HIS:NE2	3:C:69:VAL:HG23	0.75	1.97	16	3
2:B:62:PHE:CE1	2:B:73:ALA:HB1	0.75	2.16	20	6
1:A:11:THR:OG1	3:C:95:ILE:HD13	0.75	1.81	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:HD13	3:C:103:LEU:HG	0.75	1.57	18	9
3:C:31:VAL:CG2	3:C:36:ALA:HB2	0.75	2.12	8	11
1:A:4:LEU:HD11	3:C:103:LEU:CD2	0.75	2.12	8	7
3:C:106:ALA:O	3:C:110:LEU:HD13	0.75	1.80	3	1
2:B:44:LEU:HD23	2:B:77:LEU:CD2	0.75	2.12	13	3
3:C:38:THR:HG22	3:C:76:TYR:OH	0.74	1.82	12	1
1:A:4:LEU:C	3:C:107:ALA:HB1	0.74	2.03	3	15
3:C:72:LYS:HG3	3:C:99:ILE:HD12	0.74	1.59	17	3
1:A:5:GLN:HA	3:C:107:ALA:HB1	0.74	1.58	18	9
3:C:23:SER:HB2	3:C:70:LEU:HD23	0.74	1.59	3	1
3:C:38:THR:HG22	3:C:80:LYS:HD2	0.74	1.58	19	1
3:C:69:VAL:HG21	3:C:102:GLU:HB3	0.74	1.57	14	11
2:B:3:VAL:HG21	2:B:57:LEU:CD2	0.74	2.10	19	2
2:B:22:SER:O	2:B:23:THR:CG2	0.74	2.35	13	4
2:B:43:ARG:HG3	2:B:50:LEU:HD11	0.74	1.58	15	1
3:C:99:ILE:O	3:C:100:ALA:HB2	0.74	1.80	18	20
3:C:69:VAL:HG22	3:C:103:LEU:HG	0.74	1.59	6	3
3:C:70:LEU:CD1	3:C:71:SER:N	0.74	2.48	12	17
1:A:11:THR:HG21	3:C:95:ILE:HG21	0.73	1.59	3	5
2:B:8:ARG:HB3	2:B:90:ILE:HD13	0.73	1.60	11	8
2:B:77:LEU:HD22	2:B:77:LEU:N	0.73	1.97	8	3
3:C:43:LYS:O	3:C:46:LEU:HD23	0.73	1.83	14	1
2:B:51:LEU:HD23	2:B:52:ASP:N	0.73	1.98	11	2
2:B:23:THR:CB	2:B:57:LEU:HD13	0.73	2.14	19	3
2:B:13:THR:HG21	3:C:29:PHE:CE2	0.73	2.19	11	3
2:B:7:ILE:CD1	2:B:77:LEU:HD13	0.73	2.13	1	1
2:B:43:ARG:HD2	2:B:50:LEU:HD21	0.73	1.59	12	1
1:A:5:GLN:N	3:C:107:ALA:HB1	0.73	1.99	19	18
2:B:45:TYR:CZ	2:B:50:LEU:HD13	0.73	2.19	8	3
2:B:18:ALA:HB1	2:B:22:SER:HB2	0.73	1.59	4	1
3:C:70:LEU:HD12	3:C:70:LEU:C	0.73	2.03	1	6
2:B:24:VAL:CG1	2:B:51:LEU:HD22	0.73	2.13	11	1
2:B:43:ARG:HB2	2:B:78:ALA:HB3	0.73	1.61	17	2
2:B:78:ALA:HB2	2:B:87:ALA:HB3	0.73	1.59	3	2
2:B:14:ILE:HG13	3:C:30:ILE:HD12	0.73	1.58	5	1
2:B:3:VAL:CG1	2:B:57:LEU:HD23	0.73	2.13	14	2
3:C:43:LYS:HA	3:C:46:LEU:HD13	0.73	1.59	12	1
2:B:13:THR:HG23	3:C:27:HIS:CE1	0.73	2.19	18	1
3:C:69:VAL:HG13	3:C:103:LEU:HD11	0.72	1.61	2	7
2:B:5:LEU:HD12	2:B:73:ALA:CB	0.72	2.14	11	2
2:B:23:THR:HG21	2:B:57:LEU:CB	0.72	2.11	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:69:VAL:HG13	3:C:103:LEU:HD12	0.72	1.61	1	2
1:A:1:VAL:HG12	3:C:83:TYR:CB	0.72	2.14	6	3
1:A:1:VAL:HG21	3:C:80:LYS:HA	0.72	1.60	8	10
1:A:4:LEU:HD12	3:C:73:VAL:N	0.72	2.00	10	11
2:B:5:LEU:O	2:B:16:THR:HG22	0.72	1.84	5	16
2:B:23:THR:HG23	2:B:26:GLU:CB	0.72	2.15	9	4
2:B:44:LEU:CB	2:B:51:LEU:HD21	0.72	2.15	10	1
2:B:31:VAL:HG13	2:B:77:LEU:HD11	0.71	1.60	18	2
2:B:7:ILE:HD12	2:B:77:LEU:HD11	0.71	1.62	20	4
3:C:65:ILE:CG1	3:C:106:ALA:HB2	0.71	2.15	14	4
3:C:20:LYS:C	3:C:21:LEU:HD23	0.71	2.05	9	18
3:C:65:ILE:HG12	3:C:106:ALA:HB2	0.71	1.62	9	3
2:B:3:VAL:HG21	2:B:63:THR:OG1	0.71	1.85	12	2
1:A:4:LEU:CD1	3:C:103:LEU:HD13	0.71	2.10	9	1
2:B:5:LEU:N	2:B:5:LEU:HD22	0.71	2.01	20	1
2:B:9:ARG:HD2	2:B:77:LEU:HD13	0.71	1.62	2	1
2:B:31:VAL:HG11	2:B:42:GLN:NE2	0.71	2.00	1	2
2:B:23:THR:HG21	2:B:57:LEU:CD2	0.71	2.15	12	1
2:B:57:LEU:HD23	2:B:62:PHE:CG	0.71	2.21	7	1
1:A:3:THR:HG22	3:C:38:THR:O	0.71	1.86	14	1
3:C:73:VAL:HG21	3:C:110:LEU:HD13	0.71	1.63	16	7
2:B:8:ARG:CB	2:B:90:ILE:HD13	0.71	2.15	11	3
2:B:5:LEU:CD2	2:B:27:LEU:HD23	0.71	2.15	18	1
2:B:7:ILE:HG21	2:B:77:LEU:HD11	0.70	1.60	7	5
2:B:8:ARG:N	2:B:77:LEU:HD21	0.70	2.01	16	2
2:B:62:PHE:C	2:B:63:THR:HG22	0.70	2.05	2	2
2:B:5:LEU:CD1	2:B:73:ALA:HB3	0.70	2.16	4	2
2:B:8:ARG:HB3	2:B:90:ILE:HG21	0.70	1.63	10	5
3:C:29:PHE:CD2	3:C:70:LEU:HD21	0.70	2.22	6	1
1:A:4:LEU:HD23	3:C:103:LEU:HD13	0.70	1.63	19	1
2:B:31:VAL:CG2	2:B:77:LEU:HD11	0.70	2.16	3	1
2:B:87:ALA:O	2:B:88:LEU:CB	0.70	2.39	5	15
3:C:35:HIS:NE2	3:C:78:THR:HG23	0.70	2.02	11	1
3:C:35:HIS:CG	3:C:78:THR:HG22	0.70	2.21	1	3
3:C:42:ILE:CG2	3:C:46:LEU:HD23	0.70	2.17	2	1
3:C:79:TYR:CE2	3:C:83:TYR:CZ	0.70	2.80	18	4
2:B:44:LEU:HD23	2:B:77:LEU:HD22	0.70	1.62	5	2
2:B:30:ILE:O	2:B:34:ILE:HG23	0.70	1.87	16	7
2:B:3:VAL:HG22	2:B:67:ALA:HB1	0.70	1.63	16	3
2:B:23:THR:CG2	2:B:57:LEU:HD22	0.70	2.17	12	1
3:C:21:LEU:HD11	3:C:31:VAL:HG21	0.70	1.63	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:34:ILE:HD11	3:C:18:TYR:CE2	0.69	2.21	1	1
2:B:43:ARG:CG	2:B:50:LEU:HD11	0.69	2.16	15	1
2:B:14:ILE:HD11	3:C:30:ILE:HD11	0.69	1.64	20	2
2:B:14:ILE:HD12	2:B:34:ILE:HG21	0.69	1.64	6	1
3:C:79:TYR:CZ	3:C:83:TYR:CE1	0.69	2.79	19	2
2:B:62:PHE:CG	2:B:62:PHE:O	0.69	2.46	12	2
3:C:46:LEU:HD12	3:C:46:LEU:C	0.69	2.07	2	3
3:C:79:TYR:CE2	3:C:83:TYR:CE1	0.69	2.80	11	2
2:B:93:PHE:CZ	3:C:27:HIS:CE1	0.69	2.81	13	1
3:C:79:TYR:CZ	3:C:83:TYR:CZ	0.69	2.80	13	5
2:B:68:ARG:HB2	2:B:69:PRO:HD2	0.69	1.65	6	5
1:A:1:VAL:HG23	3:C:76:TYR:HE1	0.69	1.45	8	7
3:C:19:VAL:HG23	3:C:46:LEU:CD2	0.69	2.17	18	1
2:B:5:LEU:HD11	2:B:62:PHE:CE1	0.69	2.21	18	4
2:B:3:VAL:HG22	2:B:63:THR:O	0.69	1.88	5	1
3:C:79:TYR:CZ	3:C:83:TYR:CE2	0.69	2.80	4	4
2:B:77:LEU:O	2:B:87:ALA:CB	0.69	2.41	16	6
3:C:38:THR:HG21	3:C:80:LYS:HB3	0.69	1.62	15	7
2:B:31:VAL:HG21	2:B:77:LEU:HD11	0.69	1.63	5	2
2:B:88:LEU:HD13	2:B:88:LEU:O	0.69	1.87	5	1
3:C:104:LEU:HD13	3:C:104:LEU:C	0.69	2.08	7	5
3:C:19:VAL:CG2	3:C:46:LEU:HD13	0.69	2.14	17	1
3:C:23:SER:CB	3:C:70:LEU:HD23	0.69	2.18	14	5
2:B:4:PHE:O	2:B:67:ALA:HB3	0.68	1.88	2	3
3:C:72:LYS:CB	3:C:103:LEU:HD21	0.68	2.17	17	4
3:C:69:VAL:HG22	3:C:103:LEU:CG	0.68	2.17	6	2
1:A:11:THR:CG2	3:C:95:ILE:HG21	0.68	2.17	3	6
3:C:65:ILE:CD1	3:C:106:ALA:HB1	0.68	2.19	5	9
2:B:77:LEU:O	2:B:87:ALA:HB1	0.68	1.87	18	9
2:B:51:LEU:HD12	2:B:51:LEU:C	0.68	2.08	10	1
2:B:4:PHE:O	2:B:5:LEU:HD22	0.68	1.87	10	6
2:B:8:ARG:NE	2:B:90:ILE:HG21	0.68	2.04	15	5
3:C:38:THR:OG1	3:C:77:PHE:CD1	0.68	2.47	4	15
3:C:67:SER:O	3:C:70:LEU:HG	0.68	1.88	17	6
1:A:4:LEU:HD22	1:A:4:LEU:O	0.68	1.88	8	7
1:A:1:VAL:HG13	3:C:80:LYS:HD3	0.68	1.66	11	1
2:B:68:ARG:CB	2:B:69:PRO:HD2	0.68	2.19	20	15
2:B:3:VAL:HG11	2:B:57:LEU:CD2	0.68	2.18	16	2
1:A:4:LEU:CD2	3:C:103:LEU:HD22	0.68	2.18	19	1
2:B:5:LEU:HD23	2:B:27:LEU:HD13	0.68	1.63	19	3
2:B:31:VAL:HG21	2:B:77:LEU:CD1	0.68	2.19	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:VAL:CG2	3:C:104:LEU:HD13	0.68	2.18	15	2
2:B:19:LYS:O	2:B:57:LEU:HD13	0.68	1.88	15	3
1:A:3:THR:HG22	3:C:38:THR:HG22	0.68	1.66	9	1
3:C:21:LEU:HD11	3:C:31:VAL:HG22	0.68	1.65	12	1
2:B:3:VAL:HG11	2:B:57:LEU:HD13	0.68	1.65	8	3
2:B:27:LEU:HD13	2:B:28:LYS:N	0.68	2.04	5	3
3:C:74:CYS:O	3:C:77:PHE:HB2	0.67	1.89	18	20
2:B:45:TYR:CZ	2:B:88:LEU:HD11	0.67	2.24	16	3
2:B:63:THR:OG1	2:B:64:SER:N	0.67	2.26	2	17
3:C:76:TYR:CD1	3:C:93:PHE:CE1	0.67	2.82	19	1
2:B:7:ILE:HD13	2:B:77:LEU:HD11	0.67	1.65	6	3
2:B:8:ARG:CD	2:B:90:ILE:HG21	0.67	2.18	15	5
2:B:77:LEU:N	2:B:77:LEU:CD2	0.67	2.48	15	4
3:C:79:TYR:CE1	3:C:83:TYR:CG	0.67	2.82	11	1
2:B:78:ALA:CB	2:B:88:LEU:CD2	0.67	2.73	14	16
3:C:37:LEU:HD13	3:C:37:LEU:C	0.67	2.09	9	2
2:B:51:LEU:HD12	2:B:62:PHE:CZ	0.67	2.24	9	1
3:C:69:VAL:HG21	3:C:102:GLU:HB2	0.67	1.67	19	7
2:B:5:LEU:HD22	2:B:57:LEU:HD11	0.67	1.67	11	1
3:C:21:LEU:HG	3:C:29:PHE:O	0.67	1.89	20	20
3:C:73:VAL:HG21	3:C:110:LEU:HD11	0.67	1.66	5	1
3:C:30:ILE:HD12	3:C:30:ILE:C	0.67	2.10	18	1
2:B:23:THR:O	2:B:24:VAL:C	0.67	2.31	11	13
2:B:24:VAL:HA	2:B:27:LEU:HD21	0.67	1.65	14	1
1:A:1:VAL:HG13	3:C:80:LYS:CG	0.66	2.20	4	2
2:B:22:SER:O	2:B:23:THR:CB	0.66	2.43	16	14
3:C:66:PRO:CG	3:C:68:HIS:CE1	0.66	2.79	16	3
1:A:1:VAL:CG1	3:C:83:TYR:CB	0.66	2.73	5	5
3:C:37:LEU:HD22	3:C:43:LYS:CB	0.66	2.21	5	1
2:B:34:ILE:HG13	2:B:35:LEU:HD12	0.66	1.66	20	3
1:A:2:ALA:O	3:C:76:TYR:CZ	0.66	2.49	11	13
2:B:24:VAL:HG11	2:B:52:ASP:O	0.66	1.90	5	4
3:C:19:VAL:HG22	3:C:60:VAL:HG23	0.66	1.68	5	13
2:B:24:VAL:CG1	2:B:51:LEU:HD21	0.66	2.20	9	2
3:C:69:VAL:HG13	3:C:103:LEU:CD2	0.66	2.20	9	2
2:B:23:THR:C	2:B:24:VAL:HG23	0.66	2.11	12	1
1:A:12:VAL:HG21	3:C:104:LEU:HB2	0.66	1.67	18	1
3:C:37:LEU:HD12	3:C:43:LYS:HG3	0.66	1.66	19	1
2:B:22:SER:C	2:B:23:THR:HG22	0.66	2.11	17	10
2:B:7:ILE:HD13	2:B:77:LEU:CG	0.66	2.20	8	12
1:A:1:VAL:HG12	3:C:83:TYR:CG	0.66	2.25	16	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:VAL:CG2	3:C:104:LEU:HD12	0.66	2.21	4	1
2:B:3:VAL:CG1	2:B:57:LEU:HD22	0.66	2.18	4	3
3:C:46:LEU:HD21	3:C:58:ASN:OD1	0.66	1.91	7	1
3:C:33:ARG:HD2	3:C:46:LEU:HD13	0.66	1.64	10	1
3:C:18:TYR:N	3:C:18:TYR:CD1	0.66	2.62	1	2
2:B:93:PHE:CD1	2:B:93:PHE:N	0.66	2.63	10	9
1:A:11:THR:HG21	3:C:95:ILE:CG2	0.66	2.20	3	7
3:C:19:VAL:HG12	3:C:31:VAL:CG2	0.65	2.21	17	5
3:C:21:LEU:HD11	3:C:31:VAL:CG1	0.65	2.21	15	4
2:B:24:VAL:HG11	2:B:53:ASP:OD1	0.65	1.90	13	1
1:A:7:LEU:HD23	3:C:93:PHE:HB3	0.65	1.68	17	1
2:B:31:VAL:CG1	2:B:37:ARG:HB2	0.65	2.22	2	13
3:C:19:VAL:HG23	3:C:58:ASN:C	0.65	2.11	1	6
2:B:34:ILE:CD1	2:B:35:LEU:HD12	0.65	2.21	20	9
1:A:4:LEU:HD22	3:C:103:LEU:HD22	0.65	1.67	19	1
3:C:100:ALA:HA	3:C:103:LEU:HD22	0.65	1.68	13	8
2:B:23:THR:HG23	2:B:26:GLU:HB2	0.65	1.67	9	3
3:C:18:TYR:CD2	3:C:30:ILE:CG2	0.65	2.80	14	3
1:A:12:VAL:CG1	3:C:104:LEU:HD13	0.65	2.21	18	2
2:B:76:GLY:HA2	2:B:90:ILE:HD11	0.65	1.69	10	1
2:B:23:THR:HB	2:B:57:LEU:HD23	0.65	1.68	4	2
2:B:31:VAL:HG12	2:B:37:ARG:HB3	0.65	1.69	4	2
1:A:1:VAL:HG22	3:C:76:TYR:CE1	0.65	2.25	12	1
2:B:13:THR:HG21	3:C:29:PHE:CZ	0.65	2.27	17	1
3:C:69:VAL:O	3:C:73:VAL:HG12	0.65	1.92	16	3
3:C:101:LEU:C	3:C:101:LEU:HD13	0.65	2.12	15	1
3:C:39:SER:CB	3:C:77:PHE:CZ	0.65	2.80	1	19
2:B:5:LEU:HD11	2:B:62:PHE:CE2	0.65	2.26	2	1
3:C:42:ILE:HD12	3:C:77:PHE:CE2	0.65	2.27	16	1
2:B:79:PHE:N	2:B:79:PHE:CD1	0.65	2.64	4	2
3:C:42:ILE:HD13	3:C:77:PHE:CE2	0.65	2.27	13	5
3:C:46:LEU:HD13	3:C:58:ASN:OD1	0.65	1.90	5	1
1:A:7:LEU:CD1	3:C:93:PHE:CE2	0.65	2.78	11	3
3:C:95:ILE:HG23	3:C:100:ALA:HB2	0.65	1.69	14	7
1:A:4:LEU:HD11	3:C:103:LEU:CD1	0.65	2.15	9	1
2:B:3:VAL:HG23	2:B:63:THR:O	0.64	1.91	3	3
3:C:21:LEU:HD12	3:C:74:CYS:SG	0.64	2.33	12	5
3:C:69:VAL:HG13	3:C:103:LEU:HD23	0.64	1.69	9	3
2:B:20:GLU:HA	2:B:57:LEU:HD11	0.64	1.67	4	1
2:B:8:ARG:HD2	2:B:90:ILE:HG21	0.64	1.67	11	1
2:B:3:VAL:HG21	2:B:57:LEU:HD21	0.64	1.67	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:THR:HG23	3:C:95:ILE:HG22	0.64	1.68	10	4
3:C:37:LEU:HD22	3:C:43:LYS:HB3	0.64	1.67	5	1
3:C:27:HIS:CD2	3:C:28:GLU:N	0.64	2.66	18	1
2:B:14:ILE:HG21	2:B:34:ILE:HD13	0.64	1.70	5	1
3:C:38:THR:HG23	3:C:80:LYS:CD	0.64	2.23	9	1
2:B:14:ILE:HG12	3:C:30:ILE:CD1	0.64	2.23	20	16
1:A:4:LEU:CD1	3:C:73:VAL:HB	0.64	2.20	15	7
2:B:37:ARG:CZ	2:B:79:PHE:CD1	0.64	2.81	3	2
2:B:13:THR:CG2	3:C:29:PHE:CZ	0.64	2.81	17	1
1:A:2:ALA:O	3:C:76:TYR:CE2	0.64	2.51	2	15
2:B:5:LEU:CD2	2:B:27:LEU:HD13	0.64	2.23	2	4
2:B:10:HIS:CE1	2:B:89:CYS:O	0.64	2.51	12	15
3:C:103:LEU:O	3:C:107:ALA:HB3	0.64	1.92	1	6
2:B:57:LEU:HD23	2:B:62:PHE:CD2	0.64	2.27	2	3
3:C:65:ILE:CG1	3:C:106:ALA:HB1	0.64	2.23	13	10
2:B:31:VAL:HG12	2:B:37:ARG:CB	0.64	2.21	17	3
3:C:65:ILE:HD13	3:C:106:ALA:HB1	0.64	1.70	4	2
2:B:14:ILE:CD1	3:C:30:ILE:CG1	0.64	2.76	20	1
3:C:60:VAL:CG1	3:C:62:PHE:CZ	0.64	2.80	14	8
3:C:69:VAL:CG2	3:C:103:LEU:HD13	0.64	2.23	2	1
1:A:7:LEU:HD22	3:C:93:PHE:HB2	0.64	1.70	9	1
2:B:51:LEU:HD23	2:B:51:LEU:C	0.64	2.13	9	1
2:B:51:LEU:HD12	2:B:51:LEU:O	0.64	1.91	10	1
3:C:46:LEU:HD22	3:C:58:ASN:CA	0.64	2.22	16	3
2:B:78:ALA:CB	2:B:88:LEU:HD21	0.64	2.23	3	2
3:C:35:HIS:CD2	3:C:78:THR:CG2	0.64	2.80	20	8
3:C:19:VAL:HG13	3:C:31:VAL:HG22	0.64	1.68	15	4
2:B:34:ILE:HD13	2:B:34:ILE:C	0.64	2.13	17	2
2:B:37:ARG:NH2	2:B:79:PHE:CZ	0.64	2.66	18	1
3:C:93:PHE:CE1	3:C:94:PRO:O	0.64	2.51	18	1
1:A:4:LEU:HD22	3:C:103:LEU:HB3	0.63	1.68	4	3
1:A:2:ALA:O	3:C:76:TYR:CE1	0.63	2.51	12	13
2:B:7:ILE:HG12	2:B:75:VAL:HG22	0.63	1.68	17	13
2:B:77:LEU:CD2	2:B:77:LEU:N	0.63	2.61	17	1
1:A:4:LEU:HD22	3:C:73:VAL:HB	0.63	1.70	19	1
2:B:21:SER:O	2:B:56:THR:HG22	0.63	1.93	16	1
3:C:42:ILE:HG23	3:C:46:LEU:CD1	0.63	2.23	17	1
3:C:19:VAL:CG2	3:C:46:LEU:HD21	0.63	2.24	18	1
2:B:34:ILE:CD1	3:C:18:TYR:CE2	0.63	2.81	1	1
3:C:39:SER:OG	3:C:77:PHE:CZ	0.63	2.51	1	4
3:C:69:VAL:CG2	3:C:103:LEU:CD1	0.63	2.76	20	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:43:ARG:N	2:B:78:ALA:O	0.63	2.32	19	16
2:B:77:LEU:N	2:B:77:LEU:HD12	0.63	2.09	6	1
2:B:44:LEU:HD23	2:B:75:VAL:CG2	0.63	2.24	1	2
2:B:78:ALA:HB3	2:B:88:LEU:CD2	0.63	2.24	2	1
2:B:37:ARG:CD	2:B:79:PHE:CE1	0.63	2.82	6	2
2:B:7:ILE:HD11	2:B:77:LEU:HD11	0.63	1.69	17	2
2:B:42:GLN:NE2	2:B:79:PHE:CZ	0.63	2.67	14	1
1:A:11:THR:CG2	3:C:95:ILE:HG22	0.63	2.24	9	3
3:C:18:TYR:CD2	3:C:30:ILE:HG21	0.63	2.29	2	3
1:A:12:VAL:HG11	3:C:104:LEU:CD1	0.63	2.24	6	3
2:B:44:LEU:HD23	2:B:77:LEU:HD23	0.63	1.71	10	2
2:B:37:ARG:CG	2:B:79:PHE:CE2	0.63	2.82	5	1
3:C:96:ALA:HB1	3:C:97:PRO:CD	0.62	2.24	10	10
1:A:7:LEU:CD2	3:C:93:PHE:CB	0.62	2.77	17	2
1:A:4:LEU:HD13	3:C:107:ALA:HB2	0.62	1.71	3	3
2:B:62:PHE:CD1	2:B:62:PHE:N	0.62	2.67	8	2
2:B:78:ALA:HB1	2:B:88:LEU:CD2	0.62	2.24	14	4
2:B:23:THR:CG2	2:B:57:LEU:HD13	0.62	2.24	10	3
3:C:35:HIS:CD2	3:C:77:PHE:HB3	0.62	2.29	10	4
3:C:60:VAL:HG12	3:C:62:PHE:CE1	0.62	2.29	18	6
2:B:44:LEU:HD21	2:B:75:VAL:HB	0.62	1.69	11	1
2:B:34:ILE:CG1	2:B:35:LEU:N	0.62	2.63	19	8
3:C:19:VAL:CG1	3:C:31:VAL:CG2	0.62	2.78	13	14
2:B:27:LEU:HD22	2:B:27:LEU:C	0.62	2.14	5	3
1:A:5:GLN:CA	3:C:107:ALA:HB1	0.62	2.23	14	9
3:C:38:THR:HG22	3:C:80:LYS:CG	0.62	2.25	11	4
2:B:24:VAL:HA	2:B:27:LEU:HD11	0.62	1.71	14	1
3:C:38:THR:OG1	3:C:77:PHE:CG	0.62	2.52	1	4
1:A:1:VAL:HG21	3:C:80:LYS:CA	0.62	2.23	8	6
2:B:43:ARG:HG2	2:B:50:LEU:HD21	0.62	1.70	6	1
2:B:66:THR:O	2:B:67:ALA:C	0.62	2.38	19	2
2:B:5:LEU:HD23	2:B:27:LEU:CD1	0.62	2.25	19	1
2:B:5:LEU:O	2:B:16:THR:O	0.62	2.18	1	20
2:B:67:ALA:HB1	2:B:73:ALA:CB	0.62	2.25	2	2
3:C:70:LEU:HD13	3:C:71:SER:CA	0.62	2.24	19	14
2:B:4:PHE:CE1	2:B:15:PHE:CE2	0.62	2.88	15	1
2:B:10:HIS:O	2:B:12:THR:OG1	0.62	2.18	13	20
2:B:44:LEU:HA	2:B:76:GLY:O	0.62	1.94	16	20
3:C:103:LEU:O	3:C:107:ALA:N	0.62	2.28	16	15
3:C:19:VAL:CG1	3:C:36:ALA:HB2	0.62	2.24	19	3
2:B:63:THR:CG2	2:B:64:SER:N	0.62	2.62	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:31:VAL:HG22	2:B:77:LEU:CD2	0.62	2.25	2	1
1:A:3:THR:HG21	1:A:5:GLN:OE1	0.62	1.95	3	1
2:B:24:VAL:HG13	2:B:51:LEU:HD22	0.62	1.72	5	1
2:B:3:VAL:HG21	2:B:62:PHE:O	0.62	1.94	20	2
2:B:8:ARG:C	2:B:90:ILE:HD12	0.62	2.15	5	6
2:B:9:ARG:CZ	2:B:35:LEU:HD21	0.62	2.24	3	1
2:B:57:LEU:HD13	2:B:62:PHE:CB	0.62	2.25	5	1
2:B:62:PHE:O	2:B:66:THR:HG22	0.62	1.95	5	1
2:B:7:ILE:CD1	2:B:77:LEU:CD1	0.62	2.78	20	3
3:C:19:VAL:CG1	3:C:31:VAL:HG23	0.61	2.25	16	14
3:C:35:HIS:O	3:C:77:PHE:CG	0.61	2.53	14	9
2:B:8:ARG:CG	2:B:74:THR:HG23	0.61	2.25	5	5
1:A:7:LEU:HD22	3:C:93:PHE:CZ	0.61	2.29	12	1
3:C:31:VAL:HG11	3:C:35:HIS:CD2	0.61	2.30	14	1
2:B:22:SER:O	2:B:23:THR:O	0.61	2.18	12	1
3:C:18:TYR:O	3:C:18:TYR:CD1	0.61	2.53	2	3
3:C:29:PHE:CB	3:C:70:LEU:HD21	0.61	2.25	10	1
3:C:103:LEU:N	3:C:103:LEU:HD12	0.61	2.11	12	6
1:A:7:LEU:CD1	3:C:93:PHE:CG	0.61	2.83	6	1
2:B:5:LEU:HD13	2:B:57:LEU:HD21	0.61	1.72	1	1
3:C:30:ILE:HD12	3:C:30:ILE:N	0.61	2.10	14	7
3:C:21:LEU:N	3:C:29:PHE:O	0.61	2.27	9	14
3:C:99:ILE:HD12	3:C:100:ALA:N	0.61	2.10	3	1
2:B:24:VAL:HG12	2:B:51:LEU:CD1	0.61	2.25	10	1
2:B:44:LEU:CD1	2:B:51:LEU:CB	0.61	2.78	11	1
2:B:15:PHE:CD2	3:C:31:VAL:HG12	0.61	2.31	19	1
2:B:9:ARG:HB3	2:B:12:THR:O	0.61	1.96	19	9
3:C:38:THR:CG2	3:C:80:LYS:CB	0.61	2.79	17	6
3:C:21:LEU:HD22	3:C:60:VAL:HG21	0.61	1.71	12	19
2:B:21:SER:O	2:B:56:THR:CG2	0.61	2.47	12	4
3:C:95:ILE:HG23	3:C:100:ALA:HB1	0.61	1.73	1	4
2:B:24:VAL:HG11	2:B:53:ASP:HA	0.61	1.72	6	9
3:C:28:GLU:C	3:C:29:PHE:CD1	0.61	2.74	19	3
2:B:62:PHE:HZ	2:B:73:ALA:HB1	0.61	1.52	12	1
2:B:79:PHE:CD1	2:B:86:GLU:HB2	0.61	2.31	14	1
2:B:3:VAL:HG13	2:B:5:LEU:HD21	0.61	1.71	20	1
2:B:10:HIS:C	2:B:12:THR:N	0.61	2.43	14	20
2:B:45:TYR:CE2	2:B:88:LEU:HD11	0.61	2.31	1	2
3:C:35:HIS:CE1	3:C:78:THR:CG2	0.61	2.83	12	3
2:B:10:HIS:NE2	2:B:89:CYS:O	0.61	2.34	7	17
2:B:41:GLU:O	2:B:79:PHE:CD2	0.61	2.54	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:18:TYR:CE2	3:C:30:ILE:HG21	0.61	2.30	14	3
2:B:76:GLY:O	2:B:77:LEU:HD22	0.61	1.96	13	2
2:B:23:THR:CG2	2:B:24:VAL:HG13	0.61	2.23	16	1
2:B:35:LEU:HD22	2:B:77:LEU:HD13	0.61	1.70	18	1
3:C:99:ILE:O	3:C:100:ALA:HB3	0.61	1.96	17	12
2:B:16:THR:OG1	2:B:30:ILE:CD1	0.60	2.49	1	8
1:A:4:LEU:CD2	3:C:103:LEU:HD23	0.60	2.26	11	6
2:B:67:ALA:O	2:B:68:ARG:HB3	0.60	1.94	11	2
1:A:4:LEU:O	1:A:4:LEU:CD2	0.60	2.49	8	19
2:B:7:ILE:CG2	2:B:77:LEU:CD1	0.60	2.79	19	5
2:B:5:LEU:HD22	2:B:27:LEU:HD22	0.60	1.74	6	1
3:C:101:LEU:HD13	3:C:101:LEU:O	0.60	1.97	15	1
2:B:23:THR:O	2:B:25:PHE:N	0.60	2.35	12	16
2:B:87:ALA:O	2:B:88:LEU:HB2	0.60	1.95	3	11
2:B:90:ILE:O	2:B:92:PRO:HD3	0.60	1.95	17	16
3:C:95:ILE:CG2	3:C:100:ALA:CB	0.60	2.79	3	9
2:B:10:HIS:CD2	2:B:89:CYS:O	0.60	2.55	5	3
3:C:69:VAL:HG22	3:C:103:LEU:HD23	0.60	1.71	9	1
2:B:13:THR:CG2	3:C:29:PHE:CE2	0.60	2.84	13	2
2:B:42:GLN:CG	2:B:79:PHE:CE2	0.60	2.85	12	1
3:C:29:PHE:CD2	3:C:70:LEU:HD11	0.60	2.32	10	2
2:B:8:ARG:N	2:B:75:VAL:O	0.60	2.32	4	13
3:C:38:THR:HB	3:C:77:PHE:CD1	0.60	2.32	9	11
3:C:93:PHE:O	3:C:93:PHE:CD1	0.60	2.54	11	6
2:B:14:ILE:CG1	3:C:30:ILE:CD1	0.60	2.79	20	2
2:B:57:LEU:CD1	2:B:62:PHE:CB	0.60	2.79	5	1
2:B:41:GLU:O	2:B:79:PHE:CG	0.60	2.55	2	1
2:B:3:VAL:CG2	2:B:67:ALA:CB	0.60	2.80	10	11
2:B:3:VAL:HG13	2:B:67:ALA:CB	0.60	2.25	4	2
2:B:20:GLU:HA	2:B:57:LEU:HD21	0.60	1.72	4	1
2:B:24:VAL:HG13	2:B:51:LEU:HG	0.60	1.73	12	1
3:C:23:SER:HB3	3:C:70:LEU:HD23	0.60	1.73	14	1
1:A:3:THR:C	3:C:76:TYR:CD2	0.60	2.75	9	7
2:B:31:VAL:CG1	2:B:37:ARG:CB	0.60	2.80	19	5
3:C:68:HIS:CE1	3:C:99:ILE:CG1	0.60	2.84	4	2
3:C:103:LEU:N	3:C:103:LEU:HD13	0.60	2.12	18	4
3:C:39:SER:O	3:C:41:THR:N	0.60	2.35	3	12
1:A:3:THR:O	3:C:76:TYR:CD2	0.60	2.54	20	7
2:B:39:PRO:O	2:B:40:ASP:CB	0.60	2.49	10	4
3:C:27:HIS:CG	3:C:28:GLU:N	0.60	2.69	13	1
1:A:1:VAL:HG13	3:C:80:LYS:HG3	0.60	1.74	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:6:MET:N	2:B:73:ALA:O	0.60	2.35	6	15
2:B:9:ARG:CD	2:B:35:LEU:CD1	0.60	2.80	2	1
2:B:45:TYR:CA	2:B:49:GLN:O	0.60	2.49	11	17
2:B:88:LEU:CD1	2:B:88:LEU:O	0.60	2.50	15	5
2:B:23:THR:CB	2:B:57:LEU:HD23	0.60	2.26	4	1
3:C:65:ILE:CD1	3:C:106:ALA:CB	0.60	2.80	20	4
2:B:5:LEU:HD22	2:B:27:LEU:HD21	0.60	1.74	18	1
2:B:61:GLY:O	2:B:62:PHE:CG	0.59	2.55	1	3
3:C:31:VAL:HB	3:C:35:HIS:CD2	0.59	2.31	10	3
2:B:5:LEU:C	2:B:16:THR:HG22	0.59	2.18	3	10
3:C:70:LEU:C	3:C:70:LEU:CD1	0.59	2.67	18	16
3:C:27:HIS:CD2	3:C:67:SER:CB	0.59	2.85	7	1
2:B:4:PHE:CB	2:B:68:ARG:CG	0.59	2.80	9	1
2:B:34:ILE:HG22	2:B:35:LEU:HG	0.59	1.74	12	2
2:B:8:ARG:HB3	2:B:90:ILE:CD1	0.59	2.27	5	14
2:B:31:VAL:O	2:B:36:LYS:N	0.59	2.36	16	20
2:B:45:TYR:CE2	2:B:88:LEU:CD1	0.59	2.86	1	1
3:C:79:TYR:CD2	3:C:83:TYR:CE2	0.59	2.90	12	2
2:B:88:LEU:O	2:B:88:LEU:CD1	0.59	2.50	5	1
3:C:42:ILE:CD1	3:C:77:PHE:CE2	0.59	2.86	16	2
1:A:12:VAL:CB	3:C:104:LEU:HD13	0.59	2.26	18	1
2:B:3:VAL:CG1	2:B:5:LEU:CD2	0.59	2.81	4	2
2:B:43:ARG:CB	2:B:78:ALA:HB3	0.59	2.27	17	3
2:B:44:LEU:HD23	2:B:77:LEU:HD21	0.59	1.73	13	1
2:B:37:ARG:NH2	2:B:79:PHE:CD1	0.59	2.71	19	1
2:B:68:ARG:CB	2:B:69:PRO:CD	0.59	2.80	2	18
2:B:23:THR:OG1	2:B:24:VAL:HG22	0.59	1.97	10	2
2:B:14:ILE:CG1	3:C:30:ILE:HD11	0.59	2.27	20	1
3:C:38:THR:CB	3:C:77:PHE:CD1	0.59	2.85	5	14
2:B:8:ARG:CB	2:B:90:ILE:HG21	0.59	2.27	10	6
2:B:45:TYR:CE1	2:B:50:LEU:HD13	0.59	2.32	11	3
2:B:5:LEU:CD2	2:B:27:LEU:CD1	0.59	2.80	13	2
3:C:19:VAL:HG23	3:C:58:ASN:O	0.59	1.98	1	2
3:C:46:LEU:CD2	3:C:58:ASN:ND2	0.59	2.66	1	1
2:B:3:VAL:HG23	2:B:67:ALA:CB	0.59	2.26	13	3
2:B:4:PHE:CE1	2:B:15:PHE:CE1	0.59	2.91	14	1
3:C:60:VAL:HG11	3:C:62:PHE:CZ	0.59	2.33	9	6
2:B:67:ALA:C	2:B:68:ARG:CG	0.59	2.71	17	4
2:B:9:ARG:CZ	2:B:35:LEU:CD2	0.59	2.81	3	1
2:B:30:ILE:O	2:B:34:ILE:HD12	0.59	1.98	14	3
3:C:109:PHE:CD1	3:C:109:PHE:C	0.59	2.76	10	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:38:THR:HG22	3:C:80:LYS:HG2	0.59	1.74	13	3
1:A:1:VAL:CG2	3:C:76:TYR:CD1	0.59	2.86	12	1
3:C:35:HIS:O	3:C:38:THR:OG1	0.58	2.21	16	18
2:B:5:LEU:CD1	2:B:62:PHE:CZ	0.58	2.83	2	1
3:C:66:PRO:HG2	3:C:68:HIS:CE1	0.58	2.33	3	2
2:B:8:ARG:O	2:B:77:LEU:CD1	0.58	2.49	6	1
1:A:7:LEU:HD13	3:C:93:PHE:CE1	0.58	2.32	8	1
3:C:79:TYR:CZ	3:C:83:TYR:CD2	0.58	2.91	11	1
3:C:46:LEU:HD11	3:C:60:VAL:HG22	0.58	1.73	17	1
2:B:57:LEU:HD23	2:B:62:PHE:HB3	0.58	1.73	20	1
3:C:103:LEU:CD1	3:C:103:LEU:N	0.58	2.65	20	11
2:B:93:PHE:CG	3:C:67:SER:OG	0.58	2.55	3	2
2:B:63:THR:HG23	2:B:64:SER:N	0.58	2.12	6	4
1:A:15:HIS:N	1:A:15:HIS:CD2	0.58	2.70	13	1
2:B:69:PRO:O	3:C:75:MET:HE3	0.58	1.98	17	1
2:B:10:HIS:O	2:B:11:LYS:CG	0.58	2.52	9	2
3:C:35:HIS:NE2	3:C:78:THR:CG2	0.58	2.67	15	4
3:C:39:SER:HB3	3:C:77:PHE:CZ	0.58	2.34	13	11
2:B:9:ARG:CD	2:B:35:LEU:HD21	0.58	2.26	7	1
3:C:65:ILE:CG1	3:C:106:ALA:CB	0.58	2.81	13	6
3:C:69:VAL:HG22	3:C:103:LEU:HD21	0.58	1.74	9	1
3:C:35:HIS:CE1	3:C:74:CYS:O	0.58	2.56	14	3
1:A:1:VAL:HG22	3:C:76:TYR:HE1	0.58	1.56	12	1
2:B:5:LEU:HD23	2:B:27:LEU:HD22	0.58	1.73	13	1
2:B:23:THR:HA	2:B:57:LEU:HD12	0.58	1.71	16	1
1:A:4:LEU:CD1	3:C:73:VAL:HA	0.58	2.28	19	1
1:A:4:LEU:HD22	3:C:103:LEU:HG	0.58	1.75	2	1
3:C:39:SER:HB2	3:C:77:PHE:CZ	0.58	2.34	2	12
2:B:3:VAL:CG2	2:B:63:THR:CA	0.58	2.81	5	1
3:C:76:TYR:CE1	3:C:79:TYR:CD2	0.58	2.91	19	2
1:A:11:THR:CG2	3:C:95:ILE:CG2	0.58	2.81	19	7
2:B:23:THR:CG2	2:B:26:GLU:CG	0.58	2.81	8	2
2:B:45:TYR:CG	2:B:49:GLN:O	0.58	2.57	11	6
2:B:5:LEU:HD22	2:B:27:LEU:HD13	0.58	1.76	1	1
2:B:14:ILE:HG12	3:C:30:ILE:HB	0.58	1.74	8	18
2:B:68:ARG:N	2:B:72:PRO:HA	0.58	2.13	2	4
2:B:30:ILE:HG23	2:B:34:ILE:HD12	0.58	1.75	5	1
2:B:9:ARG:HG3	2:B:35:LEU:HD21	0.58	1.76	13	1
1:A:7:LEU:N	1:A:7:LEU:CD2	0.58	2.66	7	2
2:B:4:PHE:O	2:B:67:ALA:CB	0.58	2.51	2	15
1:A:7:LEU:HD13	3:C:93:PHE:HB3	0.58	1.76	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:67:ALA:N	2:B:71:ALA:O	0.58	2.36	11	2
3:C:21:LEU:CD2	3:C:60:VAL:HG21	0.58	2.29	20	20
3:C:39:SER:O	3:C:111:ASP:CB	0.58	2.52	10	7
3:C:79:TYR:OH	3:C:83:TYR:CE2	0.58	2.57	2	2
2:B:46:LYS:O	2:B:48:ASP:N	0.58	2.37	5	6
1:A:3:THR:HG21	3:C:112:CYS:OXT	0.58	1.99	4	1
3:C:107:ALA:O	3:C:110:LEU:CD2	0.58	2.52	5	1
2:B:8:ARG:O	2:B:77:LEU:CD2	0.58	2.51	16	2
1:A:1:VAL:CG2	3:C:76:TYR:CE1	0.58	2.87	12	5
2:B:34:ILE:CG1	2:B:35:LEU:CD1	0.58	2.80	6	7
1:A:4:LEU:O	3:C:107:ALA:HB1	0.58	1.99	9	2
2:B:92:PRO:O	3:C:27:HIS:CE1	0.58	2.57	19	1
2:B:9:ARG:CB	2:B:12:THR:O	0.57	2.52	1	16
3:C:33:ARG:O	3:C:37:LEU:N	0.57	2.37	5	11
2:B:45:TYR:CD2	2:B:49:GLN:O	0.57	2.57	11	16
2:B:79:PHE:CG	2:B:79:PHE:O	0.57	2.57	7	2
3:C:23:SER:HA	3:C:62:PHE:O	0.57	1.99	3	3
2:B:14:ILE:HG13	3:C:30:ILE:HD13	0.57	1.75	6	2
3:C:19:VAL:CG1	3:C:31:VAL:HG22	0.57	2.29	8	6
2:B:4:PHE:CE2	2:B:17:ASP:OD2	0.57	2.57	9	1
2:B:57:LEU:HD11	2:B:62:PHE:CE2	0.57	2.34	12	1
3:C:76:TYR:CE2	3:C:93:PHE:HB3	0.57	2.34	18	1
3:C:43:LYS:CD	3:C:44:ALA:N	0.57	2.67	5	2
2:B:3:VAL:HG23	2:B:20:GLU:HG3	0.57	1.75	5	1
2:B:24:VAL:HG13	2:B:51:LEU:HD21	0.57	1.74	6	1
3:C:23:SER:OG	3:C:70:LEU:HD21	0.57	1.99	1	1
3:C:70:LEU:C	3:C:70:LEU:CD2	0.57	2.70	5	12
1:A:3:THR:HA	3:C:76:TYR:CZ	0.57	2.34	6	5
2:B:8:ARG:NE	2:B:90:ILE:CG2	0.57	2.68	15	4
3:C:35:HIS:O	3:C:77:PHE:CD1	0.57	2.57	12	1
3:C:39:SER:CB	3:C:77:PHE:CE1	0.57	2.88	11	9
2:B:18:ALA:CB	2:B:22:SER:O	0.57	2.53	4	2
2:B:66:THR:O	2:B:73:ALA:N	0.57	2.37	6	3
2:B:15:PHE:CE2	3:C:78:THR:HG21	0.57	2.34	11	2
3:C:18:TYR:CE1	3:C:32:LYS:HG2	0.57	2.35	13	1
2:B:57:LEU:HD13	2:B:62:PHE:CG	0.57	2.34	5	1
2:B:78:ALA:O	2:B:79:PHE:CD1	0.57	2.58	9	2
3:C:63:ARG:CZ	3:C:63:ARG:CB	0.57	2.82	18	1
3:C:76:TYR:CE2	3:C:93:PHE:CB	0.57	2.88	18	1
2:B:7:ILE:CB	2:B:14:ILE:HG22	0.57	2.30	16	4
2:B:57:LEU:HD13	2:B:62:PHE:HB2	0.57	1.77	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:HD11	3:C:103:LEU:HD23	0.57	1.75	8	3
3:C:106:ALA:O	3:C:110:LEU:HD12	0.57	2.00	9	3
1:A:12:VAL:HG11	3:C:104:LEU:HG	0.57	1.77	11	1
1:A:1:VAL:HB	3:C:83:TYR:CG	0.57	2.35	20	1
2:B:23:THR:O	2:B:26:GLU:N	0.57	2.38	10	10
2:B:24:VAL:CG1	2:B:55:LYS:O	0.57	2.52	19	3
2:B:5:LEU:CD1	2:B:73:ALA:CB	0.57	2.82	11	1
2:B:8:ARG:HG2	2:B:90:ILE:HG21	0.57	1.76	16	3
2:B:5:LEU:HD23	2:B:27:LEU:CD2	0.57	2.29	13	1
2:B:7:ILE:HD12	2:B:31:VAL:CG2	0.57	2.29	14	1
2:B:30:ILE:O	2:B:34:ILE:CG2	0.57	2.52	4	4
2:B:78:ALA:CB	2:B:87:ALA:O	0.57	2.52	8	3
2:B:4:PHE:CB	2:B:67:ALA:O	0.57	2.53	5	1
3:C:76:TYR:C	3:C:76:TYR:CD1	0.57	2.78	7	2
3:C:34:GLU:OE2	3:C:81:VAL:HG22	0.57	2.00	6	1
2:B:16:THR:CG2	2:B:30:ILE:HD13	0.57	2.29	10	3
3:C:33:ARG:CD	3:C:46:LEU:HD13	0.57	2.30	10	1
3:C:35:HIS:CE1	3:C:78:THR:OG1	0.57	2.57	13	1
3:C:79:TYR:OH	3:C:83:TYR:CZ	0.57	2.57	13	2
3:C:18:TYR:CD2	3:C:30:ILE:HD13	0.57	2.35	18	1
1:A:5:GLN:OE1	1:A:6:HIS:CE1	0.56	2.57	1	1
2:B:8:ARG:HD2	2:B:74:THR:HG21	0.56	1.77	10	7
3:C:18:TYR:CE2	3:C:32:LYS:HE3	0.56	2.35	4	1
2:B:44:LEU:CD2	2:B:75:VAL:HG23	0.56	2.30	11	2
3:C:67:SER:HA	3:C:70:LEU:HD21	0.56	1.76	16	4
3:C:79:TYR:O	3:C:83:TYR:CD1	0.56	2.58	1	1
2:B:23:THR:HG23	2:B:26:GLU:CG	0.56	2.30	8	2
3:C:18:TYR:HA	3:C:32:LYS:HA	0.56	1.78	1	2
2:B:3:VAL:HG12	2:B:20:GLU:N	0.56	2.15	2	4
2:B:30:ILE:O	2:B:34:ILE:HG22	0.56	1.99	2	4
3:C:37:LEU:HD12	3:C:43:LYS:HD3	0.56	1.77	4	1
2:B:35:LEU:HD13	2:B:77:LEU:HD13	0.56	1.75	7	1
2:B:46:LYS:HB3	2:B:51:LEU:HD12	0.56	1.78	11	2
3:C:103:LEU:HD13	3:C:103:LEU:N	0.56	2.15	20	2
3:C:68:HIS:NE2	3:C:99:ILE:CD1	0.56	2.69	12	1
1:A:7:LEU:HD22	1:A:7:LEU:H	0.56	1.60	15	1
3:C:65:ILE:HG23	3:C:69:VAL:HB	0.56	1.76	17	1
2:B:88:LEU:HD13	2:B:88:LEU:N	0.56	2.14	3	2
3:C:43:LYS:CG	3:C:44:ALA:N	0.56	2.69	1	7
2:B:78:ALA:HB3	2:B:88:LEU:HD22	0.56	1.75	2	1
3:C:18:TYR:CD1	3:C:18:TYR:C	0.56	2.77	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:18:TYR:CE1	3:C:32:LYS:CG	0.56	2.89	13	1
3:C:21:LEU:HD11	3:C:31:VAL:HG11	0.56	1.76	15	3
2:B:56:THR:O	2:B:60:CYS:CB	0.56	2.54	9	12
1:A:1:VAL:HG11	3:C:80:LYS:CA	0.56	2.29	3	5
3:C:101:LEU:HD12	3:C:102:GLU:HG3	0.56	1.76	9	1
3:C:23:SER:CB	3:C:65:ILE:O	0.56	2.54	10	2
3:C:62:PHE:CE1	3:C:110:LEU:HD11	0.56	2.36	12	1
3:C:68:HIS:C	3:C:68:HIS:CD2	0.56	2.78	12	1
2:B:62:PHE:HE1	2:B:73:ALA:HB1	0.56	1.54	20	1
2:B:8:ARG:CG	2:B:90:ILE:CG2	0.56	2.77	17	4
1:A:8:CYS:SG	1:A:9:ARG:N	0.56	2.79	9	13
2:B:64:SER:O	2:B:65:GLN:CB	0.56	2.54	6	6
1:A:7:LEU:CD1	3:C:76:TYR:CE2	0.56	2.89	20	2
1:A:7:LEU:CD2	3:C:93:PHE:HB2	0.56	2.31	17	2
2:B:38:PRO:O	2:B:42:GLN:CB	0.56	2.54	11	2
1:A:7:LEU:HB3	3:C:93:PHE:CZ	0.56	2.36	12	1
3:C:38:THR:CG2	3:C:76:TYR:CZ	0.56	2.89	12	1
3:C:31:VAL:CG1	3:C:35:HIS:CD2	0.56	2.89	14	1
3:C:19:VAL:HG23	3:C:46:LEU:HD21	0.56	1.77	18	1
2:B:57:LEU:HD23	2:B:62:PHE:HB2	0.56	1.76	20	3
2:B:24:VAL:HG11	2:B:52:ASP:C	0.56	2.20	12	1
2:B:3:VAL:CG2	2:B:57:LEU:CD2	0.56	2.81	19	1
2:B:7:ILE:HG12	2:B:75:VAL:CG2	0.56	2.30	11	19
3:C:66:PRO:HB2	3:C:68:HIS:CE1	0.56	2.36	1	1
3:C:103:LEU:O	3:C:104:LEU:C	0.56	2.44	6	15
2:B:3:VAL:HG12	2:B:5:LEU:CD2	0.56	2.31	4	1
1:A:7:LEU:HD22	3:C:93:PHE:CE2	0.56	2.36	12	1
1:A:1:VAL:HG11	3:C:80:LYS:HG2	0.56	1.78	16	1
3:C:35:HIS:CE1	3:C:78:THR:CB	0.56	2.88	12	2
3:C:103:LEU:N	3:C:103:LEU:CD1	0.56	2.68	15	3
3:C:68:HIS:CE1	3:C:99:ILE:HG13	0.56	2.36	4	2
2:B:8:ARG:O	2:B:77:LEU:HD21	0.56	2.01	16	2
2:B:3:VAL:O	2:B:18:ALA:O	0.56	2.23	9	8
2:B:37:ARG:HD2	2:B:79:PHE:CE2	0.56	2.35	4	1
2:B:13:THR:CG2	3:C:27:HIS:NE2	0.56	2.69	18	1
1:A:11:THR:OG1	3:C:95:ILE:CG2	0.55	2.54	3	10
2:B:23:THR:CB	2:B:57:LEU:CD1	0.55	2.79	16	1
3:C:93:PHE:CE1	3:C:95:ILE:HG13	0.55	2.37	18	1
3:C:65:ILE:HG12	3:C:69:VAL:HG11	0.55	1.78	2	5
2:B:8:ARG:HB2	2:B:74:THR:HG23	0.55	1.77	3	1
2:B:7:ILE:HD13	2:B:77:LEU:CD1	0.55	2.31	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:13:THR:HG23	3:C:27:HIS:NE2	0.55	2.16	18	1
3:C:37:LEU:HD12	3:C:43:LYS:HB2	0.55	1.77	20	1
3:C:21:LEU:CD2	3:C:60:VAL:CG2	0.55	2.84	11	20
3:C:42:ILE:CG1	3:C:60:VAL:HG11	0.55	2.31	18	4
3:C:38:THR:CG2	3:C:80:LYS:CD	0.55	2.85	3	3
1:A:1:VAL:HG12	3:C:83:TYR:CD2	0.55	2.37	10	6
3:C:35:HIS:CE1	3:C:77:PHE:HB2	0.55	2.36	18	2
3:C:23:SER:CB	3:C:25:ASP:OD2	0.55	2.54	11	1
3:C:110:LEU:O	3:C:111:ASP:O	0.55	2.24	16	4
2:B:4:PHE:CE1	2:B:17:ASP:OD2	0.55	2.59	13	2
3:C:21:LEU:CD1	3:C:74:CYS:SG	0.55	2.95	20	7
3:C:32:LYS:O	3:C:33:ARG:C	0.55	2.44	13	20
3:C:39:SER:HB3	3:C:42:ILE:HD12	0.55	1.77	5	3
2:B:13:THR:OG1	3:C:29:PHE:CG	0.55	2.55	15	1
3:C:35:HIS:CE1	3:C:78:THR:HB	0.55	2.37	12	2
2:B:7:ILE:HD12	2:B:77:LEU:CD1	0.55	2.32	20	2
3:C:36:ALA:O	3:C:39:SER:OG	0.55	2.25	1	2
3:C:103:LEU:O	3:C:107:ALA:CB	0.55	2.55	11	8
2:B:19:LYS:O	2:B:57:LEU:CD1	0.55	2.55	20	5
2:B:3:VAL:CG1	2:B:5:LEU:HD21	0.55	2.32	4	1
3:C:67:SER:HA	3:C:70:LEU:HG	0.55	1.78	17	2
3:C:42:ILE:CG1	3:C:60:VAL:CG1	0.55	2.85	11	3
3:C:38:THR:CB	3:C:77:PHE:HA	0.55	2.32	13	11
2:B:67:ALA:O	2:B:68:ARG:CB	0.55	2.53	19	9
2:B:13:THR:OG1	3:C:29:PHE:CD2	0.55	2.60	15	4
2:B:14:ILE:CG1	3:C:30:ILE:HD13	0.55	2.29	15	5
3:C:31:VAL:CB	3:C:35:HIS:CD2	0.55	2.90	14	2
3:C:38:THR:O	3:C:38:THR:HG22	0.55	2.00	14	2
3:C:30:ILE:O	3:C:30:ILE:CD1	0.55	2.53	18	1
2:B:9:ARG:CZ	2:B:86:GLU:OE2	0.55	2.54	1	1
1:A:11:THR:CB	3:C:95:ILE:HG21	0.55	2.31	3	7
3:C:60:VAL:CG1	3:C:62:PHE:CE1	0.55	2.90	18	3
2:B:34:ILE:HD13	2:B:35:LEU:CA	0.55	2.31	17	2
1:A:7:LEU:HD12	3:C:95:ILE:HD12	0.55	1.78	18	1
3:C:38:THR:HG23	3:C:80:LYS:HG3	0.55	1.77	20	1
3:C:66:PRO:CB	3:C:68:HIS:CE1	0.55	2.89	1	1
2:B:8:ARG:HG2	2:B:74:THR:HG23	0.55	1.77	13	3
2:B:14:ILE:CG2	2:B:14:ILE:O	0.55	2.55	9	7
3:C:93:PHE:O	3:C:95:ILE:HD12	0.55	2.02	7	1
2:B:4:PHE:CZ	2:B:15:PHE:CE2	0.55	2.95	15	1
3:C:35:HIS:HD2	3:C:78:THR:HG23	0.55	1.55	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:5:LEU:N	2:B:5:LEU:CD2	0.55	2.70	20	2
1:A:1:VAL:HG12	3:C:83:TYR:CD1	0.55	2.37	7	2
2:B:44:LEU:CD2	2:B:77:LEU:HD21	0.55	2.32	13	1
3:C:27:HIS:N	3:C:27:HIS:CD2	0.55	2.74	16	2
2:B:34:ILE:HD11	2:B:35:LEU:HD12	0.54	1.80	8	8
3:C:100:ALA:CA	3:C:103:LEU:HD12	0.54	2.32	6	3
2:B:34:ILE:HG13	2:B:35:LEU:CD1	0.54	2.32	10	7
2:B:14:ILE:HG13	2:B:34:ILE:HD13	0.54	1.79	7	3
2:B:8:ARG:O	2:B:77:LEU:HD23	0.54	2.02	9	3
3:C:79:TYR:CE2	3:C:83:TYR:OH	0.54	2.60	12	3
2:B:31:VAL:HG13	2:B:35:LEU:HB2	0.54	1.79	13	1
1:A:4:LEU:CD1	3:C:73:VAL:CA	0.54	2.84	1	7
3:C:20:LYS:O	3:C:60:VAL:N	0.54	2.38	6	11
2:B:45:TYR:CB	2:B:49:GLN:O	0.54	2.55	2	8
2:B:93:PHE:CB	3:C:67:SER:OG	0.54	2.55	11	3
3:C:24:SER:N	3:C:62:PHE:O	0.54	2.40	12	3
1:A:1:VAL:N	3:C:83:TYR:CD1	0.54	2.75	6	1
2:B:8:ARG:O	2:B:77:LEU:HG	0.54	2.02	16	2
3:C:41:THR:HG23	3:C:111:ASP:OD1	0.54	2.02	19	1
3:C:35:HIS:O	3:C:77:PHE:HB3	0.54	2.02	17	17
2:B:6:MET:O	2:B:75:VAL:CG1	0.54	2.55	5	8
2:B:66:THR:O	2:B:73:ALA:CB	0.54	2.54	4	5
1:A:1:VAL:CG1	3:C:83:TYR:HB2	0.54	2.32	16	5
2:B:76:GLY:CA	2:B:90:ILE:HD11	0.54	2.31	10	1
3:C:68:HIS:NE2	3:C:99:ILE:HD11	0.54	2.17	12	1
2:B:56:THR:O	2:B:60:CYS:N	0.54	2.41	3	10
3:C:39:SER:C	3:C:41:THR:H	0.54	2.05	9	12
3:C:79:TYR:CE2	3:C:83:TYR:CE2	0.54	2.95	4	3
1:A:1:VAL:CG1	3:C:80:LYS:CD	0.54	2.82	11	1
1:A:1:VAL:HB	3:C:83:TYR:CD2	0.54	2.37	14	1
2:B:18:ALA:CB	2:B:27:LEU:HD11	0.54	2.31	18	1
3:C:69:VAL:CG1	3:C:103:LEU:CD1	0.54	2.78	1	4
3:C:19:VAL:HG13	3:C:21:LEU:HD21	0.54	1.79	11	13
3:C:35:HIS:O	3:C:77:PHE:CB	0.54	2.56	10	10
2:B:46:LYS:CG	2:B:46:LYS:O	0.54	2.56	12	2
2:B:63:THR:O	2:B:66:THR:CG2	0.54	2.54	6	2
3:C:46:LEU:CD2	3:C:58:ASN:HA	0.54	2.33	18	3
1:A:6:HIS:O	1:A:9:ARG:CG	0.54	2.56	16	1
2:B:13:THR:CG2	3:C:27:HIS:CE1	0.54	2.90	18	1
1:A:11:THR:O	1:A:15:HIS:N	0.54	2.40	1	3
3:C:69:VAL:CG2	3:C:102:GLU:CB	0.54	2.81	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:GLN:CB	3:C:111:ASP:OD2	0.54	2.56	5	1
2:B:42:GLN:CA	2:B:78:ALA:O	0.54	2.55	5	1
2:B:37:ARG:CZ	2:B:79:PHE:CE1	0.54	2.91	10	1
1:A:7:LEU:HD22	3:C:93:PHE:CE1	0.54	2.38	13	1
2:B:7:ILE:CD1	2:B:31:VAL:CG2	0.54	2.85	14	1
1:A:1:VAL:HG23	3:C:76:TYR:CZ	0.54	2.37	19	1
2:B:14:ILE:HG13	2:B:34:ILE:CD1	0.54	2.32	20	11
1:A:11:THR:OG1	3:C:95:ILE:CB	0.54	2.56	14	5
3:C:42:ILE:HG22	3:C:46:LEU:HD23	0.54	1.78	2	1
2:B:2:ASP:O	2:B:64:SER:CB	0.54	2.56	5	1
2:B:62:PHE:O	2:B:66:THR:CG2	0.54	2.56	6	2
1:A:1:VAL:HG11	3:C:83:TYR:HB2	0.54	1.79	17	2
1:A:11:THR:OG1	3:C:100:ALA:HB3	0.54	2.03	15	1
2:B:6:MET:O	2:B:75:VAL:N	0.54	2.39	20	13
1:A:1:VAL:CG1	3:C:80:LYS:CG	0.54	2.86	4	1
2:B:23:THR:HG21	2:B:57:LEU:HG	0.54	1.79	5	1
2:B:57:LEU:CD2	2:B:62:PHE:CB	0.54	2.85	8	3
2:B:28:LYS:O	2:B:37:ARG:NH1	0.54	2.41	15	1
2:B:38:PRO:O	2:B:42:GLN:CG	0.54	2.56	14	4
2:B:24:VAL:CG1	2:B:52:ASP:O	0.54	2.56	5	1
3:C:21:LEU:HD23	3:C:21:LEU:N	0.54	2.17	9	9
2:B:8:ARG:HB3	2:B:90:ILE:HG23	0.54	1.80	6	2
3:C:27:HIS:CG	3:C:67:SER:HB2	0.54	2.38	7	1
2:B:8:ARG:O	2:B:77:LEU:CG	0.54	2.56	16	2
3:C:79:TYR:OH	3:C:83:TYR:CE1	0.54	2.58	19	1
1:A:3:THR:CG2	3:C:38:THR:O	0.54	2.56	2	3
3:C:43:LYS:HA	3:C:46:LEU:HD21	0.54	1.79	8	3
2:B:57:LEU:HA	2:B:62:PHE:CD1	0.54	2.37	4	1
2:B:34:ILE:HD11	2:B:35:LEU:CD1	0.54	2.33	6	8
2:B:5:LEU:HD13	2:B:73:ALA:CB	0.54	2.29	7	1
2:B:23:THR:OG1	2:B:57:LEU:HD12	0.54	2.02	16	1
2:B:34:ILE:CD1	2:B:35:LEU:N	0.54	2.61	17	2
2:B:68:ARG:CG	2:B:69:PRO:HD2	0.53	2.33	18	11
3:C:39:SER:O	3:C:110:LEU:O	0.53	2.26	2	6
2:B:24:VAL:CG2	2:B:55:LYS:O	0.53	2.56	10	9
1:A:3:THR:O	3:C:76:TYR:CE2	0.53	2.60	11	6
1:A:5:GLN:CG	3:C:108:ASN:OD1	0.53	2.56	6	2
2:B:46:LYS:O	2:B:49:GLN:CB	0.53	2.56	16	3
2:B:13:THR:CG2	3:C:27:HIS:HE2	0.53	2.15	18	1
2:B:24:VAL:CB	2:B:53:ASP:HA	0.53	2.33	14	13
2:B:87:ALA:C	2:B:88:LEU:CD2	0.53	2.76	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:63:THR:O	2:B:64:SER:CB	0.53	2.56	2	4
3:C:19:VAL:HG12	3:C:31:VAL:HG23	0.53	1.81	13	9
3:C:42:ILE:HG22	3:C:46:LEU:CD2	0.53	2.33	2	1
1:A:1:VAL:HB	3:C:83:TYR:CB	0.53	2.33	14	4
2:B:27:LEU:C	2:B:27:LEU:CD1	0.53	2.73	4	2
3:C:41:THR:OG1	3:C:110:LEU:CA	0.53	2.56	12	4
2:B:44:LEU:HD21	2:B:75:VAL:CB	0.53	2.33	11	1
3:C:25:ASP:OD2	3:C:67:SER:N	0.53	2.41	11	1
1:A:3:THR:O	1:A:5:GLN:N	0.53	2.41	17	2
1:A:7:LEU:CB	3:C:93:PHE:CZ	0.53	2.90	12	1
3:C:42:ILE:HD13	3:C:77:PHE:HZ	0.53	1.60	12	1
1:A:11:THR:OG1	3:C:100:ALA:CB	0.53	2.56	15	1
2:B:37:ARG:HD3	2:B:79:PHE:CE1	0.53	2.37	17	1
1:A:7:LEU:HD12	3:C:95:ILE:CD1	0.53	2.33	18	1
3:C:19:VAL:CG2	3:C:46:LEU:CD2	0.53	2.86	18	1
1:A:8:CYS:SG	3:C:104:LEU:N	0.53	2.81	11	7
3:C:22:ILE:CG1	3:C:28:GLU:OE1	0.53	2.56	2	2
3:C:45:MET:O	3:C:45:MET:CE	0.53	2.56	3	1
2:B:3:VAL:HG21	2:B:57:LEU:HD13	0.53	1.81	4	1
2:B:9:ARG:C	2:B:90:ILE:HG23	0.53	2.24	17	4
2:B:23:THR:HG21	2:B:57:LEU:N	0.53	2.18	4	1
2:B:11:LYS:O	3:C:28:GLU:N	0.53	2.40	7	3
2:B:37:ARG:CG	2:B:79:PHE:CZ	0.53	2.91	5	1
3:C:68:HIS:HB3	3:C:99:ILE:HD13	0.53	1.81	6	2
2:B:3:VAL:HG13	2:B:5:LEU:HD23	0.53	1.79	7	1
3:C:105:MET:O	3:C:109:PHE:CB	0.53	2.55	10	7
3:C:33:ARG:HG3	3:C:46:LEU:HD23	0.53	1.81	11	1
3:C:98:GLU:CA	3:C:98:GLU:OE1	0.53	2.55	1	2
3:C:19:VAL:HG22	3:C:60:VAL:CG2	0.53	2.33	5	8
3:C:65:ILE:CG2	3:C:69:VAL:CG1	0.53	2.86	4	3
2:B:37:ARG:HG2	2:B:79:PHE:CD2	0.53	2.38	5	1
3:C:41:THR:OG1	3:C:111:ASP:N	0.53	2.42	5	2
3:C:41:THR:HG23	3:C:110:LEU:O	0.53	2.02	10	1
3:C:20:LYS:HA	3:C:30:ILE:HA	0.53	1.80	18	3
3:C:66:PRO:HG2	3:C:69:VAL:CG2	0.53	2.33	3	4
2:B:37:ARG:HG3	2:B:79:PHE:CE1	0.53	2.39	5	4
3:C:35:HIS:HD1	3:C:78:THR:HG22	0.53	1.62	5	1
1:A:2:ALA:HB1	1:A:6:HIS:CD2	0.53	2.38	6	1
1:A:3:THR:HG23	1:A:5:GLN:HB3	0.53	1.80	7	2
2:B:44:LEU:C	2:B:44:LEU:CD1	0.53	2.72	11	1
3:C:38:THR:HG22	3:C:76:TYR:CZ	0.53	2.37	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:99:ILE:HD13	3:C:100:ALA:N	0.53	2.18	14	4
3:C:38:THR:OG1	3:C:80:LYS:CD	0.53	2.57	14	1
2:B:13:THR:HB	3:C:29:PHE:CE1	0.53	2.38	15	1
2:B:23:THR:OG1	2:B:57:LEU:N	0.53	2.42	19	1
3:C:42:ILE:O	3:C:45:MET:CG	0.53	2.57	2	1
1:A:8:CYS:HB2	3:C:104:LEU:N	0.53	2.18	15	3
2:B:5:LEU:HD22	2:B:5:LEU:N	0.53	2.19	17	4
2:B:34:ILE:HG22	2:B:35:LEU:HD12	0.53	1.79	11	1
3:C:35:HIS:CE1	3:C:78:THR:HG23	0.53	2.39	13	1
3:C:82:ARG:CZ	3:C:83:TYR:CE1	0.53	2.91	19	1
2:B:4:PHE:HB2	2:B:68:ARG:N	0.53	2.19	12	6
2:B:5:LEU:HD13	2:B:57:LEU:HD11	0.53	1.81	5	1
2:B:8:ARG:HD3	2:B:74:THR:HG21	0.53	1.81	12	2
2:B:91:GLU:O	2:B:93:PHE:CE1	0.53	2.61	16	1
2:B:14:ILE:HD11	3:C:30:ILE:CD1	0.53	2.33	20	1
3:C:106:ALA:O	3:C:110:LEU:CD1	0.53	2.57	1	7
2:B:7:ILE:HG23	2:B:77:LEU:CD1	0.53	2.33	14	4
3:C:35:HIS:CD2	3:C:77:PHE:CB	0.53	2.92	10	2
2:B:23:THR:OG1	2:B:57:LEU:CD1	0.53	2.57	16	1
3:C:41:THR:O	3:C:45:MET:CG	0.53	2.57	15	5
1:A:4:LEU:CD1	3:C:103:LEU:CD2	0.53	2.86	6	1
2:B:80:ARG:CD	2:B:80:ARG:O	0.53	2.57	10	1
3:C:41:THR:CG2	3:C:110:LEU:O	0.53	2.57	10	1
3:C:27:HIS:CE1	3:C:28:GLU:O	0.53	2.62	13	1
3:C:23:SER:OG	3:C:70:LEU:HD23	0.53	2.04	14	2
3:C:63:ARG:CZ	3:C:63:ARG:HB3	0.53	2.34	18	1
2:B:5:LEU:O	2:B:16:THR:CG2	0.53	2.56	18	6
2:B:25:PHE:CD1	2:B:25:PHE:C	0.53	2.82	20	4
3:C:60:VAL:CG1	3:C:62:PHE:CE2	0.53	2.92	10	2
2:B:45:TYR:HA	2:B:49:GLN:O	0.53	2.04	17	16
2:B:37:ARG:HG2	2:B:79:PHE:CE1	0.53	2.38	9	2
2:B:53:ASP:N	2:B:53:ASP:OD1	0.53	2.42	8	1
2:B:30:ILE:HG23	2:B:34:ILE:HD13	0.53	1.80	14	4
3:C:19:VAL:CG1	3:C:21:LEU:HD21	0.53	2.34	9	2
2:B:3:VAL:HG11	2:B:63:THR:OG1	0.53	2.04	12	1
2:B:32:GLU:HA	2:B:36:LYS:HA	0.52	1.81	20	10
2:B:68:ARG:CB	2:B:69:PRO:HD3	0.52	2.34	9	3
2:B:68:ARG:HB3	2:B:69:PRO:CD	0.52	2.34	2	1
3:C:39:SER:HB3	3:C:77:PHE:CE1	0.52	2.39	10	3
3:C:67:SER:O	3:C:70:LEU:CD1	0.52	2.57	7	5
3:C:70:LEU:HD12	3:C:71:SER:CA	0.52	2.34	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:65:ILE:CG2	3:C:69:VAL:HG11	0.52	2.34	4	1
2:B:44:LEU:CD1	2:B:51:LEU:HB2	0.52	2.34	11	1
1:A:4:LEU:CD1	3:C:103:LEU:HG	0.52	2.33	10	12
2:B:24:VAL:O	2:B:28:LYS:CG	0.52	2.57	1	1
3:C:67:SER:HA	3:C:70:LEU:CD2	0.52	2.33	1	6
2:B:77:LEU:N	2:B:87:ALA:HB2	0.52	2.19	3	1
2:B:37:ARG:HG3	2:B:79:PHE:CZ	0.52	2.40	5	1
3:C:109:PHE:CD1	3:C:110:LEU:N	0.52	2.77	5	1
1:A:8:CYS:SG	3:C:103:LEU:CB	0.52	2.98	11	1
2:B:41:GLU:N	2:B:42:GLN:OE1	0.52	2.42	14	1
2:B:42:GLN:OE1	2:B:77:LEU:HD21	0.52	2.04	18	1
3:C:35:HIS:O	3:C:77:PHE:CD2	0.52	2.63	18	1
2:B:77:LEU:C	2:B:87:ALA:HB2	0.52	2.25	3	2
1:A:11:THR:OG1	3:C:95:ILE:CD1	0.52	2.57	3	2
3:C:42:ILE:CD1	3:C:77:PHE:CZ	0.52	2.93	13	8
2:B:14:ILE:HD12	2:B:34:ILE:HD13	0.52	1.82	6	1
1:A:8:CYS:HB3	3:C:107:ALA:CB	0.52	2.34	9	1
2:B:44:LEU:HB3	2:B:51:LEU:CD2	0.52	2.31	10	1
3:C:35:HIS:CG	3:C:77:PHE:HB3	0.52	2.39	10	2
2:B:42:GLN:HG2	2:B:79:PHE:CE2	0.52	2.40	12	1
3:C:22:ILE:CD1	3:C:28:GLU:OE1	0.52	2.57	12	1
2:B:45:TYR:N	2:B:76:GLY:O	0.52	2.43	15	1
2:B:86:GLU:O	2:B:87:ALA:HB3	0.52	2.03	16	1
2:B:23:THR:HA	2:B:56:THR:HG23	0.52	1.81	2	1
1:A:3:THR:CG2	1:A:5:GLN:OE1	0.52	2.57	3	1
3:C:32:LYS:O	3:C:35:HIS:N	0.52	2.42	19	7
3:C:38:THR:CG2	3:C:38:THR:O	0.52	2.57	10	1
2:B:93:PHE:CB	3:C:67:SER:HG	0.52	2.15	12	1
2:B:24:VAL:CG1	2:B:53:ASP:OD1	0.52	2.58	13	1
3:C:35:HIS:CE1	3:C:77:PHE:HB3	0.52	2.40	13	1
3:C:93:PHE:CD2	3:C:94:PRO:HD2	0.52	2.39	18	1
3:C:19:VAL:O	3:C:30:ILE:HA	0.52	2.05	18	10
3:C:23:SER:OG	3:C:70:LEU:CD2	0.52	2.58	1	1
2:B:22:SER:O	2:B:23:THR:HB	0.52	2.03	20	11
2:B:62:PHE:C	2:B:63:THR:CG2	0.52	2.75	2	2
3:C:73:VAL:HG21	3:C:110:LEU:CD1	0.52	2.33	14	4
2:B:31:VAL:CG2	2:B:77:LEU:CD1	0.52	2.81	3	1
3:C:35:HIS:CE1	3:C:78:THR:HA	0.52	2.40	20	5
2:B:38:PRO:O	2:B:42:GLN:NE2	0.52	2.42	4	1
3:C:25:ASP:OD1	3:C:67:SER:N	0.52	2.42	5	1
2:B:14:ILE:HD13	3:C:30:ILE:CD1	0.52	2.33	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:CD1	3:C:73:VAL:N	0.52	2.72	1	7
3:C:95:ILE:CG2	3:C:100:ALA:HB1	0.52	2.35	1	1
2:B:66:THR:O	2:B:68:ARG:N	0.52	2.41	2	1
3:C:100:ALA:CA	3:C:103:LEU:CD1	0.52	2.87	5	2
2:B:4:PHE:HB2	2:B:68:ARG:CG	0.52	2.33	9	1
2:B:16:THR:CG2	2:B:30:ILE:CD1	0.52	2.87	10	3
2:B:67:ALA:HB2	2:B:73:ALA:HB2	0.52	1.82	11	1
3:C:25:ASP:OD1	3:C:27:HIS:CG	0.52	2.63	11	1
3:C:27:HIS:NE2	3:C:28:GLU:O	0.52	2.43	13	1
3:C:76:TYR:CD2	3:C:93:PHE:CD1	0.52	2.97	16	1
3:C:33:ARG:CG	3:C:46:LEU:HD22	0.52	2.34	20	1
2:B:8:ARG:HG3	2:B:90:ILE:CG2	0.52	2.35	1	2
2:B:67:ALA:O	2:B:68:ARG:CD	0.52	2.57	1	3
3:C:42:ILE:HG23	3:C:46:LEU:HD23	0.52	1.81	2	1
2:B:31:VAL:CG1	2:B:37:ARG:HB3	0.52	2.35	19	6
3:C:99:ILE:HD12	3:C:100:ALA:H	0.52	1.61	3	1
2:B:34:ILE:HG23	3:C:30:ILE:CD1	0.52	2.35	5	1
2:B:24:VAL:HG21	2:B:53:ASP:HA	0.52	1.80	7	3
1:A:7:LEU:HD13	3:C:76:TYR:HE2	0.52	1.65	10	1
2:B:7:ILE:CD1	2:B:77:LEU:HD22	0.52	2.26	15	1
2:B:18:ALA:HB1	2:B:27:LEU:HD11	0.52	1.82	18	1
2:B:5:LEU:HD22	2:B:23:THR:HA	0.52	1.81	19	1
2:B:45:TYR:CE1	2:B:50:LEU:HD12	0.52	2.40	10	2
1:A:8:CYS:CB	3:C:103:LEU:HB3	0.52	2.35	2	1
2:B:55:LYS:CD	2:B:60:CYS:SG	0.52	2.98	2	1
2:B:57:LEU:HD23	2:B:62:PHE:CE2	0.52	2.39	2	1
3:C:69:VAL:CG2	3:C:102:GLU:HB2	0.52	2.35	3	10
1:A:9:ARG:O	1:A:13:ASN:ND2	0.52	2.43	4	1
3:C:27:HIS:CD2	3:C:27:HIS:N	0.52	2.77	4	3
3:C:31:VAL:HB	3:C:35:HIS:CG	0.52	2.39	16	6
3:C:67:SER:O	3:C:70:LEU:N	0.52	2.43	20	4
2:B:64:SER:O	2:B:65:GLN:HB2	0.52	2.05	6	4
2:B:51:LEU:O	2:B:51:LEU:CD1	0.52	2.57	10	1
2:B:10:HIS:CE1	2:B:91:GLU:OE1	0.52	2.62	15	1
2:B:29:ARG:O	2:B:33:GLY:N	0.52	2.43	17	2
2:B:51:LEU:HD12	2:B:52:ASP:N	0.52	2.20	18	1
2:B:44:LEU:HD23	2:B:75:VAL:HG21	0.52	1.82	1	1
3:C:79:TYR:CZ	3:C:83:TYR:OH	0.52	2.61	1	1
3:C:23:SER:O	3:C:25:ASP:N	0.52	2.42	12	2
1:A:7:LEU:CD1	3:C:93:PHE:HB2	0.52	2.34	15	2
2:B:46:LYS:N	2:B:49:GLN:O	0.52	2.43	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:66:THR:O	2:B:71:ALA:O	0.52	2.28	5	1
3:C:107:ALA:O	3:C:110:LEU:HD23	0.52	2.05	5	1
2:B:5:LEU:HB3	2:B:16:THR:HG23	0.52	1.81	18	9
2:B:32:GLU:HA	2:B:36:LYS:CA	0.52	2.35	7	10
2:B:77:LEU:O	2:B:87:ALA:HB2	0.52	2.05	1	1
2:B:42:GLN:HB3	2:B:79:PHE:CZ	0.52	2.40	2	1
3:C:38:THR:CG2	3:C:80:LYS:CG	0.52	2.88	3	2
3:C:38:THR:HB	3:C:76:TYR:CE2	0.52	2.40	6	2
3:C:39:SER:C	3:C:41:THR:N	0.52	2.63	15	12
2:B:21:SER:HA	2:B:56:THR:HG21	0.52	1.81	4	1
3:C:100:ALA:N	3:C:103:LEU:CD1	0.52	2.73	5	2
2:B:25:PHE:CZ	2:B:53:ASP:OD2	0.52	2.63	6	1
3:C:42:ILE:HG12	3:C:60:VAL:CG1	0.52	2.35	18	2
3:C:38:THR:O	3:C:38:THR:CG2	0.52	2.57	14	1
2:B:68:ARG:NH2	3:C:78:THR:OG1	0.52	2.42	19	1
3:C:38:THR:O	3:C:77:PHE:CE1	0.51	2.63	1	2
2:B:66:THR:O	2:B:67:ALA:HB2	0.51	2.05	3	1
2:B:93:PHE:HB3	3:C:27:HIS:CG	0.51	2.39	3	2
3:C:38:THR:HG23	3:C:80:LYS:HD2	0.51	1.81	9	1
2:B:23:THR:OG1	2:B:56:THR:HA	0.51	2.05	10	3
2:B:44:LEU:CB	2:B:51:LEU:CD2	0.51	2.88	10	1
3:C:43:LYS:O	3:C:46:LEU:CD2	0.51	2.57	14	1
2:B:9:ARG:HB2	2:B:77:LEU:CD1	0.51	2.34	15	1
3:C:33:ARG:HG3	3:C:46:LEU:HD22	0.51	1.82	20	1
2:B:45:TYR:O	2:B:75:VAL:HA	0.51	2.05	5	15
2:B:8:ARG:CD	2:B:74:THR:HG21	0.51	2.35	6	3
2:B:8:ARG:HB3	2:B:90:ILE:CG1	0.51	2.35	19	7
2:B:3:VAL:HG13	2:B:5:LEU:CD2	0.51	2.35	7	3
3:C:93:PHE:CD1	3:C:93:PHE:C	0.51	2.84	11	4
1:A:1:VAL:HG11	3:C:83:TYR:CB	0.51	2.36	9	1
1:A:11:THR:HG23	3:C:95:ILE:CG2	0.51	2.35	10	2
3:C:79:TYR:CD1	3:C:79:TYR:C	0.51	2.84	11	1
3:C:39:SER:CB	3:C:110:LEU:O	0.51	2.57	13	1
3:C:67:SER:O	3:C:69:VAL:N	0.51	2.43	17	1
2:B:23:THR:O	2:B:24:VAL:HG13	0.51	2.05	19	1
2:B:14:ILE:HG12	3:C:30:ILE:CB	0.51	2.36	16	6
2:B:22:SER:C	2:B:23:THR:OG1	0.51	2.47	12	3
3:C:66:PRO:HB2	3:C:68:HIS:CD2	0.51	2.40	3	1
3:C:95:ILE:HG23	3:C:100:ALA:HB3	0.51	1.82	3	2
1:A:1:VAL:CG1	3:C:80:LYS:HG2	0.51	2.35	4	3
1:A:7:LEU:HD11	3:C:93:PHE:N	0.51	2.19	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:37:ARG:HB3	2:B:79:PHE:CE2	0.51	2.39	5	1
2:B:23:THR:HA	2:B:56:THR:HG22	0.51	1.83	6	1
3:C:108:ASN:OD1	3:C:108:ASN:N	0.51	2.42	6	1
3:C:62:PHE:CZ	3:C:110:LEU:HD21	0.51	2.40	7	1
2:B:14:ILE:CG1	2:B:34:ILE:HD12	0.51	2.35	8	3
2:B:47:ASP:N	2:B:47:ASP:OD1	0.51	2.43	8	2
3:C:19:VAL:HG12	3:C:31:VAL:HG22	0.51	1.82	17	2
2:B:23:THR:HG21	2:B:57:LEU:H	0.51	1.66	10	1
2:B:44:LEU:HD22	2:B:45:TYR:H	0.51	1.64	11	1
2:B:8:ARG:HG2	2:B:90:ILE:CG2	0.51	2.35	16	3
2:B:14:ILE:CD1	3:C:30:ILE:CD1	0.51	2.84	18	2
3:C:76:TYR:CE1	3:C:93:PHE:CD1	0.51	2.99	19	1
2:B:46:LYS:HG3	2:B:62:PHE:CE2	0.51	2.40	20	1
1:A:11:THR:OG1	3:C:95:ILE:HB	0.51	2.06	11	5
2:B:9:ARG:HB3	2:B:12:THR:HB	0.51	1.82	18	15
2:B:14:ILE:CD1	3:C:30:ILE:HB	0.51	2.36	16	9
3:C:45:MET:O	3:C:45:MET:HE3	0.51	2.06	3	1
3:C:18:TYR:CE2	3:C:32:LYS:CE	0.51	2.92	4	1
2:B:78:ALA:HA	2:B:87:ALA:CB	0.51	2.34	8	2
2:B:1:MET:SD	2:B:2:ASP:N	0.51	2.83	17	1
2:B:7:ILE:CD1	2:B:77:LEU:CD2	0.51	2.75	2	3
2:B:23:THR:CG2	2:B:57:LEU:N	0.51	2.73	4	1
2:B:10:HIS:NE2	2:B:89:CYS:HB2	0.51	2.20	5	5
3:C:38:THR:HB	3:C:77:PHE:HD1	0.51	1.65	16	7
3:C:108:ASN:HA	3:C:111:ASP:OD1	0.51	2.05	5	1
2:B:76:GLY:C	2:B:77:LEU:HD12	0.51	2.25	6	1
1:A:3:THR:HA	3:C:76:TYR:CE2	0.51	2.41	7	2
2:B:23:THR:CG2	2:B:57:LEU:HB2	0.51	2.35	12	1
2:B:37:ARG:NH2	2:B:86:GLU:OE1	0.51	2.43	14	1
2:B:91:GLU:OE1	2:B:91:GLU:CA	0.51	2.56	15	1
1:A:1:VAL:CG1	3:C:80:LYS:HD2	0.51	2.35	11	2
2:B:37:ARG:HB3	2:B:79:PHE:CZ	0.51	2.41	5	1
3:C:37:LEU:O	3:C:37:LEU:CD1	0.51	2.57	5	3
3:C:38:THR:HG21	3:C:77:PHE:HA	0.51	1.82	5	1
1:A:2:ALA:O	3:C:76:TYR:CD2	0.51	2.64	19	2
1:A:7:LEU:CD2	3:C:93:PHE:HB3	0.51	2.36	10	2
2:B:7:ILE:CD1	2:B:75:VAL:CG2	0.51	2.89	11	2
2:B:42:GLN:O	2:B:43:ARG:NE	0.51	2.44	11	1
2:B:20:GLU:N	2:B:20:GLU:OE1	0.51	2.43	12	2
2:B:93:PHE:CE1	3:C:27:HIS:ND1	0.51	2.79	13	1
2:B:44:LEU:CD2	2:B:77:LEU:HD23	0.51	2.35	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:43:ARG:CG	2:B:50:LEU:CD1	0.51	2.88	15	1
2:B:45:TYR:CE1	2:B:88:LEU:HD11	0.51	2.41	16	1
2:B:14:ILE:CD1	3:C:30:ILE:HG12	0.51	2.35	20	1
2:B:9:ARG:NH2	2:B:86:GLU:OE2	0.51	2.43	14	3
3:C:38:THR:OG1	3:C:77:PHE:CB	0.51	2.59	1	2
3:C:97:PRO:O	3:C:98:GLU:CB	0.51	2.57	18	4
3:C:69:VAL:CG2	3:C:103:LEU:HG	0.51	2.32	6	2
1:A:15:HIS:CD2	1:A:15:HIS:O	0.51	2.64	6	1
3:C:62:PHE:CE1	3:C:110:LEU:CD2	0.51	2.94	13	1
3:C:60:VAL:HG12	3:C:62:PHE:CZ	0.51	2.41	14	1
1:A:3:THR:HG22	1:A:4:LEU:H	0.51	1.66	18	1
3:C:72:LYS:HG2	3:C:103:LEU:HD21	0.51	1.82	2	3
3:C:21:LEU:HB3	3:C:62:PHE:CE2	0.51	2.41	4	7
2:B:79:PHE:C	2:B:86:GLU:CG	0.51	2.79	10	1
3:C:30:ILE:HD12	3:C:30:ILE:H	0.51	1.65	11	2
3:C:42:ILE:HG12	3:C:60:VAL:HG11	0.51	1.81	18	2
2:B:30:ILE:HG23	2:B:34:ILE:CD1	0.51	2.36	5	5
2:B:68:ARG:HB3	2:B:69:PRO:HD2	0.51	1.83	18	12
3:C:36:ALA:HB3	3:C:42:ILE:HG21	0.51	1.76	12	4
2:B:6:MET:SD	2:B:15:PHE:CE1	0.51	3.04	4	2
2:B:8:ARG:CG	2:B:74:THR:CG2	0.51	2.89	13	4
2:B:57:LEU:CD1	2:B:62:PHE:HB2	0.51	2.36	5	1
2:B:8:ARG:HD2	2:B:74:THR:CG2	0.51	2.36	15	4
3:C:43:LYS:C	3:C:43:LYS:CD	0.51	2.79	7	3
2:B:50:LEU:HD13	2:B:51:LEU:N	0.51	2.21	16	1
1:A:4:LEU:HD11	3:C:73:VAL:HA	0.51	1.81	19	1
2:B:37:ARG:NH2	2:B:79:PHE:CE1	0.51	2.79	19	1
2:B:7:ILE:CG2	2:B:14:ILE:HG22	0.51	2.35	17	4
2:B:3:VAL:CG2	2:B:63:THR:HA	0.51	2.36	5	1
2:B:8:ARG:HG3	2:B:74:THR:CG2	0.51	2.35	20	3
1:A:7:LEU:CD1	3:C:93:PHE:CZ	0.51	2.84	8	1
3:C:65:ILE:HG12	3:C:106:ALA:CB	0.51	2.35	8	4
2:B:4:PHE:CD1	2:B:4:PHE:N	0.51	2.79	19	3
2:B:24:VAL:CG1	2:B:51:LEU:HD13	0.51	2.36	10	1
2:B:24:VAL:O	2:B:27:LEU:HG	0.51	2.06	14	1
2:B:42:GLN:O	2:B:42:GLN:NE2	0.51	2.43	16	1
2:B:31:VAL:HG12	2:B:37:ARG:CG	0.51	2.36	17	1
3:C:77:PHE:O	3:C:81:VAL:CG2	0.50	2.57	2	1
2:B:67:ALA:HA	2:B:72:PRO:HA	0.50	1.82	5	10
2:B:79:PHE:CD1	2:B:86:GLU:OE2	0.50	2.65	4	1
2:B:23:THR:CG2	2:B:57:LEU:HG	0.50	2.35	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:68:ARG:N	2:B:69:PRO:CD	0.50	2.74	5	1
2:B:4:PHE:CB	2:B:68:ARG:HG3	0.50	2.36	9	2
3:C:39:SER:HB2	3:C:77:PHE:CE1	0.50	2.41	16	2
2:B:42:GLN:CD	2:B:77:LEU:CD2	0.50	2.80	18	1
3:C:19:VAL:O	3:C:30:ILE:CA	0.50	2.59	20	1
3:C:46:LEU:C	3:C:46:LEU:CD1	0.50	2.80	2	2
3:C:61:ASN:O	3:C:61:ASN:ND2	0.50	2.44	7	1
2:B:27:LEU:N	2:B:27:LEU:HD22	0.50	2.21	8	1
2:B:17:ASP:OD1	2:B:18:ALA:N	0.50	2.44	19	2
2:B:9:ARG:HD3	2:B:35:LEU:CD1	0.50	2.36	2	1
2:B:11:LYS:HA	3:C:27:HIS:CE1	0.50	2.40	3	1
2:B:46:LYS:HD3	2:B:62:PHE:CE1	0.50	2.41	3	1
2:B:42:GLN:HA	2:B:78:ALA:O	0.50	2.06	9	6
2:B:23:THR:HB	2:B:57:LEU:N	0.50	2.21	16	1
3:C:63:ARG:HB2	3:C:63:ARG:NH1	0.50	2.21	18	1
3:C:72:LYS:HD3	3:C:99:ILE:HG21	0.50	1.83	18	1
2:B:3:VAL:CG2	2:B:63:THR:O	0.50	2.59	8	3
2:B:14:ILE:O	2:B:14:ILE:CG2	0.50	2.60	15	13
2:B:16:THR:OG1	2:B:30:ILE:HD12	0.50	2.07	2	5
2:B:8:ARG:HB3	2:B:90:ILE:CG2	0.50	2.37	8	8
2:B:78:ALA:HB2	2:B:88:LEU:CA	0.50	2.36	2	1
3:C:72:LYS:HB3	3:C:103:LEU:CD2	0.50	2.36	5	2
1:A:3:THR:HA	3:C:76:TYR:CE1	0.50	2.42	6	1
2:B:22:SER:O	2:B:23:THR:OG1	0.50	2.29	12	1
2:B:69:PRO:O	3:C:75:MET:CE	0.50	2.58	17	1
3:C:43:LYS:HG3	3:C:44:ALA:N	0.50	2.22	1	7
1:A:5:GLN:HA	3:C:107:ALA:CB	0.50	2.36	10	9
2:B:8:ARG:HD3	2:B:13:THR:HG23	0.50	1.82	3	1
2:B:45:TYR:O	2:B:76:GLY:N	0.50	2.39	3	1
2:B:93:PHE:HB2	3:C:67:SER:CB	0.50	2.37	3	2
2:B:68:ARG:N	2:B:69:PRO:HD2	0.50	2.21	5	1
2:B:37:ARG:HB2	2:B:79:PHE:CE2	0.50	2.42	15	1
3:C:101:LEU:C	3:C:101:LEU:CD1	0.50	2.80	15	1
2:B:20:GLU:O	2:B:57:LEU:CB	0.50	2.59	16	1
2:B:24:VAL:HG23	2:B:25:PHE:N	0.50	2.21	16	1
3:C:104:LEU:HD13	3:C:105:MET:N	0.50	2.21	17	1
2:B:68:ARG:HB3	2:B:69:PRO:HD3	0.50	1.83	2	4
2:B:14:ILE:HG13	2:B:34:ILE:CG1	0.50	2.36	9	4
3:C:69:VAL:CG2	3:C:103:LEU:HD11	0.50	2.34	4	1
2:B:44:LEU:CD2	2:B:75:VAL:CG2	0.50	2.90	7	2
3:C:69:VAL:CG1	3:C:103:LEU:HD23	0.50	2.37	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:72:LYS:NZ	3:C:94:PRO:O	0.50	2.44	19	2
2:B:57:LEU:HG	2:B:62:PHE:CG	0.50	2.41	10	1
3:C:65:ILE:HG12	3:C:106:ALA:HB1	0.50	1.83	13	3
3:C:35:HIS:CD2	3:C:81:VAL:HG21	0.50	2.42	12	1
3:C:35:HIS:CE1	3:C:78:THR:N	0.50	2.80	13	1
2:B:24:VAL:CA	2:B:27:LEU:HD21	0.50	2.36	14	1
3:C:39:SER:HB2	3:C:42:ILE:HD12	0.50	1.83	19	1
2:B:2:ASP:OD2	3:C:82:ARG:CZ	0.50	2.59	20	1
1:A:7:LEU:CD1	3:C:93:PHE:CB	0.50	2.88	4	3
2:B:79:PHE:HB2	2:B:86:GLU:HB2	0.50	1.82	2	2
1:A:2:ALA:O	3:C:76:TYR:CD1	0.50	2.65	6	2
2:B:41:GLU:O	2:B:79:PHE:CA	0.50	2.59	10	6
3:C:108:ASN:O	3:C:111:ASP:OD1	0.50	2.30	5	2
1:A:7:LEU:CD2	3:C:93:PHE:O	0.50	2.60	5	1
3:C:66:PRO:CD	3:C:102:GLU:OE1	0.50	2.60	11	1
2:B:8:ARG:HG3	2:B:90:ILE:HG23	0.50	1.84	1	1
2:B:22:SER:OG	2:B:23:THR:N	0.50	2.44	17	5
3:C:67:SER:O	3:C:68:HIS:C	0.50	2.49	17	11
3:C:72:LYS:CG	3:C:103:LEU:HD21	0.50	2.37	2	3
2:B:9:ARG:NH2	2:B:86:GLU:CD	0.50	2.66	14	2
3:C:38:THR:CG2	3:C:80:LYS:HD3	0.50	2.36	3	3
3:C:104:LEU:C	3:C:104:LEU:CD2	0.50	2.80	6	2
2:B:79:PHE:CE1	2:B:86:GLU:HG3	0.50	2.42	18	2
2:B:5:LEU:CD2	2:B:57:LEU:HD11	0.50	2.35	11	1
3:C:39:SER:CA	3:C:77:PHE:CZ	0.50	2.95	1	2
2:B:24:VAL:CG1	2:B:53:ASP:HA	0.50	2.37	4	13
3:C:41:THR:OG1	3:C:112:CYS:N	0.50	2.45	5	1
2:B:64:SER:C	2:B:65:GLN:CG	0.50	2.80	12	3
3:C:38:THR:CG2	3:C:80:LYS:HB3	0.50	2.37	6	4
3:C:104:LEU:O	3:C:108:ASN:ND2	0.50	2.45	6	1
3:C:106:ALA:O	3:C:110:LEU:CG	0.50	2.60	9	3
2:B:14:ILE:HD13	2:B:15:PHE:N	0.50	2.20	20	4
3:C:41:THR:OG1	3:C:110:LEU:HA	0.50	2.07	19	4
2:B:57:LEU:CD2	2:B:62:PHE:CD2	0.50	2.95	11	1
2:B:4:PHE:CB	2:B:68:ARG:N	0.50	2.75	15	1
2:B:93:PHE:CD2	3:C:67:SER:HB3	0.50	2.42	18	1
2:B:14:ILE:CG1	3:C:30:ILE:HB	0.49	2.37	6	11
2:B:92:PRO:O	2:B:93:PHE:O	0.49	2.30	12	5
2:B:10:HIS:CE1	2:B:89:CYS:HB2	0.49	2.42	9	4
2:B:77:LEU:O	2:B:87:ALA:O	0.49	2.29	11	2
2:B:22:SER:O	2:B:56:THR:HG22	0.49	2.07	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:75:MET:HG2	3:C:93:PHE:CZ	0.49	2.42	17	1
2:B:35:LEU:HD22	2:B:79:PHE:HZ	0.49	1.66	1	1
3:C:98:GLU:OE1	3:C:98:GLU:HA	0.49	2.07	1	3
3:C:109:PHE:CD2	3:C:110:LEU:HD23	0.49	2.42	13	2
2:B:61:GLY:C	2:B:62:PHE:CD1	0.49	2.86	3	1
3:C:35:HIS:CD2	3:C:78:THR:HG1	0.49	2.25	4	2
2:B:42:GLN:CB	2:B:78:ALA:O	0.49	2.60	5	1
2:B:7:ILE:CD1	2:B:75:VAL:HG21	0.49	2.37	11	1
3:C:35:HIS:CE1	3:C:78:THR:HG1	0.49	2.25	14	1
2:B:8:ARG:HD3	2:B:90:ILE:HG21	0.49	1.82	15	1
3:C:38:THR:CG2	3:C:80:LYS:HD2	0.49	2.36	19	1
2:B:37:ARG:CG	2:B:42:GLN:HB2	0.49	2.37	15	2
2:B:23:THR:HB	2:B:57:LEU:CD2	0.49	2.37	5	1
1:A:7:LEU:O	3:C:95:ILE:CD1	0.49	2.60	12	2
2:B:23:THR:CG2	2:B:26:GLU:HB2	0.49	2.36	9	2
2:B:42:GLN:HG3	2:B:79:PHE:CE1	0.49	2.42	17	1
3:C:100:ALA:HA	3:C:103:LEU:CD2	0.49	2.38	18	5
2:B:31:VAL:HG13	2:B:37:ARG:HG3	0.49	1.84	2	1
3:C:70:LEU:CD1	3:C:70:LEU:C	0.49	2.78	3	1
2:B:37:ARG:CZ	2:B:42:GLN:HB2	0.49	2.38	4	1
2:B:67:ALA:O	2:B:68:ARG:HB2	0.49	2.07	5	2
2:B:20:GLU:OE1	2:B:20:GLU:N	0.49	2.45	9	1
3:C:40:GLY:N	3:C:112:CYS:O	0.49	2.46	9	1
2:B:23:THR:OG1	2:B:57:LEU:HB2	0.49	2.07	12	1
2:B:27:LEU:N	2:B:27:LEU:HD12	0.49	2.22	18	1
3:C:39:SER:OG	3:C:41:THR:OG1	0.49	2.31	3	1
1:A:3:THR:CG2	3:C:112:CYS:OXT	0.49	2.61	4	1
3:C:38:THR:CG2	3:C:80:LYS:HG2	0.49	2.37	7	2
3:C:79:TYR:CD2	3:C:83:TYR:CE1	0.49	3.00	11	1
2:B:62:PHE:O	2:B:62:PHE:CD1	0.49	2.65	12	1
2:B:42:GLN:HA	2:B:79:PHE:HA	0.49	1.82	18	2
3:C:38:THR:HB	3:C:76:TYR:CE1	0.49	2.43	15	1
2:B:14:ILE:HG12	3:C:30:ILE:HG12	0.49	1.83	20	2
3:C:19:VAL:HG23	3:C:46:LEU:HD22	0.49	1.82	18	1
1:A:9:ARG:NH2	3:C:108:ASN:OD1	0.49	2.46	19	1
2:B:86:GLU:O	2:B:87:ALA:O	0.49	2.31	3	3
2:B:41:GLU:O	2:B:79:PHE:HA	0.49	2.07	10	11
2:B:44:LEU:HD13	2:B:51:LEU:HD22	0.49	1.83	3	1
2:B:69:PRO:HB2	3:C:79:TYR:CE1	0.49	2.42	12	2
3:C:69:VAL:CG1	3:C:103:LEU:HD11	0.49	2.37	4	1
3:C:38:THR:CB	3:C:77:PHE:HD1	0.49	2.21	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:104:LEU:C	3:C:104:LEU:HD23	0.49	2.27	6	1
3:C:67:SER:O	3:C:70:LEU:CG	0.49	2.60	17	2
1:A:8:CYS:CB	3:C:107:ALA:HB3	0.49	2.38	9	1
3:C:69:VAL:CG2	3:C:103:LEU:HD23	0.49	2.38	9	1
1:A:7:LEU:HG	3:C:93:PHE:CB	0.49	2.37	15	2
1:A:9:ARG:HA	1:A:12:VAL:CG2	0.49	2.38	11	2
2:B:16:THR:OG1	2:B:30:ILE:HG13	0.49	2.08	5	13
2:B:46:LYS:HE2	2:B:62:PHE:CZ	0.49	2.43	3	1
3:C:66:PRO:HB2	3:C:68:HIS:NE2	0.49	2.23	3	1
1:A:9:ARG:NH1	1:A:13:ASN:OD1	0.49	2.44	4	1
3:C:17:MET:CB	3:C:33:ARG:HB2	0.49	2.38	16	2
2:B:57:LEU:HG	2:B:62:PHE:CB	0.49	2.38	16	4
3:C:104:LEU:C	3:C:104:LEU:CD1	0.49	2.80	7	5
3:C:76:TYR:O	3:C:80:LYS:HB3	0.49	2.06	11	3
2:B:37:ARG:O	2:B:37:ARG:NE	0.49	2.46	15	1
2:B:15:PHE:CB	3:C:30:ILE:O	0.49	2.60	1	1
2:B:62:PHE:O	2:B:63:THR:CB	0.49	2.58	2	1
2:B:45:TYR:CZ	2:B:50:LEU:HG	0.49	2.43	3	2
2:B:88:LEU:O	2:B:88:LEU:HD13	0.49	2.07	15	2
2:B:3:VAL:C	2:B:4:PHE:CD1	0.49	2.86	19	1
1:A:5:GLN:OE1	1:A:6:HIS:ND1	0.49	2.46	1	1
2:B:9:ARG:HD3	2:B:35:LEU:HD11	0.49	1.85	2	1
2:B:37:ARG:NH1	2:B:79:PHE:CE1	0.49	2.80	3	1
1:A:3:THR:HG21	3:C:111:ASP:CG	0.49	2.28	13	2
3:C:43:LYS:HA	3:C:46:LEU:HD12	0.49	1.84	9	1
2:B:13:THR:HB	3:C:29:PHE:CZ	0.49	2.42	18	2
2:B:5:LEU:CD1	2:B:62:PHE:CD1	0.49	2.91	18	2
2:B:37:ARG:HG2	2:B:79:PHE:CD1	0.49	2.43	1	1
2:B:44:LEU:HD23	2:B:75:VAL:HG23	0.49	1.84	7	4
3:C:39:SER:O	3:C:111:ASP:HB3	0.49	2.08	14	4
3:C:39:SER:OG	3:C:110:LEU:O	0.49	2.31	5	3
3:C:42:ILE:HG13	3:C:60:VAL:CG1	0.49	2.38	15	2
2:B:31:VAL:HG22	2:B:35:LEU:HD13	0.49	1.84	16	1
1:A:5:GLN:NE2	3:C:112:CYS:O	0.49	2.46	20	1
2:B:5:LEU:C	2:B:16:THR:CG2	0.48	2.81	3	6
3:C:38:THR:C	3:C:77:PHE:CE1	0.48	2.87	1	3
2:B:57:LEU:HD13	2:B:62:PHE:CD2	0.48	2.43	5	1
3:C:68:HIS:CD2	3:C:99:ILE:HD13	0.48	2.43	5	1
3:C:69:VAL:HA	3:C:72:LYS:HB2	0.48	1.84	19	3
3:C:18:TYR:CE1	3:C:32:LYS:N	0.48	2.80	8	1
2:B:23:THR:HG22	2:B:57:LEU:HD22	0.48	1.84	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:73:VAL:HG21	3:C:110:LEU:CD2	0.48	2.38	10	1
3:C:110:LEU:O	3:C:111:ASP:CB	0.48	2.60	20	3
1:A:7:LEU:HD13	3:C:93:PHE:HE2	0.48	1.62	12	1
3:C:68:HIS:ND1	3:C:99:ILE:CG1	0.48	2.76	14	1
2:B:92:PRO:O	3:C:27:HIS:ND1	0.48	2.45	19	1
2:B:5:LEU:CB	2:B:27:LEU:HD11	0.48	2.38	20	1
2:B:10:HIS:O	2:B:11:LYS:HG2	0.48	2.09	9	2
3:C:20:LYS:HG3	3:C:59:GLU:CB	0.48	2.39	18	2
3:C:110:LEU:O	3:C:111:ASP:C	0.48	2.50	7	3
1:A:7:LEU:HD12	3:C:93:PHE:HB3	0.48	1.84	2	1
3:C:79:TYR:CE1	3:C:83:TYR:CZ	0.48	3.01	2	1
3:C:35:HIS:ND1	3:C:77:PHE:HB3	0.48	2.23	16	5
2:B:37:ARG:HG2	2:B:79:PHE:CE2	0.48	2.44	5	1
3:C:38:THR:HG23	3:C:80:LYS:CE	0.48	2.38	9	1
2:B:68:ARG:HG3	2:B:69:PRO:N	0.48	2.22	11	1
3:C:76:TYR:CG	3:C:93:PHE:CE1	0.48	3.01	16	1
3:C:46:LEU:HD21	3:C:58:ASN:ND2	0.48	2.21	1	1
2:B:68:ARG:HB2	2:B:69:PRO:CD	0.48	2.38	11	2
3:C:41:THR:OG1	3:C:110:LEU:C	0.48	2.52	10	6
3:C:41:THR:OG1	3:C:111:ASP:CA	0.48	2.62	5	1
2:B:4:PHE:N	2:B:67:ALA:HB1	0.48	2.22	6	1
2:B:5:LEU:HD22	2:B:27:LEU:HD11	0.48	1.86	13	1
2:B:62:PHE:O	2:B:66:THR:OG1	0.48	2.31	16	2
3:C:79:TYR:CZ	3:C:83:TYR:CG	0.48	3.01	11	1
2:B:34:ILE:C	2:B:34:ILE:CD1	0.48	2.80	17	2
3:C:82:ARG:NH2	3:C:83:TYR:CE1	0.48	2.81	19	1
2:B:88:LEU:O	2:B:88:LEU:HD12	0.48	2.09	2	3
1:A:12:VAL:HG23	1:A:13:ASN:N	0.48	2.23	6	3
1:A:4:LEU:HG	3:C:93:PHE:CD2	0.48	2.43	9	2
2:B:57:LEU:HD11	2:B:62:PHE:HE2	0.48	1.67	12	1
3:C:62:PHE:CE1	3:C:110:LEU:HD21	0.48	2.43	13	1
2:B:23:THR:HB	2:B:57:LEU:CA	0.48	2.39	16	1
3:C:65:ILE:O	3:C:65:ILE:HG22	0.48	2.06	17	2
2:B:92:PRO:O	2:B:93:PHE:C	0.48	2.52	18	1
2:B:14:ILE:HG12	3:C:30:ILE:CG1	0.48	2.38	20	6
2:B:68:ARG:NH2	3:C:82:ARG:HB2	0.48	2.24	2	1
2:B:11:LYS:O	3:C:28:GLU:CG	0.48	2.62	6	1
3:C:21:LEU:C	3:C:22:ILE:HD12	0.48	2.28	15	2
3:C:18:TYR:CE1	3:C:32:LYS:HG3	0.48	2.43	16	2
3:C:76:TYR:CD1	3:C:93:PHE:CD1	0.48	3.01	19	1
2:B:67:ALA:HB1	2:B:73:ALA:HB3	0.48	1.85	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:GLN:HG3	3:C:108:ASN:HA	0.48	1.85	18	5
3:C:21:LEU:HD22	3:C:60:VAL:CG2	0.48	2.38	8	5
3:C:35:HIS:CE1	3:C:81:VAL:HG21	0.48	2.44	5	1
3:C:100:ALA:HA	3:C:103:LEU:CD1	0.48	2.38	5	2
2:B:65:GLN:OE1	2:B:66:THR:HG23	0.48	2.09	8	1
3:C:79:TYR:OH	3:C:83:TYR:OH	0.48	2.31	8	1
2:B:5:LEU:CD2	2:B:57:LEU:CD2	0.48	2.89	10	1
2:B:4:PHE:CD1	2:B:68:ARG:HA	0.48	2.44	17	1
3:C:39:SER:OG	3:C:77:PHE:CE1	0.48	2.65	20	1
1:A:8:CYS:SG	3:C:104:LEU:CA	0.48	3.01	1	3
2:B:15:PHE:CE1	3:C:35:HIS:CD2	0.48	3.02	1	1
3:C:106:ALA:O	3:C:110:LEU:HG	0.48	2.08	4	11
3:C:20:LYS:HG3	3:C:59:GLU:HA	0.48	1.84	18	4
1:A:1:VAL:HG13	3:C:80:LYS:HG2	0.48	1.86	4	1
1:A:5:GLN:HB2	3:C:111:ASP:OD2	0.48	2.09	5	1
3:C:67:SER:HA	3:C:70:LEU:CG	0.48	2.39	17	2
2:B:6:MET:HE2	2:B:13:THR:HG22	0.48	1.85	11	1
2:B:67:ALA:CA	2:B:71:ALA:O	0.48	2.62	11	1
2:B:46:LYS:NZ	2:B:49:GLN:OE1	0.48	2.47	12	1
2:B:46:LYS:CB	2:B:51:LEU:HD22	0.48	2.32	16	1
2:B:5:LEU:HB3	2:B:16:THR:CG2	0.48	2.38	12	11
2:B:9:ARG:CD	2:B:35:LEU:HD11	0.48	2.38	2	1
2:B:38:PRO:O	2:B:42:GLN:HG2	0.48	2.09	7	3
3:C:69:VAL:O	3:C:73:VAL:CG1	0.48	2.62	20	3
3:C:105:MET:O	3:C:109:PHE:HB2	0.48	2.08	10	4
2:B:14:ILE:HD11	3:C:18:TYR:CZ	0.48	2.44	17	2
2:B:13:THR:OG1	3:C:28:GLU:O	0.48	2.31	15	3
3:C:96:ALA:CB	3:C:97:PRO:HD2	0.48	2.32	10	1
3:C:99:ILE:HD13	3:C:100:ALA:H	0.48	1.66	14	4
2:B:24:VAL:HA	2:B:27:LEU:CD2	0.48	2.36	14	1
2:B:37:ARG:HB2	2:B:79:PHE:CZ	0.48	2.44	15	1
3:C:41:THR:OG1	3:C:110:LEU:O	0.48	2.31	18	1
3:C:82:ARG:NE	3:C:83:TYR:CD1	0.48	2.81	19	1
3:C:18:TYR:CD2	3:C:32:LYS:HE2	0.48	2.44	4	1
3:C:43:LYS:CD	3:C:43:LYS:C	0.48	2.82	5	1
1:A:4:LEU:O	1:A:4:LEU:HD23	0.48	2.09	9	1
3:C:46:LEU:CD2	3:C:58:ASN:HB3	0.48	2.39	9	1
2:B:7:ILE:HD13	2:B:77:LEU:HG	0.48	1.86	18	3
3:C:35:HIS:CE1	3:C:77:PHE:CB	0.48	2.96	13	2
2:B:24:VAL:HG23	2:B:25:PHE:H	0.48	1.69	19	2
1:A:7:LEU:HG	3:C:93:PHE:CE2	0.47	2.44	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:21:LEU:HD21	3:C:31:VAL:HG22	0.47	1.86	16	3
3:C:32:LYS:HG2	3:C:35:HIS:CB	0.47	2.39	14	1
3:C:68:HIS:ND1	3:C:99:ILE:HG12	0.47	2.23	14	1
2:B:51:LEU:HD13	2:B:62:PHE:HE2	0.47	1.68	18	1
3:C:80:LYS:CD	3:C:80:LYS:C	0.47	2.82	20	1
1:A:7:LEU:N	1:A:7:LEU:HD22	0.47	2.24	7	2
2:B:3:VAL:HG21	2:B:62:PHE:HB3	0.47	1.86	1	1
2:B:9:ARG:HB2	2:B:12:THR:O	0.47	2.09	5	3
2:B:57:LEU:CD2	2:B:62:PHE:CE2	0.47	2.97	2	1
1:A:7:LEU:HD13	3:C:93:PHE:HB2	0.47	1.85	4	2
2:B:5:LEU:CB	2:B:16:THR:HG23	0.47	2.39	7	2
2:B:5:LEU:HD22	2:B:57:LEU:HD21	0.47	1.85	15	1
2:B:68:ARG:HE	2:B:71:ALA:HB3	0.47	1.67	3	1
2:B:79:PHE:CD1	2:B:79:PHE:O	0.47	2.67	3	1
3:C:97:PRO:O	3:C:98:GLU:CG	0.47	2.62	12	2
3:C:94:PRO:C	3:C:95:ILE:HD13	0.47	2.30	4	1
2:B:66:THR:O	2:B:66:THR:HG23	0.47	2.08	6	2
3:C:27:HIS:CD2	3:C:67:SER:HB2	0.47	2.43	7	1
1:A:4:LEU:HG	3:C:93:PHE:CE2	0.47	2.45	9	1
2:B:34:ILE:HD11	3:C:18:TYR:CE1	0.47	2.44	9	1
2:B:46:LYS:HB2	2:B:62:PHE:CE2	0.47	2.44	9	1
2:B:23:THR:OG1	2:B:57:LEU:CG	0.47	2.63	16	1
3:C:33:ARG:HG3	3:C:43:LYS:HZ3	0.47	1.68	19	1
3:C:20:LYS:HB3	3:C:30:ILE:HG22	0.47	1.85	20	1
2:B:67:ALA:HB1	2:B:73:ALA:HB2	0.47	1.86	2	2
3:C:65:ILE:HG23	3:C:69:VAL:HG11	0.47	1.87	10	3
2:B:34:ILE:HG13	2:B:35:LEU:N	0.47	2.23	13	6
3:C:27:HIS:CD2	3:C:67:SER:HB3	0.47	2.43	7	1
3:C:68:HIS:CD2	3:C:99:ILE:HG12	0.47	2.44	10	2
2:B:57:LEU:CD2	2:B:62:PHE:HB2	0.47	2.39	8	2
2:B:57:LEU:O	2:B:62:PHE:N	0.47	2.41	11	3
2:B:78:ALA:C	2:B:79:PHE:CD1	0.47	2.87	12	2
3:C:97:PRO:C	3:C:98:GLU:CG	0.47	2.81	18	1
3:C:29:PHE:CG	3:C:70:LEU:HD11	0.47	2.44	19	1
3:C:27:HIS:O	3:C:28:GLU:OE2	0.47	2.33	2	5
2:B:4:PHE:HB3	2:B:68:ARG:N	0.47	2.24	4	3
3:C:31:VAL:HB	3:C:35:HIS:ND1	0.47	2.25	19	3
2:B:44:LEU:CD2	2:B:77:LEU:CD2	0.47	2.93	5	2
2:B:93:PHE:HB3	3:C:27:HIS:CD2	0.47	2.45	5	1
1:A:3:THR:HG21	3:C:111:ASP:CB	0.47	2.39	6	1
2:B:79:PHE:CZ	2:B:86:GLU:OE1	0.47	2.67	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:42:ILE:HA	3:C:45:MET:CG	0.47	2.39	7	1
3:C:37:LEU:HA	3:C:43:LYS:CG	0.47	2.39	19	1
1:A:1:VAL:HB	3:C:83:TYR:CD1	0.47	2.44	20	1
2:B:4:PHE:HB2	2:B:68:ARG:CA	0.47	2.38	15	6
2:B:13:THR:O	3:C:30:ILE:CD1	0.47	2.57	15	5
2:B:13:THR:OG1	2:B:93:PHE:CZ	0.47	2.58	1	1
2:B:6:MET:CB	2:B:73:ALA:O	0.47	2.62	10	2
2:B:10:HIS:ND1	2:B:91:GLU:HB2	0.47	2.24	3	1
2:B:11:LYS:HA	3:C:27:HIS:ND1	0.47	2.24	18	3
3:C:26:GLY:O	3:C:27:HIS:CD2	0.47	2.67	3	1
2:B:38:PRO:O	2:B:42:GLN:HG3	0.47	2.09	4	1
2:B:23:THR:O	2:B:24:VAL:HB	0.47	2.09	20	3
2:B:77:LEU:N	2:B:77:LEU:CD1	0.47	2.77	6	1
3:C:72:LYS:O	3:C:93:PHE:CE2	0.47	2.67	9	2
2:B:22:SER:C	2:B:23:THR:CG2	0.47	2.81	14	2
3:C:107:ALA:O	3:C:111:ASP:OD1	0.47	2.32	8	2
2:B:57:LEU:CD2	2:B:62:PHE:CG	0.47	2.92	11	1
3:C:17:MET:SD	3:C:33:ARG:CD	0.47	3.03	16	1
2:B:31:VAL:HG13	2:B:77:LEU:CD1	0.47	2.39	20	1
1:A:5:GLN:HG3	3:C:108:ASN:CB	0.47	2.40	19	3
2:B:35:LEU:HD22	2:B:79:PHE:CZ	0.47	2.45	1	1
2:B:67:ALA:O	2:B:68:ARG:HD3	0.47	2.09	1	3
3:C:22:ILE:HG13	3:C:28:GLU:OE1	0.47	2.10	5	3
3:C:27:HIS:O	3:C:28:GLU:OE1	0.47	2.32	1	2
3:C:39:SER:O	3:C:110:LEU:C	0.47	2.52	1	2
3:C:37:LEU:HD12	3:C:43:LYS:CB	0.47	2.40	2	1
3:C:101:LEU:HD23	3:C:102:GLU:N	0.47	2.24	2	1
2:B:8:ARG:CD	2:B:90:ILE:HG23	0.47	2.40	3	1
2:B:13:THR:OG1	3:C:29:PHE:CE1	0.47	2.67	4	1
2:B:37:ARG:NE	2:B:42:GLN:CB	0.47	2.78	4	1
3:C:38:THR:O	3:C:112:CYS:OXT	0.47	2.33	4	1
1:A:4:LEU:CD2	1:A:8:CYS:HB3	0.47	2.40	5	1
2:B:34:ILE:HG22	2:B:35:LEU:N	0.47	2.24	5	2
2:B:38:PRO:O	2:B:79:PHE:CZ	0.47	2.68	5	1
2:B:43:ARG:HD3	2:B:50:LEU:HD21	0.47	1.85	12	1
2:B:57:LEU:HB3	2:B:63:THR:CB	0.47	2.40	12	1
2:B:93:PHE:CB	3:C:67:SER:CB	0.47	2.92	12	1
2:B:78:ALA:HB1	2:B:88:LEU:HD23	0.47	1.85	14	1
3:C:26:GLY:O	3:C:27:HIS:HB3	0.47	2.09	17	1
3:C:46:LEU:HD21	3:C:59:GLU:O	0.47	2.09	17	1
3:C:17:MET:HB2	3:C:33:ARG:CB	0.47	2.40	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:VAL:HB	3:C:83:TYR:HB2	0.47	1.86	9	6
3:C:42:ILE:O	3:C:46:LEU:N	0.47	2.45	3	3
2:B:80:ARG:O	2:B:80:ARG:CG	0.47	2.62	10	1
3:C:76:TYR:O	3:C:80:LYS:CB	0.47	2.63	11	1
3:C:36:ALA:HA	3:C:77:PHE:CD1	0.47	2.44	12	1
1:A:7:LEU:HD22	3:C:76:TYR:CE2	0.47	2.44	17	1
1:A:4:LEU:CD2	3:C:103:LEU:HG	0.47	2.40	2	1
2:B:13:THR:HB	3:C:29:PHE:CD1	0.47	2.44	2	1
3:C:42:ILE:O	3:C:45:MET:HG2	0.47	2.10	2	1
3:C:43:LYS:HA	3:C:46:LEU:CG	0.47	2.40	2	1
2:B:46:LYS:HE3	2:B:51:LEU:HD12	0.47	1.87	3	1
2:B:4:PHE:CZ	2:B:68:ARG:NH2	0.47	2.83	5	1
3:C:37:LEU:CD2	3:C:43:LYS:CB	0.47	2.93	5	1
2:B:79:PHE:HB2	2:B:86:GLU:CG	0.47	2.40	15	2
3:C:65:ILE:CG1	3:C:69:VAL:HG11	0.47	2.40	6	2
2:B:39:PRO:O	2:B:41:GLU:OE1	0.47	2.33	8	1
2:B:62:PHE:O	2:B:63:THR:O	0.47	2.31	16	2
1:A:4:LEU:N	1:A:4:LEU:HD12	0.47	2.25	19	1
2:B:2:ASP:OD2	3:C:82:ARG:NH2	0.47	2.48	20	1
2:B:37:ARG:O	2:B:42:GLN:OE1	0.47	2.33	20	1
3:C:20:LYS:CB	3:C:30:ILE:HG22	0.47	2.39	20	1
3:C:19:VAL:O	3:C:31:VAL:N	0.47	2.48	18	5
3:C:39:SER:CB	3:C:42:ILE:CD1	0.47	2.90	19	4
3:C:70:LEU:O	3:C:74:CYS:SG	0.47	2.73	2	7
2:B:56:THR:O	2:B:60:CYS:HB2	0.47	2.10	17	14
3:C:66:PRO:HD2	3:C:69:VAL:CB	0.47	2.40	14	2
2:B:45:TYR:CE1	2:B:50:LEU:HG	0.47	2.45	6	2
2:B:86:GLU:OE1	2:B:87:ALA:HB2	0.47	2.10	9	1
3:C:72:LYS:HG3	3:C:99:ILE:CD1	0.47	2.40	15	3
2:B:64:SER:O	2:B:65:GLN:HB3	0.47	2.10	12	1
3:C:34:GLU:HA	3:C:37:LEU:HB2	0.47	1.86	12	1
3:C:31:VAL:HG11	3:C:35:HIS:NE2	0.47	2.24	14	1
2:B:37:ARG:HG3	2:B:42:GLN:HG3	0.47	1.87	15	1
3:C:23:SER:OG	3:C:65:ILE:O	0.47	2.34	16	1
3:C:33:ARG:HG2	3:C:34:GLU:N	0.47	2.25	19	1
3:C:28:GLU:O	3:C:29:PHE:CD1	0.46	2.68	3	3
2:B:52:ASP:OD1	2:B:52:ASP:N	0.46	2.48	4	1
2:B:25:PHE:CE2	2:B:53:ASP:HB2	0.46	2.44	6	1
2:B:68:ARG:NH2	2:B:70:GLN:NE2	0.46	2.63	8	1
3:C:108:ASN:O	3:C:112:CYS:N	0.46	2.47	8	1
2:B:1:MET:O	2:B:20:GLU:OE1	0.46	2.33	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:9:ARG:HD2	2:B:35:LEU:HD22	0.46	1.85	9	1
3:C:46:LEU:CD2	3:C:58:ASN:CB	0.46	2.93	9	1
1:A:7:LEU:HD21	3:C:93:PHE:HB2	0.46	1.87	10	1
2:B:38:PRO:O	2:B:42:GLN:OE1	0.46	2.33	20	1
2:B:5:LEU:CD1	2:B:57:LEU:CD2	0.46	2.85	1	1
2:B:9:ARG:NE	2:B:86:GLU:OE2	0.46	2.49	1	1
2:B:44:LEU:HB2	2:B:51:LEU:HB3	0.46	1.87	16	2
1:A:5:GLN:O	1:A:8:CYS:SG	0.46	2.72	15	6
3:C:45:MET:SD	3:C:59:GLU:O	0.46	2.74	3	1
2:B:1:MET:O	2:B:2:ASP:OD1	0.46	2.34	5	1
2:B:34:ILE:HG12	2:B:35:LEU:HD12	0.46	1.85	6	2
3:C:33:ARG:HG3	3:C:34:GLU:N	0.46	2.25	6	1
3:C:72:LYS:O	3:C:93:PHE:CZ	0.46	2.69	9	2
2:B:23:THR:OG1	2:B:57:LEU:HG	0.46	2.10	16	1
3:C:72:LYS:HE2	3:C:103:LEU:HD11	0.46	1.87	19	1
3:C:42:ILE:O	3:C:46:LEU:HD12	0.46	2.11	1	1
2:B:9:ARG:HD3	2:B:35:LEU:CD2	0.46	2.41	2	1
1:A:1:VAL:HG13	3:C:80:LYS:HD2	0.46	1.82	11	2
2:B:67:ALA:C	2:B:68:ARG:HG2	0.46	2.31	8	3
1:A:7:LEU:HD22	3:C:95:ILE:CG1	0.46	2.40	4	1
2:B:42:GLN:HB2	2:B:78:ALA:O	0.46	2.11	5	1
2:B:45:TYR:CD2	2:B:49:GLN:C	0.46	2.89	11	1
2:B:60:CYS:HG	2:B:62:PHE:HE2	0.46	1.51	15	2
2:B:8:ARG:HD3	2:B:74:THR:CG2	0.46	2.41	1	3
2:B:13:THR:CG2	3:C:29:PHE:CE1	0.46	2.98	1	1
2:B:61:GLY:O	2:B:62:PHE:CD2	0.46	2.68	14	3
3:C:26:GLY:O	3:C:28:GLU:OE2	0.46	2.33	11	3
1:A:6:HIS:O	1:A:9:ARG:HG3	0.46	2.10	16	2
2:B:57:LEU:HB2	2:B:62:PHE:CB	0.46	2.40	4	1
2:B:37:ARG:NH1	2:B:79:PHE:CD2	0.46	2.83	8	1
2:B:23:THR:HB	2:B:57:LEU:CB	0.46	2.41	16	1
2:B:34:ILE:HG13	3:C:30:ILE:HG21	0.46	1.87	17	1
3:C:63:ARG:CB	3:C:63:ARG:NH1	0.46	2.79	18	1
2:B:43:ARG:O	2:B:77:LEU:HA	0.46	2.10	1	2
2:B:4:PHE:CG	2:B:68:ARG:HD3	0.46	2.45	2	1
3:C:19:VAL:CG2	3:C:60:VAL:CG2	0.46	2.94	2	5
3:C:66:PRO:CB	3:C:68:HIS:NE2	0.46	2.77	3	1
3:C:72:LYS:CE	3:C:99:ILE:HG21	0.46	2.40	4	1
2:B:13:THR:O	3:C:29:PHE:HA	0.46	2.11	6	2
2:B:64:SER:O	2:B:64:SER:OG	0.46	2.34	6	2
3:C:105:MET:O	3:C:109:PHE:HB3	0.46	2.10	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:VAL:CG1	3:C:83:TYR:HB3	0.46	2.39	6	1
2:B:14:ILE:CB	2:B:34:ILE:HD12	0.46	2.41	8	1
2:B:16:THR:CB	2:B:30:ILE:HD13	0.46	2.40	9	3
2:B:44:LEU:CB	2:B:51:LEU:CB	0.46	2.94	16	1
2:B:93:PHE:HB3	3:C:67:SER:CB	0.46	2.41	18	1
3:C:38:THR:OG1	3:C:77:PHE:CA	0.46	2.64	1	2
3:C:42:ILE:O	3:C:46:LEU:CB	0.46	2.64	3	1
2:B:93:PHE:CZ	3:C:71:SER:OG	0.46	2.66	5	1
3:C:110:LEU:HD23	3:C:110:LEU:C	0.46	2.31	5	1
2:B:66:THR:HG23	2:B:73:ALA:HB2	0.46	1.88	6	1
2:B:24:VAL:CG2	2:B:53:ASP:HA	0.46	2.39	16	2
3:C:37:LEU:C	3:C:37:LEU:CD1	0.46	2.82	9	1
1:A:3:THR:C	1:A:5:GLN:N	0.46	2.69	17	2
3:C:18:TYR:CD1	3:C:32:LYS:HG2	0.46	2.46	13	1
3:C:18:TYR:CD1	3:C:32:LYS:HG3	0.46	2.45	16	1
3:C:42:ILE:HD12	3:C:77:PHE:CZ	0.46	2.46	16	1
3:C:46:LEU:CD2	3:C:59:GLU:N	0.46	2.78	17	1
1:A:7:LEU:HD11	3:C:76:TYR:CE2	0.46	2.45	20	1
3:C:107:ALA:HA	3:C:110:LEU:HD12	0.46	1.88	1	3
1:A:9:ARG:HG3	1:A:10:LYS:N	0.46	2.25	16	2
2:B:78:ALA:CB	2:B:88:LEU:N	0.46	2.73	2	1
2:B:7:ILE:HG21	2:B:77:LEU:CD1	0.46	2.37	4	1
2:B:20:GLU:O	2:B:57:LEU:HG	0.46	2.11	4	1
2:B:4:PHE:CB	2:B:68:ARG:HB2	0.46	2.41	5	1
2:B:32:GLU:O	2:B:36:LYS:HA	0.46	2.10	13	9
3:C:21:LEU:CD2	3:C:21:LEU:N	0.46	2.79	5	4
1:A:3:THR:HG22	3:C:38:THR:CG2	0.46	2.38	9	1
1:A:4:LEU:HB2	3:C:73:VAL:HA	0.46	1.87	9	1
3:C:35:HIS:CD2	3:C:78:THR:HA	0.46	2.45	12	1
3:C:36:ALA:HA	3:C:77:PHE:CG	0.46	2.46	12	1
1:A:12:VAL:O	1:A:15:HIS:O	0.46	2.33	17	1
3:C:19:VAL:HG13	3:C:21:LEU:CD2	0.46	2.41	17	1
2:B:48:ASP:OD1	2:B:48:ASP:O	0.46	2.34	16	4
3:C:69:VAL:O	3:C:70:LEU:C	0.46	2.54	2	3
1:A:13:ASN:O	1:A:14:GLY:C	0.46	2.55	3	3
1:A:5:GLN:CG	3:C:108:ASN:HA	0.46	2.41	14	3
2:B:93:PHE:HB3	3:C:27:HIS:ND1	0.46	2.26	12	1
3:C:111:ASP:O	3:C:112:CYS:OXT	0.46	2.34	12	1
2:B:37:ARG:CG	2:B:42:GLN:HG3	0.46	2.40	15	1
2:B:23:THR:HG22	2:B:24:VAL:HG22	0.46	1.86	16	1
2:B:27:LEU:N	2:B:27:LEU:CD1	0.46	2.78	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:9:ARG:NE	2:B:86:GLU:CD	0.46	2.69	1	1
1:A:5:GLN:HA	1:A:8:CYS:SG	0.46	2.51	5	2
3:C:33:ARG:O	3:C:37:LEU:HB2	0.46	2.11	10	4
2:B:38:PRO:O	2:B:42:GLN:HB2	0.46	2.11	11	2
2:B:38:PRO:O	2:B:42:GLN:CD	0.46	2.54	14	1
3:C:21:LEU:N	3:C:21:LEU:CD2	0.46	2.79	14	1
3:C:42:ILE:HG23	3:C:60:VAL:CG2	0.46	2.41	16	1
2:B:20:GLU:OE1	2:B:58:GLY:CA	0.46	2.64	18	1
3:C:17:MET:O	3:C:18:TYR:CD1	0.46	2.69	20	1
3:C:101:LEU:HD23	3:C:101:LEU:O	0.46	2.10	1	1
2:B:41:GLU:O	2:B:79:PHE:HB2	0.46	2.10	18	6
3:C:23:SER:HB2	3:C:70:LEU:CD2	0.46	2.41	16	2
3:C:23:SER:C	3:C:25:ASP:N	0.46	2.67	12	3
2:B:67:ALA:HA	2:B:73:ALA:N	0.46	2.26	5	1
2:B:57:LEU:HB3	2:B:62:PHE:CB	0.46	2.40	11	1
3:C:23:SER:HB3	3:C:25:ASP:OD2	0.46	2.11	11	1
2:B:63:THR:HG22	2:B:64:SER:N	0.46	2.24	12	1
2:B:24:VAL:HG11	2:B:53:ASP:CA	0.46	2.41	20	2
1:A:4:LEU:HD21	3:C:103:LEU:CD2	0.46	2.36	15	2
1:A:4:LEU:O	1:A:8:CYS:SG	0.46	2.74	19	1
1:A:3:THR:CG2	3:C:112:CYS:HA	0.45	2.42	1	1
2:B:31:VAL:CG2	2:B:77:LEU:CD2	0.45	2.94	2	1
3:C:61:ASN:OD1	3:C:61:ASN:O	0.45	2.35	13	2
3:C:98:GLU:OE1	3:C:98:GLU:O	0.45	2.34	5	1
2:B:75:VAL:HG22	2:B:77:LEU:HD21	0.45	1.87	8	1
3:C:96:ALA:CB	3:C:97:PRO:CD	0.45	2.92	10	2
2:B:47:ASP:O	2:B:49:GLN:N	0.45	2.49	10	1
1:A:8:CYS:SG	3:C:100:ALA:O	0.45	2.74	11	1
3:C:25:ASP:OD2	3:C:67:SER:HB2	0.45	2.11	11	2
2:B:5:LEU:CD2	2:B:27:LEU:CD2	0.45	2.81	18	2
3:C:70:LEU:CD1	3:C:71:SER:HB2	0.45	2.41	13	1
3:C:78:THR:O	3:C:81:VAL:CG2	0.45	2.54	16	1
2:B:44:LEU:HD21	2:B:77:LEU:HD21	0.45	1.86	20	1
3:C:19:VAL:O	3:C:30:ILE:HB	0.45	2.11	20	1
2:B:62:PHE:O	2:B:63:THR:C	0.45	2.55	1	2
2:B:8:ARG:O	2:B:90:ILE:CD1	0.45	2.63	9	3
1:A:4:LEU:CG	3:C:73:VAL:HB	0.45	2.41	3	2
2:B:11:LYS:CG	3:C:28:GLU:HG2	0.45	2.42	5	1
2:B:23:THR:O	2:B:24:VAL:CB	0.45	2.65	20	3
2:B:67:ALA:CA	2:B:72:PRO:HA	0.45	2.41	5	1
1:A:4:LEU:HD12	3:C:73:VAL:CG1	0.45	2.42	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:ARG:HA	1:A:12:VAL:HG22	0.45	1.87	11	1
2:B:52:ASP:N	2:B:52:ASP:OD1	0.45	2.48	11	1
3:C:68:HIS:CE1	3:C:99:ILE:HG12	0.45	2.46	11	1
1:A:12:VAL:HG21	3:C:104:LEU:CG	0.45	2.37	17	1
3:C:68:HIS:CD2	3:C:69:VAL:N	0.45	2.84	1	1
1:A:7:LEU:CD1	3:C:93:PHE:N	0.45	2.79	4	1
2:B:14:ILE:HD13	3:C:30:ILE:O	0.45	2.11	4	1
3:C:70:LEU:O	3:C:74:CYS:HB2	0.45	2.11	17	4
2:B:64:SER:O	2:B:65:GLN:CD	0.45	2.55	19	2
2:B:66:THR:OG1	2:B:69:PRO:HG2	0.45	2.11	9	1
3:C:39:SER:O	3:C:111:ASP:HB2	0.45	2.11	18	2
3:C:66:PRO:HG3	3:C:102:GLU:OE2	0.45	2.12	11	1
3:C:68:HIS:CG	3:C:69:VAL:N	0.45	2.84	12	1
3:C:99:ILE:CD1	3:C:100:ALA:N	0.45	2.79	14	4
2:B:20:GLU:OE2	2:B:58:GLY:CA	0.45	2.65	14	1
2:B:37:ARG:HG3	2:B:79:PHE:CD1	0.45	2.46	16	1
2:B:3:VAL:O	2:B:17:ASP:OD1	0.45	2.34	19	1
3:C:110:LEU:O	3:C:111:ASP:HB2	0.45	2.10	20	1
2:B:28:LYS:CE	2:B:39:PRO:HB3	0.45	2.42	2	2
3:C:19:VAL:CG1	3:C:36:ALA:CB	0.45	2.95	2	1
2:B:27:LEU:C	2:B:27:LEU:CD2	0.45	2.83	5	2
3:C:97:PRO:O	3:C:98:GLU:HB2	0.45	2.11	16	2
2:B:34:ILE:CD1	2:B:35:LEU:CD1	0.45	2.94	10	6
3:C:36:ALA:HA	3:C:77:PHE:CD2	0.45	2.46	10	1
2:B:23:THR:HG21	2:B:57:LEU:CG	0.45	2.42	12	1
1:A:5:GLN:OE1	3:C:112:CYS:SG	0.45	2.74	14	1
2:B:8:ARG:H	2:B:77:LEU:HD21	0.45	1.69	16	1
3:C:20:LYS:CE	3:C:59:GLU:HB2	0.45	2.40	18	1
3:C:93:PHE:CD1	3:C:95:ILE:HG13	0.45	2.46	18	1
2:B:4:PHE:CE1	2:B:17:ASP:OD1	0.45	2.70	2	1
2:B:13:THR:OG1	3:C:29:PHE:CZ	0.45	2.66	4	1
3:C:22:ILE:O	3:C:62:PHE:HB2	0.45	2.11	4	4
3:C:18:TYR:CD1	3:C:32:LYS:HA	0.45	2.47	19	2
3:C:33:ARG:CG	3:C:34:GLU:N	0.45	2.80	6	1
2:B:3:VAL:HG12	2:B:18:ALA:O	0.45	2.11	7	1
3:C:38:THR:HB	3:C:77:PHE:HA	0.45	1.87	14	1
2:B:11:LYS:O	3:C:28:GLU:HG2	0.45	2.12	6	2
1:A:1:VAL:H1	3:C:83:TYR:HB3	0.45	1.72	3	1
3:C:65:ILE:HD11	3:C:106:ALA:HB2	0.45	1.87	7	1
1:A:3:THR:OG1	1:A:4:LEU:N	0.45	2.50	11	1
2:B:37:ARG:O	2:B:37:ARG:CD	0.45	2.64	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:97:PRO:O	3:C:98:GLU:OE1	0.45	2.35	19	1
2:B:5:LEU:HG	2:B:27:LEU:HD11	0.45	1.89	20	1
2:B:6:MET:O	2:B:74:THR:HA	0.45	2.11	11	4
3:C:41:THR:O	3:C:45:MET:HG2	0.45	2.11	3	3
2:B:52:ASP:OD1	2:B:52:ASP:O	0.45	2.34	4	1
3:C:41:THR:HB	3:C:110:LEU:O	0.45	2.12	5	1
1:A:12:VAL:CG2	1:A:13:ASN:N	0.45	2.80	11	2
1:A:6:HIS:O	1:A:10:LYS:CG	0.45	2.65	8	1
2:B:6:MET:CE	2:B:13:THR:CG2	0.45	2.94	11	1
3:C:23:SER:HB2	3:C:65:ILE:O	0.45	2.12	14	2
3:C:38:THR:HG1	3:C:77:PHE:HD1	0.45	1.52	12	1
3:C:95:ILE:HG12	3:C:100:ALA:HB1	0.45	1.88	19	2
2:B:24:VAL:CG1	2:B:51:LEU:HD12	0.45	2.41	16	1
2:B:14:ILE:CG1	3:C:30:ILE:HG12	0.45	2.41	20	1
2:B:23:THR:C	2:B:25:PHE:N	0.45	2.69	14	7
2:B:44:LEU:CB	2:B:51:LEU:HB3	0.45	2.42	9	4
2:B:93:PHE:HA	3:C:27:HIS:ND1	0.45	2.27	1	1
3:C:21:LEU:HD23	3:C:60:VAL:CG2	0.45	2.42	1	4
1:A:8:CYS:SG	3:C:104:LEU:HA	0.45	2.52	5	4
2:B:4:PHE:HB3	2:B:67:ALA:O	0.45	2.11	5	1
2:B:8:ARG:CD	2:B:74:THR:CG2	0.45	2.95	7	3
2:B:14:ILE:HB	2:B:34:ILE:HD12	0.45	1.89	8	1
2:B:19:LYS:O	2:B:22:SER:N	0.45	2.43	10	1
2:B:7:ILE:HD11	2:B:27:LEU:HD21	0.45	1.89	11	1
3:C:27:HIS:HE2	3:C:29:PHE:HD2	0.45	1.55	13	1
2:B:46:LYS:NZ	2:B:60:CYS:O	0.45	2.43	14	1
2:B:47:ASP:OD1	2:B:47:ASP:N	0.45	2.50	14	1
3:C:109:PHE:CD2	3:C:110:LEU:CD1	0.45	3.00	15	1
2:B:15:PHE:O	3:C:18:TYR:OH	0.45	2.32	17	1
2:B:42:GLN:HG2	2:B:43:ARG:N	0.45	2.27	17	1
3:C:60:VAL:O	3:C:61:ASN:ND2	0.45	2.50	18	1
2:B:22:SER:O	2:B:24:VAL:CG2	0.45	2.50	19	1
2:B:61:GLY:C	2:B:62:PHE:CD2	0.45	2.90	1	1
3:C:39:SER:OG	3:C:77:PHE:CE2	0.45	2.58	1	1
1:A:8:CYS:CB	3:C:103:LEU:CB	0.45	2.95	2	1
3:C:69:VAL:HA	3:C:72:LYS:CB	0.45	2.41	13	2
2:B:2:ASP:O	2:B:64:SER:HB3	0.45	2.11	5	1
2:B:37:ARG:CB	2:B:79:PHE:CZ	0.45	3.00	5	1
2:B:37:ARG:HD3	2:B:79:PHE:CD1	0.45	2.47	6	1
3:C:29:PHE:CD1	3:C:29:PHE:N	0.45	2.84	19	2
2:B:9:ARG:HG2	2:B:12:THR:CB	0.45	2.42	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:28:LYS:CD	2:B:39:PRO:HB3	0.45	2.42	11	1
2:B:13:THR:OG1	3:C:29:PHE:CE2	0.45	2.67	12	1
2:B:35:LEU:O	2:B:37:ARG:NH1	0.45	2.50	13	1
3:C:41:THR:O	3:C:45:MET:N	0.45	2.49	15	1
2:B:46:LYS:O	2:B:47:ASP:C	0.45	2.53	16	4
3:C:72:LYS:HD3	3:C:103:LEU:CD2	0.45	2.42	17	1
2:B:52:ASP:O	2:B:55:LYS:HG3	0.45	2.12	19	1
2:B:24:VAL:O	2:B:28:LYS:HG2	0.45	2.12	1	1
3:C:38:THR:OG1	3:C:77:PHE:HA	0.45	2.11	4	7
2:B:46:LYS:O	2:B:47:ASP:HB3	0.45	2.12	9	2
2:B:3:VAL:HG21	2:B:57:LEU:CD1	0.45	2.42	4	1
3:C:64:GLU:C	3:C:65:ILE:CG1	0.45	2.85	4	1
2:B:3:VAL:HG11	2:B:57:LEU:CB	0.45	2.41	5	1
2:B:31:VAL:HG13	2:B:37:ARG:HB2	0.45	1.87	5	1
3:C:62:PHE:CD1	3:C:65:ILE:HD13	0.45	2.47	7	1
2:B:41:GLU:O	2:B:80:ARG:N	0.45	2.49	8	1
2:B:67:ALA:CB	2:B:73:ALA:HB2	0.45	2.42	9	1
2:B:31:VAL:HG21	2:B:77:LEU:CD2	0.45	2.42	10	1
2:B:39:PRO:O	2:B:40:ASP:HB2	0.45	2.11	10	1
3:C:35:HIS:NE2	3:C:77:PHE:CB	0.45	2.80	10	1
3:C:95:ILE:HG12	3:C:100:ALA:CB	0.45	2.42	13	2
3:C:45:MET:SD	3:C:61:ASN:OD1	0.45	2.74	16	1
1:A:1:VAL:CG1	3:C:80:LYS:HG3	0.44	2.42	2	3
3:C:27:HIS:C	3:C:28:GLU:OE2	0.44	2.55	12	3
3:C:103:LEU:CD1	3:C:103:LEU:H	0.44	2.26	17	4
2:B:8:ARG:C	2:B:90:ILE:CD1	0.44	2.85	9	3
3:C:110:LEU:O	3:C:110:LEU:HG	0.44	2.12	5	1
2:B:66:THR:O	2:B:72:PRO:C	0.44	2.56	6	1
2:B:78:ALA:C	2:B:79:PHE:CG	0.44	2.90	6	2
2:B:24:VAL:HG12	2:B:51:LEU:HD13	0.44	1.89	10	1
2:B:51:LEU:C	2:B:51:LEU:CD1	0.44	2.79	10	1
2:B:68:ARG:HG2	2:B:69:PRO:HD2	0.44	1.89	15	4
2:B:38:PRO:O	2:B:42:GLN:HB3	0.44	2.11	11	2
3:C:23:SER:HB2	3:C:25:ASP:OD2	0.44	2.12	11	1
3:C:19:VAL:HG13	3:C:31:VAL:CG2	0.44	2.42	16	1
2:B:41:GLU:HG3	2:B:80:ARG:CG	0.44	2.41	20	1
2:B:9:ARG:NH1	2:B:77:LEU:HB3	0.44	2.27	10	1
3:C:37:LEU:O	3:C:37:LEU:CD2	0.44	2.56	10	1
3:C:109:PHE:CD1	3:C:109:PHE:O	0.44	2.70	16	1
2:B:44:LEU:CD2	2:B:77:LEU:HG	0.44	2.43	18	1
2:B:51:LEU:HD12	2:B:52:ASP:H	0.44	1.71	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:86:GLU:OE1	2:B:88:LEU:HD23	0.44	2.11	19	1
2:B:47:ASP:O	2:B:48:ASP:C	0.44	2.55	20	11
3:C:19:VAL:HA	3:C:58:ASN:O	0.44	2.12	5	12
2:B:35:LEU:O	2:B:37:ARG:NE	0.44	2.43	12	2
1:A:13:ASN:O	1:A:15:HIS:N	0.44	2.50	11	2
2:B:35:LEU:CD1	2:B:77:LEU:HD13	0.44	2.43	7	1
3:C:66:PRO:HD3	3:C:102:GLU:OE1	0.44	2.13	7	2
2:B:43:ARG:HG3	2:B:50:LEU:HD21	0.44	1.89	9	1
3:C:18:TYR:O	3:C:58:ASN:CG	0.44	2.56	9	1
2:B:37:ARG:NE	2:B:79:PHE:CE1	0.44	2.85	10	1
2:B:24:VAL:HA	2:B:27:LEU:CD1	0.44	2.40	14	1
3:C:18:TYR:CE2	3:C:30:ILE:CG2	0.44	3.00	14	1
3:C:34:GLU:O	3:C:37:LEU:N	0.44	2.50	14	1
2:B:51:LEU:HD11	2:B:62:PHE:HE2	0.44	1.71	16	1
2:B:3:VAL:HG12	2:B:19:LYS:C	0.44	2.33	17	1
2:B:64:SER:O	2:B:65:GLN:OE1	0.44	2.35	20	1
3:C:25:ASP:OD1	3:C:27:HIS:CE1	0.44	2.70	20	1
3:C:72:LYS:NZ	3:C:99:ILE:HG12	0.44	2.27	1	1
2:B:44:LEU:O	2:B:51:LEU:N	0.44	2.42	7	1
1:A:8:CYS:SG	3:C:103:LEU:HB2	0.44	2.53	11	1
2:B:7:ILE:CG1	2:B:75:VAL:CG2	0.44	2.95	11	1
1:A:4:LEU:CD2	1:A:8:CYS:HB2	0.44	2.43	16	1
2:B:6:MET:SD	2:B:74:THR:OG1	0.44	2.74	20	1
1:A:1:VAL:HB	3:C:83:TYR:HB3	0.44	1.90	8	2
2:B:93:PHE:HA	3:C:27:HIS:CE1	0.44	2.47	8	3
3:C:27:HIS:HB2	3:C:67:SER:CB	0.44	2.43	1	1
2:B:9:ARG:CD	2:B:35:LEU:HD13	0.44	2.42	2	1
3:C:72:LYS:HG2	3:C:99:ILE:CG2	0.44	2.43	4	1
2:B:7:ILE:HD13	2:B:77:LEU:HD23	0.44	1.90	5	1
1:A:1:VAL:N	3:C:83:TYR:CG	0.44	2.85	6	1
2:B:25:PHE:CE2	2:B:53:ASP:OD2	0.44	2.71	6	1
1:A:6:HIS:O	1:A:10:LYS:HG2	0.44	2.13	8	1
3:C:105:MET:SD	3:C:105:MET:O	0.44	2.76	8	1
1:A:4:LEU:CG	3:C:103:LEU:HD23	0.44	2.43	11	1
2:B:57:LEU:HB3	2:B:62:PHE:HB2	0.44	1.89	11	2
2:B:68:ARG:HG3	2:B:69:PRO:CD	0.44	2.42	11	1
3:C:67:SER:HA	3:C:70:LEU:HB3	0.44	1.88	2	2
3:C:72:LYS:HE3	3:C:99:ILE:CG1	0.44	2.42	4	1
2:B:39:PRO:O	2:B:40:ASP:HB3	0.44	2.11	8	1
1:A:3:THR:HG23	3:C:112:CYS:SG	0.44	2.53	9	1
3:C:63:ARG:O	3:C:64:GLU:HG2	0.44	2.12	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:42:GLN:OE1	2:B:43:ARG:C	0.44	2.56	12	1
3:C:34:GLU:O	3:C:35:HIS:C	0.44	2.56	14	1
2:B:42:GLN:O	2:B:42:GLN:OE1	0.44	2.34	15	1
2:B:31:VAL:CG1	2:B:42:GLN:OE1	0.44	2.58	18	1
2:B:14:ILE:HD11	3:C:30:ILE:CG1	0.44	2.42	20	1
2:B:57:LEU:CD2	2:B:62:PHE:HB3	0.44	2.43	20	1
2:B:14:ILE:HD11	3:C:30:ILE:CG2	0.44	2.43	7	2
3:C:18:TYR:CA	3:C:32:LYS:HA	0.44	2.43	1	1
2:B:46:LYS:O	2:B:46:LYS:HG3	0.44	2.13	12	4
2:B:37:ARG:CG	2:B:79:PHE:CE1	0.44	3.00	6	1
2:B:14:ILE:CG1	2:B:34:ILE:HG12	0.44	2.43	9	1
1:A:4:LEU:CD2	3:C:103:LEU:HB3	0.44	2.42	17	2
3:C:76:TYR:N	3:C:93:PHE:CZ	0.44	2.85	16	1
1:A:7:LEU:HD23	3:C:93:PHE:CB	0.44	2.35	17	1
3:C:17:MET:HG2	3:C:33:ARG:NH1	0.44	2.28	18	1
2:B:46:LYS:HE3	2:B:60:CYS:SG	0.44	2.53	20	1
2:B:15:PHE:HB2	3:C:30:ILE:O	0.44	2.12	2	5
1:A:1:VAL:CG1	3:C:80:LYS:HA	0.44	2.40	3	2
2:B:45:TYR:CE1	2:B:50:LEU:CD1	0.44	3.01	8	3
2:B:4:PHE:HB2	2:B:67:ALA:O	0.44	2.13	9	2
3:C:79:TYR:O	3:C:83:TYR:HB2	0.44	2.13	11	1
2:B:43:ARG:HD3	2:B:50:LEU:HD11	0.44	1.90	12	1
3:C:20:LYS:N	3:C:20:LYS:CD	0.44	2.80	13	1
2:B:32:GLU:OE1	2:B:32:GLU:O	0.44	2.35	17	1
3:C:20:LYS:HB2	3:C:28:GLU:OE2	0.44	2.12	18	1
3:C:30:ILE:C	3:C:30:ILE:CD1	0.44	2.81	18	1
3:C:79:TYR:O	3:C:82:ARG:HG3	0.44	2.13	19	1
2:B:18:ALA:HB2	2:B:27:LEU:HD21	0.44	1.90	1	1
2:B:78:ALA:HA	2:B:86:GLU:HB2	0.44	1.89	1	1
2:B:4:PHE:CD1	2:B:17:ASP:OD1	0.44	2.71	2	1
3:C:43:LYS:HA	3:C:46:LEU:CD2	0.44	2.42	8	3
3:C:45:MET:HG3	3:C:46:LEU:N	0.44	2.26	3	2
3:C:101:LEU:O	3:C:104:LEU:HB3	0.44	2.13	5	2
3:C:35:HIS:NE2	3:C:77:PHE:HB2	0.44	2.28	10	1
3:C:58:ASN:O	3:C:58:ASN:OD1	0.44	2.36	11	1
2:B:23:THR:CB	2:B:57:LEU:HB2	0.44	2.43	12	1
2:B:86:GLU:O	2:B:87:ALA:C	0.44	2.56	12	4
1:A:7:LEU:HD23	3:C:76:TYR:HE2	0.44	1.72	18	1
2:B:42:GLN:HA	2:B:79:PHE:CA	0.44	2.43	18	1
2:B:5:LEU:HB2	2:B:16:THR:HG23	0.44	1.89	20	1
3:C:39:SER:HA	3:C:77:PHE:CE1	0.43	2.48	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:7:ILE:CD1	2:B:77:LEU:HG	0.43	2.42	18	2
3:C:34:GLU:O	3:C:37:LEU:HB3	0.43	2.12	20	2
2:B:62:PHE:CE2	2:B:73:ALA:HB1	0.43	2.48	4	1
3:C:38:THR:O	3:C:76:TYR:OH	0.43	2.32	6	1
3:C:111:ASP:CG	3:C:111:ASP:O	0.43	2.57	6	2
2:B:79:PHE:O	2:B:86:GLU:OE2	0.43	2.35	7	1
2:B:79:PHE:C	2:B:86:GLU:HG2	0.43	2.34	10	1
3:C:60:VAL:HG12	3:C:62:PHE:CE2	0.43	2.47	10	1
2:B:5:LEU:HD22	2:B:57:LEU:CD1	0.43	2.40	11	1
2:B:46:LYS:HB3	2:B:51:LEU:CD1	0.43	2.43	12	2
3:C:19:VAL:N	3:C:31:VAL:O	0.43	2.41	11	2
1:A:1:VAL:HG21	3:C:80:LYS:HB2	0.43	1.89	12	1
3:C:17:MET:HB3	3:C:33:ARG:CB	0.43	2.43	14	1
2:B:13:THR:CB	3:C:29:PHE:CE1	0.43	3.01	15	1
3:C:20:LYS:HG3	3:C:59:GLU:CA	0.43	2.43	18	1
2:B:65:GLN:HG2	2:B:70:GLN:CB	0.43	2.43	19	1
3:C:95:ILE:CG1	3:C:100:ALA:CB	0.43	2.96	19	1
2:B:14:ILE:HG13	2:B:34:ILE:HG12	0.43	1.89	9	3
2:B:8:ARG:NH1	2:B:74:THR:OG1	0.43	2.51	5	1
2:B:37:ARG:CB	2:B:79:PHE:CE2	0.43	3.01	5	1
1:A:1:VAL:HG11	3:C:80:LYS:HG3	0.43	1.89	6	1
1:A:1:VAL:CG2	3:C:80:LYS:HA	0.43	2.43	6	2
3:C:39:SER:OG	3:C:110:LEU:HB3	0.43	2.13	9	1
3:C:72:LYS:HD3	3:C:93:PHE:CE2	0.43	2.48	9	1
2:B:13:THR:HB	3:C:27:HIS:CE1	0.43	2.48	13	1
3:C:33:ARG:NH1	3:C:43:LYS:HB2	0.43	2.28	13	1
3:C:93:PHE:CE1	3:C:95:ILE:CG1	0.43	3.00	18	1
3:C:35:HIS:NE2	3:C:78:THR:HB	0.43	2.28	20	1
3:C:38:THR:HG21	3:C:80:LYS:HB2	0.43	1.89	20	1
2:B:35:LEU:O	2:B:36:LYS:CB	0.43	2.67	5	4
3:C:41:THR:OG1	3:C:111:ASP:C	0.43	2.56	5	1
3:C:41:THR:O	3:C:45:MET:HG3	0.43	2.12	19	3
3:C:43:LYS:CE	3:C:44:ALA:N	0.43	2.82	9	1
2:B:24:VAL:N	2:B:27:LEU:HD12	0.43	2.28	10	1
2:B:20:GLU:OE2	2:B:58:GLY:HA3	0.43	2.12	14	1
2:B:5:LEU:HD22	2:B:27:LEU:CD1	0.43	2.43	2	2
2:B:32:GLU:HA	2:B:37:ARG:N	0.43	2.29	3	9
2:B:67:ALA:HA	2:B:71:ALA:O	0.43	2.13	2	3
2:B:68:ARG:HG2	2:B:69:PRO:N	0.43	2.29	2	1
3:C:45:MET:CE	3:C:45:MET:C	0.43	2.86	3	1
2:B:16:THR:OG1	2:B:30:ILE:CG1	0.43	2.66	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:87:ALA:O	2:B:88:LEU:HB3	0.43	2.10	5	1
3:C:17:MET:HB2	3:C:33:ARG:HD2	0.43	1.90	6	1
3:C:41:THR:OG1	3:C:109:PHE:O	0.43	2.33	9	1
3:C:72:LYS:HG2	3:C:99:ILE:CD1	0.43	2.44	10	1
2:B:45:TYR:CZ	2:B:88:LEU:HD21	0.43	2.48	13	1
3:C:66:PRO:CD	3:C:69:VAL:HG21	0.43	2.34	17	1
3:C:68:HIS:HB3	3:C:99:ILE:HD11	0.43	1.89	17	1
1:A:7:LEU:CB	3:C:95:ILE:HD11	0.43	2.31	18	1
3:C:108:ASN:O	3:C:111:ASP:O	0.43	2.36	20	1
2:B:18:ALA:CB	2:B:27:LEU:HD21	0.43	2.44	1	1
3:C:30:ILE:N	3:C:30:ILE:CD1	0.43	2.78	14	4
2:B:4:PHE:CD1	2:B:68:ARG:HD3	0.43	2.48	2	1
1:A:1:VAL:CB	3:C:83:TYR:HB2	0.43	2.43	9	3
2:B:4:PHE:HB3	2:B:68:ARG:HB2	0.43	1.91	5	1
2:B:79:PHE:N	2:B:86:GLU:HB3	0.43	2.28	10	1
2:B:93:PHE:HB3	3:C:67:SER:OG	0.43	2.13	12	1
2:B:65:GLN:CG	2:B:70:GLN:HB2	0.43	2.43	19	1
3:C:17:MET:HG2	3:C:33:ARG:CD	0.43	2.44	20	1
1:A:3:THR:HB	3:C:112:CYS:HA	0.43	1.91	1	2
2:B:66:THR:C	2:B:71:ALA:O	0.43	2.56	5	1
2:B:65:GLN:CG	2:B:66:THR:N	0.43	2.82	9	1
2:B:5:LEU:HD13	2:B:57:LEU:CD1	0.43	2.43	11	1
3:C:22:ILE:HD11	3:C:28:GLU:OE1	0.43	2.13	12	1
2:B:57:LEU:N	2:B:57:LEU:CD1	0.43	2.82	14	1
3:C:20:LYS:HA	3:C:30:ILE:CA	0.43	2.44	20	1
2:B:87:ALA:O	2:B:89:CYS:N	0.43	2.51	3	2
2:B:35:LEU:O	2:B:36:LYS:HB2	0.43	2.13	14	3
3:C:27:HIS:CB	3:C:67:SER:HB2	0.43	2.44	7	2
2:B:65:GLN:HG2	2:B:66:THR:OG1	0.43	2.13	9	1
3:C:39:SER:HA	3:C:111:ASP:O	0.43	2.13	16	1
2:B:65:GLN:CG	2:B:70:GLN:CB	0.43	2.97	19	1
3:C:76:TYR:O	3:C:80:LYS:HB2	0.43	2.14	1	1
2:B:9:ARG:HD2	2:B:35:LEU:CD1	0.43	2.44	2	1
2:B:21:SER:O	2:B:22:SER:O	0.43	2.37	6	2
2:B:68:ARG:HH21	2:B:71:ALA:HB3	0.43	1.74	8	1
2:B:46:LYS:HG2	2:B:51:LEU:CA	0.43	2.44	11	1
2:B:78:ALA:CA	2:B:87:ALA:O	0.43	2.67	11	1
2:B:5:LEU:HG	2:B:23:THR:HG22	0.43	1.91	12	1
2:B:20:GLU:CD	2:B:21:SER:N	0.43	2.72	12	1
2:B:9:ARG:HG2	2:B:12:THR:OG1	0.43	2.14	15	2
2:B:46:LYS:HB2	2:B:51:LEU:HD12	0.43	1.89	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:48:ASP:N	2:B:48:ASP:OD1	0.43	2.52	17	1
1:A:11:THR:O	1:A:15:HIS:CB	0.43	2.67	1	1
2:B:79:PHE:HB2	2:B:86:GLU:CB	0.43	2.43	2	2
2:B:24:VAL:HA	2:B:27:LEU:HD12	0.43	1.91	6	1
2:B:17:ASP:HB2	3:C:32:LYS:NZ	0.43	2.29	7	1
2:B:51:LEU:CD1	2:B:62:PHE:CE2	0.43	2.90	9	1
2:B:79:PHE:O	2:B:79:PHE:CG	0.43	2.72	10	1
2:B:44:LEU:HD22	2:B:45:TYR:N	0.43	2.27	11	1
3:C:66:PRO:HG3	3:C:102:GLU:OE1	0.43	2.14	11	1
1:A:7:LEU:HD22	1:A:7:LEU:N	0.43	2.26	15	1
2:B:37:ARG:HG3	2:B:42:GLN:CG	0.43	2.44	15	1
2:B:23:THR:OG1	2:B:62:PHE:CD2	0.43	2.70	16	1
2:B:13:THR:O	3:C:29:PHE:CD1	0.43	2.72	18	1
2:B:42:GLN:HA	2:B:79:PHE:CB	0.43	2.43	18	1
2:B:51:LEU:HD13	2:B:62:PHE:CE2	0.43	2.47	18	1
3:C:39:SER:HA	3:C:111:ASP:HB2	0.43	1.91	20	1
1:A:5:GLN:NE2	3:C:112:CYS:HA	0.43	2.29	2	1
2:B:31:VAL:HG13	2:B:37:ARG:CG	0.43	2.44	2	1
2:B:43:ARG:CZ	2:B:80:ARG:HD2	0.43	2.44	2	1
3:C:100:ALA:CA	3:C:103:LEU:HD22	0.43	2.44	4	4
1:A:1:VAL:HG12	3:C:83:TYR:HB3	0.43	1.85	6	1
1:A:3:THR:HG21	3:C:111:ASP:OD2	0.43	2.13	6	1
2:B:91:GLU:OE1	2:B:91:GLU:O	0.43	2.37	7	1
3:C:35:HIS:ND1	3:C:81:VAL:HG21	0.43	2.29	8	1
2:B:57:LEU:CB	2:B:62:PHE:HB2	0.43	2.44	11	3
3:C:103:LEU:HD12	3:C:103:LEU:H	0.43	1.74	11	1
2:B:57:LEU:HB3	2:B:63:THR:OG1	0.43	2.14	12	1
2:B:6:MET:HB3	2:B:73:ALA:O	0.43	2.14	15	3
3:C:97:PRO:O	3:C:98:GLU:HB3	0.43	2.12	18	2
3:C:66:PRO:HG2	3:C:69:VAL:HB	0.42	1.91	1	1
2:B:45:TYR:CZ	2:B:50:LEU:CD1	0.42	2.99	8	2
3:C:70:LEU:HD13	3:C:71:SER:CB	0.42	2.43	2	1
2:B:51:LEU:O	2:B:51:LEU:CG	0.42	2.67	10	1
3:C:60:VAL:C	3:C:61:ASN:OD1	0.42	2.57	10	1
2:B:93:PHE:CD2	2:B:93:PHE:N	0.42	2.87	11	1
3:C:43:LYS:CA	3:C:46:LEU:HD13	0.42	2.38	12	1
3:C:45:MET:O	3:C:46:LEU:C	0.42	2.56	15	2
2:B:44:LEU:C	2:B:45:TYR:CD1	0.42	2.93	13	1
3:C:38:THR:CG2	3:C:77:PHE:O	0.42	2.56	13	1
2:B:9:ARG:HB2	2:B:77:LEU:HD11	0.42	1.90	16	2
2:B:79:PHE:CD1	2:B:79:PHE:N	0.42	2.87	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:39:SER:CB	3:C:42:ILE:HG13	0.42	2.43	16	1
2:B:68:ARG:CG	2:B:69:PRO:HD3	0.42	2.44	2	1
2:B:46:LYS:HD3	2:B:62:PHE:CZ	0.42	2.50	3	1
2:B:23:THR:O	2:B:23:THR:OG1	0.42	2.37	6	1
2:B:8:ARG:CD	2:B:74:THR:HG23	0.42	2.44	7	1
2:B:62:PHE:O	2:B:63:THR:OG1	0.42	2.33	7	1
3:C:25:ASP:OD2	3:C:67:SER:CB	0.42	2.67	11	2
2:B:76:GLY:O	2:B:77:LEU:CD2	0.42	2.67	13	1
1:A:8:CYS:O	1:A:11:THR:OG1	0.42	2.33	16	1
2:B:8:ARG:O	2:B:90:ILE:HD11	0.42	2.15	9	2
2:B:20:GLU:CA	2:B:57:LEU:HD21	0.42	2.43	4	1
3:C:97:PRO:O	3:C:98:GLU:CD	0.42	2.58	4	2
3:C:111:ASP:O	3:C:112:CYS:C	0.42	2.57	4	3
2:B:24:VAL:CB	2:B:55:LYS:O	0.42	2.67	5	1
3:C:110:LEU:HD23	3:C:111:ASP:N	0.42	2.29	5	1
3:C:17:MET:HB2	3:C:33:ARG:CD	0.42	2.45	6	1
3:C:37:LEU:O	3:C:37:LEU:HD22	0.42	2.15	9	2
2:B:15:PHE:HD2	3:C:31:VAL:HG12	0.42	1.74	10	1
3:C:110:LEU:N	3:C:110:LEU:CD1	0.42	2.83	12	1
2:B:64:SER:O	2:B:68:ARG:NE	0.42	2.52	15	1
1:A:4:LEU:O	1:A:8:CYS:HB3	0.42	2.14	19	2
2:B:34:ILE:HD11	3:C:18:TYR:CD2	0.42	2.49	1	1
2:B:53:ASP:OD1	2:B:53:ASP:C	0.42	2.58	7	2
3:C:18:TYR:HA	3:C:33:ARG:N	0.42	2.28	1	1
3:C:75:MET:O	3:C:79:TYR:HB2	0.42	2.14	6	5
3:C:101:LEU:O	3:C:104:LEU:HB2	0.42	2.14	6	2
2:B:69:PRO:HB2	3:C:79:TYR:CD1	0.42	2.50	3	1
3:C:24:SER:O	3:C:25:ASP:CB	0.42	2.66	3	2
3:C:109:PHE:HD2	3:C:110:LEU:HD12	0.42	1.73	3	1
2:B:93:PHE:CE1	3:C:29:PHE:CZ	0.42	3.07	4	1
1:A:5:GLN:HG3	3:C:108:ASN:OD1	0.42	2.14	6	1
3:C:72:LYS:CG	3:C:103:LEU:HD11	0.42	2.38	9	1
2:B:35:LEU:O	2:B:36:LYS:HB3	0.42	2.14	19	3
2:B:68:ARG:CZ	2:B:69:PRO:HD2	0.42	2.44	11	1
1:A:5:GLN:HB2	3:C:107:ALA:O	0.42	2.14	14	1
3:C:109:PHE:O	3:C:111:ASP:N	0.42	2.48	14	1
2:B:2:ASP:N	2:B:2:ASP:OD1	0.42	2.47	15	1
1:A:12:VAL:HA	1:A:15:HIS:CD2	0.42	2.49	16	1
2:B:41:GLU:OE2	2:B:80:ARG:O	0.42	2.37	16	1
3:C:25:ASP:CG	3:C:67:SER:OG	0.42	2.57	19	1
2:B:61:GLY:C	2:B:62:PHE:CG	0.42	2.92	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:110:LEU:O	3:C:111:ASP:HB3	0.42	2.13	2	2
2:B:20:GLU:HA	2:B:57:LEU:HB2	0.42	1.91	3	1
3:C:43:LYS:C	3:C:43:LYS:HD3	0.42	2.35	5	1
2:B:27:LEU:N	2:B:27:LEU:CD2	0.42	2.81	8	1
2:B:44:LEU:HB2	2:B:51:LEU:HD22	0.42	1.92	9	1
1:A:7:LEU:O	3:C:95:ILE:HD12	0.42	2.13	12	1
2:B:45:TYR:N	2:B:45:TYR:CD1	0.42	2.87	14	1
2:B:7:ILE:HA	2:B:75:VAL:HG22	0.42	1.92	15	1
2:B:25:PHE:O	2:B:28:LYS:HB2	0.42	2.14	17	2
3:C:30:ILE:CD1	3:C:30:ILE:N	0.42	2.83	15	1
1:A:1:VAL:CG1	3:C:83:TYR:CG	0.42	3.02	20	1
1:A:7:LEU:HG	3:C:93:PHE:CZ	0.42	2.49	3	1
2:B:5:LEU:CB	2:B:16:THR:CG2	0.42	2.98	7	1
3:C:104:LEU:O	3:C:108:ASN:CG	0.42	2.57	14	1
2:B:9:ARG:HG3	2:B:10:HIS:N	0.42	2.29	15	1
2:B:65:GLN:O	2:B:71:ALA:HB3	0.42	2.15	18	1
2:B:20:GLU:HA	2:B:57:LEU:CD1	0.42	2.41	4	1
2:B:79:PHE:O	2:B:86:GLU:CG	0.42	2.67	5	1
3:C:38:THR:CG2	3:C:77:PHE:HA	0.42	2.44	5	1
3:C:111:ASP:OD1	3:C:111:ASP:C	0.42	2.56	5	1
1:A:5:GLN:HG3	3:C:108:ASN:ND2	0.42	2.30	7	1
2:B:17:ASP:HB2	3:C:32:LYS:CE	0.42	2.44	7	1
3:C:18:TYR:CZ	3:C:32:LYS:HE3	0.42	2.50	8	1
2:B:56:THR:OG1	2:B:59:GLU:HB2	0.42	2.15	16	2
1:A:1:VAL:HG11	3:C:80:LYS:CB	0.42	2.45	12	1
2:B:5:LEU:HB3	2:B:27:LEU:HD11	0.42	1.90	12	1
2:B:76:GLY:CA	2:B:77:LEU:HD23	0.42	2.43	16	1
3:C:42:ILE:HG22	3:C:43:LYS:HD2	0.42	1.92	19	1
3:C:39:SER:CA	3:C:77:PHE:CE1	0.42	3.02	2	1
1:A:7:LEU:HD22	3:C:95:ILE:HD11	0.42	1.91	4	1
2:B:62:PHE:HE2	2:B:73:ALA:HB1	0.42	1.75	4	1
3:C:32:LYS:O	3:C:36:ALA:N	0.42	2.52	5	1
3:C:35:HIS:ND1	3:C:78:THR:HA	0.42	2.30	5	1
3:C:40:GLY:N	3:C:111:ASP:HA	0.42	2.30	6	1
3:C:65:ILE:CD1	3:C:106:ALA:HB2	0.42	2.44	7	1
2:B:45:TYR:HB3	2:B:49:GLN:O	0.42	2.14	14	1
2:B:47:ASP:O	2:B:48:ASP:HB3	0.42	2.14	16	1
1:A:1:VAL:CB	3:C:83:TYR:CG	0.42	3.03	20	1
2:B:34:ILE:HG12	2:B:35:LEU:N	0.42	2.29	20	1
2:B:70:GLN:O	2:B:72:PRO:HD3	0.42	2.15	2	1
2:B:78:ALA:HB2	2:B:87:ALA:CB	0.42	2.37	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:68:HIS:ND1	3:C:99:ILE:HD13	0.42	2.30	3	1
1:A:9:ARG:O	1:A:13:ASN:CG	0.42	2.58	4	1
2:B:8:ARG:C	2:B:77:LEU:HD13	0.42	2.31	6	1
3:C:20:LYS:O	3:C:20:LYS:CG	0.42	2.68	6	1
2:B:1:MET:O	2:B:1:MET:CG	0.42	2.68	8	1
2:B:48:ASP:O	2:B:49:GLN:NE2	0.42	2.52	9	1
2:B:48:ASP:CG	2:B:48:ASP:O	0.42	2.58	10	1
3:C:35:HIS:NE2	3:C:78:THR:CB	0.42	2.83	15	1
3:C:22:ILE:CD1	3:C:28:GLU:HB2	0.42	2.45	18	1
3:C:76:TYR:HA	3:C:79:TYR:HB3	0.42	1.92	19	1
2:B:48:ASP:O	2:B:48:ASP:CG	0.42	2.57	4	2
3:C:19:VAL:C	3:C:30:ILE:HG23	0.42	2.35	1	1
3:C:46:LEU:O	3:C:58:ASN:ND2	0.42	2.52	2	1
3:C:23:SER:HB3	3:C:65:ILE:O	0.42	2.15	3	1
2:B:23:THR:HG21	2:B:57:LEU:CA	0.42	2.45	4	1
2:B:11:LYS:HG2	3:C:28:GLU:HG2	0.42	1.90	5	1
1:A:4:LEU:CD1	3:C:103:LEU:HD23	0.42	2.43	8	2
3:C:28:GLU:C	3:C:29:PHE:CG	0.42	2.93	9	1
2:B:24:VAL:HB	2:B:53:ASP:HA	0.42	1.91	14	1
1:A:3:THR:O	1:A:4:LEU:C	0.42	2.58	17	1
3:C:40:GLY:HA3	3:C:111:ASP:CB	0.41	2.44	2	2
3:C:46:LEU:HD23	3:C:58:ASN:ND2	0.41	2.28	1	1
2:B:9:ARG:HD3	2:B:35:LEU:HD21	0.41	1.92	2	1
3:C:17:MET:HB2	3:C:33:ARG:HB2	0.41	1.92	2	1
3:C:42:ILE:HA	3:C:45:MET:HG2	0.41	1.91	2	1
2:B:48:ASP:O	2:B:48:ASP:OD2	0.41	2.38	4	1
2:B:79:PHE:CE1	2:B:86:GLU:OE1	0.41	2.73	7	1
1:A:2:ALA:HB1	1:A:6:HIS:HB3	0.41	1.92	11	1
1:A:8:CYS:SG	3:C:103:LEU:C	0.41	2.98	11	2
2:B:8:ARG:CD	2:B:90:ILE:CG2	0.41	2.98	14	1
3:C:41:THR:HG1	3:C:111:ASP:N	0.41	2.13	14	1
1:A:7:LEU:HG	3:C:93:PHE:CD2	0.41	2.50	15	1
3:C:39:SER:OG	3:C:42:ILE:HG13	0.41	2.15	16	1
3:C:65:ILE:HG12	3:C:69:VAL:CG1	0.41	2.44	19	1
2:B:14:ILE:HD11	3:C:18:TYR:CE2	0.41	2.50	20	1
2:B:14:ILE:CG1	3:C:30:ILE:CG1	0.41	2.98	20	1
3:C:22:ILE:HG12	3:C:28:GLU:OE1	0.41	2.15	2	5
2:B:3:VAL:CG2	2:B:63:THR:C	0.41	2.81	5	1
2:B:11:LYS:O	3:C:28:GLU:CB	0.41	2.68	6	1
2:B:13:THR:C	3:C:30:ILE:HD12	0.41	2.34	9	1
2:B:14:ILE:HG22	2:B:14:ILE:O	0.41	2.14	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:88:LEU:HD22	2:B:88:LEU:N	0.41	2.29	1	1
1:A:4:LEU:O	3:C:107:ALA:CB	0.41	2.67	3	1
2:B:9:ARG:N	2:B:90:ILE:HG23	0.41	2.30	4	2
2:B:24:VAL:HG23	2:B:57:LEU:HD23	0.41	1.92	5	1
2:B:9:ARG:HG3	2:B:77:LEU:HD22	0.41	1.90	6	1
1:A:3:THR:CG2	1:A:5:GLN:HB3	0.41	2.44	7	1
2:B:13:THR:HB	3:C:29:PHE:CE2	0.41	2.50	10	1
2:B:62:PHE:CZ	2:B:73:ALA:CB	0.41	2.81	12	1
2:B:40:ASP:C	2:B:40:ASP:OD1	0.41	2.58	14	1
2:B:7:ILE:HB	2:B:14:ILE:CG2	0.41	2.43	18	2
2:B:23:THR:HB	2:B:57:LEU:HD12	0.41	1.83	16	1
2:B:46:LYS:NZ	2:B:61:GLY:O	0.41	2.51	16	1
2:B:37:ARG:HD2	2:B:79:PHE:CZ	0.41	2.50	17	1
3:C:95:ILE:CG1	3:C:100:ALA:HB2	0.41	2.45	19	1
2:B:37:ARG:C	2:B:42:GLN:OE1	0.41	2.58	20	1
2:B:6:MET:HG3	2:B:15:PHE:CE1	0.41	2.50	2	1
2:B:55:LYS:CG	2:B:59:GLU:HB3	0.41	2.45	4	1
3:C:18:TYR:CG	3:C:32:LYS:HE2	0.41	2.50	4	1
2:B:44:LEU:HD22	2:B:75:VAL:HG21	0.41	1.92	7	1
2:B:42:GLN:NE2	2:B:44:LEU:HG	0.41	2.30	10	1
2:B:62:PHE:HA	2:B:66:THR:OG1	0.41	2.15	10	1
2:B:46:LYS:O	2:B:49:GLN:HB2	0.41	2.14	14	3
3:C:73:VAL:CG2	3:C:110:LEU:HD12	0.41	2.33	13	1
2:B:37:ARG:CG	2:B:42:GLN:CB	0.41	2.98	15	1
2:B:65:GLN:HG2	2:B:70:GLN:HB3	0.41	1.93	19	1
2:B:65:GLN:HG3	2:B:70:GLN:HB2	0.41	1.93	19	1
2:B:78:ALA:CB	2:B:86:GLU:HG2	0.41	2.36	19	1
1:A:8:CYS:HB3	3:C:103:LEU:HB3	0.41	1.90	2	1
3:C:24:SER:O	3:C:25:ASP:HB3	0.41	2.15	3	1
3:C:35:HIS:NE2	3:C:78:THR:OG1	0.41	2.43	16	2
3:C:58:ASN:OD1	3:C:58:ASN:N	0.41	2.52	4	2
2:B:57:LEU:HA	2:B:62:PHE:HB2	0.41	1.93	6	1
3:C:21:LEU:N	3:C:21:LEU:HD23	0.41	2.30	7	1
2:B:3:VAL:CG1	2:B:57:LEU:HD13	0.41	2.43	8	1
1:A:10:LYS:O	1:A:14:GLY:N	0.41	2.50	9	1
2:B:68:ARG:HD2	3:C:78:THR:CB	0.41	2.45	9	1
2:B:24:VAL:HG13	2:B:51:LEU:CG	0.41	2.43	12	1
2:B:46:LYS:CE	2:B:49:GLN:OE1	0.41	2.69	12	1
2:B:24:VAL:HG23	2:B:55:LYS:O	0.41	2.14	15	2
3:C:61:ASN:O	3:C:61:ASN:CG	0.41	2.59	16	1
3:C:72:LYS:HD3	3:C:99:ILE:CG2	0.41	2.45	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:43:ARG:NH1	2:B:86:GLU:OE1	0.41	2.53	20	1
2:B:46:LYS:CE	2:B:60:CYS:SG	0.41	3.08	20	1
3:C:19:VAL:CG2	3:C:58:ASN:O	0.41	2.68	1	1
2:B:68:ARG:NH1	2:B:69:PRO:HD3	0.41	2.31	2	1
2:B:37:ARG:NE	2:B:42:GLN:HB2	0.41	2.30	4	1
2:B:20:GLU:HA	2:B:57:LEU:CB	0.41	2.45	6	1
2:B:4:PHE:HB3	2:B:68:ARG:CG	0.41	2.45	9	1
1:A:7:LEU:HD13	3:C:76:TYR:CE2	0.41	2.48	10	1
2:B:9:ARG:HG2	2:B:12:THR:HB	0.41	1.93	11	1
2:B:51:LEU:HD23	2:B:52:ASP:H	0.41	1.75	11	1
2:B:34:ILE:HG13	2:B:35:LEU:CG	0.41	2.46	13	1
3:C:22:ILE:HD12	3:C:22:ILE:N	0.41	2.30	15	1
3:C:17:MET:SD	3:C:33:ARG:HD3	0.41	2.55	16	1
1:A:4:LEU:HD22	3:C:73:VAL:CB	0.41	2.42	19	1
2:B:46:LYS:CE	2:B:62:PHE:CZ	0.41	3.03	3	1
2:B:57:LEU:HB3	2:B:62:PHE:O	0.41	2.16	3	1
3:C:17:MET:HB3	3:C:33:ARG:HB2	0.41	1.91	5	1
2:B:65:GLN:O	2:B:68:ARG:HD3	0.41	2.15	6	1
1:A:5:GLN:OE1	3:C:111:ASP:HA	0.41	2.16	9	1
2:B:43:ARG:NH1	2:B:80:ARG:NH2	0.41	2.69	9	1
3:C:46:LEU:HD23	3:C:58:ASN:HB3	0.41	1.92	9	1
3:C:40:GLY:HA3	3:C:111:ASP:OD2	0.41	2.16	11	1
2:B:79:PHE:O	2:B:86:GLU:HG2	0.41	2.16	12	1
1:A:3:THR:HG23	1:A:5:GLN:H	0.41	1.75	13	1
2:B:4:PHE:CE1	2:B:15:PHE:CD1	0.41	3.08	14	1
2:B:3:VAL:CG1	2:B:20:GLU:N	0.41	2.84	17	1
2:B:11:LYS:HA	3:C:27:HIS:HB2	0.41	1.92	17	1
1:A:4:LEU:O	1:A:8:CYS:CB	0.41	2.68	19	1
3:C:60:VAL:O	3:C:61:ASN:OD1	0.41	2.38	19	1
3:C:97:PRO:O	3:C:98:GLU:HG2	0.41	2.16	1	1
3:C:38:THR:HG21	3:C:81:VAL:HG23	0.41	1.93	2	1
3:C:60:VAL:HG11	3:C:62:PHE:CE2	0.41	2.51	2	1
3:C:66:PRO:CG	3:C:68:HIS:NE2	0.41	2.84	3	1
2:B:24:VAL:HG11	2:B:51:LEU:HD21	0.41	1.93	9	1
3:C:33:ARG:HG3	3:C:46:LEU:HD21	0.41	1.93	12	1
2:B:31:VAL:HG12	2:B:37:ARG:HG3	0.41	1.92	17	1
2:B:10:HIS:CD2	2:B:91:GLU:HB2	0.41	2.50	1	1
1:A:4:LEU:HD22	3:C:103:LEU:CG	0.41	2.45	2	1
2:B:45:TYR:CE1	2:B:88:LEU:HD21	0.41	2.51	2	1
2:B:62:PHE:O	2:B:62:PHE:CD2	0.41	2.74	2	1
3:C:37:LEU:O	3:C:37:LEU:HG	0.41	2.16	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:66:PRO:HG3	3:C:102:GLU:CD	0.41	2.37	2	1
2:B:78:ALA:CB	2:B:87:ALA:HB3	0.41	2.41	3	1
2:B:23:THR:CB	2:B:57:LEU:HB3	0.41	2.46	4	1
2:B:37:ARG:CD	2:B:79:PHE:CE2	0.41	3.04	4	1
3:C:75:MET:CB	3:C:93:PHE:CZ	0.41	3.03	4	1
2:B:30:ILE:HD13	2:B:30:ILE:HA	0.41	1.71	6	2
2:B:76:GLY:C	2:B:77:LEU:CD2	0.41	2.80	9	1
3:C:39:SER:OG	3:C:42:ILE:CD1	0.41	2.68	10	1
3:C:79:TYR:CE1	3:C:83:TYR:CD1	0.41	3.09	11	1
3:C:33:ARG:HD3	3:C:46:LEU:CD2	0.41	2.46	13	1
3:C:68:HIS:CE1	3:C:99:ILE:HB	0.41	2.51	13	1
2:B:24:VAL:HA	2:B:27:LEU:CG	0.41	2.46	14	1
2:B:93:PHE:CB	3:C:67:SER:HB2	0.41	2.46	14	1
2:B:13:THR:CB	3:C:29:PHE:CZ	0.41	3.04	15	1
2:B:42:GLN:CD	2:B:42:GLN:C	0.41	2.80	15	2
2:B:57:LEU:HG	2:B:62:PHE:HB3	0.41	1.91	16	1
2:B:88:LEU:HD13	2:B:88:LEU:HA	0.41	1.66	16	1
1:A:2:ALA:HB3	3:C:76:TYR:OH	0.41	2.15	17	1
2:B:42:GLN:CD	2:B:77:LEU:HD21	0.41	2.37	18	1
3:C:80:LYS:O	3:C:80:LYS:HD3	0.41	2.16	20	1
2:B:78:ALA:HA	2:B:86:GLU:CB	0.41	2.46	1	1
3:C:42:ILE:O	3:C:46:LEU:HG	0.41	2.15	2	1
3:C:72:LYS:HE3	3:C:99:ILE:CD1	0.41	2.46	4	1
2:B:38:PRO:O	2:B:79:PHE:CE1	0.41	2.74	5	1
3:C:23:SER:OG	3:C:66:PRO:C	0.41	2.59	7	1
2:B:23:THR:CG2	2:B:26:GLU:HG3	0.41	2.46	8	1
1:A:4:LEU:CD2	1:A:4:LEU:C	0.41	2.89	11	1
2:B:13:THR:HG22	3:C:29:PHE:CZ	0.41	2.50	13	1
2:B:43:ARG:HG2	2:B:50:LEU:CD1	0.41	2.46	15	1
2:B:2:ASP:OD1	2:B:3:VAL:N	0.41	2.54	17	1
2:B:19:LYS:HB2	2:B:22:SER:OG	0.40	2.16	1	1
2:B:4:PHE:H	2:B:67:ALA:HB1	0.40	1.77	4	1
2:B:43:ARG:O	2:B:78:ALA:N	0.40	2.47	5	1
2:B:25:PHE:O	2:B:28:LYS:HB3	0.40	2.16	9	2
2:B:24:VAL:CG2	2:B:56:THR:HA	0.40	2.46	11	1
1:A:8:CYS:HB2	3:C:104:LEU:CA	0.40	2.46	15	2
2:B:47:ASP:OD2	2:B:62:PHE:CD1	0.40	2.74	12	1
2:B:93:PHE:HB2	3:C:67:SER:HB2	0.40	1.92	14	1
3:C:25:ASP:OD2	3:C:27:HIS:CE1	0.40	2.74	15	1
2:B:20:GLU:CD	2:B:63:THR:HB	0.40	2.37	18	1
2:B:35:LEU:HD13	2:B:77:LEU:CD2	0.40	2.46	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:17:ASP:HB3	3:C:32:LYS:NZ	0.40	2.31	2	1
1:A:4:LEU:C	3:C:107:ALA:CB	0.40	2.85	3	1
3:C:64:GLU:OE2	3:C:109:PHE:CE2	0.40	2.75	3	1
3:C:32:LYS:O	3:C:35:HIS:HB3	0.40	2.16	4	1
2:B:27:LEU:O	2:B:30:ILE:HB	0.40	2.16	5	1
2:B:34:ILE:HG12	2:B:35:LEU:H	0.40	1.76	7	1
2:B:14:ILE:CG1	2:B:34:ILE:CD1	0.40	2.99	8	1
3:C:104:LEU:HD13	3:C:104:LEU:O	0.40	2.16	8	1
3:C:28:GLU:HG2	3:C:29:PHE:N	0.40	2.31	9	1
2:B:31:VAL:O	2:B:35:LEU:N	0.40	2.54	13	1
1:A:13:ASN:OD1	1:A:13:ASN:C	0.40	2.59	16	1
3:C:93:PHE:CZ	3:C:94:PRO:O	0.40	2.73	18	1
2:B:92:PRO:HB2	2:B:93:PHE:CD1	0.40	2.51	19	1
2:B:44:LEU:CD2	2:B:75:VAL:HG21	0.40	2.45	1	1
3:C:17:MET:O	3:C:33:ARG:N	0.40	2.45	1	1
3:C:66:PRO:HG2	3:C:68:HIS:NE2	0.40	2.32	1	1
1:A:7:LEU:HD12	3:C:93:PHE:CB	0.40	2.46	2	1
2:B:41:GLU:O	2:B:79:PHE:CB	0.40	2.69	2	1
3:C:42:ILE:CG2	3:C:46:LEU:CD2	0.40	2.94	2	1
2:B:46:LYS:O	2:B:49:GLN:HG2	0.40	2.16	3	1
3:C:23:SER:C	3:C:25:ASP:H	0.40	2.19	3	1
3:C:111:ASP:O	3:C:111:ASP:OD2	0.40	2.39	3	1
2:B:41:GLU:C	2:B:42:GLN:CD	0.40	2.80	4	1
2:B:69:PRO:HA	3:C:79:TYR:CD1	0.40	2.52	5	1
2:B:9:ARG:HD2	2:B:35:LEU:CD2	0.40	2.38	7	1
2:B:17:ASP:HB2	3:C:32:LYS:HE2	0.40	1.93	7	1
3:C:64:GLU:O	3:C:65:ILE:HG13	0.40	2.17	8	1
2:B:29:ARG:NH1	2:B:29:ARG:HG3	0.40	2.32	9	1
2:B:57:LEU:CA	2:B:62:PHE:HB2	0.40	2.46	15	1
3:C:61:ASN:O	3:C:61:ASN:OD1	0.40	2.40	15	1
3:C:109:PHE:CD2	3:C:110:LEU:HD12	0.40	2.52	15	1
2:B:20:GLU:O	2:B:57:LEU:HB2	0.40	2.16	16	1
2:B:62:PHE:CD1	2:B:73:ALA:CB	0.40	3.04	20	1
2:B:44:LEU:CD1	2:B:51:LEU:HD22	0.40	2.46	3	1
3:C:17:MET:C	3:C:18:TYR:CD1	0.40	2.95	3	1
3:C:38:THR:O	3:C:112:CYS:O	0.40	2.40	4	1
2:B:32:GLU:CA	2:B:36:LYS:HA	0.40	2.46	20	2
2:B:37:ARG:NH2	2:B:86:GLU:OE2	0.40	2.55	9	1
2:B:7:ILE:HG21	2:B:77:LEU:HD12	0.40	1.92	18	1
1:A:5:GLN:O	1:A:9:ARG:HG3	0.40	2.17	19	1
2:B:6:MET:HB2	2:B:73:ALA:O	0.40	2.17	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:101:LEU:HD23	3:C:101:LEU:C	0.40	2.36	1	1
3:C:97:PRO:O	3:C:98:GLU:HG3	0.40	2.16	3	1
3:C:21:LEU:HD21	3:C:31:VAL:CG2	0.40	2.46	7	1
3:C:35:HIS:CD2	3:C:77:PHE:CD2	0.40	3.09	10	1
2:B:32:GLU:HB2	2:B:37:ARG:NH1	0.40	2.31	15	1
3:C:104:LEU:CD1	3:C:105:MET:N	0.40	2.84	17	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	13/40 (32%)	12±1 (90±5%)	1±1 (9±6%)	0±0 (2±3%)	14	59
2	B	87/118 (74%)	70±2 (81±2%)	10±2 (12±3%)	6±3 (7±3%)	2	15
3	C	74/96 (77%)	64±2 (87±3%)	6±1 (8±2%)	4±1 (5±1%)	3	23
All	All	3480/5080 (69%)	2925 (84%)	343 (10%)	212 (6%)	3	20

All 32 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	11	LYS	20
3	C	98	GLU	20
3	C	100	ALA	20
2	B	23	THR	14
2	B	68	ARG	14
2	B	22	SER	13
3	C	40	GLY	12
3	C	111	ASP	10
3	C	58	ASN	9
2	B	93	PHE	8
2	B	47	ASP	8
2	B	87	ALA	6
2	B	63	THR	6

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Mol	Chain	Res	Type	Models (Total)
2	B	86	GLU	6
2	B	24	VAL	6
2	B	70	GLN	5
2	B	67	ALA	4
2	B	69	PRO	4
2	B	92	PRO	4
1	A	3	THR	3
2	B	40	ASP	3
2	B	65	GLN	3
2	B	64	SER	2
3	C	24	SER	2
3	C	110	LEU	2
3	C	104	LEU	2
2	B	61	GLY	1
2	B	48	ASP	1
1	A	4	LEU	1
3	C	26	GLY	1
3	C	27	HIS	1
3	C	68	HIS	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	13/36 (36%)	9±1 (68±11%)	4±1 (32±11%)	1 14
2	B	77/103 (75%)	50±4 (65±5%)	27±4 (35±5%)	1 9
3	C	68/85 (80%)	43±3 (64±5%)	25±3 (36±5%)	1 8
All	All	3160/4480 (71%)	2043 (65%)	1117 (35%)	1 9

All 137 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)
2	B	7	ILE	20
2	B	12	THR	20
2	B	14	ILE	20
2	B	88	LEU	20

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Mol	Chain	Res	Type	Models (Total)
3	C	73	VAL	20
3	C	76	TYR	20
3	C	21	LEU	18
2	B	68	ARG	17
2	B	23	THR	16
3	C	24	SER	16
3	C	72	LYS	16
3	C	70	LEU	16
2	B	56	THR	15
3	C	20	LYS	15
2	B	19	LYS	15
2	B	8	ARG	14
2	B	9	ARG	14
2	B	59	GLU	14
3	C	93	PHE	14
2	B	15	PHE	14
2	B	35	LEU	14
3	C	38	THR	14
2	B	64	SER	13
3	C	39	SER	13
3	C	42	ILE	13
2	B	36	LYS	12
3	C	29	PHE	12
3	C	74	CYS	12
1	A	9	ARG	11
2	B	34	ILE	11
2	B	66	THR	11
3	C	18	TYR	11
3	C	32	LYS	11
3	C	82	ARG	11
3	C	98	GLU	11
3	C	103	LEU	11
2	B	29	ARG	11
2	B	37	ARG	11
3	C	34	GLU	11
3	C	65	ILE	11
1	A	7	LEU	11
3	C	77	PHE	11
2	B	49	GLN	10
3	C	45	MET	10
2	B	42	GLN	10
2	B	27	LEU	10

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Mol	Chain	Res	Type	Models (Total)
3	C	17	MET	10
3	C	99	ILE	10
1	A	10	LYS	10
2	B	1	MET	9
2	B	46	LYS	9
3	C	23	SER	9
3	C	35	HIS	9
3	C	41	THR	9
3	C	63	ARG	9
1	A	4	LEU	9
3	C	43	LYS	9
3	C	79	TYR	9
3	C	78	THR	9
1	A	5	GLN	8
1	A	6	HIS	8
2	B	55	LYS	8
2	B	70	GLN	8
3	C	37	LEU	8
2	B	25	PHE	8
2	B	43	ARG	8
3	C	25	ASP	8
3	C	67	SER	8
3	C	71	SER	8
3	C	80	LYS	8
2	B	65	GLN	7
2	B	80	ARG	7
2	B	86	GLU	7
1	A	3	THR	7
1	A	13	ASN	7
2	B	13	THR	7
2	B	62	PHE	7
2	B	32	GLU	7
2	B	75	VAL	7
2	B	4	PHE	6
2	B	11	LYS	6
2	B	91	GLU	6
2	B	40	ASP	6
2	B	52	ASP	6
1	A	15	HIS	6
2	B	6	MET	6
2	B	28	LYS	6
2	B	50	LEU	6

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Mol	Chain	Res	Type	Models (Total)
2	B	2	ASP	6
3	C	101	LEU	6
2	B	51	LEU	6
3	C	33	ARG	6
3	C	111	ASP	6
3	C	46	LEU	5
3	C	59	GLU	5
2	B	41	GLU	5
2	B	21	SER	5
1	A	11	THR	5
2	B	24	VAL	5
2	B	57	LEU	5
3	C	75	MET	5
2	B	20	GLU	5
3	C	22	ILE	4
3	C	104	LEU	4
3	C	105	MET	4
2	B	26	GLU	4
2	B	47	ASP	4
3	C	112	CYS	4
3	C	64	GLU	4
2	B	16	THR	4
2	B	63	THR	3
2	B	74	THR	3
2	B	77	LEU	3
2	B	22	SER	3
2	B	48	ASP	3
3	C	68	HIS	3
2	B	44	LEU	2
2	B	3	VAL	2
2	B	60	CYS	2
2	B	93	PHE	2
2	B	79	PHE	2
3	C	109	PHE	2
2	B	5	LEU	2
2	B	30	ILE	2
2	B	53	ASP	2
3	C	102	GLU	2
3	C	19	VAL	2
3	C	30	ILE	2
3	C	58	ASN	2
3	C	95	ILE	2

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Mol	Chain	Res	Type	Models (Total)
2	B	45	TYR	2
3	C	27	HIS	1
3	C	108	ASN	1
3	C	110	LEU	1
3	C	28	GLU	1
3	C	69	VAL	1
3	C	83	TYR	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided