Full wwPDB NMR Structure Validation Report (i)

Feb 19, 2022 – 11:15 PM EST

PDB ID	:	1TBA
Title	:	SOLUTION STRUCTURE OF A TBP-TAFII230 COMPLEX: PROTEIN MIMICRY OF THE MINOR GROOVE SURFACE OF THE TATA BOX UNWOUND BY TBP, NMR, 25 STRUCTURES
Authors	:	Liu, D.; Ishima, R.; Tong, K.I.; Bagby, S.; Kokubo, T.; Muhandiram, D.R.; Kay, L.E.; Nakatani, Y.; Ikura, M.
Deposited on	:	1998-08-16

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

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

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

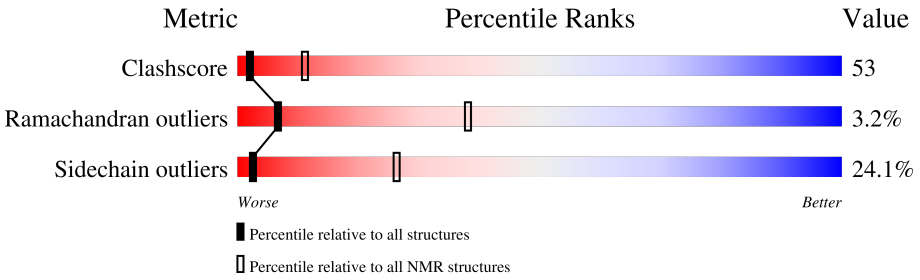
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	67	10% 37% 13% . 36%
2	B	180	37% 55% 7% .

2 Ensemble composition and analysis

This entry contains 25 models. Model 3 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:18-A:35, A:50-A:74, B:63-B:240 (221)	0.45	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3881 atoms, of which 1974 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	67	969	299	478	82	109	1	0

- Molecule 2 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	180	2912	921	1496	242	247	6	0

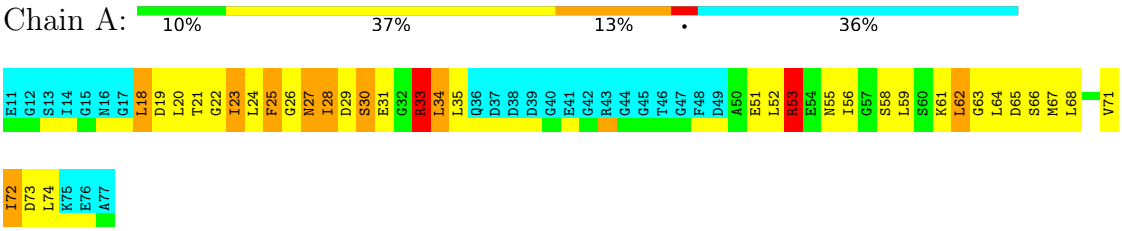
4 Residue-property plots

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.

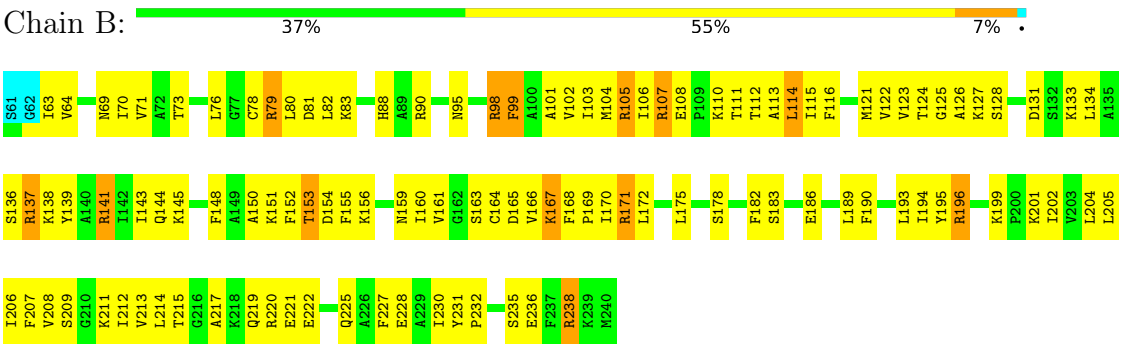
• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

Chain A:



• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

Chain B:



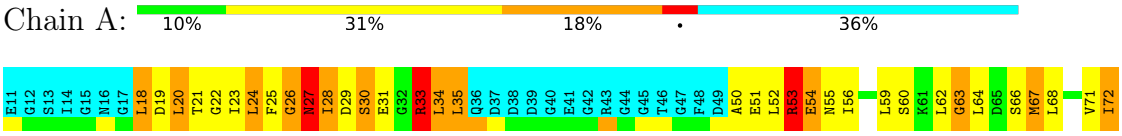
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

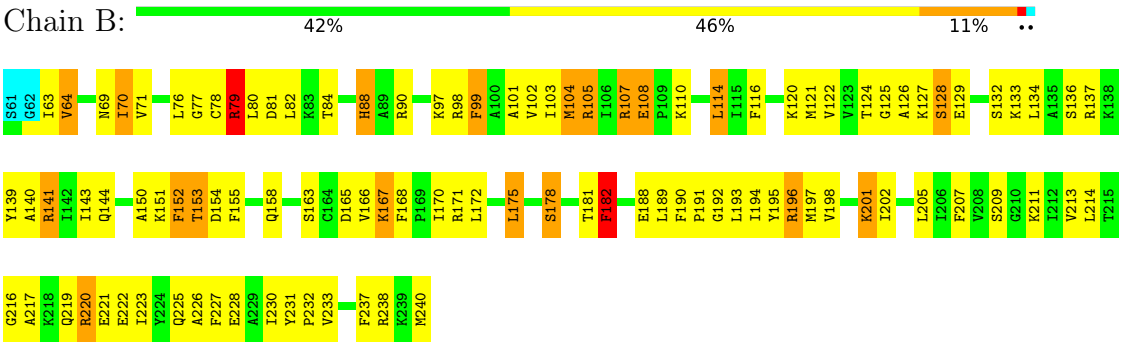
4.2.1 Score per residue for model 1

• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

Chain A:

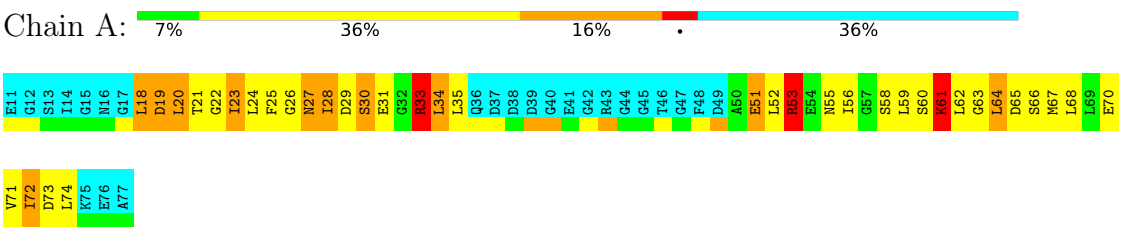


• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

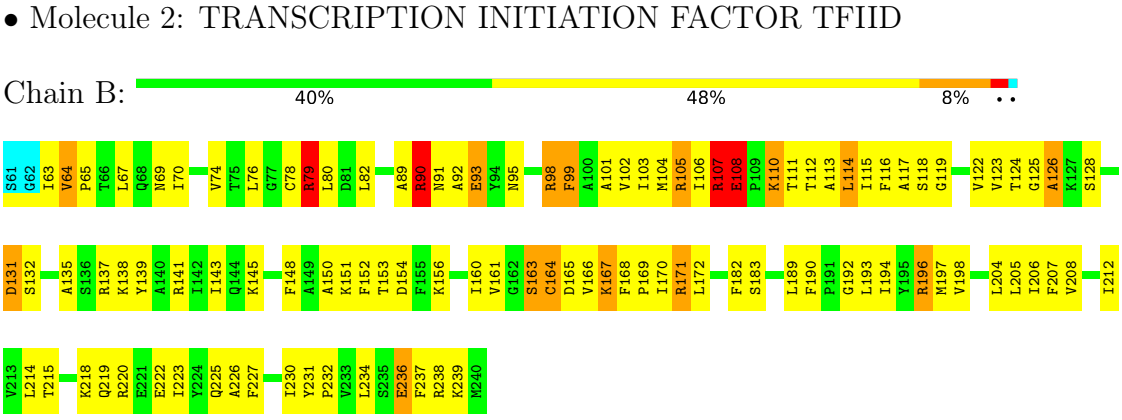


4.2.2 Score per residue for model 2

• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

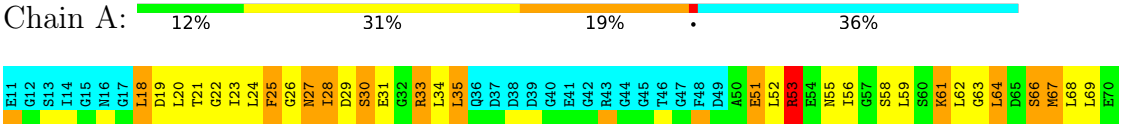


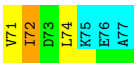
• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID



4.2.3 Score per residue for model 3 (medoid)

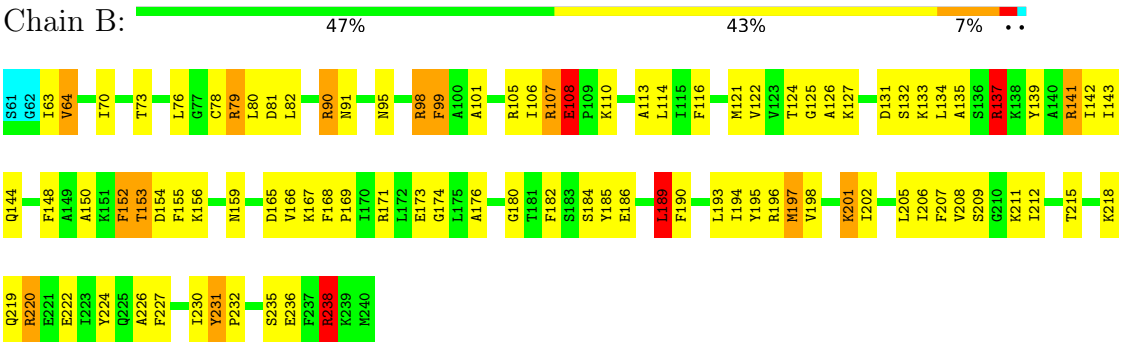
• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN





• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

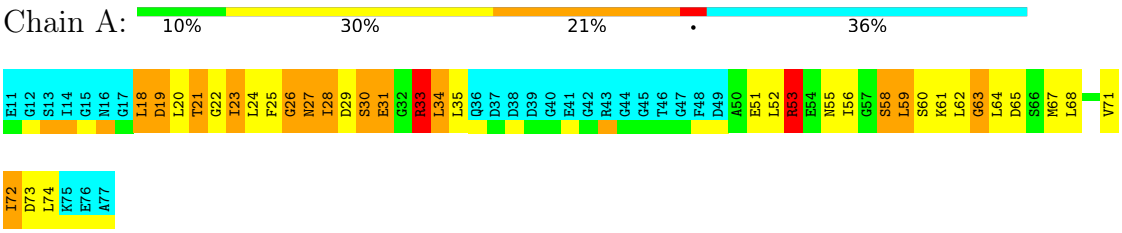
Chain B:



4.2.4 Score per residue for model 4

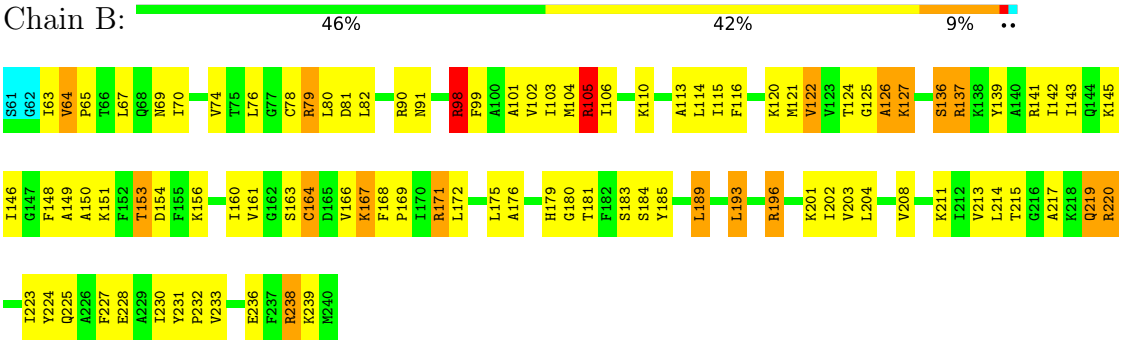
• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

Chain A:



• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

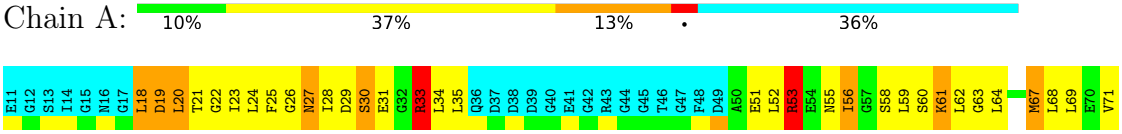
Chain B:



4.2.5 Score per residue for model 5

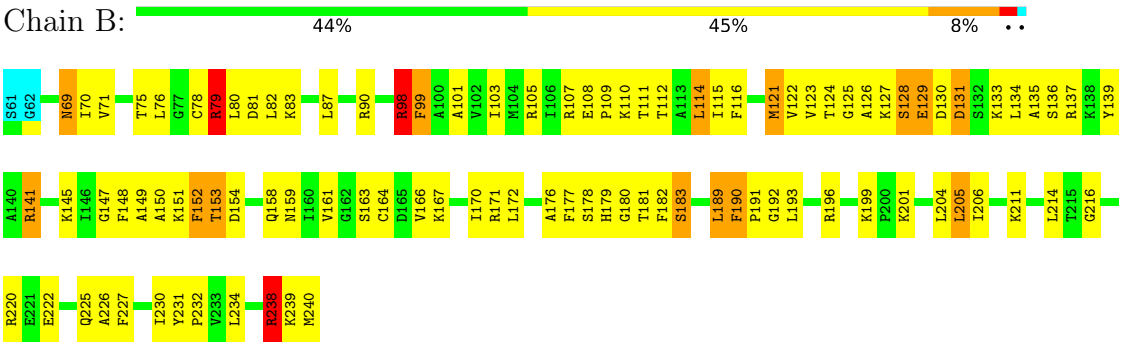
• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

Chain A:



• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

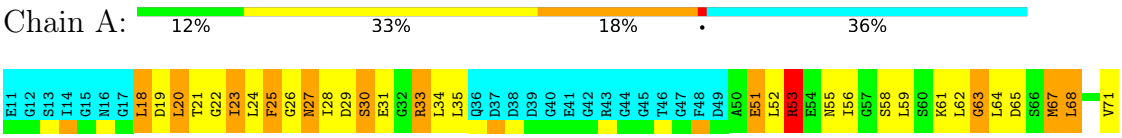
Chain B:



4.2.6 Score per residue for model 6

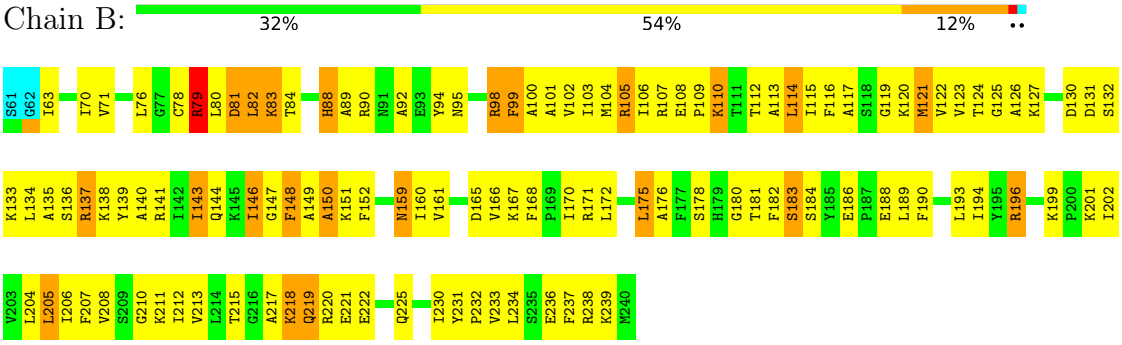
• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

Chain A:



• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

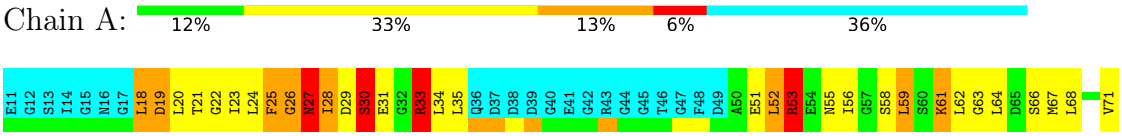
Chain B:

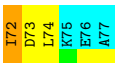


4.2.7 Score per residue for model 7

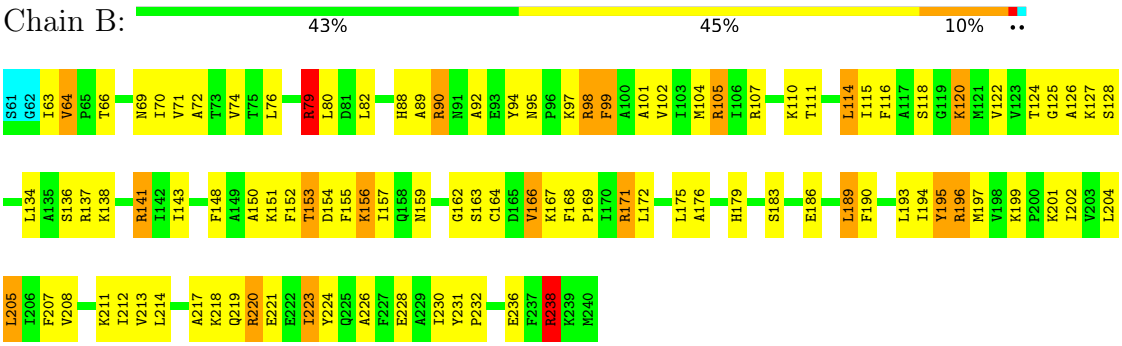
• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

Chain A:



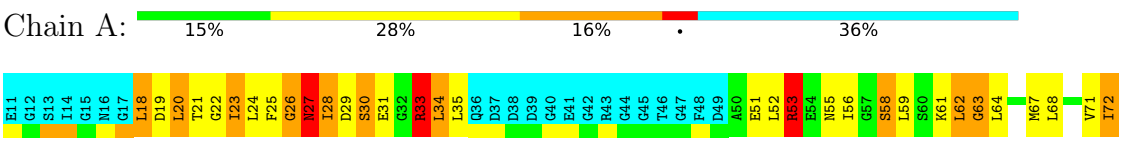


• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

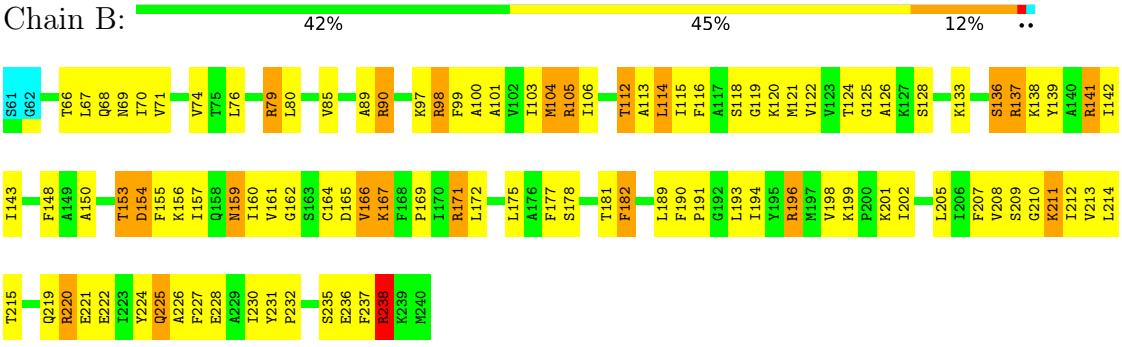


4.2.8 Score per residue for model 8

• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

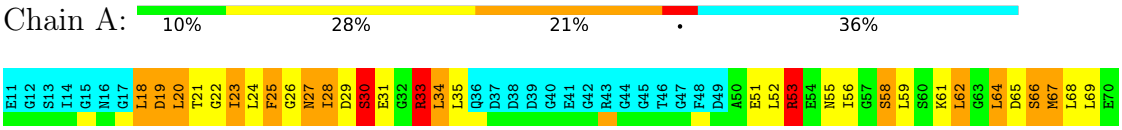


• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID



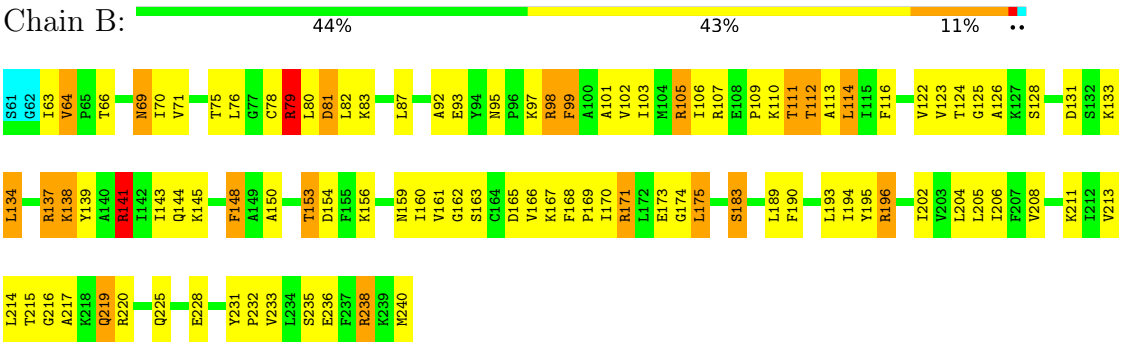
4.2.9 Score per residue for model 9

• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN



• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

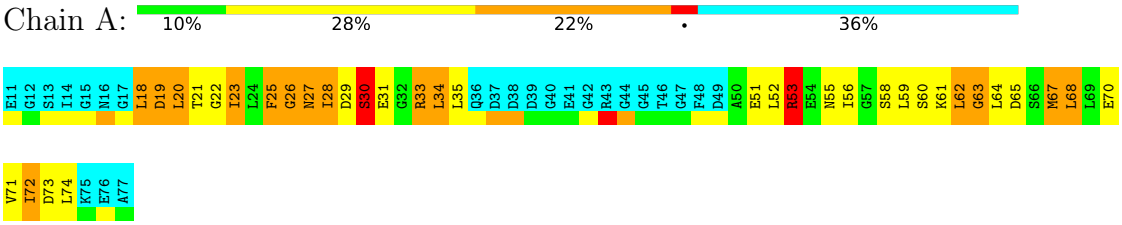
Chain B:



4.2.10 Score per residue for model 10

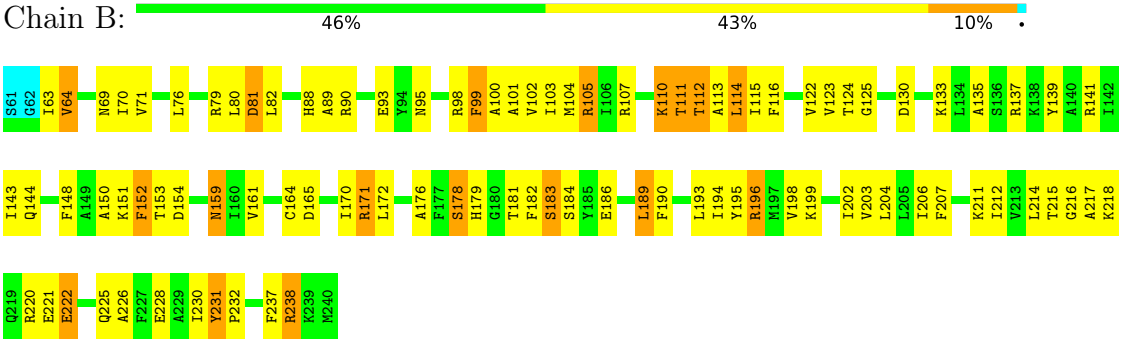
• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

Chain A:



• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

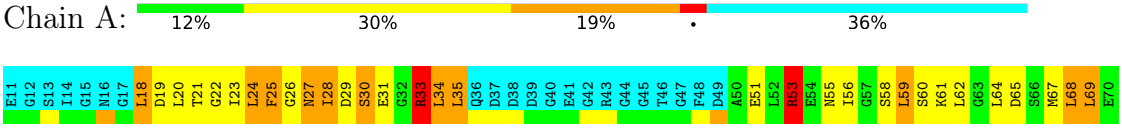
Chain B:

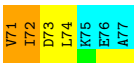


4.2.11 Score per residue for model 11

• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

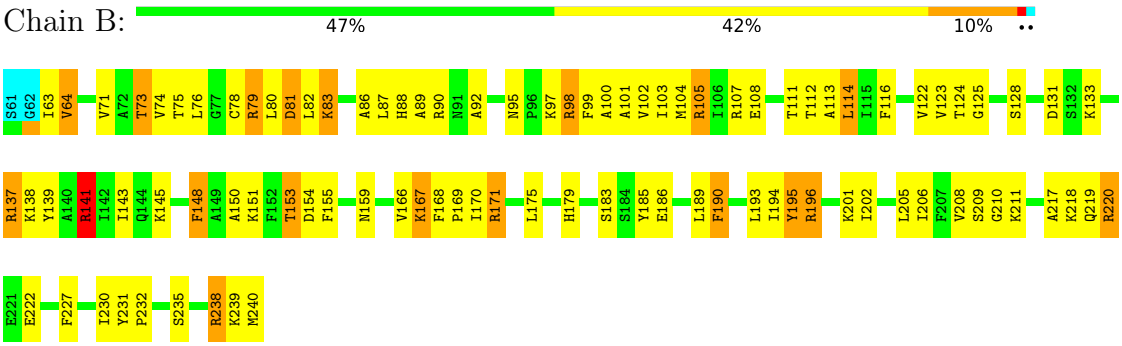
Chain A:





• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

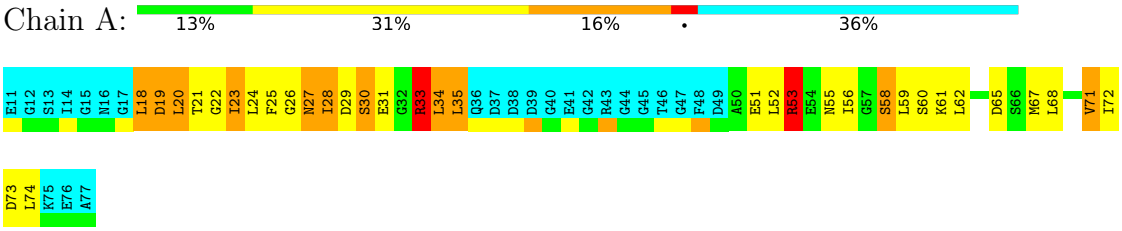
Chain B:



4.2.12 Score per residue for model 12

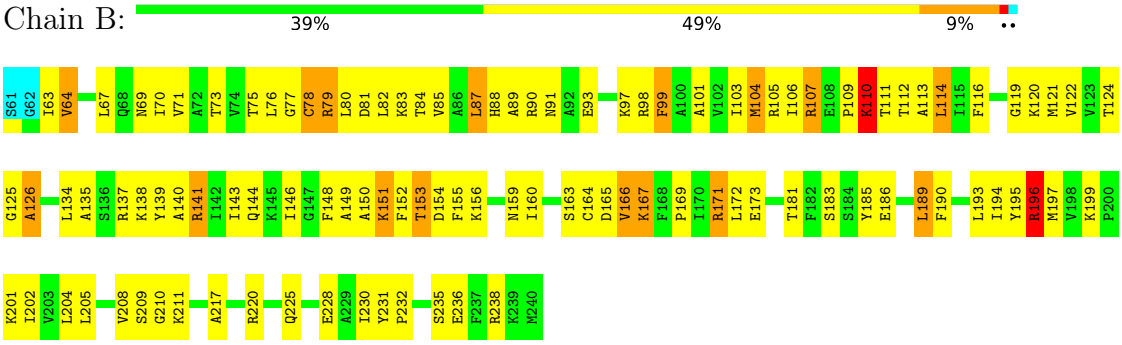
• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

Chain A:



• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

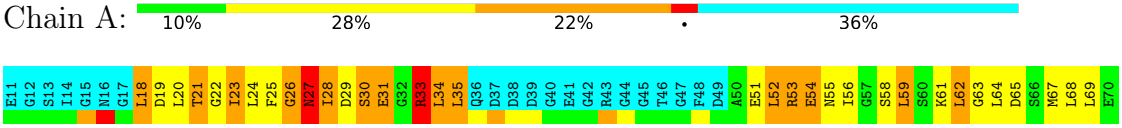
Chain B:

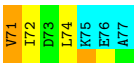


4.2.13 Score per residue for model 13

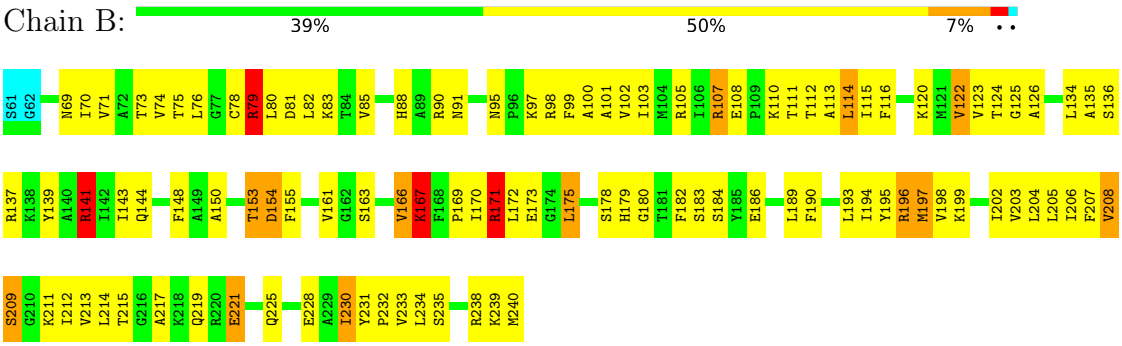
• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

Chain A:



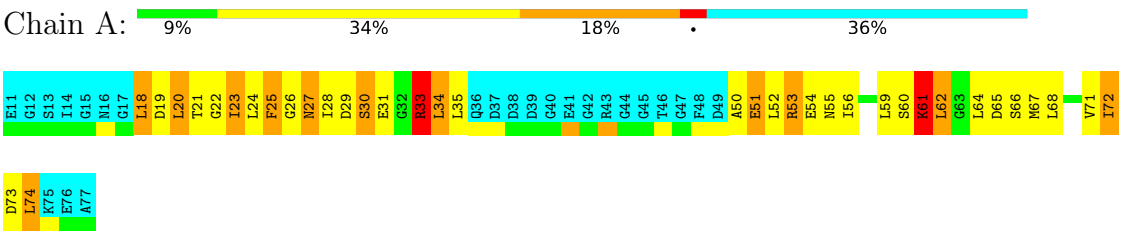


• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

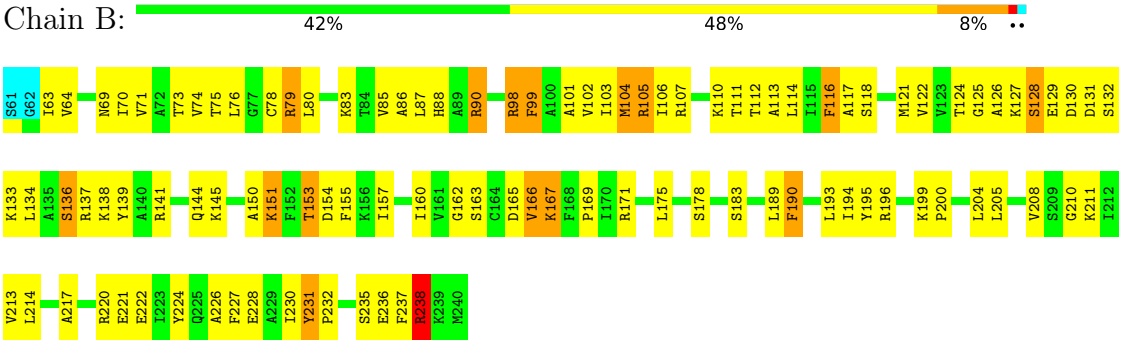


4.2.14 Score per residue for model 14

• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

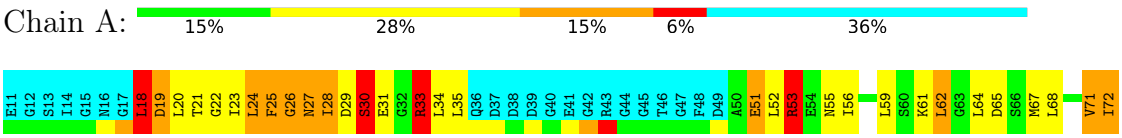


• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

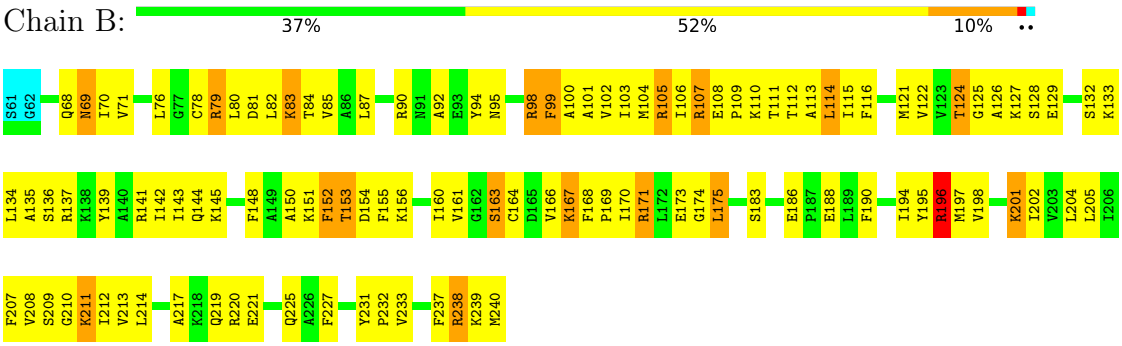


4.2.15 Score per residue for model 15

• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

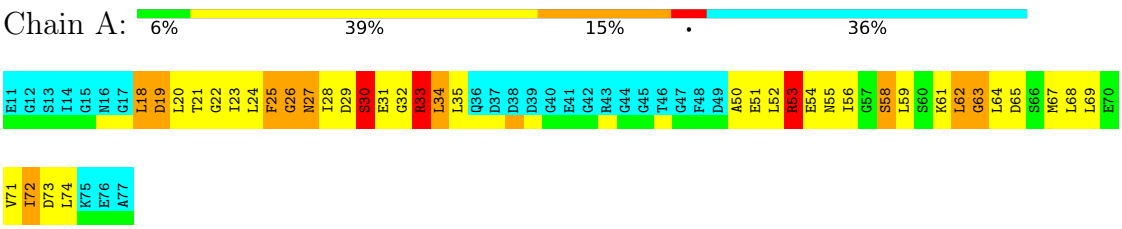


• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

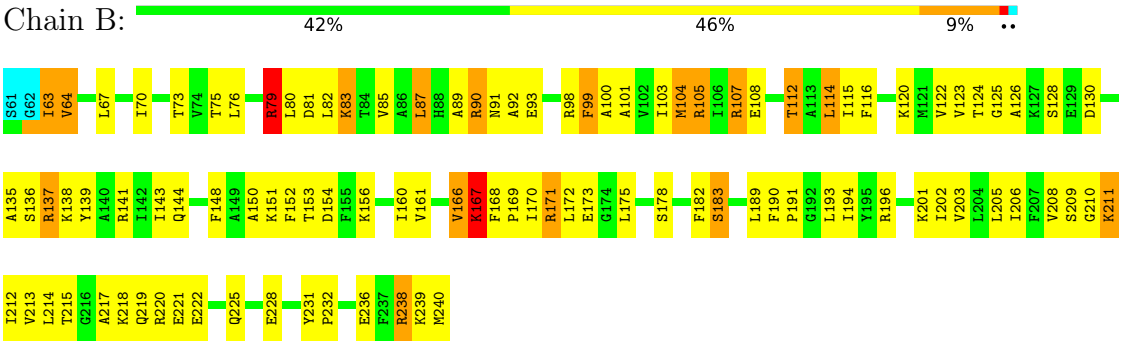


4.2.16 Score per residue for model 16

• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

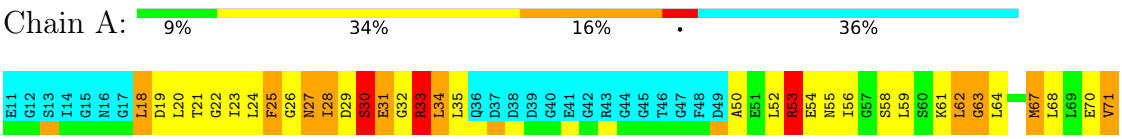


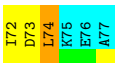
• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID



4.2.17 Score per residue for model 17

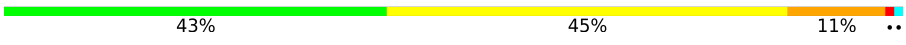
• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

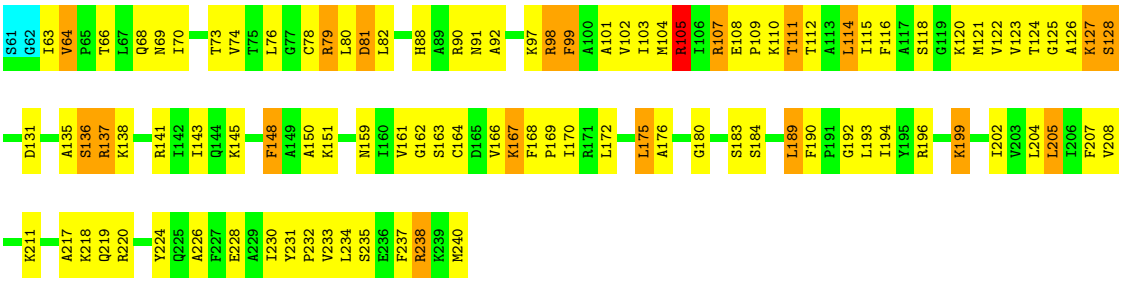




• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

Chain B:

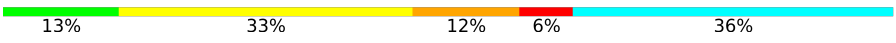


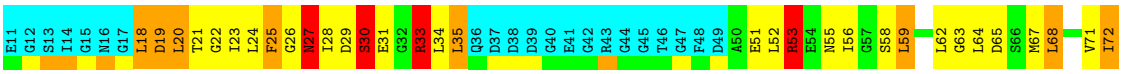


4.2.18 Score per residue for model 18

• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

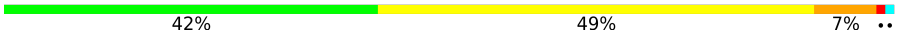
Chain A:

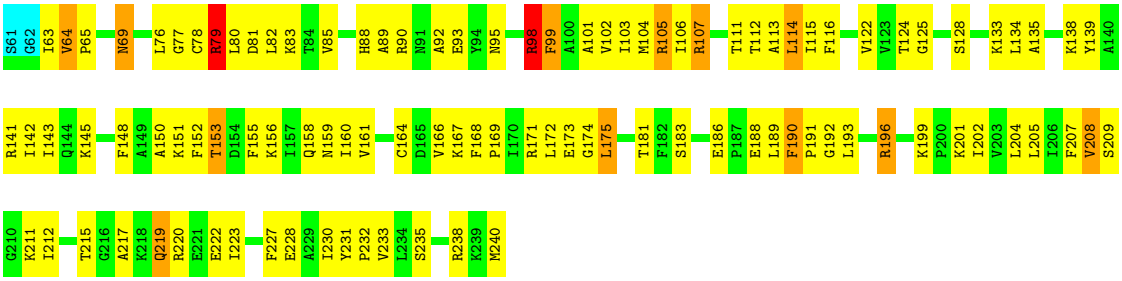




• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

Chain B:

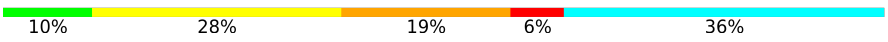


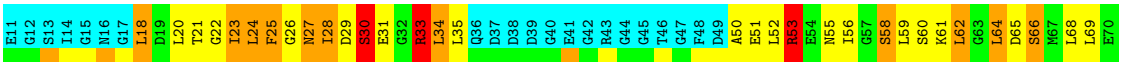


4.2.19 Score per residue for model 19

• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

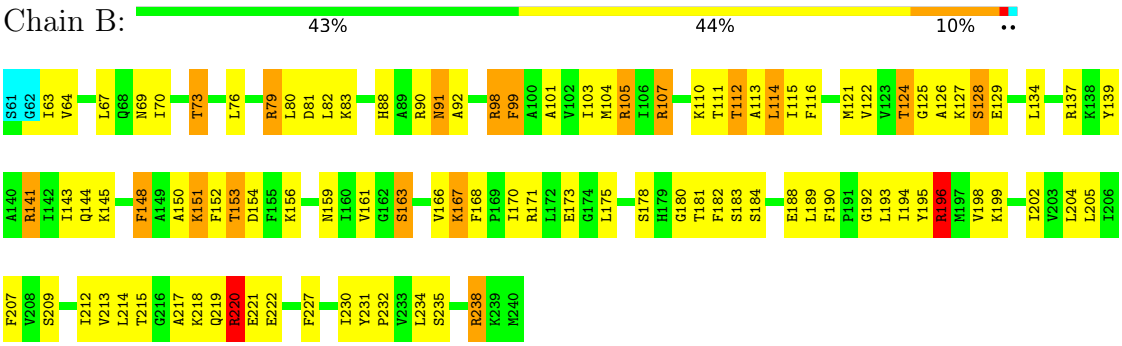
Chain A:





• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

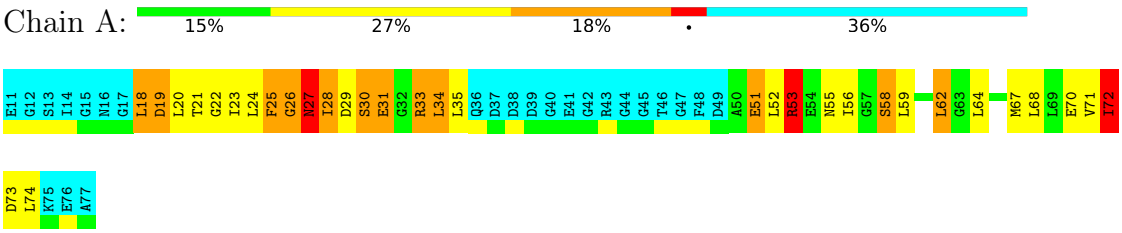
Chain B:



4.2.20 Score per residue for model 20

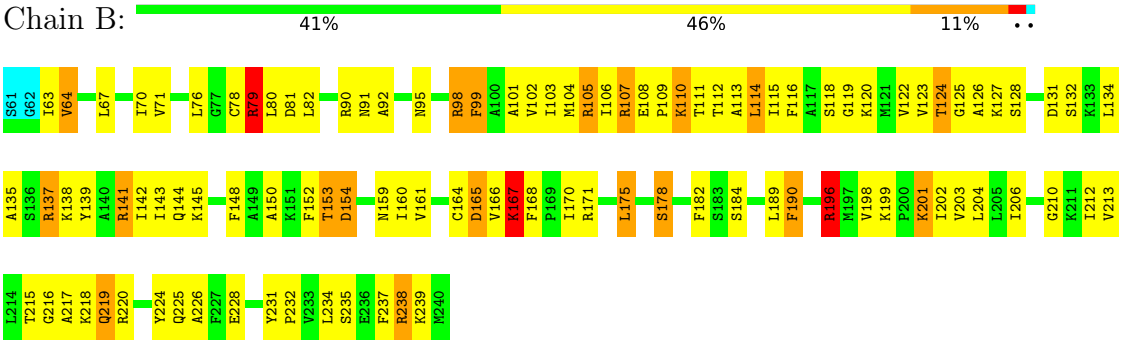
• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

Chain A:



• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

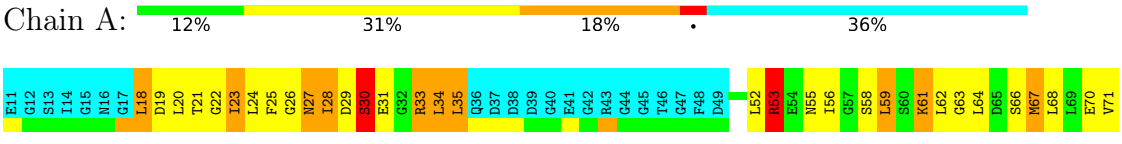
Chain B:

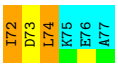


4.2.21 Score per residue for model 21

• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

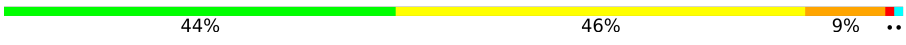
Chain A:

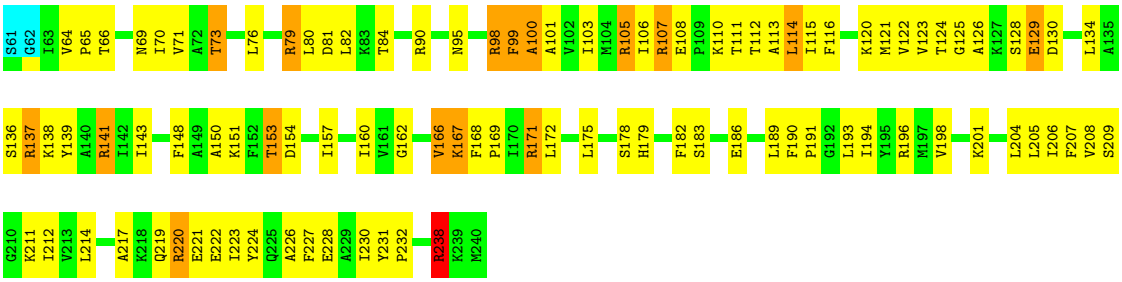




• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

Chain B:

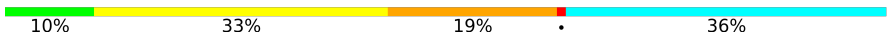


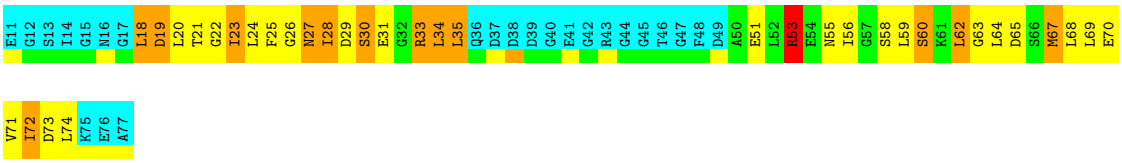


4.2.22 Score per residue for model 22

• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

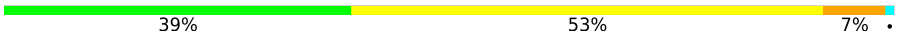
Chain A:

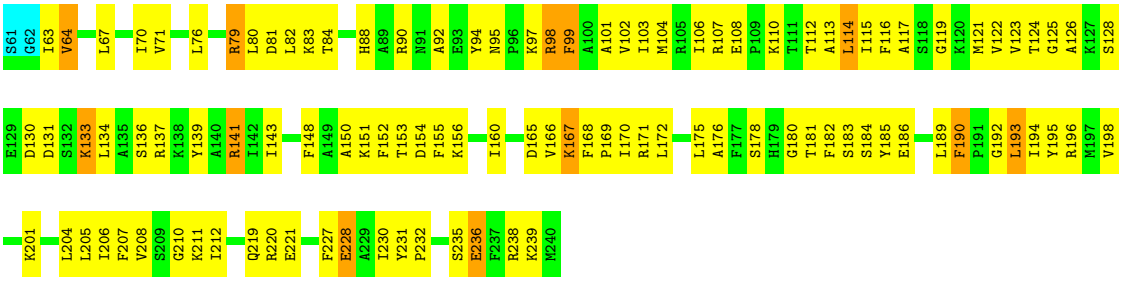




• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

Chain B:

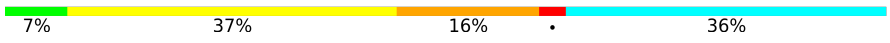


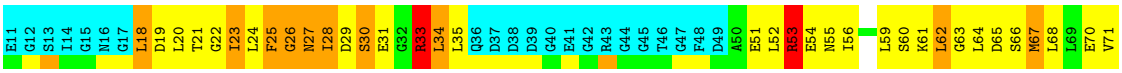


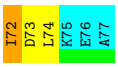
4.2.23 Score per residue for model 23

• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

Chain A:

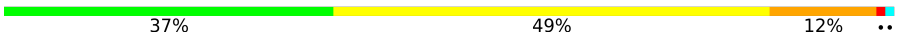


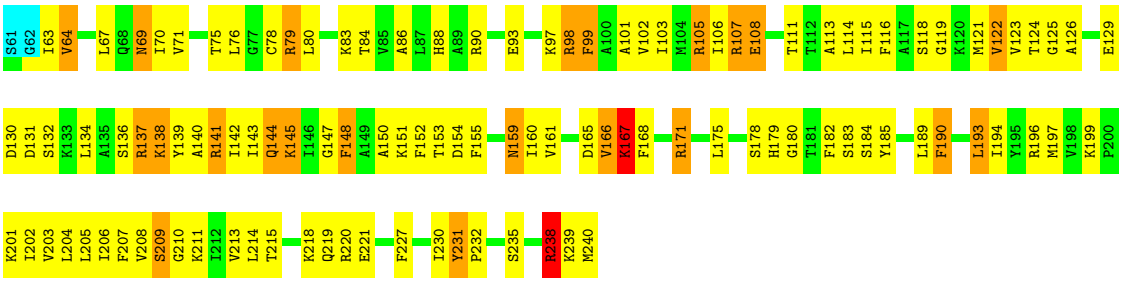




• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

Chain B:

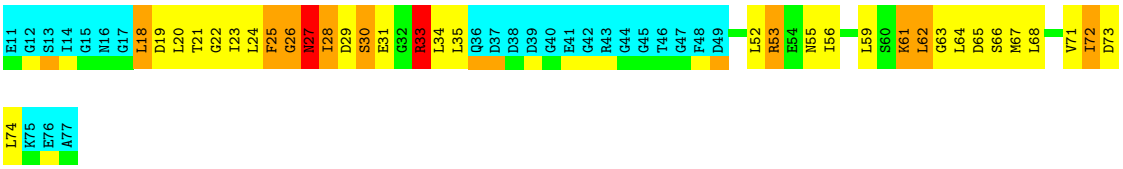




4.2.24 Score per residue for model 24

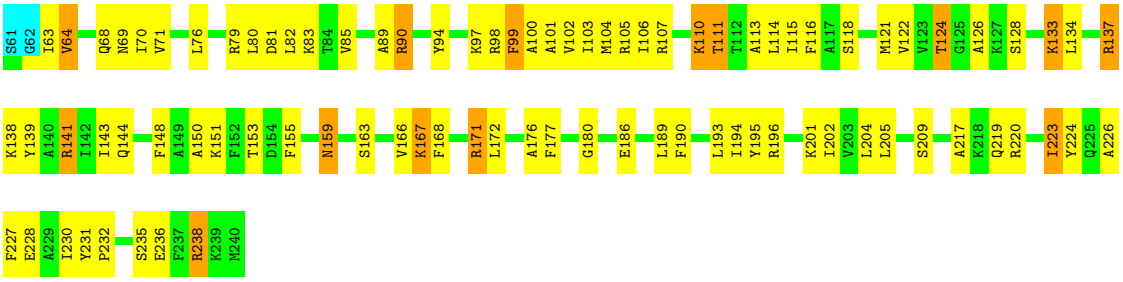
• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

Chain A:



• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

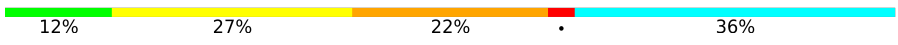
Chain B:

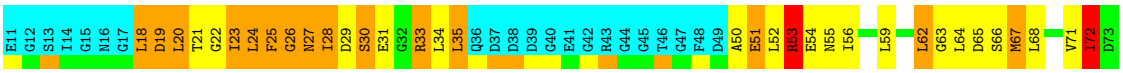


4.2.25 Score per residue for model 25

• Molecule 1: TRANSCRIPTION INITIATION FACTOR IID 230K CHAIN

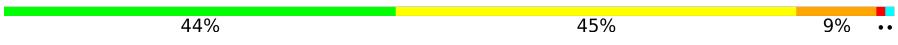
Chain A:





• Molecule 2: TRANSCRIPTION INITIATION FACTOR TFIID

Chain B:



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 25 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.06±0.01	0±0/326 (0.0± 0.0%)	1.25±0.01	0±0/439 (0.0± 0.0%)
2	B	1.02±0.00	0±0/1433 (0.0± 0.0%)	1.25±0.00	0±0/1929 (0.0± 0.0%)
All	All	1.03	0/43975 (0.0%)	1.25	1/59200 (0.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.9±0.3
2	B	0.0±0.0	10.4±0.9
All	All	0	306

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	150	ALA	N-CA-CB	-5.80	101.97	110.10	6	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
2	B	238	ARG	Sidechain	25
1	A	53	ARG	Sidechain	24
2	B	90	ARG	Sidechain	24
2	B	141	ARG	Sidechain	24
2	B	171	ARG	Sidechain	24
2	B	196	ARG	Sidechain	24

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Mol	Chain	Res	Type	Group	Models (Total)
2	B	220	ARG	Sidechain	24
1	A	33	ARG	Sidechain	23
2	B	79	ARG	Sidechain	23
2	B	98	ARG	Sidechain	23
2	B	105	ARG	Sidechain	23
2	B	107	ARG	Sidechain	23
2	B	137	ARG	Sidechain	22

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	325	341	341	112±14
2	B	1406	1486	1486	106±16
All	All	43275	45675	45675	4746

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 53.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ILE:HD11	1:A:74:LEU:HD12	1.11	1.13	1	18
2:B:76:LEU:HD22	2:B:150:ALA:HB1	1.11	1.15	10	21
2:B:99:PHE:CE2	2:B:101:ALA:HB3	1.09	1.83	17	12
1:A:18:LEU:HD21	1:A:20:LEU:HD21	1.09	1.18	1	23
1:A:74:LEU:HD11	2:B:101:ALA:HB2	1.05	1.26	11	13
1:A:74:LEU:CD1	2:B:101:ALA:HB2	1.04	1.83	10	20
2:B:143:ILE:CG2	2:B:149:ALA:HB3	1.04	1.82	6	1
1:A:59:LEU:HD21	2:B:190:PHE:CE1	1.04	1.88	12	2
2:B:170:ILE:HD13	2:B:234:LEU:HD22	1.04	1.29	17	3
1:A:59:LEU:HD22	1:A:62:LEU:HD11	1.02	1.17	19	2
2:B:166:VAL:HG21	2:B:170:ILE:HD11	1.02	1.30	19	9
1:A:74:LEU:HD11	2:B:101:ALA:CB	1.01	1.85	11	9
1:A:34:LEU:HD22	1:A:35:LEU:N	1.00	1.70	1	3
2:B:143:ILE:HG21	2:B:149:ALA:CB	0.99	1.86	6	1
1:A:59:LEU:HD23	1:A:62:LEU:HD11	0.98	1.29	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:LEU:HD11	1:A:64:LEU:CD1	0.96	1.89	18	14
1:A:59:LEU:CD2	1:A:62:LEU:HD11	0.95	1.90	19	2
1:A:59:LEU:HD22	2:B:190:PHE:CE2	0.95	1.96	11	2
2:B:99:PHE:CZ	2:B:101:ALA:HB3	0.94	1.98	7	6
1:A:72:ILE:HD11	1:A:74:LEU:CD1	0.94	1.93	24	11
2:B:143:ILE:HG21	2:B:149:ALA:HB3	0.93	0.96	6	1
1:A:71:VAL:HG12	2:B:122:VAL:HG11	0.93	1.38	18	20
2:B:204:LEU:HD21	2:B:226:ALA:HB1	0.92	1.37	20	9
1:A:34:LEU:HD13	1:A:35:LEU:N	0.92	1.78	18	3
1:A:59:LEU:HD21	2:B:190:PHE:CE2	0.92	2.00	15	5
2:B:161:VAL:HG22	2:B:215:THR:OG1	0.92	1.65	13	10
2:B:76:LEU:CD1	2:B:80:LEU:HD11	0.91	1.94	3	20
1:A:18:LEU:HD12	1:A:19:ASP:N	0.91	1.80	8	10
1:A:25:PHE:CZ	2:B:205:LEU:HD13	0.91	2.00	17	6
2:B:170:ILE:HD12	2:B:209:SER:CB	0.91	1.95	13	1
1:A:27:ASN:ND2	1:A:35:LEU:HD11	0.91	1.80	2	7
2:B:76:LEU:HD12	2:B:80:LEU:HD11	0.90	1.43	10	17
1:A:24:LEU:HD13	1:A:67:MET:SD	0.90	2.06	16	4
1:A:74:LEU:HD22	2:B:100:ALA:HB3	0.90	1.43	15	2
2:B:183:SER:OG	2:B:193:LEU:HD21	0.90	1.66	16	6
1:A:72:ILE:CD1	1:A:74:LEU:HD12	0.90	1.96	24	20
1:A:27:ASN:OD1	1:A:35:LEU:HD11	0.90	1.67	19	6
2:B:92:ALA:HB2	2:B:104:MET:SD	0.90	2.07	20	1
1:A:62:LEU:HD12	1:A:63:GLY:N	0.89	1.83	8	5
1:A:18:LEU:HD23	1:A:72:ILE:CG1	0.89	1.98	17	22
1:A:18:LEU:HD23	1:A:72:ILE:CD1	0.89	1.98	2	25
1:A:74:LEU:HD11	2:B:116:PHE:CD1	0.89	2.02	22	9
1:A:18:LEU:HD23	1:A:72:ILE:HD13	0.88	1.41	22	20
1:A:27:ASN:OD1	1:A:35:LEU:HD21	0.88	1.68	24	3
1:A:21:THR:HG22	1:A:56:ILE:HG23	0.88	1.44	1	5
2:B:82:LEU:HD22	2:B:102:VAL:HG23	0.87	1.45	17	12
2:B:193:LEU:HD23	2:B:194:ILE:N	0.87	1.84	19	5
1:A:74:LEU:HD11	2:B:116:PHE:CE1	0.87	2.05	18	2
1:A:18:LEU:HD13	1:A:30:SER:HB2	0.87	1.44	12	6
2:B:146:ILE:HG21	2:B:148:PHE:CE2	0.87	2.04	12	1
1:A:20:LEU:HD13	1:A:23:ILE:HG21	0.86	1.46	6	14
1:A:18:LEU:CD2	1:A:20:LEU:HD21	0.86	1.98	24	17
2:B:143:ILE:HG21	2:B:150:ALA:HB2	0.86	1.47	1	13
1:A:18:LEU:CD2	1:A:20:LEU:HD22	0.86	2.01	11	1
1:A:74:LEU:HD13	2:B:101:ALA:HB2	0.86	1.44	12	8
1:A:58:SER:O	2:B:189:LEU:HD11	0.86	1.69	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:LEU:O	1:A:56:ILE:HD12	0.86	1.70	24	2
1:A:20:LEU:HD11	1:A:23:ILE:CG1	0.86	2.01	11	1
2:B:170:ILE:HD12	2:B:209:SER:CA	0.85	2.01	13	1
1:A:53:ARG:HA	1:A:56:ILE:HD12	0.85	1.46	2	23
1:A:18:LEU:HD23	1:A:72:ILE:HG12	0.85	1.49	17	20
2:B:79:ARG:O	2:B:80:LEU:HD23	0.84	1.71	20	18
1:A:27:ASN:HB2	2:B:124:THR:HG23	0.84	1.49	17	5
1:A:71:VAL:O	2:B:122:VAL:HG21	0.84	1.73	9	17
2:B:85:VAL:HG22	2:B:148:PHE:CE2	0.84	2.08	15	3
1:A:18:LEU:HD21	1:A:20:LEU:HD22	0.84	1.48	11	1
1:A:59:LEU:HD23	1:A:62:LEU:HD21	0.83	1.50	15	6
1:A:18:LEU:HD22	2:B:99:PHE:CD2	0.83	2.07	7	7
1:A:62:LEU:HD22	1:A:62:LEU:O	0.83	1.72	24	1
1:A:18:LEU:HD21	1:A:20:LEU:CD2	0.83	2.03	1	14
2:B:78:CYS:SG	2:B:149:ALA:HB3	0.83	2.12	4	2
2:B:185:TYR:HB2	2:B:193:LEU:HD12	0.83	1.50	11	3
2:B:76:LEU:HD22	2:B:149:ALA:C	0.82	1.94	6	1
1:A:74:LEU:CD2	2:B:101:ALA:HB2	0.82	2.03	19	2
1:A:62:LEU:N	1:A:62:LEU:HD13	0.82	1.89	20	2
2:B:201:LYS:O	2:B:202:ILE:HD13	0.82	1.73	6	5
1:A:59:LEU:HD22	1:A:62:LEU:CD1	0.82	2.04	19	1
1:A:62:LEU:HD13	2:B:194:ILE:HD13	0.82	1.50	15	8
2:B:175:LEU:HD21	2:B:233:VAL:HG12	0.82	1.51	1	4
1:A:20:LEU:HD12	1:A:71:VAL:HB	0.82	1.52	24	17
2:B:101:ALA:HB1	2:B:115:ILE:O	0.82	1.75	21	6
1:A:28:ILE:HD12	1:A:29:ASP:O	0.81	1.74	14	5
2:B:71:VAL:HG22	2:B:124:THR:HB	0.81	1.50	15	8
2:B:71:VAL:HG22	2:B:124:THR:CB	0.80	2.05	22	8
1:A:74:LEU:HD22	2:B:101:ALA:HB2	0.80	1.53	19	2
1:A:23:ILE:HG12	1:A:28:ILE:HD12	0.80	1.52	15	2
1:A:34:LEU:C	1:A:34:LEU:HD22	0.80	1.97	20	1
1:A:18:LEU:O	1:A:68:LEU:HD11	0.80	1.75	20	3
1:A:72:ILE:CG1	1:A:74:LEU:HD13	0.80	2.05	21	4
1:A:23:ILE:HG22	1:A:71:VAL:HG11	0.80	1.53	11	2
1:A:20:LEU:HD22	1:A:23:ILE:HG13	0.79	1.52	3	15
2:B:182:PHE:CE1	2:B:198:VAL:HG22	0.79	2.12	20	4
1:A:20:LEU:HD11	1:A:72:ILE:HB	0.79	1.53	24	16
2:B:176:ALA:HB2	2:B:193:LEU:HD11	0.79	1.54	4	1
1:A:59:LEU:HD23	1:A:62:LEU:HD12	0.79	1.55	5	2
2:B:193:LEU:O	2:B:205:LEU:HD13	0.79	1.78	5	2
2:B:114:LEU:HD12	2:B:122:VAL:CG1	0.78	2.09	12	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:166:VAL:HG11	2:B:234:LEU:HD13	0.78	1.54	19	1
1:A:62:LEU:HD13	1:A:62:LEU:N	0.78	1.94	13	1
2:B:170:ILE:HD12	2:B:209:SER:HA	0.78	1.55	13	1
1:A:23:ILE:HG23	2:B:124:THR:HG21	0.77	1.56	15	2
1:A:62:LEU:HD22	2:B:194:ILE:HD13	0.77	1.57	19	3
2:B:114:LEU:HD12	2:B:116:PHE:CE1	0.77	2.13	22	2
2:B:76:LEU:HD22	2:B:149:ALA:O	0.77	1.78	6	1
2:B:140:ALA:HB1	2:B:144:GLN:NE2	0.77	1.94	12	2
1:A:27:ASN:CB	2:B:124:THR:HG23	0.77	2.08	16	12
2:B:181:THR:HG23	2:B:182:PHE:CD2	0.77	2.15	6	1
1:A:20:LEU:HD13	1:A:23:ILE:CG2	0.76	2.10	6	6
2:B:152:PHE:O	2:B:153:THR:HG23	0.76	1.81	18	6
1:A:52:LEU:HD22	1:A:53:ARG:N	0.76	1.96	13	1
1:A:18:LEU:CD2	1:A:72:ILE:HD13	0.76	2.11	14	19
1:A:58:SER:HB3	2:B:189:LEU:HD11	0.76	1.57	3	1
2:B:202:ILE:HD11	2:B:217:ALA:HB2	0.76	1.57	25	3
1:A:28:ILE:HG22	1:A:34:LEU:HD22	0.76	1.55	18	2
1:A:21:THR:OG1	1:A:68:LEU:HD21	0.76	1.81	9	1
2:B:106:ILE:HG23	2:B:139:TYR:CE1	0.75	2.16	3	9
1:A:52:LEU:N	1:A:52:LEU:HD13	0.75	1.95	13	1
1:A:34:LEU:HD13	1:A:56:ILE:HD13	0.75	1.57	15	4
2:B:70:ILE:HB	2:B:126:ALA:HB3	0.75	1.56	2	11
2:B:204:LEU:N	2:B:204:LEU:HD12	0.75	1.95	23	10
1:A:62:LEU:HD11	2:B:189:LEU:CD2	0.75	2.12	21	1
2:B:110:LYS:O	2:B:111:THR:HG23	0.75	1.80	10	7
2:B:109:PRO:HG2	2:B:135:ALA:HB2	0.75	1.57	15	4
1:A:24:LEU:HD22	1:A:67:MET:HG2	0.75	1.57	17	8
2:B:144:GLN:HG2	2:B:150:ALA:HB1	0.75	1.57	6	2
1:A:61:LYS:HG3	1:A:62:LEU:HD23	0.75	1.55	10	3
1:A:56:ILE:HA	1:A:59:LEU:HD12	0.75	1.58	17	14
2:B:211:LYS:O	2:B:212:ILE:HD13	0.74	1.82	10	6
2:B:175:LEU:HD11	2:B:233:VAL:CG1	0.74	2.12	18	3
2:B:204:LEU:HD12	2:B:204:LEU:N	0.74	1.96	19	2
1:A:64:LEU:HD12	1:A:68:LEU:HD21	0.74	1.59	19	2
2:B:170:ILE:CD1	2:B:234:LEU:HD22	0.74	2.12	17	2
2:B:202:ILE:HD11	2:B:217:ALA:CB	0.74	2.12	25	4
2:B:214:LEU:N	2:B:214:LEU:HD12	0.74	1.96	4	9
1:A:20:LEU:HD11	1:A:23:ILE:HG12	0.74	1.59	11	1
1:A:71:VAL:CG1	2:B:122:VAL:HG11	0.74	2.12	3	6
1:A:24:LEU:HD11	1:A:64:LEU:HD12	0.74	1.59	17	7
1:A:23:ILE:CG2	1:A:71:VAL:HG11	0.73	2.12	11	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LEU:HD23	1:A:62:LEU:CD1	0.73	2.12	5	3
2:B:143:ILE:N	2:B:143:ILE:HD13	0.73	1.98	6	1
1:A:20:LEU:HD23	1:A:72:ILE:CG2	0.73	2.13	11	1
1:A:62:LEU:HD22	1:A:62:LEU:C	0.73	2.04	24	3
2:B:172:LEU:HD22	2:B:193:LEU:HB2	0.73	1.58	13	5
1:A:24:LEU:CD1	1:A:64:LEU:HD12	0.73	2.12	20	1
1:A:19:ASP:O	1:A:20:LEU:HD23	0.73	1.83	7	3
1:A:34:LEU:HD23	1:A:35:LEU:N	0.73	1.99	25	5
1:A:34:LEU:HD13	1:A:34:LEU:C	0.73	2.04	6	6
1:A:24:LEU:HD13	1:A:67:MET:HG2	0.73	1.58	25	8
2:B:189:LEU:HD23	2:B:190:PHE:N	0.73	1.99	19	3
1:A:35:LEU:C	1:A:35:LEU:HD12	0.72	2.04	17	11
1:A:74:LEU:HD13	2:B:100:ALA:O	0.72	1.83	13	2
2:B:196:ARG:HG2	2:B:203:VAL:HG22	0.72	1.60	10	1
2:B:113:ALA:HB2	2:B:139:TYR:CE2	0.72	2.20	25	9
1:A:24:LEU:HD11	1:A:64:LEU:HD11	0.72	1.62	7	4
1:A:24:LEU:HD22	1:A:67:MET:HB3	0.72	1.59	8	4
1:A:28:ILE:HD12	1:A:29:ASP:C	0.72	2.04	6	6
1:A:34:LEU:HD13	1:A:34:LEU:O	0.72	1.85	1	2
2:B:93:GLU:O	2:B:103:ILE:HD12	0.72	1.84	12	4
2:B:112:THR:HG22	2:B:124:THR:HG23	0.71	1.60	13	8
1:A:29:ASP:HA	2:B:103:ILE:HG21	0.71	1.61	13	5
1:A:23:ILE:HG21	1:A:71:VAL:HG11	0.71	1.61	7	2
1:A:62:LEU:HD12	1:A:63:GLY:H	0.71	1.45	17	3
2:B:76:LEU:HD23	2:B:151:LYS:O	0.71	1.86	6	6
2:B:99:PHE:CZ	2:B:101:ALA:HB2	0.71	2.19	21	1
2:B:103:ILE:CD1	2:B:114:LEU:HD13	0.71	2.16	24	2
1:A:24:LEU:HA	2:B:71:VAL:HG21	0.71	1.63	21	2
2:B:172:LEU:HD22	2:B:193:LEU:CB	0.71	2.16	24	6
2:B:67:LEU:HD22	2:B:160:ILE:CG2	0.70	2.15	8	8
2:B:76:LEU:HD22	2:B:150:ALA:CB	0.70	2.07	10	2
2:B:204:LEU:HD22	2:B:230:ILE:HG13	0.70	1.63	7	4
1:A:34:LEU:HD22	1:A:35:LEU:H	0.70	1.42	16	3
1:A:23:ILE:N	1:A:28:ILE:HG21	0.70	2.02	7	4
1:A:59:LEU:HD12	1:A:59:LEU:O	0.70	1.86	21	4
2:B:202:ILE:CD1	2:B:217:ALA:HB2	0.70	2.16	25	6
2:B:176:ALA:HB2	2:B:193:LEU:CD1	0.70	2.15	3	2
1:A:68:LEU:O	1:A:72:ILE:HG22	0.70	1.86	13	7
2:B:212:ILE:HG22	2:B:214:LEU:HD11	0.70	1.64	15	2
2:B:205:LEU:C	2:B:206:ILE:HD13	0.70	2.07	9	1
2:B:67:LEU:HD22	2:B:160:ILE:HG22	0.70	1.63	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:202:ILE:HD12	2:B:217:ALA:HB2	0.70	1.62	17	8
2:B:217:ALA:HB3	2:B:223:ILE:HD12	0.70	1.63	7	1
1:A:20:LEU:HD13	1:A:23:ILE:CB	0.70	2.17	15	3
1:A:62:LEU:HD22	1:A:63:GLY:N	0.70	2.02	22	2
1:A:20:LEU:HD22	1:A:23:ILE:CG1	0.69	2.17	5	11
1:A:18:LEU:HD11	1:A:30:SER:CA	0.69	2.17	15	5
1:A:18:LEU:HD22	2:B:99:PHE:CE2	0.69	2.21	7	2
2:B:139:TYR:HA	2:B:142:ILE:HD12	0.69	1.65	15	6
2:B:170:ILE:HD13	2:B:206:ILE:CG2	0.69	2.18	10	1
1:A:72:ILE:HD12	2:B:116:PHE:CZ	0.69	2.23	21	7
2:B:196:ARG:HD3	2:B:203:VAL:HG22	0.69	1.64	16	1
1:A:68:LEU:C	1:A:68:LEU:HD13	0.69	2.07	21	13
2:B:112:THR:CG2	2:B:124:THR:HG23	0.68	2.17	13	5
2:B:183:SER:HB3	2:B:193:LEU:HD21	0.68	1.63	7	1
1:A:59:LEU:CD1	1:A:62:LEU:HD21	0.68	2.19	20	1
1:A:71:VAL:HG12	2:B:122:VAL:CG1	0.68	2.15	10	8
2:B:190:PHE:CE2	2:B:205:LEU:HD11	0.68	2.23	7	3
2:B:143:ILE:CG2	2:B:150:ALA:HB2	0.68	2.18	1	7
1:A:18:LEU:HD12	1:A:18:LEU:O	0.68	1.89	16	1
1:A:18:LEU:HB2	2:B:99:PHE:CG	0.68	2.24	8	9
1:A:58:SER:C	2:B:189:LEU:HD11	0.68	2.09	5	1
2:B:76:LEU:HD13	2:B:149:ALA:HA	0.68	1.64	6	1
2:B:214:LEU:HD12	2:B:214:LEU:N	0.68	2.03	15	3
1:A:72:ILE:HD13	2:B:114:LEU:HD13	0.68	1.65	6	2
2:B:205:LEU:HD12	2:B:213:VAL:HB	0.68	1.64	15	3
1:A:21:THR:OG1	1:A:68:LEU:HD12	0.68	1.89	5	2
1:A:68:LEU:C	1:A:68:LEU:HD23	0.68	2.09	5	3
2:B:67:LEU:HD11	2:B:220:ARG:HD2	0.68	1.65	19	1
1:A:18:LEU:CB	2:B:99:PHE:CG	0.68	2.77	16	10
1:A:18:LEU:HD12	1:A:19:ASP:H	0.68	1.48	20	7
1:A:23:ILE:N	1:A:28:ILE:CG2	0.67	2.58	20	18
1:A:24:LEU:HD12	1:A:24:LEU:O	0.67	1.88	8	2
1:A:18:LEU:HD11	1:A:30:SER:O	0.67	1.89	5	5
1:A:28:ILE:O	1:A:28:ILE:HD13	0.67	1.89	20	3
2:B:202:ILE:HD11	2:B:222:GLU:OE1	0.67	1.89	8	2
2:B:99:PHE:CZ	2:B:101:ALA:CB	0.67	2.76	21	2
2:B:170:ILE:HD12	2:B:209:SER:HB3	0.67	1.66	13	1
1:A:74:LEU:HD12	2:B:101:ALA:HB2	0.67	1.66	13	6
2:B:193:LEU:C	2:B:193:LEU:HD23	0.67	2.09	24	5
1:A:20:LEU:HD23	1:A:72:ILE:HB	0.67	1.66	11	1
1:A:72:ILE:O	1:A:72:ILE:HG23	0.67	1.88	18	23

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ILE:HD12	2:B:116:PHE:CE1	0.67	2.24	24	11
1:A:62:LEU:CD1	2:B:194:ILE:HG21	0.67	2.19	1	3
1:A:22:GLY:HA3	1:A:28:ILE:HG21	0.67	1.67	20	3
1:A:27:ASN:HB2	2:B:112:THR:HG22	0.67	1.64	21	4
1:A:20:LEU:N	1:A:68:LEU:HD21	0.67	2.05	20	2
1:A:22:GLY:C	1:A:28:ILE:HG21	0.66	2.10	1	11
1:A:66:SER:HA	1:A:69:LEU:HD21	0.66	1.67	9	3
2:B:76:LEU:HD13	2:B:150:ALA:HB1	0.66	1.65	19	1
1:A:52:LEU:HD13	1:A:52:LEU:H	0.66	1.48	13	1
1:A:34:LEU:HD22	1:A:34:LEU:C	0.66	2.08	1	1
1:A:18:LEU:N	2:B:99:PHE:CZ	0.66	2.62	2	8
2:B:88:HIS:HB2	2:B:146:ILE:HD11	0.66	1.67	6	1
1:A:28:ILE:HG22	1:A:34:LEU:HA	0.66	1.68	16	6
1:A:18:LEU:N	2:B:99:PHE:CE1	0.66	2.63	12	7
1:A:62:LEU:HD23	1:A:62:LEU:N	0.66	2.04	12	7
1:A:62:LEU:HB2	1:A:64:LEU:HD23	0.66	1.67	19	1
1:A:21:THR:HG21	1:A:59:LEU:HB2	0.66	1.68	15	8
2:B:143:ILE:HG21	2:B:150:ALA:CB	0.66	2.20	11	4
1:A:27:ASN:ND2	1:A:35:LEU:HD12	0.66	2.06	22	4
2:B:227:PHE:CZ	2:B:231:TYR:CD1	0.66	2.84	4	1
2:B:114:LEU:HD12	2:B:122:VAL:HB	0.65	1.69	15	3
2:B:160:ILE:HD12	2:B:219:GLN:O	0.65	1.91	4	5
2:B:76:LEU:HD13	2:B:149:ALA:CB	0.65	2.21	6	1
1:A:74:LEU:HD13	2:B:101:ALA:CB	0.65	2.21	18	2
2:B:99:PHE:CZ	2:B:103:ILE:HD11	0.65	2.26	23	5
2:B:176:ALA:HB2	2:B:193:LEU:HD12	0.65	1.66	3	2
2:B:143:ILE:HG22	2:B:148:PHE:CB	0.65	2.22	19	11
1:A:18:LEU:CD2	1:A:72:ILE:CD1	0.65	2.73	18	11
1:A:21:THR:N	1:A:68:LEU:HD21	0.65	2.06	6	3
2:B:76:LEU:HD13	2:B:150:ALA:CB	0.65	2.21	19	1
1:A:18:LEU:CB	2:B:99:PHE:CD2	0.65	2.80	8	3
1:A:27:ASN:ND2	2:B:124:THR:HG23	0.65	2.07	15	3
1:A:20:LEU:HD23	1:A:72:ILE:CB	0.65	2.21	11	1
1:A:64:LEU:HD22	1:A:64:LEU:N	0.65	2.06	20	1
2:B:76:LEU:HD11	2:B:121:MET:CG	0.65	2.22	6	1
2:B:190:PHE:CZ	2:B:205:LEU:HD22	0.64	2.27	14	2
1:A:24:LEU:HD13	1:A:67:MET:CG	0.64	2.22	11	3
1:A:52:LEU:C	1:A:56:ILE:HD12	0.64	2.12	24	2
1:A:74:LEU:CD1	2:B:116:PHE:CD1	0.64	2.80	2	8
1:A:21:THR:HG21	1:A:56:ILE:O	0.64	1.92	4	2
1:A:23:ILE:HD13	1:A:28:ILE:HG23	0.64	1.68	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:76:LEU:HD13	2:B:149:ALA:CA	0.64	2.22	6	1
1:A:62:LEU:N	1:A:62:LEU:HD23	0.64	2.07	19	1
2:B:76:LEU:HD13	2:B:80:LEU:HD11	0.64	1.70	8	11
2:B:175:LEU:HD21	2:B:233:VAL:CG1	0.64	2.23	9	3
2:B:195:TYR:CD2	2:B:230:ILE:HD13	0.64	2.27	3	1
1:A:35:LEU:HD12	1:A:35:LEU:C	0.64	2.12	4	5
1:A:23:ILE:HG12	1:A:28:ILE:HG23	0.64	1.70	15	7
2:B:223:ILE:HG22	2:B:224:TYR:N	0.64	2.08	24	2
1:A:20:LEU:HD11	1:A:23:ILE:HG13	0.64	1.69	11	1
1:A:59:LEU:CD2	1:A:62:LEU:HD21	0.63	2.23	1	1
1:A:74:LEU:CB	2:B:99:PHE:CE2	0.63	2.81	13	5
1:A:27:ASN:HD21	1:A:35:LEU:HD11	0.63	1.53	9	2
1:A:20:LEU:CD1	1:A:23:ILE:CG1	0.63	2.75	11	1
2:B:113:ALA:HB2	2:B:139:TYR:CD2	0.63	2.28	25	2
1:A:18:LEU:CD2	1:A:20:LEU:CD2	0.63	2.76	18	11
1:A:21:THR:OG1	1:A:68:LEU:HD23	0.63	1.93	17	10
2:B:170:ILE:HD13	2:B:234:LEU:CD2	0.63	2.17	17	1
2:B:114:LEU:HD12	2:B:116:PHE:HE1	0.63	1.49	22	2
2:B:116:PHE:N	2:B:116:PHE:CD1	0.63	2.65	14	11
1:A:18:LEU:HD21	2:B:114:LEU:HD22	0.63	1.70	2	4
2:B:114:LEU:HD12	2:B:116:PHE:CZ	0.63	2.28	6	2
1:A:59:LEU:HD21	2:B:190:PHE:HE1	0.63	1.49	12	1
1:A:59:LEU:HA	1:A:62:LEU:HD21	0.63	1.70	17	2
1:A:74:LEU:CB	2:B:99:PHE:CZ	0.63	2.81	13	2
2:B:182:PHE:CE1	2:B:198:VAL:CG2	0.63	2.81	22	4
1:A:20:LEU:CD1	1:A:23:ILE:HG21	0.63	2.20	6	3
2:B:74:VAL:HG21	2:B:136:SER:OG	0.63	1.93	17	4
1:A:72:ILE:HG13	1:A:74:LEU:HD12	0.63	1.70	19	1
2:B:172:LEU:HD21	2:B:206:ILE:HG22	0.63	1.70	2	1
1:A:20:LEU:HD13	1:A:23:ILE:HG13	0.63	1.71	1	6
2:B:190:PHE:HE2	2:B:205:LEU:HD11	0.63	1.53	7	1
1:A:27:ASN:HB3	2:B:124:THR:HG23	0.63	1.71	18	5
2:B:64:VAL:CG1	2:B:224:TYR:CZ	0.63	2.82	20	1
2:B:144:GLN:CG	2:B:150:ALA:CB	0.63	2.77	6	1
1:A:53:ARG:CA	1:A:56:ILE:HD12	0.63	2.23	2	21
1:A:24:LEU:HD22	1:A:67:MET:CG	0.63	2.23	17	5
2:B:70:ILE:HG12	2:B:160:ILE:HG23	0.62	1.70	9	4
2:B:70:ILE:HG22	2:B:126:ALA:HB3	0.62	1.70	1	1
2:B:166:VAL:HG21	2:B:170:ILE:CD1	0.62	2.18	19	2
1:A:25:PHE:CE2	1:A:52:LEU:HD21	0.62	2.29	7	1
1:A:74:LEU:HB3	2:B:99:PHE:CZ	0.62	2.30	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:172:LEU:HD11	2:B:208:VAL:HG23	0.62	1.71	16	1
1:A:27:ASN:ND2	1:A:27:ASN:N	0.62	2.47	20	4
2:B:116:PHE:CD1	2:B:116:PHE:N	0.62	2.66	12	12
1:A:22:GLY:HA3	1:A:34:LEU:HD12	0.62	1.71	15	3
1:A:28:ILE:HD13	1:A:28:ILE:C	0.62	2.14	20	8
2:B:182:PHE:CZ	2:B:198:VAL:CG2	0.62	2.83	19	3
2:B:76:LEU:HB3	2:B:149:ALA:HB3	0.62	1.70	12	1
2:B:143:ILE:HD12	2:B:143:ILE:N	0.62	2.10	15	2
2:B:106:ILE:HD11	2:B:111:THR:OG1	0.62	1.95	15	2
1:A:74:LEU:CD1	2:B:99:PHE:CD2	0.62	2.83	3	3
1:A:18:LEU:HB3	2:B:99:PHE:CD2	0.62	2.30	18	11
1:A:72:ILE:CD1	2:B:114:LEU:HD13	0.62	2.23	6	1
1:A:59:LEU:HD11	2:B:190:PHE:CE1	0.62	2.28	7	1
1:A:28:ILE:HG22	1:A:34:LEU:HD12	0.62	1.70	9	2
2:B:170:ILE:CD1	2:B:209:SER:CB	0.62	2.76	13	1
1:A:71:VAL:HG12	2:B:122:VAL:HG21	0.62	1.72	25	1
2:B:194:ILE:HG12	2:B:205:LEU:HD21	0.62	1.72	16	1
1:A:56:ILE:CA	1:A:59:LEU:HD12	0.62	2.25	8	13
2:B:190:PHE:CE2	2:B:194:ILE:CG1	0.62	2.83	21	3
1:A:62:LEU:HD13	1:A:62:LEU:H	0.62	1.54	13	3
2:B:115:ILE:HG23	2:B:120:LYS:O	0.62	1.94	17	1
1:A:62:LEU:HD13	2:B:194:ILE:CD1	0.62	2.23	3	2
2:B:182:PHE:CZ	2:B:198:VAL:HG22	0.61	2.30	8	2
2:B:99:PHE:CD2	2:B:101:ALA:HB3	0.61	2.29	22	4
1:A:62:LEU:HD22	2:B:194:ILE:HD12	0.61	1.72	25	2
1:A:74:LEU:CD1	2:B:116:PHE:CE1	0.61	2.83	18	2
1:A:23:ILE:HD13	2:B:124:THR:HG21	0.61	1.72	2	8
2:B:196:ARG:CG	2:B:203:VAL:HG22	0.61	2.24	10	1
2:B:82:LEU:CD1	2:B:117:ALA:HB2	0.61	2.25	22	1
2:B:203:VAL:C	2:B:204:LEU:HD12	0.61	2.14	23	3
1:A:59:LEU:CD2	1:A:62:LEU:HD12	0.61	2.24	5	1
1:A:27:ASN:C	1:A:28:ILE:HG22	0.61	2.16	15	2
2:B:76:LEU:HD11	2:B:121:MET:SD	0.61	2.36	6	1
2:B:227:PHE:CZ	2:B:231:TYR:CE2	0.61	2.88	3	2
1:A:21:THR:CG2	1:A:56:ILE:HG23	0.61	2.25	18	2
1:A:24:LEU:HD21	1:A:68:LEU:CD2	0.61	2.26	19	1
1:A:18:LEU:CD1	1:A:30:SER:CB	0.60	2.79	22	3
1:A:62:LEU:N	1:A:62:LEU:CD1	0.60	2.62	20	3
1:A:72:ILE:CD1	1:A:74:LEU:CD1	0.60	2.79	19	3
2:B:103:ILE:HD12	2:B:114:LEU:HD13	0.60	1.72	24	2
1:A:74:LEU:HD11	2:B:101:ALA:HB3	0.60	1.71	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:GLY:CA	1:A:28:ILE:HG21	0.60	2.26	20	1
2:B:70:ILE:CD1	2:B:160:ILE:HG23	0.60	2.27	15	3
2:B:168:PHE:CD1	2:B:168:PHE:N	0.60	2.68	4	4
1:A:26:GLY:O	1:A:28:ILE:HG23	0.60	1.96	18	4
1:A:62:LEU:HD11	2:B:189:LEU:HD21	0.60	1.72	21	1
1:A:59:LEU:HD23	1:A:62:LEU:CD2	0.60	2.25	15	2
2:B:202:ILE:HD13	2:B:217:ALA:HB2	0.60	1.74	16	2
1:A:27:ASN:N	1:A:27:ASN:OD1	0.60	2.35	12	10
2:B:227:PHE:HA	2:B:230:ILE:HG22	0.60	1.72	2	11
2:B:80:LEU:CD2	2:B:149:ALA:HB2	0.60	2.26	6	1
1:A:20:LEU:HG	1:A:72:ILE:HG21	0.60	1.73	19	15
2:B:92:ALA:HB2	2:B:104:MET:HG3	0.60	1.71	19	5
1:A:25:PHE:HZ	2:B:205:LEU:HD13	0.60	1.54	8	7
1:A:28:ILE:CG2	1:A:34:LEU:HD12	0.60	2.27	17	3
1:A:23:ILE:CD1	1:A:28:ILE:CD1	0.60	2.79	17	1
1:A:28:ILE:HB	1:A:34:LEU:HA	0.60	1.73	4	19
2:B:143:ILE:HG22	2:B:148:PHE:HB2	0.60	1.74	19	11
2:B:111:THR:HG22	2:B:125:GLY:C	0.60	2.18	9	4
1:A:64:LEU:O	1:A:68:LEU:HD12	0.60	1.97	18	1
2:B:202:ILE:CD1	2:B:217:ALA:CB	0.59	2.80	17	3
2:B:231:TYR:N	2:B:232:PRO:CD	0.59	2.65	2	25
1:A:62:LEU:HD23	2:B:194:ILE:HD13	0.59	1.74	24	1
1:A:21:THR:N	1:A:68:LEU:CD2	0.59	2.66	8	13
1:A:18:LEU:CB	2:B:99:PHE:CD1	0.59	2.85	15	4
2:B:211:LYS:O	2:B:212:ILE:HD12	0.59	1.97	15	2
1:A:74:LEU:HD21	2:B:116:PHE:HB3	0.59	1.74	2	5
2:B:70:ILE:HG21	2:B:132:SER:OG	0.59	1.96	3	1
1:A:34:LEU:CD1	1:A:56:ILE:HD13	0.59	2.28	3	1
2:B:189:LEU:O	2:B:189:LEU:HD23	0.59	1.97	24	5
1:A:21:THR:N	1:A:68:LEU:HD23	0.59	2.13	21	1
1:A:62:LEU:HD22	2:B:194:ILE:CD1	0.59	2.26	19	5
1:A:23:ILE:HD12	2:B:114:LEU:HD11	0.59	1.75	10	4
1:A:61:LYS:C	1:A:62:LEU:HD23	0.59	2.18	2	6
2:B:183:SER:HB2	2:B:193:LEU:HD21	0.59	1.73	17	5
1:A:24:LEU:HD12	1:A:24:LEU:C	0.59	2.18	8	1
2:B:205:LEU:O	2:B:206:ILE:HD13	0.59	1.98	23	2
1:A:27:ASN:N	1:A:27:ASN:ND2	0.59	2.50	13	1
1:A:74:LEU:CD1	2:B:101:ALA:CB	0.59	2.80	25	13
2:B:143:ILE:CG2	2:B:148:PHE:CB	0.59	2.81	19	15
1:A:72:ILE:HD13	2:B:114:LEU:CD1	0.59	2.27	13	2
2:B:99:PHE:CZ	2:B:101:ALA:O	0.59	2.55	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:63:ILE:HG22	2:B:164:CYS:SG	0.59	2.37	4	2
2:B:114:LEU:HD23	2:B:114:LEU:N	0.59	2.12	11	4
2:B:149:ALA:O	2:B:150:ALA:HB3	0.59	1.97	12	1
1:A:18:LEU:HD13	2:B:99:PHE:CD1	0.59	2.32	25	1
1:A:20:LEU:N	1:A:68:LEU:CD2	0.59	2.66	20	2
1:A:23:ILE:CD1	1:A:71:VAL:HG11	0.59	2.27	20	1
2:B:99:PHE:CE1	2:B:101:ALA:O	0.58	2.56	5	8
2:B:88:HIS:CB	2:B:146:ILE:HD11	0.58	2.28	6	1
2:B:202:ILE:HD11	2:B:222:GLU:HG2	0.58	1.74	10	1
1:A:28:ILE:O	2:B:112:THR:HG21	0.58	1.97	14	3
1:A:18:LEU:HB2	2:B:99:PHE:CD1	0.58	2.33	15	1
1:A:64:LEU:CD2	1:A:64:LEU:N	0.58	2.65	17	14
2:B:166:VAL:O	2:B:168:PHE:CD2	0.58	2.56	2	10
2:B:231:TYR:N	2:B:232:PRO:HD2	0.58	2.13	18	25
1:A:28:ILE:C	1:A:28:ILE:HD13	0.58	2.17	2	9
1:A:23:ILE:CA	1:A:28:ILE:HG23	0.58	2.27	13	5
1:A:23:ILE:N	1:A:28:ILE:HG23	0.58	2.13	12	10
1:A:24:LEU:C	1:A:24:LEU:HD12	0.58	2.19	23	3
2:B:143:ILE:N	2:B:143:ILE:HD12	0.58	2.14	9	3
1:A:62:LEU:CD1	2:B:194:ILE:CD1	0.58	2.81	3	1
1:A:20:LEU:CB	1:A:68:LEU:CD2	0.58	2.81	10	2
1:A:64:LEU:N	1:A:64:LEU:CD2	0.58	2.66	20	5
1:A:55:ASN:OD1	2:B:190:PHE:CD2	0.58	2.57	2	2
1:A:28:ILE:HG22	1:A:34:LEU:CD2	0.58	2.29	6	2
2:B:160:ILE:HD12	2:B:219:GLN:N	0.58	2.14	6	1
1:A:52:LEU:N	1:A:52:LEU:CD1	0.58	2.67	13	1
2:B:208:VAL:O	2:B:209:SER:CB	0.58	2.52	13	1
1:A:27:ASN:ND2	2:B:125:GLY:CA	0.58	2.67	21	13
2:B:65:PRO:HG2	2:B:223:ILE:HG22	0.58	1.74	2	2
2:B:168:PHE:O	2:B:168:PHE:CD1	0.58	2.57	11	5
2:B:80:LEU:HD12	2:B:116:PHE:O	0.58	1.99	12	1
1:A:18:LEU:HD11	1:A:30:SER:CB	0.58	2.28	15	2
1:A:74:LEU:HB2	2:B:99:PHE:CD2	0.58	2.34	15	2
1:A:74:LEU:HB2	2:B:99:PHE:CE1	0.58	2.33	21	1
1:A:67:MET:O	1:A:71:VAL:HG23	0.58	1.99	3	5
1:A:23:ILE:CD1	1:A:28:ILE:HG23	0.58	2.29	24	2
1:A:68:LEU:CD1	1:A:68:LEU:N	0.58	2.67	9	1
1:A:30:SER:HB3	2:B:103:ILE:HD11	0.58	1.75	13	1
2:B:114:LEU:HD12	2:B:114:LEU:O	0.58	1.99	17	1
1:A:23:ILE:HG12	1:A:28:ILE:HD13	0.57	1.76	13	5
2:B:114:LEU:N	2:B:114:LEU:CD2	0.57	2.67	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:LEU:CD2	1:A:74:LEU:N	0.57	2.67	21	4
1:A:29:ASP:O	1:A:31:GLU:N	0.57	2.37	15	25
2:B:114:LEU:O	2:B:116:PHE:CE1	0.57	2.57	16	7
2:B:143:ILE:HG23	2:B:148:PHE:CB	0.57	2.30	15	3
2:B:63:ILE:O	2:B:227:PHE:CE2	0.57	2.58	14	1
2:B:73:THR:HG23	2:B:122:VAL:HG22	0.57	1.77	21	2
1:A:26:GLY:O	1:A:27:ASN:O	0.57	2.22	1	10
1:A:18:LEU:HD13	1:A:30:SER:CB	0.57	2.25	12	7
1:A:19:ASP:HA	1:A:68:LEU:HD11	0.57	1.76	24	3
2:B:212:ILE:CD1	2:B:212:ILE:N	0.57	2.67	16	2
2:B:175:LEU:HD11	2:B:195:TYR:CE2	0.57	2.34	13	1
2:B:207:PHE:C	2:B:208:VAL:HG23	0.57	2.20	13	1
1:A:72:ILE:CG1	1:A:74:LEU:HD12	0.57	2.29	19	3
2:B:183:SER:OG	2:B:195:TYR:CD2	0.57	2.57	25	1
2:B:112:THR:CG2	2:B:124:THR:CG2	0.57	2.82	6	3
2:B:143:ILE:N	2:B:143:ILE:CD1	0.57	2.67	10	5
2:B:74:VAL:HG21	2:B:136:SER:HB3	0.57	1.75	4	1
2:B:99:PHE:CE1	2:B:101:ALA:HB3	0.57	2.34	11	1
2:B:76:LEU:HD12	2:B:119:GLY:O	0.57	1.99	6	6
1:A:52:LEU:HD12	1:A:52:LEU:O	0.57	1.99	7	1
1:A:25:PHE:CE1	1:A:52:LEU:CD1	0.57	2.87	24	5
2:B:190:PHE:CE1	2:B:192:GLY:O	0.57	2.57	5	1
1:A:18:LEU:HB3	2:B:99:PHE:CG	0.57	2.34	15	6
2:B:143:ILE:O	2:B:146:ILE:N	0.57	2.37	6	1
2:B:80:LEU:HD22	2:B:148:PHE:HD2	0.57	1.60	9	1
1:A:52:LEU:HD21	2:B:205:LEU:CD1	0.57	2.28	16	3
1:A:55:ASN:OD1	2:B:190:PHE:CD1	0.57	2.57	22	1
2:B:214:LEU:HD12	2:B:214:LEU:H	0.57	1.60	15	2
1:A:23:ILE:HD12	2:B:114:LEU:HD23	0.57	1.77	8	2
2:B:213:VAL:C	2:B:214:LEU:HD12	0.57	2.20	1	7
2:B:214:LEU:N	2:B:214:LEU:CD1	0.57	2.68	4	3
2:B:223:ILE:CG2	2:B:224:TYR:N	0.57	2.68	24	2
1:A:59:LEU:HD13	2:B:190:PHE:CE2	0.57	2.35	20	1
1:A:26:GLY:O	1:A:27:ASN:C	0.56	2.44	18	19
2:B:144:GLN:HG3	2:B:150:ALA:HB3	0.56	1.77	13	1
2:B:182:PHE:CE2	2:B:198:VAL:CG2	0.56	2.87	21	1
1:A:74:LEU:HD21	2:B:116:PHE:CD1	0.56	2.35	18	1
1:A:27:ASN:CG	1:A:35:LEU:HD11	0.56	2.20	10	5
1:A:27:ASN:OD1	2:B:125:GLY:N	0.56	2.39	4	1
1:A:25:PHE:HE2	1:A:52:LEU:HD21	0.56	1.58	7	1
2:B:211:LYS:C	2:B:212:ILE:HD12	0.56	2.20	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:GLY:O	1:A:28:ILE:N	0.56	2.39	14	5
2:B:190:PHE:CE2	2:B:194:ILE:HG13	0.56	2.36	21	2
1:A:24:LEU:CD1	1:A:64:LEU:CD1	0.56	2.83	20	1
1:A:20:LEU:CD1	1:A:72:ILE:HB	0.56	2.31	20	19
2:B:182:PHE:CD1	2:B:198:VAL:HG22	0.56	2.35	3	1
2:B:189:LEU:HD23	2:B:190:PHE:HB2	0.56	1.77	19	6
1:A:21:THR:HG23	1:A:64:LEU:HB3	0.56	1.75	11	1
1:A:74:LEU:O	2:B:99:PHE:CE2	0.56	2.58	12	1
1:A:68:LEU:N	1:A:68:LEU:HD23	0.56	2.15	13	3
2:B:82:LEU:HD11	2:B:117:ALA:HB2	0.56	1.76	22	1
2:B:76:LEU:O	2:B:151:LYS:CB	0.56	2.53	6	2
1:A:25:PHE:CZ	2:B:205:LEU:CD1	0.56	2.86	17	4
2:B:172:LEU:O	2:B:176:ALA:HB2	0.56	2.01	10	1
1:A:18:LEU:CD1	1:A:30:SER:O	0.56	2.54	5	7
1:A:18:LEU:CD1	1:A:30:SER:HB2	0.56	2.31	4	7
1:A:74:LEU:HB2	2:B:99:PHE:CE2	0.56	2.35	15	5
2:B:113:ALA:HB1	2:B:122:VAL:O	0.56	2.01	6	3
1:A:21:THR:HG23	1:A:64:LEU:CB	0.56	2.31	11	1
2:B:75:THR:HG23	2:B:120:LYS:HG3	0.56	1.78	13	1
2:B:99:PHE:C	2:B:99:PHE:CD1	0.56	2.78	20	8
1:A:28:ILE:CB	1:A:33:ARG:O	0.56	2.54	4	10
1:A:24:LEU:O	2:B:161:VAL:HG22	0.56	2.01	25	2
2:B:103:ILE:N	2:B:103:ILE:HD13	0.56	2.16	15	1
1:A:74:LEU:HB2	2:B:99:PHE:CD1	0.56	2.36	21	1
1:A:23:ILE:CG2	1:A:71:VAL:CG1	0.55	2.83	11	3
2:B:112:THR:HG22	2:B:124:THR:CG2	0.55	2.31	16	2
2:B:182:PHE:CE1	2:B:198:VAL:HG21	0.55	2.36	10	1
1:A:74:LEU:CB	2:B:99:PHE:CD2	0.55	2.89	15	1
2:B:80:LEU:HD13	2:B:143:ILE:HD13	0.55	1.78	19	2
2:B:166:VAL:HG11	2:B:234:LEU:CD1	0.55	2.28	19	1
2:B:104:MET:SD	2:B:142:ILE:HD13	0.55	2.42	4	1
1:A:68:LEU:N	1:A:68:LEU:HD12	0.55	2.16	9	1
1:A:28:ILE:HD13	1:A:28:ILE:O	0.55	2.02	2	10
1:A:20:LEU:HB2	1:A:68:LEU:CD2	0.55	2.32	10	2
1:A:30:SER:OG	2:B:99:PHE:CE2	0.55	2.56	11	1
1:A:72:ILE:HD12	1:A:74:LEU:HD12	0.55	1.78	12	2
2:B:82:LEU:HD11	2:B:100:ALA:O	0.55	2.01	15	2
2:B:85:VAL:CG2	2:B:148:PHE:CE2	0.55	2.88	15	1
1:A:25:PHE:CZ	2:B:205:LEU:HD12	0.55	2.36	16	1
1:A:74:LEU:HD12	2:B:99:PHE:CG	0.55	2.36	21	1
2:B:116:PHE:CD2	2:B:120:LYS:O	0.55	2.59	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:166:VAL:HG23	2:B:168:PHE:O	0.55	2.01	22	5
2:B:103:ILE:H	2:B:103:ILE:HD12	0.55	1.62	10	2
1:A:71:VAL:O	2:B:122:VAL:CG2	0.55	2.54	20	2
2:B:112:THR:CG2	2:B:113:ALA:N	0.55	2.69	8	4
1:A:23:ILE:CB	2:B:124:THR:HG21	0.55	2.32	20	1
1:A:26:GLY:O	1:A:28:ILE:CG2	0.55	2.54	6	4
1:A:23:ILE:HG22	2:B:124:THR:HG21	0.55	1.78	20	1
1:A:18:LEU:N	1:A:74:LEU:HD11	0.55	2.16	21	1
1:A:23:ILE:HG12	1:A:28:ILE:CG1	0.55	2.32	5	6
1:A:20:LEU:CD1	1:A:71:VAL:HB	0.55	2.31	12	17
1:A:56:ILE:N	1:A:59:LEU:HD12	0.55	2.17	13	8
1:A:23:ILE:CD1	2:B:114:LEU:HD21	0.55	2.32	15	2
1:A:25:PHE:CE1	1:A:52:LEU:HD13	0.55	2.37	4	7
2:B:195:TYR:CD2	2:B:230:ILE:HD11	0.55	2.37	24	1
1:A:20:LEU:O	1:A:24:LEU:HD23	0.54	2.01	15	5
1:A:22:GLY:O	1:A:26:GLY:N	0.54	2.40	21	16
2:B:81:ASP:O	2:B:85:VAL:HG23	0.54	2.02	12	1
1:A:27:ASN:OD1	1:A:35:LEU:CG	0.54	2.55	18	1
1:A:21:THR:HG23	1:A:56:ILE:HG23	0.54	1.79	19	1
2:B:160:ILE:HD12	2:B:219:GLN:CA	0.54	2.32	6	1
1:A:67:MET:O	1:A:71:VAL:CG2	0.54	2.56	15	3
2:B:166:VAL:O	2:B:167:LYS:CB	0.54	2.56	2	15
2:B:89:ALA:HB3	2:B:92:ALA:HB3	0.54	1.77	7	5
1:A:23:ILE:CG1	1:A:28:ILE:HG23	0.54	2.32	15	2
1:A:27:ASN:OD1	2:B:125:GLY:CA	0.54	2.56	4	1
1:A:30:SER:OG	2:B:103:ILE:CD1	0.54	2.56	6	1
2:B:99:PHE:CE1	2:B:101:ALA:HB2	0.54	2.37	21	1
1:A:18:LEU:CA	2:B:99:PHE:CE1	0.54	2.91	2	3
1:A:59:LEU:HD21	2:B:190:PHE:CZ	0.54	2.38	22	3
1:A:27:ASN:ND2	1:A:35:LEU:HD21	0.54	2.17	19	2
2:B:99:PHE:O	2:B:101:ALA:N	0.54	2.39	21	1
1:A:18:LEU:CA	2:B:99:PHE:CD1	0.54	2.90	16	4
1:A:26:GLY:O	1:A:34:LEU:CD1	0.54	2.56	23	2
1:A:74:LEU:HB3	2:B:99:PHE:CE2	0.54	2.37	8	2
1:A:59:LEU:HD12	1:A:62:LEU:HD21	0.54	1.79	20	1
1:A:62:LEU:HD13	2:B:194:ILE:HG21	0.54	1.79	23	3
1:A:55:ASN:O	1:A:59:LEU:N	0.54	2.40	20	7
2:B:160:ILE:HD12	2:B:219:GLN:C	0.54	2.23	4	3
2:B:170:ILE:N	2:B:209:SER:CB	0.54	2.70	13	1
1:A:24:LEU:HD22	1:A:67:MET:SD	0.54	2.43	7	1
2:B:172:LEU:CD1	2:B:191:PRO:O	0.54	2.56	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:LEU:O	1:A:20:LEU:N	0.54	2.41	10	7
1:A:64:LEU:HD12	1:A:64:LEU:O	0.54	2.03	9	1
1:A:65:ASP:O	1:A:68:LEU:CB	0.54	2.56	2	2
2:B:126:ALA:HB1	2:B:131:ASP:HB3	0.54	1.79	5	2
2:B:113:ALA:HB2	2:B:139:TYR:CZ	0.54	2.38	4	2
2:B:75:THR:OG1	2:B:154:ASP:CB	0.54	2.56	9	1
1:A:25:PHE:HE1	2:B:213:VAL:HG11	0.54	1.63	20	3
2:B:206:ILE:HG13	2:B:212:ILE:HD12	0.54	1.80	3	2
1:A:35:LEU:C	1:A:35:LEU:CD1	0.54	2.77	17	12
2:B:190:PHE:CD2	2:B:194:ILE:HD11	0.54	2.37	19	3
1:A:18:LEU:O	1:A:19:ASP:CB	0.54	2.54	16	2
2:B:178:SER:OG	2:B:237:PHE:CZ	0.53	2.58	1	2
2:B:166:VAL:CG2	2:B:168:PHE:O	0.53	2.57	24	4
2:B:144:GLN:HG3	2:B:150:ALA:CB	0.53	2.33	6	1
2:B:82:LEU:CD1	2:B:100:ALA:O	0.53	2.57	15	4
1:A:72:ILE:HG13	1:A:74:LEU:HD13	0.53	1.76	21	1
1:A:20:LEU:H	1:A:68:LEU:HD21	0.53	1.63	4	2
1:A:59:LEU:O	1:A:59:LEU:CD1	0.53	2.56	21	4
2:B:189:LEU:O	2:B:189:LEU:CG	0.53	2.56	18	6
2:B:172:LEU:CD1	2:B:208:VAL:HG23	0.53	2.32	16	2
1:A:27:ASN:OD1	1:A:35:LEU:CB	0.53	2.56	18	1
1:A:27:ASN:ND2	2:B:125:GLY:HA2	0.53	2.18	22	13
1:A:18:LEU:HB2	2:B:99:PHE:CD2	0.53	2.38	8	2
1:A:74:LEU:HD21	2:B:116:PHE:HA	0.53	1.80	18	1
2:B:104:MET:SD	2:B:142:ILE:HG21	0.53	2.44	4	1
1:A:27:ASN:HB3	2:B:112:THR:HG22	0.53	1.80	20	1
2:B:126:ALA:CB	2:B:132:SER:OG	0.53	2.57	20	3
1:A:18:LEU:CG	1:A:20:LEU:HD23	0.53	2.34	10	3
1:A:18:LEU:HD11	1:A:30:SER:HA	0.53	1.81	19	4
1:A:26:GLY:O	1:A:34:LEU:CD2	0.53	2.57	1	2
2:B:155:PHE:CD1	2:B:155:PHE:C	0.53	2.81	14	6
2:B:205:LEU:HD12	2:B:207:PHE:CE1	0.53	2.39	7	1
2:B:69:ASN:O	2:B:70:ILE:CG1	0.53	2.57	17	4
1:A:72:ILE:HG12	2:B:99:PHE:CD2	0.53	2.38	15	1
2:B:85:VAL:O	2:B:89:ALA:HB2	0.53	2.03	16	4
2:B:70:ILE:N	2:B:126:ALA:O	0.53	2.42	23	13
1:A:27:ASN:OD1	1:A:27:ASN:N	0.53	2.41	19	3
1:A:30:SER:OG	2:B:103:ILE:HD11	0.53	2.03	8	5
1:A:27:ASN:O	1:A:35:LEU:CG	0.53	2.56	12	6
1:A:27:ASN:O	1:A:35:LEU:CD2	0.53	2.56	16	1
1:A:62:LEU:CD2	1:A:62:LEU:C	0.53	2.77	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ILE:HB	1:A:34:LEU:CA	0.53	2.34	20	8
2:B:204:LEU:N	2:B:204:LEU:CD1	0.53	2.66	23	6
1:A:74:LEU:N	1:A:74:LEU:CD2	0.53	2.72	6	1
2:B:168:PHE:CD1	2:B:168:PHE:C	0.53	2.82	11	6
1:A:27:ASN:HB3	2:B:125:GLY:N	0.53	2.19	17	2
2:B:76:LEU:O	2:B:151:LYS:N	0.53	2.42	12	1
1:A:59:LEU:HD22	2:B:190:PHE:CE1	0.53	2.39	21	1
1:A:28:ILE:CA	1:A:33:ARG:O	0.53	2.56	23	14
2:B:114:LEU:HD12	2:B:122:VAL:CB	0.53	2.33	2	4
2:B:169:PRO:CB	2:B:208:VAL:O	0.53	2.57	17	13
1:A:27:ASN:ND2	2:B:125:GLY:HA3	0.53	2.19	12	7
2:B:227:PHE:CE2	2:B:231:TYR:CE2	0.53	2.96	3	2
2:B:76:LEU:CD2	2:B:151:LYS:O	0.53	2.57	19	1
1:A:29:ASP:O	1:A:30:SER:C	0.53	2.48	5	25
1:A:21:THR:OG1	1:A:68:LEU:CD1	0.53	2.57	4	1
2:B:171:ARG:CG	2:B:171:ARG:O	0.53	2.56	9	2
2:B:63:ILE:HD13	2:B:165:ASP:O	0.53	2.04	14	2
2:B:70:ILE:CG1	2:B:160:ILE:HG23	0.53	2.34	9	1
2:B:190:PHE:CE2	2:B:194:ILE:CD1	0.53	2.92	9	1
1:A:24:LEU:HD11	1:A:64:LEU:HD13	0.53	1.81	11	1
1:A:68:LEU:CD2	1:A:68:LEU:C	0.53	2.77	11	1
2:B:166:VAL:CG2	2:B:209:SER:O	0.53	2.57	13	1
2:B:170:ILE:N	2:B:209:SER:HB3	0.53	2.19	13	1
1:A:18:LEU:CD2	1:A:20:LEU:HD23	0.53	2.34	18	1
1:A:30:SER:OG	2:B:99:PHE:CE1	0.53	2.58	23	2
1:A:51:GLU:O	1:A:55:ASN:ND2	0.52	2.43	2	19
1:A:28:ILE:HG12	1:A:29:ASP:N	0.52	2.17	9	18
1:A:23:ILE:CA	1:A:28:ILE:CG2	0.52	2.87	7	6
2:B:99:PHE:CE2	2:B:101:ALA:CB	0.52	2.78	22	3
2:B:144:GLN:HG3	2:B:150:ALA:HA	0.52	1.81	6	1
2:B:134:LEU:HD23	2:B:137:ARG:HD3	0.52	1.81	7	1
1:A:61:LYS:CG	1:A:61:LYS:O	0.52	2.57	19	3
1:A:21:THR:HG21	1:A:59:LEU:CB	0.52	2.34	13	5
2:B:176:ALA:O	2:B:180:GLY:CA	0.52	2.57	3	7
1:A:27:ASN:OD1	2:B:69:ASN:ND2	0.52	2.43	8	3
2:B:155:PHE:O	2:B:156:LYS:CG	0.52	2.57	8	1
2:B:189:LEU:O	2:B:189:LEU:CD2	0.52	2.57	24	4
2:B:196:ARG:CB	2:B:196:ARG:CZ	0.52	2.87	12	2
2:B:207:PHE:O	2:B:208:VAL:CB	0.52	2.55	13	1
2:B:168:PHE:C	2:B:168:PHE:CD1	0.52	2.82	23	4
1:A:22:GLY:C	1:A:28:ILE:CG2	0.52	2.77	21	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:172:LEU:HD22	2:B:193:LEU:HB3	0.52	1.80	7	3
2:B:207:PHE:O	2:B:208:VAL:HB	0.52	2.04	13	1
1:A:72:ILE:HG12	2:B:99:PHE:CE2	0.52	2.39	15	1
2:B:140:ALA:O	2:B:144:GLN:NE2	0.52	2.43	23	2
1:A:27:ASN:ND2	1:A:35:LEU:CD1	0.52	2.66	23	6
1:A:70:GLU:O	1:A:70:GLU:CG	0.52	2.57	22	5
2:B:115:ILE:C	2:B:116:PHE:CD1	0.52	2.82	8	8
2:B:63:ILE:C	2:B:64:VAL:HG23	0.52	2.25	11	3
2:B:170:ILE:HG12	2:B:234:LEU:HD22	0.52	1.81	5	1
2:B:115:ILE:HD12	2:B:115:ILE:N	0.52	2.20	7	2
2:B:68:GLN:O	2:B:69:ASN:ND2	0.52	2.43	8	1
2:B:166:VAL:HG23	2:B:167:LYS:H	0.52	1.63	20	1
2:B:152:PHE:O	2:B:152:PHE:CG	0.52	2.61	1	1
1:A:27:ASN:ND2	2:B:124:THR:O	0.52	2.41	4	3
2:B:206:ILE:HG23	2:B:212:ILE:CD1	0.52	2.35	6	2
2:B:172:LEU:O	2:B:176:ALA:CB	0.52	2.58	10	2
1:A:62:LEU:C	1:A:62:LEU:CD2	0.52	2.78	13	2
2:B:196:ARG:CD	2:B:203:VAL:HG22	0.52	2.33	16	1
2:B:172:LEU:O	2:B:193:LEU:CD1	0.52	2.57	21	1
2:B:168:PHE:CE1	2:B:170:ILE:HG13	0.52	2.39	17	1
2:B:70:ILE:HD13	2:B:160:ILE:HG23	0.52	1.80	4	1
2:B:70:ILE:HG22	2:B:71:VAL:N	0.52	2.19	8	8
2:B:110:LYS:O	2:B:111:THR:CG2	0.52	2.57	15	4
2:B:196:ARG:CG	2:B:196:ARG:O	0.52	2.58	15	1
2:B:76:LEU:HB3	2:B:149:ALA:CB	0.52	2.35	12	1
2:B:170:ILE:CD1	2:B:209:SER:HB3	0.52	2.33	13	1
1:A:18:LEU:CB	2:B:99:PHE:HB3	0.52	2.34	23	2
2:B:227:PHE:O	2:B:230:ILE:HG22	0.52	2.05	23	1
1:A:23:ILE:HA	1:A:28:ILE:HG23	0.52	1.79	4	3
1:A:67:MET:SD	2:B:216:GLY:CA	0.52	2.98	10	3
2:B:153:THR:O	2:B:154:ASP:CB	0.52	2.58	12	13
1:A:62:LEU:CD1	2:B:194:ILE:HD13	0.52	2.34	12	2
2:B:114:LEU:HB2	2:B:122:VAL:HG12	0.52	1.83	4	1
2:B:76:LEU:CG	2:B:121:MET:SD	0.52	2.97	6	1
2:B:144:GLN:NE2	2:B:150:ALA:O	0.52	2.43	9	6
1:A:24:LEU:O	2:B:161:VAL:CG2	0.52	2.58	16	4
2:B:79:ARG:CG	2:B:117:ALA:O	0.51	2.58	2	1
2:B:141:ARG:O	2:B:145:LYS:CB	0.51	2.59	23	3
2:B:74:VAL:HG12	2:B:75:THR:N	0.51	2.20	13	2
1:A:52:LEU:HB3	2:B:190:PHE:CZ	0.51	2.40	13	1
1:A:20:LEU:HD13	1:A:23:ILE:HB	0.51	1.82	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:PHE:HZ	2:B:205:LEU:HD12	0.51	1.65	16	1
2:B:160:ILE:HG22	2:B:161:VAL:N	0.51	2.19	18	1
2:B:99:PHE:CD1	2:B:99:PHE:C	0.51	2.83	21	1
2:B:65:PRO:CG	2:B:223:ILE:HG22	0.51	2.36	21	3
2:B:144:GLN:CG	2:B:150:ALA:HB1	0.51	2.27	6	1
2:B:217:ALA:CB	2:B:223:ILE:HD12	0.51	2.35	7	1
2:B:113:ALA:CB	2:B:139:TYR:CE2	0.51	2.93	11	1
2:B:137:ARG:HD2	2:B:152:PHE:CE2	0.51	2.41	16	1
1:A:64:LEU:O	1:A:68:LEU:CD1	0.51	2.58	18	1
2:B:71:VAL:HG22	2:B:124:THR:OG1	0.51	2.05	1	2
2:B:116:PHE:CD2	2:B:120:LYS:HB3	0.51	2.40	17	2
2:B:204:LEU:HD21	2:B:226:ALA:CB	0.51	2.25	20	4
1:A:62:LEU:CD2	2:B:194:ILE:HD13	0.51	2.35	12	3
1:A:27:ASN:ND2	2:B:124:THR:C	0.51	2.63	15	3
2:B:107:ARG:O	2:B:108:GLU:CG	0.51	2.58	20	1
2:B:220:ARG:HG2	2:B:224:TYR:CE1	0.51	2.41	21	1
1:A:33:ARG:CD	1:A:33:ARG:C	0.51	2.79	17	14
1:A:52:LEU:O	1:A:55:ASN:N	0.51	2.43	9	5
1:A:68:LEU:C	1:A:68:LEU:CD1	0.51	2.79	12	11
1:A:59:LEU:O	1:A:59:LEU:CG	0.51	2.59	18	3
1:A:29:ASP:N	1:A:33:ARG:O	0.51	2.43	16	16
2:B:143:ILE:CG2	2:B:148:PHE:HB2	0.51	2.36	16	11
2:B:110:LYS:C	2:B:111:THR:HG23	0.51	2.25	13	4
2:B:230:ILE:HD13	2:B:230:ILE:O	0.51	2.06	13	1
1:A:62:LEU:O	2:B:196:ARG:NH2	0.51	2.43	19	1
2:B:206:ILE:HG12	2:B:234:LEU:HD21	0.51	1.82	20	1
1:A:72:ILE:HD12	2:B:116:PHE:CE2	0.51	2.40	21	1
2:B:224:TYR:O	2:B:228:GLU:CG	0.51	2.57	21	1
1:A:28:ILE:HA	1:A:33:ARG:O	0.51	2.06	23	10
2:B:165:ASP:OD1	2:B:165:ASP:N	0.51	2.43	6	3
2:B:160:ILE:CD1	2:B:219:GLN:CA	0.51	2.89	15	2
2:B:76:LEU:CD2	2:B:150:ALA:HB1	0.51	2.27	24	3
1:A:23:ILE:CG2	2:B:124:THR:HG21	0.51	2.36	20	1
1:A:18:LEU:HD13	1:A:30:SER:HB3	0.51	1.81	22	1
2:B:130:ASP:OD1	2:B:131:ASP:N	0.51	2.43	23	1
1:A:18:LEU:CD1	1:A:30:SER:HB3	0.51	2.36	22	2
2:B:95:ASN:N	2:B:95:ASN:OD1	0.51	2.43	11	1
2:B:170:ILE:CB	2:B:209:SER:HB3	0.51	2.36	13	1
2:B:175:LEU:HD11	2:B:233:VAL:HG11	0.51	1.81	18	1
2:B:105:ARG:O	2:B:105:ARG:CG	0.51	2.59	21	1
2:B:178:SER:OG	2:B:179:HIS:ND1	0.51	2.44	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LEU:HD23	1:A:35:LEU:H	0.51	1.65	11	2
1:A:71:VAL:CG1	2:B:71:VAL:HG11	0.51	2.35	11	1
2:B:76:LEU:O	2:B:151:LYS:CG	0.51	2.58	15	1
2:B:112:THR:HG23	2:B:113:ALA:N	0.51	2.21	19	1
2:B:170:ILE:HD12	2:B:210:GLY:HA2	0.51	1.82	16	4
2:B:189:LEU:C	2:B:189:LEU:HD23	0.51	2.25	20	3
1:A:21:THR:H	1:A:68:LEU:HD21	0.51	1.65	10	1
1:A:67:MET:SD	2:B:159:ASN:ND2	0.51	2.84	18	2
1:A:71:VAL:CA	2:B:122:VAL:HG21	0.51	2.36	13	1
1:A:23:ILE:CD1	1:A:28:ILE:HD13	0.51	2.36	17	1
1:A:59:LEU:HB2	1:A:62:LEU:HD12	0.51	1.82	21	1
1:A:18:LEU:CB	2:B:99:PHE:CB	0.51	2.89	22	2
1:A:71:VAL:CG1	2:B:122:VAL:HG21	0.51	2.35	25	1
2:B:201:LYS:CG	2:B:201:LYS:O	0.51	2.59	1	1
1:A:18:LEU:CD2	1:A:30:SER:HB2	0.51	2.36	11	4
2:B:220:ARG:CG	2:B:224:TYR:CE1	0.51	2.94	3	2
1:A:58:SER:HB2	2:B:189:LEU:HD11	0.51	1.83	4	1
2:B:67:LEU:HD11	2:B:220:ARG:HG3	0.51	1.83	4	1
1:A:65:ASP:HA	1:A:68:LEU:HD22	0.51	1.83	9	1
1:A:20:LEU:CD1	1:A:23:ILE:HG12	0.51	2.33	11	1
1:A:25:PHE:CE1	2:B:213:VAL:HG11	0.51	2.41	20	2
1:A:62:LEU:CD1	1:A:62:LEU:N	0.51	2.74	24	1
2:B:135:ALA:O	2:B:139:TYR:CD2	0.50	2.64	13	8
2:B:67:LEU:HD13	2:B:70:ILE:HD11	0.50	1.81	8	1
1:A:27:ASN:O	1:A:35:LEU:CB	0.50	2.59	25	6
2:B:81:ASP:OD1	2:B:81:ASP:N	0.50	2.44	20	1
2:B:76:LEU:HA	2:B:151:LYS:CB	0.50	2.36	6	1
1:A:30:SER:OG	2:B:99:PHE:CZ	0.50	2.56	25	2
1:A:21:THR:CG2	1:A:59:LEU:CB	0.50	2.89	22	3
1:A:20:LEU:O	1:A:23:ILE:N	0.50	2.44	5	4
1:A:68:LEU:C	1:A:68:LEU:CD2	0.50	2.79	4	2
1:A:35:LEU:CD2	2:B:112:THR:OG1	0.50	2.60	8	1
1:A:74:LEU:CG	2:B:116:PHE:CD1	0.50	2.93	18	1
2:B:199:LYS:CG	2:B:199:LYS:O	0.50	2.59	20	1
1:A:23:ILE:HD11	2:B:114:LEU:HD21	0.50	1.83	25	1
1:A:74:LEU:HD12	2:B:99:PHE:HB2	0.50	1.83	5	5
2:B:190:PHE:CE2	2:B:192:GLY:HA3	0.50	2.41	5	1
1:A:28:ILE:HD12	1:A:28:ILE:C	0.50	2.26	6	2
2:B:76:LEU:HD21	2:B:121:MET:SD	0.50	2.46	6	1
2:B:144:GLN:HG3	2:B:150:ALA:CA	0.50	2.36	6	1
1:A:19:ASP:C	1:A:20:LEU:HD23	0.50	2.27	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ILE:HD11	2:B:99:PHE:HE2	0.50	1.66	8	2
2:B:151:LYS:O	2:B:152:PHE:C	0.50	2.50	15	2
1:A:62:LEU:N	1:A:62:LEU:CD2	0.50	2.72	19	4
1:A:74:LEU:O	1:A:74:LEU:HG	0.50	2.07	5	4
1:A:23:ILE:CD1	2:B:114:LEU:HD23	0.50	2.37	8	1
2:B:73:THR:HG22	2:B:122:VAL:HG22	0.50	1.83	12	1
2:B:111:THR:HG22	2:B:125:GLY:HA3	0.50	1.82	2	2
1:A:18:LEU:HB3	2:B:99:PHE:CE2	0.50	2.41	13	2
2:B:85:VAL:HG22	2:B:148:PHE:CZ	0.50	2.41	12	1
2:B:190:PHE:CD2	2:B:192:GLY:O	0.50	2.64	19	2
1:A:34:LEU:C	1:A:34:LEU:CD2	0.50	2.72	20	1
2:B:70:ILE:CB	2:B:126:ALA:HB3	0.50	2.36	4	1
2:B:168:PHE:CD1	2:B:168:PHE:O	0.50	2.65	23	5
1:A:23:ILE:HA	1:A:28:ILE:HG22	0.50	1.83	7	1
1:A:27:ASN:CB	2:B:124:THR:CG2	0.50	2.86	16	6
2:B:190:PHE:CE2	2:B:194:ILE:HD11	0.50	2.42	9	2
2:B:166:VAL:HG21	2:B:168:PHE:CE1	0.50	2.42	24	1
1:A:23:ILE:HG21	1:A:71:VAL:CG1	0.50	2.37	14	3
1:A:28:ILE:HB	1:A:33:ARG:O	0.50	2.07	6	8
2:B:170:ILE:HG21	2:B:234:LEU:CD2	0.50	2.37	6	1
2:B:66:THR:O	2:B:162:GLY:CA	0.50	2.60	9	3
1:A:71:VAL:HA	2:B:122:VAL:HG21	0.50	1.82	13	1
2:B:160:ILE:CG2	2:B:161:VAL:N	0.50	2.75	18	1
2:B:166:VAL:HB	2:B:168:PHE:CZ	0.49	2.42	6	6
1:A:21:THR:CG2	1:A:59:LEU:HB2	0.49	2.37	2	3
1:A:27:ASN:O	1:A:35:LEU:HB2	0.49	2.07	25	7
2:B:185:TYR:O	2:B:185:TYR:CD2	0.49	2.65	3	1
1:A:55:ASN:HB3	2:B:190:PHE:CE1	0.49	2.42	8	1
1:A:21:THR:N	1:A:68:LEU:HD22	0.49	2.21	13	2
1:A:25:PHE:HZ	2:B:205:LEU:HD11	0.49	1.65	14	1
2:B:82:LEU:HD13	2:B:101:ALA:HA	0.49	1.83	22	1
2:B:152:PHE:C	2:B:152:PHE:CD1	0.49	2.81	1	1
1:A:20:LEU:O	1:A:22:GLY:N	0.49	2.45	4	8
2:B:206:ILE:HD12	2:B:206:ILE:N	0.49	2.22	5	2
1:A:55:ASN:HB3	2:B:190:PHE:CE2	0.49	2.42	10	1
2:B:103:ILE:HD12	2:B:103:ILE:N	0.49	2.21	10	2
2:B:178:SER:CB	2:B:237:PHE:CZ	0.49	2.95	10	3
1:A:24:LEU:HD22	1:A:67:MET:CB	0.49	2.37	13	2
2:B:115:ILE:HG13	2:B:121:MET:CG	0.49	2.37	17	1
1:A:18:LEU:CB	2:B:99:PHE:HB2	0.49	2.37	21	1
1:A:26:GLY:O	1:A:28:ILE:HG22	0.49	2.08	12	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ILE:C	1:A:28:ILE:CD1	0.49	2.79	20	7
2:B:179:HIS:O	2:B:183:SER:N	0.49	2.45	11	5
1:A:30:SER:HB3	2:B:103:ILE:HD12	0.49	1.83	15	1
2:B:63:ILE:HG22	2:B:64:VAL:N	0.49	2.22	19	1
1:A:20:LEU:CD1	1:A:23:ILE:HG13	0.49	2.34	11	2
2:B:201:LYS:O	2:B:202:ILE:CD1	0.49	2.60	3	2
1:A:53:ARG:CD	1:A:53:ARG:C	0.49	2.81	4	3
2:B:146:ILE:CG2	2:B:148:PHE:CE2	0.49	2.90	12	1
2:B:170:ILE:CG1	2:B:209:SER:HB3	0.49	2.37	13	1
2:B:99:PHE:CD1	2:B:99:PHE:N	0.49	2.80	23	7
1:A:72:ILE:O	1:A:74:LEU:N	0.49	2.43	15	3
2:B:86:ALA:HB2	2:B:102:VAL:HG13	0.49	1.82	11	1
2:B:182:PHE:CD1	2:B:198:VAL:CG2	0.49	2.95	10	2
2:B:238:ARG:NH2	2:B:239:LYS:O	0.49	2.45	5	1
2:B:81:ASP:CB	2:B:84:THR:OG1	0.49	2.60	12	1
1:A:52:LEU:CD2	1:A:52:LEU:C	0.49	2.80	13	1
1:A:30:SER:HB3	2:B:103:ILE:CD1	0.49	2.38	15	2
1:A:20:LEU:HD22	1:A:23:ILE:HD12	0.49	1.84	25	1
2:B:63:ILE:O	2:B:64:VAL:O	0.49	2.31	9	13
1:A:62:LEU:HD11	2:B:189:LEU:HG	0.49	1.83	5	1
2:B:170:ILE:HD13	2:B:206:ILE:HG23	0.49	1.85	16	2
2:B:78:CYS:H	2:B:149:ALA:HB1	0.49	1.66	12	1
2:B:165:ASP:OD1	2:B:166:VAL:N	0.49	2.45	12	1
2:B:198:VAL:O	2:B:201:LYS:N	0.49	2.45	15	1
1:A:18:LEU:HB2	2:B:99:PHE:HB3	0.49	1.84	23	2
1:A:27:ASN:CB	1:A:35:LEU:HG	0.49	2.37	25	1
2:B:238:ARG:C	2:B:238:ARG:CD	0.49	2.81	7	1
1:A:18:LEU:HA	2:B:99:PHE:CD1	0.49	2.42	16	4
1:A:23:ILE:HA	1:A:28:ILE:CG2	0.49	2.38	7	3
1:A:27:ASN:HB3	1:A:35:LEU:CG	0.49	2.38	4	3
2:B:123:VAL:HG13	2:B:139:TYR:HE2	0.49	1.68	10	2
2:B:75:THR:HG22	2:B:77:GLY:H	0.49	1.68	12	1
2:B:175:LEU:HD11	2:B:195:TYR:HE2	0.49	1.68	13	1
2:B:101:ALA:CB	2:B:115:ILE:O	0.49	2.56	21	1
2:B:63:ILE:HD13	2:B:231:TYR:CE2	0.49	2.43	22	1
1:A:23:ILE:N	1:A:28:ILE:HG12	0.49	2.23	1	2
1:A:29:ASP:HB3	2:B:103:ILE:HG21	0.49	1.84	9	1
1:A:23:ILE:CG1	1:A:28:ILE:HD12	0.49	2.34	15	1
1:A:34:LEU:HD12	1:A:53:ARG:CG	0.49	2.38	16	1
1:A:62:LEU:HB3	2:B:194:ILE:HG21	0.49	1.83	19	1
1:A:20:LEU:CD2	1:A:23:ILE:HG13	0.48	2.38	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:179:HIS:ND1	2:B:195:TYR:OH	0.48	2.46	7	1
2:B:166:VAL:O	2:B:167:LYS:HB2	0.48	2.08	20	5
1:A:24:LEU:HD13	1:A:67:MET:CE	0.48	2.37	12	1
1:A:20:LEU:HD13	1:A:23:ILE:CD1	0.48	2.37	20	1
1:A:74:LEU:HD12	2:B:99:PHE:CB	0.48	2.37	21	1
1:A:74:LEU:HD12	2:B:99:PHE:CD1	0.48	2.43	21	1
2:B:172:LEU:HD13	2:B:191:PRO:O	0.48	2.08	1	1
1:A:25:PHE:CD1	2:B:215:THR:HG21	0.48	2.44	3	1
1:A:23:ILE:HG12	1:A:28:ILE:HG13	0.48	1.84	18	3
2:B:166:VAL:HG22	2:B:210:GLY:O	0.48	2.08	14	6
2:B:68:GLN:NE2	2:B:163:SER:HB2	0.48	2.23	15	1
2:B:109:PRO:O	2:B:111:THR:N	0.48	2.46	12	2
1:A:27:ASN:ND2	2:B:125:GLY:N	0.48	2.61	7	2
1:A:64:LEU:N	1:A:64:LEU:HD22	0.48	2.23	21	6
2:B:69:ASN:OD1	2:B:70:ILE:N	0.48	2.47	10	1
1:A:67:MET:O	1:A:71:VAL:HG22	0.48	2.07	13	1
1:A:62:LEU:C	1:A:62:LEU:HD22	0.48	2.27	20	1
2:B:222:GLU:O	2:B:226:ALA:CB	0.48	2.61	3	1
1:A:52:LEU:CD2	1:A:53:ARG:N	0.48	2.74	13	1
1:A:61:LYS:H	1:A:62:LEU:HD13	0.48	1.68	13	1
1:A:31:GLU:O	2:B:98:ARG:NH2	0.48	2.46	5	1
2:B:81:ASP:O	2:B:83:LYS:N	0.48	2.47	6	2
2:B:94:TYR:HB2	2:B:102:VAL:HG22	0.48	1.84	6	1
1:A:20:LEU:CG	1:A:23:ILE:HG13	0.48	2.39	11	1
1:A:30:SER:CB	2:B:99:PHE:CE2	0.48	2.96	11	1
1:A:30:SER:CB	2:B:103:ILE:HG12	0.48	2.38	16	1
2:B:104:MET:HB3	2:B:139:TYR:CE1	0.48	2.43	14	6
2:B:211:LYS:C	2:B:212:ILE:HD13	0.48	2.29	7	2
2:B:143:ILE:HD12	2:B:143:ILE:H	0.48	1.68	13	1
1:A:65:ASP:OD1	1:A:66:SER:N	0.48	2.46	24	1
2:B:166:VAL:HB	2:B:168:PHE:CE2	0.48	2.44	11	3
1:A:29:ASP:N	1:A:29:ASP:OD1	0.48	2.44	11	2
1:A:62:LEU:HD11	1:A:64:LEU:HD23	0.48	1.85	4	1
1:A:74:LEU:CD1	2:B:99:PHE:HB2	0.48	2.38	14	2
1:A:52:LEU:CD1	1:A:59:LEU:CD1	0.48	2.92	7	1
1:A:27:ASN:OD1	1:A:35:LEU:O	0.48	2.32	13	1
1:A:18:LEU:HG	1:A:20:LEU:CD2	0.48	2.38	15	1
1:A:34:LEU:HD22	1:A:34:LEU:O	0.48	2.07	20	1
1:A:34:LEU:C	1:A:34:LEU:CD1	0.48	2.82	18	4
1:A:18:LEU:HG	1:A:19:ASP:N	0.48	2.22	24	4
2:B:137:ARG:HG3	2:B:138:LYS:N	0.48	2.23	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:148:PHE:O	2:B:149:ALA:C	0.48	2.52	12	2
1:A:27:ASN:HB2	1:A:35:LEU:CG	0.48	2.38	7	2
2:B:183:SER:HB2	2:B:195:TYR:CD2	0.48	2.43	9	1
2:B:69:ASN:C	2:B:69:ASN:ND2	0.48	2.67	18	1
2:B:78:CYS:O	2:B:79:ARG:O	0.48	2.32	20	1
2:B:99:PHE:CD1	2:B:100:ALA:N	0.48	2.82	21	1
2:B:168:PHE:CD1	2:B:238:ARG:HG2	0.48	2.43	23	1
2:B:208:VAL:O	2:B:209:SER:HB3	0.48	2.09	13	1
1:A:27:ASN:O	1:A:35:LEU:HG	0.48	2.08	1	12
2:B:80:LEU:HD21	2:B:149:ALA:HB2	0.48	1.85	6	1
2:B:160:ILE:CD1	2:B:219:GLN:N	0.48	2.77	15	2
2:B:79:ARG:O	2:B:80:LEU:CD2	0.48	2.56	17	1
2:B:121:MET:SD	2:B:123:VAL:CG2	0.48	3.02	17	2
1:A:24:LEU:HD13	1:A:64:LEU:HD12	0.48	1.84	20	1
1:A:18:LEU:HD13	2:B:99:PHE:CE1	0.48	2.44	25	1
1:A:28:ILE:CD1	1:A:29:ASP:O	0.47	2.60	5	3
1:A:28:ILE:HG12	1:A:33:ARG:O	0.47	2.08	3	10
1:A:72:ILE:HG13	1:A:72:ILE:O	0.47	2.08	14	7
2:B:106:ILE:CG2	2:B:139:TYR:CE1	0.47	2.96	24	2
2:B:164:CYS:SG	2:B:227:PHE:CE1	0.47	3.07	5	2
2:B:98:ARG:HD2	2:B:98:ARG:N	0.47	2.24	6	1
2:B:86:ALA:HB2	2:B:102:VAL:CG1	0.47	2.39	11	1
2:B:129:GLU:HG3	2:B:157:ILE:CD1	0.47	2.39	14	1
1:A:21:THR:OG1	1:A:68:LEU:CD2	0.47	2.61	17	2
2:B:126:ALA:HB1	2:B:132:SER:OG	0.47	2.09	25	2
1:A:62:LEU:HD13	1:A:63:GLY:N	0.47	2.24	24	1
2:B:231:TYR:CD1	2:B:231:TYR:C	0.47	2.87	1	1
1:A:18:LEU:CD2	1:A:72:ILE:HG12	0.47	2.33	17	3
1:A:52:LEU:O	1:A:56:ILE:N	0.47	2.47	13	4
2:B:190:PHE:CZ	2:B:194:ILE:HD11	0.47	2.43	9	1
2:B:64:VAL:CG1	2:B:224:TYR:OH	0.47	2.62	14	2
1:A:31:GLU:HG3	2:B:103:ILE:HD13	0.47	1.85	21	1
2:B:133:LYS:CD	2:B:155:PHE:CE2	0.47	2.97	24	2
1:A:27:ASN:HB2	1:A:35:LEU:HD21	0.47	1.86	1	2
1:A:18:LEU:HD11	1:A:20:LEU:HD23	0.47	1.86	8	2
2:B:107:ARG:O	2:B:108:GLU:CB	0.47	2.61	2	2
1:A:23:ILE:HG12	1:A:28:ILE:CD1	0.47	2.40	12	7
2:B:207:PHE:CD1	2:B:207:PHE:N	0.47	2.82	10	6
2:B:193:LEU:HD23	2:B:193:LEU:C	0.47	2.29	19	2
2:B:155:PHE:C	2:B:155:PHE:CD1	0.47	2.88	15	1
1:A:62:LEU:HD12	1:A:64:LEU:HD21	0.47	1.86	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:108:GLU:O	2:B:138:LYS:CD	0.47	2.63	23	1
2:B:166:VAL:HG23	2:B:168:PHE:H	0.47	1.70	1	1
2:B:190:PHE:HZ	2:B:205:LEU:HD11	0.47	1.69	5	1
2:B:151:LYS:O	2:B:152:PHE:O	0.47	2.32	15	2
1:A:20:LEU:HD13	1:A:23:ILE:CG1	0.47	2.40	15	1
2:B:76:LEU:CD1	2:B:80:LEU:CD1	0.47	2.90	19	2
2:B:80:LEU:HD12	2:B:115:ILE:CG2	0.47	2.40	21	1
1:A:26:GLY:C	1:A:27:ASN:ND2	0.47	2.67	1	1
1:A:18:LEU:HD13	2:B:99:PHE:CE2	0.47	2.45	4	1
1:A:27:ASN:HB3	1:A:35:LEU:HG	0.47	1.86	25	3
2:B:176:ALA:O	2:B:180:GLY:N	0.47	2.48	5	2
2:B:109:PRO:CG	2:B:135:ALA:HB2	0.47	2.40	6	1
2:B:148:PHE:O	2:B:150:ALA:N	0.47	2.48	6	1
2:B:85:VAL:O	2:B:89:ALA:CB	0.47	2.62	18	5
1:A:18:LEU:CD1	1:A:19:ASP:N	0.47	2.68	12	3
2:B:154:ASP:N	2:B:154:ASP:OD1	0.47	2.47	14	1
2:B:201:LYS:O	2:B:202:ILE:CG1	0.47	2.63	18	2
1:A:20:LEU:HG	1:A:72:ILE:CG2	0.47	2.40	15	14
1:A:65:ASP:O	1:A:68:LEU:HB3	0.47	2.09	12	5
1:A:62:LEU:HD13	2:B:194:ILE:HD11	0.47	1.85	3	1
2:B:88:HIS:HB3	2:B:146:ILE:CG1	0.47	2.39	6	1
2:B:148:PHE:C	2:B:150:ALA:N	0.47	2.68	6	1
1:A:58:SER:O	1:A:61:LYS:CD	0.47	2.62	16	2
1:A:20:LEU:CD2	1:A:72:ILE:HB	0.47	2.37	11	1
1:A:53:ARG:HA	1:A:56:ILE:CD1	0.47	2.39	13	3
2:B:172:LEU:HD13	2:B:192:GLY:HA2	0.47	1.87	25	1
1:A:23:ILE:CD1	1:A:28:ILE:HG13	0.47	2.40	1	2
1:A:74:LEU:CD2	1:A:74:LEU:H	0.47	2.23	5	4
2:B:180:GLY:O	2:B:183:SER:O	0.47	2.33	5	2
2:B:181:THR:HG23	2:B:182:PHE:CD1	0.47	2.45	5	1
1:A:74:LEU:C	1:A:74:LEU:HD23	0.47	2.29	21	3
2:B:70:ILE:CG2	2:B:71:VAL:N	0.47	2.78	24	6
2:B:221:GLU:N	2:B:221:GLU:CD	0.47	2.68	8	1
1:A:30:SER:HB3	2:B:103:ILE:CG1	0.47	2.39	16	2
1:A:34:LEU:HB2	1:A:53:ARG:NE	0.47	2.25	13	1
2:B:186:GLU:O	2:B:190:PHE:N	0.47	2.47	18	2
2:B:99:PHE:CE2	2:B:103:ILE:HD11	0.47	2.45	24	3
2:B:168:PHE:CD1	2:B:238:ARG:CG	0.47	2.97	23	1
2:B:143:ILE:CG2	2:B:150:ALA:CB	0.47	2.91	1	2
2:B:195:TYR:CE2	2:B:230:ILE:HD13	0.47	2.44	3	1
1:A:18:LEU:HD13	2:B:99:PHE:CD2	0.47	2.44	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:114:LEU:N	2:B:114:LEU:HD22	0.47	2.25	4	1
1:A:71:VAL:O	2:B:114:LEU:HD12	0.47	2.10	5	2
1:A:18:LEU:HB2	2:B:99:PHE:CB	0.47	2.39	8	3
1:A:55:ASN:C	1:A:59:LEU:HD12	0.47	2.30	13	1
1:A:23:ILE:HG12	1:A:28:ILE:CG2	0.47	2.40	15	1
2:B:212:ILE:N	2:B:212:ILE:CD1	0.47	2.78	15	1
1:A:20:LEU:HD22	1:A:23:ILE:CD1	0.47	2.39	25	1
1:A:20:LEU:O	1:A:21:THR:C	0.47	2.53	5	16
2:B:63:ILE:O	2:B:64:VAL:CB	0.47	2.63	11	4
1:A:20:LEU:HD22	1:A:23:ILE:CB	0.47	2.40	12	5
2:B:103:ILE:HD12	2:B:103:ILE:H	0.47	1.69	12	2
2:B:221:GLU:CA	2:B:221:GLU:OE1	0.47	2.62	13	1
1:A:62:LEU:HD22	2:B:194:ILE:HD11	0.47	1.86	17	1
1:A:23:ILE:HG13	1:A:24:LEU:N	0.47	2.25	20	1
1:A:27:ASN:C	1:A:28:ILE:CG2	0.47	2.80	20	1
1:A:61:LYS:HG3	1:A:62:LEU:N	0.47	2.24	24	1
1:A:73:ASP:CG	1:A:73:ASP:O	0.47	2.54	20	14
2:B:205:LEU:N	2:B:205:LEU:HD22	0.47	2.25	1	1
2:B:217:ALA:HB1	2:B:222:GLU:HB2	0.47	1.87	18	6
1:A:24:LEU:HG	1:A:25:PHE:N	0.47	2.24	11	5
2:B:76:LEU:CD1	2:B:121:MET:SD	0.47	3.03	6	1
2:B:137:ARG:HA	2:B:152:PHE:CE1	0.47	2.44	7	1
1:A:73:ASP:O	1:A:73:ASP:OD1	0.47	2.33	18	3
2:B:143:ILE:HG23	2:B:148:PHE:HB2	0.47	1.86	16	3
1:A:27:ASN:HB3	2:B:124:THR:CG2	0.47	2.38	18	3
2:B:89:ALA:CB	2:B:104:MET:CE	0.47	2.92	12	1
1:A:29:ASP:OD1	1:A:29:ASP:N	0.47	2.47	13	1
1:A:59:LEU:CD2	2:B:190:PHE:CE2	0.47	2.89	15	1
2:B:190:PHE:CE2	2:B:192:GLY:C	0.47	2.89	17	1
2:B:206:ILE:CG1	2:B:212:ILE:CD1	0.47	2.93	20	1
2:B:228:GLU:N	2:B:228:GLU:OE1	0.47	2.48	22	1
1:A:62:LEU:O	1:A:62:LEU:CD2	0.47	2.56	24	1
1:A:24:LEU:HD12	2:B:215:THR:OG1	0.46	2.10	3	1
2:B:116:PHE:CG	2:B:120:LYS:O	0.46	2.68	4	1
2:B:83:LYS:O	2:B:87:LEU:CB	0.46	2.63	15	3
2:B:177:PHE:C	2:B:177:PHE:CD1	0.46	2.88	24	2
2:B:137:ARG:HA	2:B:152:PHE:CZ	0.46	2.45	7	1
2:B:195:TYR:CD1	2:B:195:TYR:C	0.46	2.89	19	2
2:B:91:ASN:OD1	2:B:91:ASN:O	0.46	2.34	16	1
1:A:34:LEU:HD12	1:A:56:ILE:HD13	0.46	1.86	22	2
1:A:18:LEU:HD23	1:A:72:ILE:CB	0.46	2.40	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:104:MET:CB	2:B:113:ALA:HB3	0.46	2.40	8	1
1:A:27:ASN:OD1	1:A:35:LEU:CD2	0.46	2.57	9	2
1:A:18:LEU:HD23	1:A:20:LEU:HD22	0.46	1.85	11	1
1:A:28:ILE:HG22	1:A:34:LEU:CD1	0.46	2.41	17	1
2:B:166:VAL:CG2	2:B:168:PHE:CE1	0.46	2.98	24	1
2:B:95:ASN:O	2:B:95:ASN:OD1	0.46	2.34	2	1
1:A:21:THR:CG2	1:A:56:ILE:O	0.46	2.63	4	1
2:B:166:VAL:O	2:B:167:LYS:HB3	0.46	2.10	9	4
1:A:18:LEU:HD21	1:A:30:SER:HB2	0.46	1.86	7	2
1:A:22:GLY:O	1:A:25:PHE:N	0.46	2.48	16	5
2:B:66:THR:O	2:B:162:GLY:HA2	0.46	2.10	9	5
1:A:52:LEU:HB3	2:B:190:PHE:CE2	0.46	2.46	13	1
1:A:18:LEU:N	2:B:99:PHE:CE2	0.46	2.83	19	1
2:B:181:THR:O	2:B:182:PHE:CG	0.46	2.68	1	1
1:A:27:ASN:ND2	1:A:35:LEU:CG	0.46	2.78	22	2
2:B:75:THR:O	2:B:151:LYS:O	0.46	2.33	12	1
1:A:59:LEU:HB2	1:A:62:LEU:CD1	0.46	2.40	18	2
1:A:23:ILE:HD11	1:A:71:VAL:HG11	0.46	1.86	20	1
2:B:172:LEU:HB3	2:B:185:TYR:CE1	0.46	2.45	4	2
2:B:76:LEU:CD1	2:B:119:GLY:O	0.46	2.63	8	2
1:A:27:ASN:HB2	1:A:35:LEU:HD11	0.46	1.88	7	1
2:B:76:LEU:CB	2:B:149:ALA:CB	0.46	2.94	12	1
2:B:81:ASP:HB3	2:B:84:THR:OG1	0.46	2.11	12	1
1:A:29:ASP:C	1:A:31:GLU:N	0.46	2.69	12	25
2:B:175:LEU:HB3	2:B:193:LEU:CD1	0.46	2.41	1	1
1:A:72:ILE:HD11	2:B:99:PHE:CE2	0.46	2.45	8	1
1:A:20:LEU:HB3	1:A:23:ILE:HD11	0.46	1.88	20	1
2:B:155:PHE:O	2:B:156:LYS:HG3	0.46	2.11	8	1
2:B:128:SER:O	2:B:129:GLU:CB	0.46	2.62	14	1
2:B:168:PHE:CE1	2:B:170:ILE:CG1	0.46	2.98	17	1
1:A:23:ILE:HD13	1:A:28:ILE:H	0.46	1.71	18	1
2:B:134:LEU:O	2:B:138:LYS:CG	0.46	2.64	21	1
2:B:81:ASP:O	2:B:82:LEU:C	0.46	2.54	6	18
2:B:175:LEU:HB3	2:B:193:LEU:HD11	0.46	1.86	1	1
2:B:74:VAL:HG11	2:B:152:PHE:CD1	0.46	2.46	2	1
2:B:186:GLU:O	2:B:190:PHE:O	0.46	2.32	6	12
1:A:64:LEU:O	1:A:68:LEU:N	0.46	2.49	16	3
1:A:52:LEU:HD21	2:B:207:PHE:HZ	0.46	1.70	8	2
1:A:68:LEU:HD23	1:A:68:LEU:O	0.46	2.11	11	1
1:A:74:LEU:HB2	2:B:99:PHE:CZ	0.46	2.46	13	1
2:B:68:GLN:O	2:B:69:ASN:OD1	0.46	2.33	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:202:ILE:CG2	2:B:203:VAL:N	0.46	2.78	25	1
2:B:103:ILE:CD1	2:B:114:LEU:HB3	0.46	2.40	1	1
2:B:197:MET:N	2:B:202:ILE:O	0.46	2.49	23	2
2:B:76:LEU:O	2:B:151:LYS:HB2	0.46	2.11	6	2
2:B:146:ILE:CG2	2:B:148:PHE:CE1	0.46	2.99	6	1
1:A:29:ASP:CB	1:A:31:GLU:HG2	0.46	2.41	7	1
2:B:113:ALA:CA	2:B:122:VAL:O	0.46	2.64	12	1
2:B:128:SER:O	2:B:130:ASP:N	0.46	2.48	14	1
1:A:26:GLY:HA2	2:B:69:ASN:ND2	0.46	2.26	15	1
2:B:64:VAL:HG13	2:B:224:TYR:CE2	0.46	2.45	20	1
2:B:193:LEU:C	2:B:193:LEU:CD2	0.46	2.82	24	1
2:B:172:LEU:HB3	2:B:185:TYR:CD1	0.46	2.46	25	1
2:B:190:PHE:CZ	2:B:205:LEU:HD11	0.46	2.45	3	3
2:B:110:LYS:CG	2:B:110:LYS:O	0.46	2.64	6	1
2:B:175:LEU:HD12	2:B:179:HIS:CD2	0.46	2.46	7	1
2:B:195:TYR:HB2	2:B:206:ILE:CD1	0.46	2.41	10	1
1:A:24:LEU:HD13	1:A:67:MET:HB3	0.46	1.88	11	1
2:B:91:ASN:ND2	2:B:105:ARG:O	0.46	2.44	12	2
2:B:144:GLN:HG2	2:B:150:ALA:CB	0.46	2.41	12	1
2:B:172:LEU:HB3	2:B:185:TYR:CE2	0.46	2.46	12	1
1:A:20:LEU:O	1:A:24:LEU:CD2	0.46	2.64	15	3
2:B:193:LEU:O	2:B:205:LEU:HD23	0.46	2.11	16	1
1:A:33:ARG:O	1:A:33:ARG:HG3	0.45	2.11	7	12
1:A:55:ASN:HB3	1:A:59:LEU:CD1	0.45	2.41	5	1
1:A:63:GLY:O	1:A:65:ASP:N	0.45	2.50	16	3
2:B:78:CYS:O	2:B:119:GLY:CA	0.45	2.64	12	1
1:A:27:ASN:HB3	1:A:35:LEU:CD2	0.45	2.41	15	1
1:A:74:LEU:HD22	2:B:101:ALA:CB	0.45	2.39	18	2
1:A:24:LEU:O	2:B:161:VAL:HG21	0.45	2.10	19	1
1:A:18:LEU:O	1:A:68:LEU:CD1	0.45	2.58	20	2
2:B:169:PRO:HB3	2:B:208:VAL:O	0.45	2.12	3	9
1:A:21:THR:O	1:A:25:PHE:HB2	0.45	2.11	13	4
2:B:70:ILE:CG2	2:B:132:SER:OG	0.45	2.64	3	1
2:B:173:GLU:HG3	2:B:174:GLY:N	0.45	2.26	15	3
2:B:106:ILE:HG12	2:B:139:TYR:CZ	0.45	2.46	20	4
2:B:185:TYR:CD1	2:B:193:LEU:HD12	0.45	2.46	4	1
1:A:18:LEU:CD2	2:B:99:PHE:CD2	0.45	2.92	7	1
2:B:67:LEU:CD2	2:B:160:ILE:CG2	0.45	2.91	8	1
2:B:74:VAL:HG22	2:B:155:PHE:HA	0.45	1.86	8	2
2:B:74:VAL:O	2:B:121:MET:N	0.45	2.49	25	2
1:A:18:LEU:HG	1:A:20:LEU:HD23	0.45	1.87	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:LEU:HD21	2:B:205:LEU:HD13	0.45	1.87	16	1
2:B:202:ILE:HG23	2:B:215:THR:O	0.45	2.11	16	1
2:B:104:MET:N	2:B:113:ALA:O	0.45	2.49	22	2
1:A:68:LEU:HD23	1:A:68:LEU:N	0.45	2.26	3	1
2:B:137:ARG:HB2	2:B:137:ARG:CZ	0.45	2.41	3	1
2:B:144:GLN:CG	2:B:150:ALA:O	0.45	2.65	19	4
1:A:18:LEU:CG	1:A:20:LEU:HD21	0.45	2.42	17	2
1:A:35:LEU:CD2	2:B:112:THR:HB	0.45	2.42	5	1
1:A:33:ARG:HD3	1:A:34:LEU:N	0.45	2.27	10	2
2:B:151:LYS:O	2:B:153:THR:HG23	0.45	2.11	10	1
2:B:179:HIS:O	2:B:183:SER:CB	0.45	2.64	21	2
1:A:18:LEU:O	1:A:19:ASP:HB2	0.45	2.11	16	1
2:B:98:ARG:N	2:B:98:ARG:HD2	0.45	2.27	17	1
2:B:95:ASN:O	2:B:98:ARG:HG3	0.45	2.11	18	1
2:B:159:ASN:ND2	2:B:216:GLY:HA2	0.45	2.27	20	1
1:A:18:LEU:HB3	1:A:74:LEU:CD1	0.45	2.41	21	1
2:B:79:ARG:HG3	2:B:117:ALA:O	0.45	2.11	2	1
2:B:104:MET:HB3	2:B:115:ILE:CD1	0.45	2.42	4	1
2:B:115:ILE:CD1	2:B:121:MET:HG3	0.45	2.41	5	1
2:B:80:LEU:HD22	2:B:148:PHE:CD2	0.45	2.45	9	1
1:A:67:MET:SD	2:B:159:ASN:OD1	0.45	2.75	11	1
2:B:88:HIS:O	2:B:90:ARG:NH2	0.45	2.50	14	1
2:B:151:LYS:O	2:B:153:THR:OG1	0.45	2.33	21	3
1:A:18:LEU:HD11	1:A:30:SER:HB2	0.45	1.89	15	1
1:A:72:ILE:HD11	1:A:74:LEU:HB3	0.45	1.87	17	1
2:B:172:LEU:HD11	2:B:207:PHE:HA	0.45	1.88	17	1
1:A:27:ASN:O	1:A:34:LEU:HA	0.45	2.12	20	1
2:B:136:SER:HB3	2:B:152:PHE:CE1	0.45	2.46	22	1
1:A:72:ILE:CD1	2:B:116:PHE:CE1	0.45	2.98	24	1
1:A:30:SER:CB	2:B:103:ILE:CG1	0.45	2.94	16	1
1:A:74:LEU:HD21	2:B:116:PHE:HD1	0.45	1.72	18	1
2:B:175:LEU:HD23	2:B:237:PHE:HB2	0.45	1.88	20	1
2:B:81:ASP:O	2:B:84:THR:N	0.45	2.49	15	3
2:B:113:ALA:HA	2:B:122:VAL:O	0.45	2.12	9	6
1:A:27:ASN:OD1	1:A:35:LEU:C	0.45	2.55	13	1
1:A:74:LEU:H	1:A:74:LEU:CD2	0.45	2.25	14	1
1:A:65:ASP:HA	1:A:68:LEU:CD1	0.45	2.42	15	2
2:B:76:LEU:HD12	2:B:80:LEU:CD1	0.45	2.41	19	1
2:B:190:PHE:CD2	2:B:194:ILE:CD1	0.45	2.99	19	1
1:A:34:LEU:O	1:A:34:LEU:HD13	0.45	2.12	20	1
1:A:70:GLU:C	1:A:71:VAL:HG23	0.45	2.31	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:LEU:CB	1:A:72:ILE:HG12	0.45	2.41	22	1
1:A:19:ASP:O	1:A:19:ASP:OD2	0.45	2.35	23	1
2:B:98:ARG:HB3	2:B:99:PHE:CD1	0.45	2.46	25	1
2:B:227:PHE:HA	2:B:230:ILE:CG2	0.45	2.41	2	2
1:A:19:ASP:OD1	1:A:19:ASP:O	0.45	2.33	3	1
2:B:83:LYS:O	2:B:87:LEU:HD23	0.45	2.11	16	1
1:A:72:ILE:HD13	2:B:114:LEU:HD22	0.45	1.88	19	1
2:B:189:LEU:HD23	2:B:189:LEU:C	0.45	2.32	19	1
2:B:195:TYR:CG	2:B:230:ILE:HD13	0.45	2.46	1	1
2:B:201:LYS:O	2:B:201:LYS:CD	0.45	2.65	1	1
2:B:99:PHE:CD1	2:B:99:PHE:O	0.45	2.69	5	1
2:B:77:GLY:HA3	2:B:151:LYS:CB	0.45	2.42	12	1
2:B:82:LEU:CD2	2:B:102:VAL:HG23	0.45	2.30	17	1
2:B:192:GLY:HA3	2:B:207:PHE:CD1	0.45	2.47	19	2
1:A:27:ASN:CA	2:B:124:THR:OG1	0.45	2.65	20	1
2:B:176:ALA:O	2:B:180:GLY:HA3	0.45	2.12	22	1
2:B:185:TYR:CD1	2:B:185:TYR:C	0.45	2.88	23	1
1:A:72:ILE:O	1:A:72:ILE:HG13	0.45	2.11	1	14
1:A:18:LEU:HA	2:B:99:PHE:CE1	0.45	2.46	9	2
1:A:28:ILE:CG1	1:A:33:ARG:O	0.45	2.65	4	2
2:B:71:VAL:HB	2:B:159:ASN:CB	0.45	2.42	7	4
2:B:128:SER:OG	2:B:129:GLU:N	0.45	2.50	5	1
2:B:102:VAL:O	2:B:114:LEU:HA	0.45	2.12	20	3
1:A:22:GLY:O	1:A:23:ILE:C	0.45	2.55	16	8
1:A:24:LEU:HD13	1:A:67:MET:CB	0.45	2.41	11	1
2:B:169:PRO:HA	2:B:209:SER:OG	0.45	2.12	13	1
1:A:59:LEU:O	1:A:62:LEU:HD12	0.45	2.12	16	1
2:B:179:HIS:O	2:B:182:PHE:N	0.45	2.45	23	1
1:A:67:MET:SD	2:B:216:GLY:HA2	0.45	2.52	10	4
2:B:195:TYR:CG	2:B:230:ILE:CD1	0.45	3.00	1	1
2:B:205:LEU:N	2:B:205:LEU:CD2	0.45	2.80	1	1
2:B:217:ALA:CB	2:B:223:ILE:HG12	0.45	2.42	21	3
2:B:125:GLY:O	2:B:126:ALA:C	0.45	2.54	4	4
1:A:27:ASN:HB3	2:B:124:THR:OG1	0.45	2.12	17	11
2:B:161:VAL:HA	2:B:214:LEU:O	0.45	2.12	23	5
2:B:75:THR:HB	2:B:154:ASP:CB	0.45	2.42	11	4
2:B:71:VAL:HG13	2:B:123:VAL:O	0.45	2.12	6	3
2:B:79:ARG:HD3	2:B:117:ALA:O	0.45	2.12	6	1
2:B:160:ILE:CD1	2:B:219:GLN:HA	0.45	2.42	6	1
1:A:26:GLY:C	1:A:27:ASN:CG	0.45	2.75	20	2
1:A:22:GLY:HA3	1:A:28:ILE:CG2	0.45	2.42	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:GLY:C	1:A:28:ILE:HG23	0.45	2.33	16	1
2:B:206:ILE:HG23	2:B:234:LEU:HD21	0.45	1.89	25	1
2:B:168:PHE:CE1	2:B:238:ARG:HB3	0.44	2.47	3	1
1:A:29:ASP:CB	2:B:103:ILE:HG21	0.44	2.43	9	1
2:B:78:CYS:O	2:B:119:GLY:HA3	0.44	2.11	12	1
2:B:172:LEU:HD11	2:B:208:VAL:HA	0.44	1.89	13	1
2:B:74:VAL:HB	2:B:121:MET:CE	0.44	2.42	17	1
2:B:111:THR:HG22	2:B:124:THR:O	0.44	2.12	17	1
2:B:114:LEU:HD12	2:B:122:VAL:HG12	0.44	1.88	18	1
2:B:201:LYS:O	2:B:202:ILE:HG13	0.44	2.12	18	1
2:B:64:VAL:CG1	2:B:224:TYR:CE2	0.44	3.01	20	1
2:B:91:ASN:O	2:B:104:MET:SD	0.44	2.75	20	1
1:A:27:ASN:HB3	1:A:35:LEU:CD1	0.44	2.41	24	1
1:A:27:ASN:OD1	1:A:35:LEU:HG	0.44	2.12	13	3
2:B:63:ILE:O	2:B:64:VAL:HB	0.44	2.12	2	16
2:B:102:VAL:HG12	2:B:103:ILE:N	0.44	2.27	1	1
2:B:93:GLU:OE2	2:B:103:ILE:CG1	0.44	2.64	2	1
2:B:123:VAL:HG12	2:B:124:THR:N	0.44	2.27	5	2
2:B:136:SER:HG	2:B:152:PHE:HE1	0.44	1.52	6	1
1:A:20:LEU:HD12	1:A:71:VAL:CB	0.44	2.35	24	2
2:B:74:VAL:HG22	2:B:155:PHE:CD1	0.44	2.46	7	1
2:B:155:PHE:CD1	2:B:156:LYS:N	0.44	2.85	7	1
2:B:194:ILE:HG13	2:B:205:LEU:CD1	0.44	2.43	12	1
1:A:52:LEU:HD22	1:A:52:LEU:C	0.44	2.32	13	1
1:A:54:GLU:OE2	1:A:55:ASN:OD1	0.44	2.35	14	2
2:B:75:THR:CB	2:B:154:ASP:HB2	0.44	2.43	14	1
1:A:27:ASN:HD22	2:B:124:THR:HG23	0.44	1.72	15	2
1:A:23:ILE:HB	2:B:124:THR:CG2	0.44	2.42	20	1
1:A:52:LEU:HD21	2:B:190:PHE:CZ	0.44	2.46	20	1
2:B:133:LYS:O	2:B:137:ARG:HG2	0.44	2.13	3	1
2:B:137:ARG:CG	2:B:138:LYS:N	0.44	2.80	6	1
2:B:170:ILE:HG21	2:B:234:LEU:HD22	0.44	1.89	6	1
2:B:197:MET:CE	2:B:230:ILE:HG12	0.44	2.42	12	2
2:B:211:LYS:C	2:B:212:ILE:CD1	0.44	2.85	15	2
1:A:31:GLU:OE1	2:B:93:GLU:OE2	0.44	2.35	9	1
1:A:30:SER:HB2	2:B:99:PHE:CE2	0.44	2.47	11	2
1:A:29:ASP:HB2	1:A:33:ARG:CG	0.44	2.42	12	1
2:B:138:LYS:N	2:B:138:LYS:HD2	0.44	2.27	18	1
1:A:24:LEU:CD2	1:A:68:LEU:HD23	0.44	2.41	13	2
2:B:98:ARG:HB3	2:B:99:PHE:CD2	0.44	2.47	4	1
2:B:69:ASN:CB	2:B:161:VAL:HB	0.44	2.42	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:ASN:O	1:A:58:SER:N	0.44	2.43	12	5
1:A:24:LEU:CD2	1:A:68:LEU:HD12	0.44	2.41	9	1
1:A:71:VAL:CG1	2:B:122:VAL:CG1	0.44	2.91	10	1
1:A:23:ILE:HD11	1:A:28:ILE:O	0.44	2.13	13	1
2:B:221:GLU:HG3	2:B:222:GLU:N	0.44	2.26	19	2
2:B:206:ILE:HG13	2:B:212:ILE:CD1	0.44	2.41	20	1
2:B:64:VAL:CG1	2:B:65:PRO:HD2	0.44	2.41	21	1
1:A:18:LEU:CD2	2:B:114:LEU:HD13	0.44	2.42	22	1
1:A:62:LEU:HG	2:B:194:ILE:CD1	0.44	2.42	22	1
2:B:236:GLU:OE1	2:B:236:GLU:CA	0.44	2.64	22	1
1:A:59:LEU:O	1:A:62:LEU:CD1	0.44	2.65	16	2
2:B:207:PHE:O	2:B:209:SER:N	0.44	2.50	23	4
1:A:28:ILE:HD12	1:A:29:ASP:N	0.44	2.28	6	2
2:B:134:LEU:O	2:B:137:ARG:HG2	0.44	2.13	7	2
2:B:70:ILE:HA	2:B:159:ASN:O	0.44	2.13	8	1
2:B:114:LEU:HD12	2:B:122:VAL:HG11	0.44	1.85	12	1
2:B:116:PHE:CD2	2:B:120:LYS:CB	0.44	3.00	17	1
2:B:84:THR:O	2:B:88:HIS:N	0.44	2.50	22	2
1:A:64:LEU:O	1:A:65:ASP:C	0.44	2.56	6	12
2:B:71:VAL:N	2:B:159:ASN:O	0.44	2.51	10	2
2:B:136:SER:O	2:B:137:ARG:C	0.44	2.56	7	2
2:B:189:LEU:O	2:B:189:LEU:HG	0.44	2.11	16	6
1:A:20:LEU:HD12	1:A:71:VAL:CG2	0.44	2.42	13	1
1:A:27:ASN:HB3	1:A:35:LEU:HD21	0.44	1.89	15	1
1:A:20:LEU:CA	1:A:23:ILE:HB	0.44	2.42	22	1
1:A:70:GLU:C	1:A:71:VAL:CG2	0.44	2.85	2	4
2:B:64:VAL:HG12	2:B:224:TYR:CE1	0.44	2.48	4	1
1:A:28:ILE:CB	1:A:34:LEU:HA	0.44	2.43	7	3
1:A:61:LYS:O	1:A:62:LEU:HD23	0.44	2.13	5	1
2:B:177:PHE:CD1	2:B:177:PHE:C	0.44	2.91	8	1
2:B:106:ILE:HG13	2:B:109:PRO:O	0.44	2.13	9	1
2:B:123:VAL:HG13	2:B:139:TYR:CE2	0.44	2.47	16	2
1:A:21:THR:CG2	1:A:22:GLY:N	0.44	2.81	19	1
2:B:136:SER:HB3	2:B:152:PHE:CZ	0.44	2.47	22	1
1:A:22:GLY:O	1:A:28:ILE:CG2	0.44	2.66	1	1
2:B:227:PHE:O	2:B:231:TYR:HB2	0.44	2.13	1	1
2:B:152:PHE:CE1	2:B:155:PHE:HB2	0.44	2.48	3	1
1:A:18:LEU:CD2	2:B:114:LEU:HD11	0.44	2.43	13	2
2:B:206:ILE:HD13	2:B:206:ILE:N	0.44	2.24	9	1
1:A:65:ASP:O	1:A:69:LEU:HD23	0.44	2.13	11	2
2:B:129:GLU:CG	2:B:157:ILE:CD1	0.44	2.96	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:162:GLY:O	2:B:163:SER:OG	0.44	2.36	14	1
2:B:104:MET:O	2:B:112:THR:HA	0.44	2.12	15	2
1:A:27:ASN:ND2	1:A:35:LEU:CB	0.44	2.81	22	1
1:A:27:ASN:HA	2:B:124:THR:CG2	0.43	2.41	7	2
1:A:73:ASP:O	1:A:73:ASP:CG	0.43	2.55	7	3
2:B:147:GLY:O	2:B:148:PHE:C	0.43	2.56	25	3
1:A:63:GLY:O	1:A:64:LEU:C	0.43	2.56	16	4
1:A:30:SER:CB	2:B:114:LEU:HD23	0.43	2.43	16	1
2:B:84:THR:HG23	2:B:88:HIS:CE1	0.43	2.48	1	1
2:B:90:ARG:HG3	2:B:91:ASN:N	0.43	2.28	2	1
2:B:220:ARG:HG2	2:B:224:TYR:CD1	0.43	2.48	3	1
2:B:70:ILE:HB	2:B:126:ALA:O	0.43	2.13	4	2
1:A:27:ASN:CG	2:B:125:GLY:HA2	0.43	2.34	7	2
1:A:35:LEU:HD12	1:A:35:LEU:O	0.43	2.13	19	2
2:B:141:ARG:NH1	2:B:141:ARG:HG3	0.43	2.27	13	1
2:B:160:ILE:CD1	2:B:219:GLN:C	0.43	2.85	15	1
2:B:152:PHE:CD1	2:B:152:PHE:O	0.43	2.71	23	1
1:A:27:ASN:HB2	1:A:35:LEU:CD1	0.43	2.43	7	1
1:A:33:ARG:C	1:A:33:ARG:HD3	0.43	2.34	13	3
1:A:61:LYS:HG3	1:A:62:LEU:CD2	0.43	2.44	7	1
1:A:20:LEU:HD21	2:B:114:LEU:HD22	0.43	1.90	10	1
2:B:89:ALA:CB	2:B:104:MET:HE1	0.43	2.43	12	1
2:B:85:VAL:HG12	2:B:102:VAL:HG11	0.43	1.89	18	3
1:A:55:ASN:ND2	2:B:190:PHE:CE1	0.43	2.86	19	1
1:A:30:SER:OG	2:B:95:ASN:ND2	0.43	2.51	2	1
2:B:93:GLU:CG	2:B:103:ILE:HB	0.43	2.43	23	2
2:B:227:PHE:O	2:B:231:TYR:N	0.43	2.50	19	4
2:B:230:ILE:HG13	2:B:234:LEU:CD1	0.43	2.44	2	1
1:A:25:PHE:CE2	1:A:52:LEU:HD13	0.43	2.49	3	1
1:A:21:THR:N	1:A:68:LEU:HG	0.43	2.28	4	2
2:B:141:ARG:O	2:B:145:LYS:HB2	0.43	2.13	5	1
2:B:68:GLN:O	2:B:69:ASN:CG	0.43	2.57	17	3
1:A:67:MET:SD	2:B:216:GLY:HA3	0.43	2.53	10	1
1:A:59:LEU:HD21	2:B:190:PHE:HE2	0.43	1.71	14	1
2:B:114:LEU:CD1	2:B:122:VAL:HB	0.43	2.43	15	1
2:B:77:GLY:O	2:B:78:CYS:SG	0.43	2.76	18	1
2:B:122:VAL:C	2:B:123:VAL:CG2	0.43	2.86	20	1
2:B:124:THR:OG1	2:B:125:GLY:N	0.43	2.51	20	1
1:A:20:LEU:HB3	1:A:23:ILE:CG2	0.43	2.43	22	1
2:B:86:ALA:HB2	2:B:102:VAL:CG2	0.43	2.44	23	1
2:B:185:TYR:O	2:B:185:TYR:CG	0.43	2.71	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ILE:HG23	2:B:124:THR:CB	0.43	2.43	25	1
1:A:20:LEU:C	1:A:22:GLY:N	0.43	2.72	4	3
1:A:52:LEU:O	1:A:53:ARG:C	0.43	2.57	9	5
2:B:142:ILE:O	2:B:146:ILE:CG1	0.43	2.67	4	1
2:B:79:ARG:HG2	2:B:80:LEU:N	0.43	2.28	16	2
2:B:82:LEU:HB3	2:B:94:TYR:CE1	0.43	2.48	7	2
2:B:196:ARG:CZ	2:B:196:ARG:HB3	0.43	2.43	12	1
1:A:72:ILE:O	1:A:74:LEU:HD22	0.43	2.13	21	2
2:B:70:ILE:HG13	2:B:128:SER:N	0.43	2.29	15	1
1:A:30:SER:HB2	2:B:114:LEU:HD23	0.43	1.91	16	1
2:B:82:LEU:HA	2:B:102:VAL:CG2	0.43	2.44	17	1
1:A:27:ASN:HA	2:B:124:THR:OG1	0.43	2.13	20	1
1:A:74:LEU:H	1:A:74:LEU:HD22	0.43	1.72	21	1
1:A:50:ALA:O	1:A:54:GLU:HG2	0.43	2.14	16	4
2:B:207:PHE:O	2:B:208:VAL:C	0.43	2.57	8	4
2:B:76:LEU:HD13	2:B:149:ALA:HB1	0.43	1.90	6	1
2:B:78:CYS:O	2:B:79:ARG:C	0.43	2.57	6	1
2:B:83:LYS:O	2:B:87:LEU:HB2	0.43	2.14	14	2
2:B:99:PHE:CD1	2:B:101:ALA:HB3	0.43	2.49	11	1
1:A:64:LEU:CD1	1:A:68:LEU:HD21	0.43	2.42	3	1
2:B:195:TYR:CE1	2:B:197:MET:SD	0.43	3.12	13	1
2:B:109:PRO:O	2:B:110:LYS:C	0.43	2.57	15	1
2:B:212:ILE:N	2:B:212:ILE:HD12	0.43	2.28	16	1
1:A:21:THR:HA	1:A:68:LEU:HD11	0.43	1.90	18	1
2:B:208:VAL:HG23	2:B:209:SER:H	0.43	1.73	18	1
2:B:80:LEU:CD2	2:B:148:PHE:HB2	0.43	2.44	6	1
2:B:140:ALA:CB	2:B:144:GLN:NE2	0.43	2.74	12	1
1:A:69:LEU:HD12	1:A:69:LEU:C	0.43	2.34	13	1
2:B:195:TYR:O	2:B:204:LEU:N	0.43	2.49	15	2
1:A:27:ASN:OD1	1:A:35:LEU:CD1	0.43	2.61	16	5
1:A:74:LEU:CB	2:B:99:PHE:CE1	0.43	3.01	21	1
2:B:196:ARG:O	2:B:197:MET:C	0.43	2.57	1	2
1:A:18:LEU:CG	1:A:19:ASP:N	0.43	2.81	5	3
2:B:175:LEU:HD22	2:B:237:PHE:CD2	0.43	2.48	15	2
1:A:59:LEU:HD22	2:B:190:PHE:CZ	0.43	2.45	11	1
2:B:106:ILE:HD13	2:B:138:LYS:HB3	0.43	1.89	12	1
2:B:143:ILE:HG22	2:B:148:PHE:HB3	0.43	1.91	19	1
2:B:123:VAL:HG21	2:B:136:SER:OG	0.43	2.14	23	1
2:B:80:LEU:HD22	2:B:148:PHE:CD1	0.43	2.48	2	1
2:B:137:ARG:CZ	2:B:137:ARG:CB	0.43	2.97	3	1
2:B:84:THR:HA	2:B:87:LEU:CD2	0.43	2.44	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:PHE:CZ	2:B:205:LEU:HD11	0.43	2.49	13	1
1:A:29:ASP:CA	2:B:103:ILE:HG21	0.43	2.41	13	1
2:B:172:LEU:CD1	2:B:208:VAL:HA	0.43	2.44	13	1
2:B:169:PRO:HA	2:B:208:VAL:O	0.43	2.14	18	3
1:A:60:SER:O	1:A:60:SER:OG	0.43	2.34	22	1
2:B:227:PHE:CA	2:B:230:ILE:HG22	0.42	2.42	2	1
1:A:24:LEU:HB2	2:B:159:ASN:ND2	0.42	2.29	19	5
2:B:88:HIS:HB2	2:B:146:ILE:CD1	0.42	2.41	6	1
2:B:218:LYS:N	2:B:222:GLU:OE2	0.42	2.51	6	1
1:A:20:LEU:HG	1:A:72:ILE:CB	0.42	2.44	10	1
2:B:89:ALA:HB1	2:B:104:MET:HE3	0.42	1.91	12	1
1:A:72:ILE:CD1	2:B:114:LEU:HD12	0.42	2.44	13	1
2:B:208:VAL:O	2:B:209:SER:C	0.42	2.55	18	1
1:A:34:LEU:HD11	1:A:53:ARG:CD	0.42	2.43	20	1
2:B:97:LYS:HE2	2:B:98:ARG:NH2	0.42	2.29	22	1
1:A:27:ASN:HB3	2:B:125:GLY:CA	0.42	2.44	1	1
2:B:107:ARG:O	2:B:108:GLU:HG2	0.42	2.15	1	1
2:B:192:GLY:HA3	2:B:207:PHE:CE2	0.42	2.49	1	1
2:B:192:GLY:HA3	2:B:207:PHE:CE1	0.42	2.49	22	4
1:A:27:ASN:OD1	1:A:35:LEU:HB2	0.42	2.15	22	4
1:A:26:GLY:HA2	2:B:69:ASN:CB	0.42	2.44	8	3
1:A:21:THR:O	1:A:21:THR:CG2	0.42	2.67	11	2
1:A:65:ASP:CA	1:A:68:LEU:HG	0.42	2.44	13	1
2:B:74:VAL:HB	2:B:121:MET:CG	0.42	2.43	14	1
1:A:20:LEU:CB	1:A:68:LEU:HA	0.42	2.44	15	1
2:B:212:ILE:HG22	2:B:214:LEU:CD1	0.42	2.39	15	1
2:B:190:PHE:CD2	2:B:194:ILE:HG13	0.42	2.48	19	1
1:A:23:ILE:CG1	1:A:24:LEU:N	0.42	2.82	20	1
1:A:33:ARG:O	1:A:33:ARG:CG	0.42	2.67	20	1
1:A:70:GLU:O	1:A:70:GLU:HG2	0.42	2.12	22	3
1:A:27:ASN:HB3	1:A:35:LEU:HD11	0.42	1.91	24	1
2:B:136:SER:OG	2:B:137:ARG:N	0.42	2.51	25	1
2:B:133:LYS:CG	2:B:155:PHE:CE2	0.42	3.03	1	1
1:A:26:GLY:O	1:A:34:LEU:HG	0.42	2.14	2	1
2:B:179:HIS:O	2:B:180:GLY:C	0.42	2.57	13	2
2:B:80:LEU:CD1	2:B:115:ILE:CG2	0.42	2.96	6	1
2:B:92:ALA:HA	2:B:103:ILE:O	0.42	2.14	9	7
1:A:72:ILE:HD13	2:B:114:LEU:HD12	0.42	1.91	13	1
2:B:205:LEU:HB2	2:B:213:VAL:CG2	0.42	2.44	13	1
1:A:29:ASP:HA	2:B:103:ILE:CG2	0.42	2.44	16	1
1:A:72:ILE:CD1	1:A:74:LEU:HB3	0.42	2.44	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:115:ILE:HG13	2:B:121:MET:CB	0.42	2.45	17	1
2:B:106:ILE:CD1	2:B:111:THR:OG1	0.42	2.65	18	1
2:B:159:ASN:HA	2:B:217:ALA:O	0.42	2.14	20	1
2:B:172:LEU:O	2:B:193:LEU:HD12	0.42	2.14	21	1
2:B:127:LYS:O	2:B:127:LYS:HG3	0.42	2.15	4	1
2:B:76:LEU:HG	2:B:121:MET:SD	0.42	2.54	6	1
2:B:178:SER:HB2	2:B:237:PHE:CZ	0.42	2.49	8	1
1:A:24:LEU:CD2	1:A:68:LEU:CD1	0.42	2.97	9	1
2:B:218:LYS:N	2:B:222:GLU:OE1	0.42	2.51	11	1
2:B:88:HIS:HB3	2:B:146:ILE:CD1	0.42	2.45	12	1
2:B:170:ILE:HG22	2:B:171:ARG:N	0.42	2.29	13	1
2:B:195:TYR:O	2:B:204:LEU:HD12	0.42	2.14	14	1
1:A:29:ASP:O	1:A:32:GLY:N	0.42	2.42	16	2
1:A:28:ILE:HG21	1:A:34:LEU:HD12	0.42	1.92	17	1
2:B:98:ARG:HD2	2:B:99:PHE:N	0.42	2.30	18	1
2:B:92:ALA:HB1	2:B:102:VAL:CG1	0.42	2.44	22	1
2:B:114:LEU:HB3	2:B:116:PHE:CZ	0.42	2.49	23	2
1:A:62:LEU:CD1	1:A:62:LEU:H	0.42	2.28	24	1
2:B:219:GLN:O	2:B:222:GLU:N	0.42	2.52	1	1
1:A:21:THR:HA	1:A:68:LEU:CD2	0.42	2.44	3	1
1:A:72:ILE:HA	2:B:116:PHE:CZ	0.42	2.49	8	1
2:B:70:ILE:CG2	2:B:157:ILE:HG23	0.42	2.44	8	1
2:B:69:ASN:ND2	2:B:161:VAL:HG21	0.42	2.28	10	1
2:B:189:LEU:CD2	2:B:190:PHE:HB2	0.42	2.44	19	1
2:B:114:LEU:CG	2:B:122:VAL:HB	0.42	2.45	20	1
1:A:61:LYS:HE2	1:A:62:LEU:HD21	0.42	1.90	21	1
1:A:55:ASN:ND2	2:B:190:PHE:CD1	0.42	2.88	25	1
2:B:103:ILE:HD13	2:B:114:LEU:HB3	0.42	1.90	1	1
2:B:65:PRO:HG3	2:B:223:ILE:O	0.42	2.15	4	1
2:B:69:ASN:ND2	2:B:124:THR:OG1	0.42	2.52	4	1
2:B:170:ILE:H	2:B:209:SER:CB	0.42	2.27	13	1
2:B:104:MET:C	2:B:105:ARG:CG	0.42	2.88	15	1
2:B:114:LEU:CD1	2:B:122:VAL:CG1	0.42	2.94	18	1
2:B:152:PHE:O	2:B:153:THR:CG2	0.42	2.62	18	1
2:B:102:VAL:O	2:B:115:ILE:N	0.42	2.52	20	1
2:B:194:ILE:HG12	2:B:205:LEU:CD2	0.42	2.44	22	1
2:B:202:ILE:HD11	2:B:217:ALA:HA	0.42	1.91	1	1
1:A:18:LEU:HD22	1:A:30:SER:HB2	0.42	1.92	3	1
2:B:179:HIS:CE1	2:B:233:VAL:HG13	0.42	2.49	4	1
1:A:52:LEU:CD1	1:A:59:LEU:HD11	0.42	2.45	7	1
1:A:66:SER:O	1:A:69:LEU:HG	0.42	2.14	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:HD12	1:A:71:VAL:HG23	0.42	1.90	13	1
2:B:166:VAL:O	2:B:167:LYS:CG	0.42	2.68	13	1
1:A:27:ASN:HB2	2:B:125:GLY:CA	0.42	2.45	15	1
1:A:27:ASN:HB3	2:B:124:THR:C	0.42	2.34	21	3
2:B:129:GLU:HG2	2:B:157:ILE:CD1	0.42	2.45	21	1
2:B:69:ASN:HA	2:B:126:ALA:O	0.42	2.15	15	3
2:B:77:GLY:C	2:B:78:CYS:SG	0.42	2.98	1	1
2:B:202:ILE:CD1	2:B:217:ALA:HA	0.42	2.45	4	4
2:B:112:THR:HB	2:B:124:THR:HG23	0.42	1.91	8	1
2:B:226:ALA:O	2:B:230:ILE:HG22	0.42	2.15	8	1
2:B:232:PRO:O	2:B:233:VAL:C	0.42	2.58	9	3
1:A:20:LEU:HB2	1:A:68:LEU:HD22	0.42	1.91	10	1
1:A:22:GLY:CA	1:A:34:LEU:HD12	0.42	2.45	15	1
2:B:195:TYR:CD1	2:B:230:ILE:HD13	0.42	2.48	1	1
1:A:27:ASN:OD1	2:B:124:THR:C	0.42	2.58	4	1
2:B:64:VAL:CG1	2:B:224:TYR:CE1	0.42	3.03	4	1
2:B:70:ILE:HB	2:B:126:ALA:CB	0.42	2.39	4	1
2:B:226:ALA:O	2:B:230:ILE:HG12	0.42	2.15	5	1
1:A:24:LEU:HD21	1:A:68:LEU:CD1	0.42	2.44	9	1
1:A:53:ARG:O	1:A:56:ILE:HB	0.42	2.15	13	1
2:B:78:CYS:SG	2:B:80:LEU:HD21	0.42	2.54	15	1
2:B:218:LYS:O	2:B:218:LYS:HG2	0.42	2.15	16	1
1:A:74:LEU:CD2	2:B:116:PHE:CD1	0.42	3.03	18	1
2:B:227:PHE:CD1	2:B:227:PHE:C	0.42	2.93	18	1
1:A:52:LEU:HD23	1:A:52:LEU:HA	0.42	1.72	1	4
1:A:20:LEU:HD11	2:B:114:LEU:HD13	0.42	1.92	5	1
2:B:88:HIS:O	2:B:89:ALA:C	0.42	2.58	10	1
2:B:217:ALA:HB1	2:B:222:GLU:CB	0.42	2.45	10	1
2:B:68:GLN:NE2	2:B:163:SER:CB	0.42	2.82	15	1
1:A:55:ASN:C	1:A:59:LEU:HD23	0.42	2.35	18	1
2:B:168:PHE:HB2	2:B:240:MET:OXT	0.42	2.15	18	1
2:B:175:LEU:HA	2:B:178:SER:OG	0.42	2.15	19	1
1:A:18:LEU:HB2	2:B:99:PHE:HB2	0.42	1.91	21	1
1:A:55:ASN:OD1	2:B:191:PRO:HD2	0.42	2.14	21	1
1:A:18:LEU:CG	1:A:72:ILE:HG12	0.42	2.44	22	1
2:B:115:ILE:HG12	2:B:121:MET:CG	0.42	2.45	24	1
2:B:160:ILE:CD1	2:B:219:GLN:O	0.41	2.68	15	2
2:B:70:ILE:O	2:B:124:THR:HA	0.41	2.15	4	3
2:B:153:THR:O	2:B:154:ASP:HB2	0.41	2.15	8	2
1:A:28:ILE:HG22	1:A:34:LEU:CG	0.41	2.45	5	1
2:B:196:ARG:HA	2:B:202:ILE:O	0.41	2.14	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:179:HIS:CG	2:B:195:TYR:OH	0.41	2.72	11	1
2:B:172:LEU:O	2:B:173:GLU:C	0.41	2.59	13	1
1:A:28:ILE:CG2	1:A:34:LEU:CD2	0.41	2.97	18	1
2:B:104:MET:SD	2:B:115:ILE:HD11	0.41	2.55	18	1
1:A:34:LEU:H	1:A:34:LEU:CD1	0.41	2.28	20	1
2:B:93:GLU:O	2:B:102:VAL:HA	0.41	2.15	23	1
2:B:114:LEU:HB2	2:B:122:VAL:HB	0.41	1.92	23	2
2:B:91:ASN:OD1	2:B:105:ARG:NH1	0.41	2.53	25	1
2:B:127:LYS:C	2:B:128:SER:OG	0.41	2.57	1	1
1:A:60:SER:O	1:A:65:ASP:OD1	0.41	2.38	4	1
2:B:152:PHE:CD2	2:B:152:PHE:O	0.41	2.73	5	1
1:A:20:LEU:CB	1:A:68:LEU:HD23	0.41	2.44	10	2
2:B:80:LEU:HD21	2:B:149:ALA:N	0.41	2.28	6	1
2:B:72:ALA:HB2	2:B:157:ILE:CG1	0.41	2.45	7	1
1:A:64:LEU:O	1:A:68:LEU:HG	0.41	2.15	13	1
2:B:173:GLU:O	2:B:174:GLY:C	0.41	2.58	18	1
2:B:159:ASN:OD1	2:B:159:ASN:C	0.41	2.59	20	1
2:B:130:ASP:N	2:B:130:ASP:OD1	0.41	2.51	25	1
2:B:219:GLN:O	2:B:220:ARG:C	0.41	2.58	1	1
1:A:18:LEU:CG	1:A:20:LEU:CD2	0.41	2.98	2	2
2:B:163:SER:HA	2:B:212:ILE:O	0.41	2.15	19	3
2:B:236:GLU:HG2	2:B:237:PHE:CE1	0.41	2.50	2	1
1:A:30:SER:OG	2:B:103:ILE:HG12	0.41	2.15	5	1
1:A:74:LEU:O	1:A:74:LEU:CG	0.41	2.69	6	2
2:B:74:VAL:CG1	2:B:75:THR:N	0.41	2.83	13	2
2:B:84:THR:HB	2:B:88:HIS:CD2	0.41	2.49	12	1
2:B:204:LEU:HD23	2:B:214:LEU:HG	0.41	1.91	13	1
1:A:30:SER:OG	2:B:103:ILE:HG13	0.41	2.15	14	2
2:B:200:PRO:HB3	2:B:222:GLU:OE2	0.41	2.16	14	1
2:B:227:PHE:CE2	2:B:231:TYR:CD2	0.41	3.08	14	1
1:A:27:ASN:CB	2:B:124:THR:OG1	0.41	2.68	17	1
2:B:180:GLY:O	2:B:181:THR:C	0.41	2.57	19	1
2:B:95:ASN:OD1	2:B:98:ARG:NH1	0.41	2.50	22	1
1:A:27:ASN:HA	2:B:124:THR:HG23	0.41	1.91	1	1
2:B:122:VAL:CG1	2:B:123:VAL:N	0.41	2.84	2	1
1:A:35:LEU:HD21	2:B:112:THR:HB	0.41	1.92	13	2
2:B:160:ILE:N	2:B:217:ALA:O	0.41	2.54	6	2
2:B:76:LEU:HD21	2:B:121:MET:HE2	0.41	1.93	8	1
2:B:77:GLY:CA	2:B:151:LYS:CE	0.41	2.99	12	1
1:A:65:ASP:HA	1:A:68:LEU:HG	0.41	1.91	19	2
2:B:86:ALA:HB2	2:B:102:VAL:HG22	0.41	1.93	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:238:ARG:NH2	2:B:238:ARG:HG2	0.41	2.31	14	1
2:B:69:ASN:O	2:B:161:VAL:N	0.41	2.48	17	2
1:A:25:PHE:CE1	1:A:52:LEU:HD11	0.41	2.49	18	1
1:A:72:ILE:CD1	1:A:74:LEU:HD13	0.41	2.43	21	1
2:B:98:ARG:NE	2:B:98:ARG:HA	0.41	2.30	25	1
1:A:62:LEU:HD11	1:A:64:LEU:CD2	0.41	2.45	4	1
2:B:166:VAL:CG1	2:B:168:PHE:CE2	0.41	3.03	7	1
2:B:111:THR:HB	2:B:124:THR:O	0.41	2.16	23	2
1:A:27:ASN:OD1	2:B:112:THR:HB	0.41	2.15	15	1
2:B:128:SER:O	2:B:129:GLU:C	0.41	2.59	15	1
2:B:76:LEU:CD1	2:B:150:ALA:HB1	0.41	2.41	19	1
1:A:23:ILE:CD1	2:B:114:LEU:CD2	0.41	2.99	25	1
1:A:27:ASN:O	1:A:35:LEU:N	0.41	2.54	25	1
2:B:90:ARG:O	2:B:91:ASN:OD1	0.41	2.38	3	1
1:A:74:LEU:N	1:A:74:LEU:HD23	0.41	2.30	5	1
2:B:153:THR:O	2:B:155:PHE:N	0.41	2.53	7	1
1:A:74:LEU:CD2	2:B:116:PHE:HB3	0.41	2.45	8	1
2:B:71:VAL:CG2	2:B:159:ASN:HB3	0.41	2.45	8	1
1:A:18:LEU:CD2	1:A:30:SER:CB	0.41	2.98	11	1
2:B:73:THR:O	2:B:154:ASP:O	0.41	2.38	11	2
2:B:140:ALA:O	2:B:144:GLN:CD	0.41	2.58	23	2
1:A:24:LEU:CD2	1:A:68:LEU:CD2	0.41	2.98	19	1
2:B:193:LEU:CD2	2:B:194:ILE:N	0.41	2.72	19	1
1:A:23:ILE:CG2	1:A:28:ILE:HG23	0.41	2.46	20	1
2:B:133:LYS:CD	2:B:155:PHE:CZ	0.41	3.04	24	1
2:B:235:SER:O	2:B:238:ARG:HG2	0.41	2.15	3	1
1:A:20:LEU:HG	1:A:72:ILE:HB	0.41	1.92	6	1
2:B:93:GLU:O	2:B:103:ILE:CD1	0.41	2.68	9	1
2:B:106:ILE:O	2:B:110:LYS:HA	0.41	2.15	12	1
1:A:23:ILE:HD11	1:A:28:ILE:CD1	0.41	2.44	17	1
2:B:91:ASN:HB2	2:B:105:ARG:O	0.41	2.16	17	1
1:A:27:ASN:CG	1:A:35:LEU:CB	0.41	2.88	22	1
2:B:99:PHE:HE2	2:B:101:ALA:HB3	0.41	1.61	23	1
2:B:225:GLN:O	2:B:226:ALA:C	0.41	2.59	1	2
2:B:114:LEU:O	2:B:121:MET:HA	0.41	2.15	4	2
2:B:114:LEU:O	2:B:121:MET:CA	0.41	2.69	4	1
1:A:23:ILE:CG1	1:A:28:ILE:HG13	0.41	2.46	6	1
2:B:183:SER:HA	2:B:194:ILE:O	0.41	2.16	14	2
1:A:56:ILE:HA	1:A:59:LEU:CD1	0.41	2.43	8	1
1:A:62:LEU:HD13	2:B:194:ILE:CG1	0.41	2.46	12	1
2:B:206:ILE:O	2:B:208:VAL:N	0.41	2.47	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:127:LYS:HG3	2:B:128:SER:N	0.41	2.30	17	1
2:B:199:LYS:HG2	2:B:199:LYS:O	0.41	2.16	17	1
2:B:71:VAL:CG2	2:B:124:THR:OG1	0.41	2.69	22	1
2:B:134:LEU:O	2:B:137:ARG:HG3	0.41	2.16	3	1
2:B:230:ILE:O	2:B:231:TYR:C	0.41	2.57	3	1
2:B:235:SER:O	2:B:238:ARG:CG	0.41	2.69	3	1
1:A:69:LEU:C	1:A:69:LEU:HD12	0.41	2.36	5	1
2:B:114:LEU:CD1	2:B:116:PHE:CZ	0.41	3.04	6	1
2:B:143:ILE:O	2:B:144:GLN:C	0.41	2.59	6	1
2:B:143:ILE:O	2:B:147:GLY:N	0.41	2.49	6	1
2:B:194:ILE:HG12	2:B:205:LEU:HD23	0.41	1.92	6	1
2:B:153:THR:O	2:B:154:ASP:C	0.41	2.58	7	1
2:B:162:GLY:N	2:B:214:LEU:O	0.41	2.48	7	1
1:A:65:ASP:O	1:A:68:LEU:HB2	0.41	2.16	9	1
2:B:173:GLU:CG	2:B:174:GLY:N	0.41	2.84	9	1
1:A:68:LEU:HD23	1:A:68:LEU:HA	0.41	1.69	10	1
2:B:164:CYS:C	2:B:165:ASP:OD1	0.41	2.58	10	1
1:A:20:LEU:HD23	1:A:72:ILE:HG21	0.41	1.86	11	1
1:A:27:ASN:CG	1:A:35:LEU:HG	0.41	2.36	22	2
1:A:72:ILE:O	1:A:72:ILE:CG2	0.41	2.65	12	1
2:B:71:VAL:HA	2:B:123:VAL:O	0.41	2.16	13	2
2:B:78:CYS:O	2:B:78:CYS:SG	0.41	2.78	13	1
2:B:114:LEU:N	2:B:122:VAL:O	0.41	2.45	13	1
2:B:79:ARG:HG2	2:B:117:ALA:O	0.41	2.16	14	1
1:A:73:ASP:OD2	1:A:73:ASP:O	0.41	2.39	15	1
1:A:18:LEU:O	1:A:18:LEU:HD12	0.41	2.15	17	1
1:A:62:LEU:HB2	1:A:64:LEU:CD2	0.41	2.43	19	1
2:B:190:PHE:CD2	2:B:194:ILE:CG1	0.41	3.04	19	1
2:B:166:VAL:HG23	2:B:167:LYS:N	0.41	2.31	20	1
2:B:63:ILE:HD13	2:B:231:TYR:HE2	0.41	1.76	22	1
1:A:68:LEU:HD13	1:A:68:LEU:C	0.41	2.36	24	1
2:B:67:LEU:HA	2:B:161:VAL:O	0.41	2.15	25	1
2:B:80:LEU:CD1	2:B:149:ALA:HB2	0.41	2.46	6	1
2:B:172:LEU:HD11	2:B:208:VAL:N	0.41	2.31	6	1
1:A:52:LEU:O	1:A:55:ASN:HB2	0.41	2.16	7	1
2:B:205:LEU:CB	2:B:213:VAL:HB	0.41	2.47	7	1
1:A:20:LEU:HB3	1:A:68:LEU:CD2	0.41	2.45	11	1
1:A:55:ASN:O	1:A:56:ILE:C	0.41	2.60	12	1
2:B:89:ALA:HB2	2:B:104:MET:HE1	0.41	1.93	12	1
1:A:52:LEU:HD12	2:B:207:PHE:HZ	0.41	1.76	13	1
2:B:104:MET:HB3	2:B:139:TYR:CD1	0.41	2.51	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:160:ILE:HD11	2:B:219:GLN:CA	0.41	2.45	15	1
1:A:51:GLU:CD	2:B:191:PRO:HG3	0.41	2.36	16	1
1:A:59:LEU:HD22	2:B:190:PHE:HE2	0.41	1.73	18	1
2:B:126:ALA:HB1	2:B:131:ASP:CB	0.41	2.46	22	1
2:B:114:LEU:HB3	2:B:116:PHE:CE1	0.41	2.50	23	2
1:A:23:ILE:HG23	2:B:124:THR:CG2	0.41	2.46	25	1
1:A:62:LEU:CD1	2:B:194:ILE:HD11	0.40	2.43	3	1
2:B:204:LEU:HA	2:B:213:VAL:O	0.40	2.16	6	1
2:B:75:THR:OG1	2:B:154:ASP:HB3	0.40	2.16	9	1
2:B:167:LYS:O	2:B:168:PHE:HB3	0.40	2.16	11	1
1:A:20:LEU:N	1:A:20:LEU:CD2	0.40	2.84	15	1
2:B:144:GLN:HG3	2:B:150:ALA:O	0.40	2.17	16	1
1:A:74:LEU:HG	1:A:74:LEU:O	0.40	2.16	21	1
1:A:27:ASN:HD22	1:A:35:LEU:HD12	0.40	1.74	22	1
2:B:106:ILE:HG12	2:B:139:TYR:OH	0.40	2.15	23	1
1:A:18:LEU:O	1:A:68:LEU:HD21	0.40	2.16	25	1
2:B:195:TYR:C	2:B:195:TYR:CD1	0.40	2.94	25	1
2:B:151:LYS:O	2:B:153:THR:N	0.40	2.54	5	1
1:A:20:LEU:CG	1:A:72:ILE:HB	0.40	2.47	10	2
2:B:213:VAL:CG1	2:B:214:LEU:N	0.40	2.84	14	1
2:B:175:LEU:CD2	2:B:237:PHE:HB2	0.40	2.46	17	1
2:B:122:VAL:C	2:B:123:VAL:HG23	0.40	2.36	20	1
2:B:189:LEU:CD2	2:B:189:LEU:O	0.40	2.69	21	1
1:A:70:GLU:OE1	2:B:159:ASN:ND2	0.40	2.55	23	1
2:B:165:ASP:HA	2:B:210:GLY:O	0.40	2.16	23	1
2:B:91:ASN:ND2	2:B:105:ARG:HG3	0.40	2.30	4	1
1:A:55:ASN:CG	2:B:190:PHE:CB	0.40	2.90	5	1
1:A:30:SER:OG	2:B:103:ILE:HD13	0.40	2.15	11	1
2:B:110:LYS:C	2:B:111:THR:CG2	0.40	2.90	13	2
2:B:82:LEU:HD13	2:B:94:TYR:CE1	0.40	2.51	15	1
1:A:28:ILE:HG22	1:A:34:LEU:HD23	0.40	1.93	16	1
2:B:172:LEU:HD21	2:B:206:ILE:O	0.40	2.17	16	1
2:B:202:ILE:HG22	2:B:203:VAL:N	0.40	2.31	20	1
1:A:62:LEU:CD2	1:A:63:GLY:N	0.40	2.79	22	1
2:B:227:PHE:O	2:B:231:TYR:CB	0.40	2.69	1	1
1:A:24:LEU:CD1	1:A:67:MET:HG2	0.40	2.43	4	1
2:B:167:LYS:HD3	2:B:167:LYS:O	0.40	2.16	7	1
2:B:175:LEU:HD13	2:B:179:HIS:HB2	0.40	1.94	13	1
1:A:61:LYS:HE2	2:B:189:LEU:CD2	0.40	2.45	14	1
1:A:19:ASP:OD1	1:A:19:ASP:N	0.40	2.54	18	1
2:B:219:GLN:CG	2:B:221:GLU:HG2	0.40	2.45	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:137:ARG:CZ	2:B:137:ARG:HB2	0.40	2.46	20	1
1:A:18:LEU:HD21	2:B:114:LEU:HD13	0.40	1.94	22	1
2:B:231:TYR:HB3	2:B:232:PRO:HD3	0.40	1.94	1	1
2:B:75:THR:O	2:B:153:THR:OG1	0.40	2.39	5	1
1:A:18:LEU:HD21	1:A:20:LEU:HD23	0.40	1.90	10	1
1:A:31:GLU:HB2	2:B:95:ASN:ND2	0.40	2.32	15	1
2:B:115:ILE:CG1	2:B:121:MET:CG	0.40	3.00	17	1
1:A:20:LEU:HB3	1:A:23:ILE:HB	0.40	1.93	22	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	43/67 (64%)	30±2 (70±4%)	9±2 (20±5%)	4±1 (10±3%)	1 10
2	B	177/180 (98%)	158±4 (89±2%)	16±3 (9±2%)	3±1 (2±1%)	14 59
All	All	5500/6175 (89%)	4709 (86%)	616 (11%)	175 (3%)	7 38

All 28 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	27	ASN	25
1	A	30	SER	24
1	A	72	ILE	18
2	B	64	VAL	17
1	A	63	GLY	15
1	A	26	GLY	12
2	B	167	LYS	12
1	A	19	ASP	7
2	B	148	PHE	7
2	B	152	PHE	6
1	A	61	LYS	4
2	B	108	GLU	3
2	B	126	ALA	3

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Mol	Chain	Res	Type	Models (Total)
2	B	201	LYS	3
2	B	238	ARG	3
2	B	189	LEU	2
1	A	21	THR	2
2	B	110	LYS	2
2	B	182	PHE	1
2	B	82	LEU	1
2	B	208	VAL	1
2	B	209	SER	1
1	A	18	LEU	1
2	B	63	ILE	1
2	B	128	SER	1
2	B	79	ARG	1
2	B	100	ALA	1
2	B	129	GLU	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	37/52 (71%)	24±2 (66±6%)	13±2 (34±6%)	1 10
2	B	151/152 (99%)	118±4 (78±2%)	33±4 (22±2%)	3 31
All	All	4700/5100 (92%)	3565 (76%)	1135 (24%)	2 26

All 131 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	18	LEU	25
1	A	53	ARG	24
1	A	28	ILE	20
1	A	33	ARG	20
2	B	99	PHE	20
1	A	25	PHE	19
2	B	114	LEU	19
2	B	153	THR	18
1	A	34	LEU	17

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Mol	Chain	Res	Type	Models (Total)
2	B	128	SER	17
2	B	167	LYS	17
2	B	98	ARG	17
2	B	238	ARG	17
2	B	105	ARG	16
2	B	175	LEU	16
2	B	211	LYS	16
2	B	134	LEU	15
2	B	141	ARG	15
2	B	228	GLU	15
1	A	58	SER	15
2	B	79	ARG	14
1	A	23	ILE	14
2	B	219	GLN	14
1	A	62	LEU	14
2	B	235	SER	14
1	A	67	MET	13
2	B	110	LYS	13
2	B	171	ARG	13
2	B	225	GLN	13
2	B	236	GLU	13
2	B	199	LYS	13
2	B	108	GLU	12
2	B	166	VAL	12
2	B	196	ARG	12
2	B	83	LYS	12
1	A	20	LEU	11
2	B	97	LYS	11
2	B	151	LYS	11
2	B	163	SER	11
2	B	69	ASN	11
2	B	107	ARG	11
2	B	156	LYS	11
2	B	189	LEU	11
2	B	127	LYS	11
2	B	133	LYS	11
1	A	19	ASP	10
1	A	60	SER	10
1	A	66	SER	10
2	B	201	LYS	10
2	B	221	GLU	10
1	A	51	GLU	10

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Mol	Chain	Res	Type	Models (Total)
1	A	61	LYS	10
2	B	138	LYS	10
2	B	239	LYS	10
2	B	184	SER	10
1	A	30	SER	10
1	A	35	LEU	9
2	B	178	SER	9
2	B	240	MET	9
2	B	78	CYS	9
2	B	131	ASP	9
2	B	145	LYS	9
2	B	218	LYS	9
2	B	95	ASN	9
2	B	183	SER	9
2	B	88	HIS	8
2	B	121	MET	8
2	B	136	SER	8
2	B	209	SER	8
2	B	164	CYS	8
2	B	205	LEU	8
2	B	73	THR	8
2	B	137	ARG	8
1	A	27	ASN	7
2	B	104	MET	7
2	B	118	SER	7
2	B	181	THR	7
2	B	190	PHE	7
2	B	159	ASN	7
2	B	132	SER	6
2	B	90	ARG	6
1	A	59	LEU	6
2	B	81	ASP	6
1	A	74	LEU	6
2	B	130	ASP	6
2	B	120	LYS	6
2	B	112	THR	6
2	B	154	ASP	6
1	A	71	VAL	6
1	A	24	LEU	5
2	B	129	GLU	5
2	B	188	GLU	5
2	B	165	ASP	5

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Mol	Chain	Res	Type	Models (Total)
2	B	231	TYR	5
2	B	111	THR	5
1	A	72	ILE	5
1	A	54	GLU	4
1	A	64	LEU	4
1	A	31	GLU	4
1	A	68	LEU	4
2	B	220	ARG	4
2	B	173	GLU	4
2	B	124	THR	4
2	B	158	GLN	3
2	B	182	PHE	3
2	B	222	GLU	3
2	B	197	MET	3
2	B	122	VAL	3
2	B	193	LEU	3
2	B	230	ILE	3
2	B	87	LEU	3
2	B	93	GLU	2
2	B	143	ILE	2
1	A	52	LEU	2
2	B	195	TYR	2
2	B	223	ILE	2
1	A	69	LEU	2
2	B	91	ASN	2
2	B	70	ILE	1
2	B	152	PHE	1
1	A	56	ILE	1
2	B	146	ILE	1
2	B	148	PHE	1
2	B	224	TYR	1
1	A	65	ASP	1
2	B	116	PHE	1
2	B	208	VAL	1
2	B	215	THR	1
2	B	94	TYR	1
2	B	144	GLN	1
2	B	168	PHE	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided