



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 05:29 AM BST

PDB ID : 2WC2  
Title : NMR STRUCTURE OF CATABOLITE ACTIVATOR PROTEIN IN THE UNLIGANDED STATE  
Authors : Popovych, N.; Tzeng, S.R.; Kalodimos, C.G.  
Deposited on : 2009-03-06

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

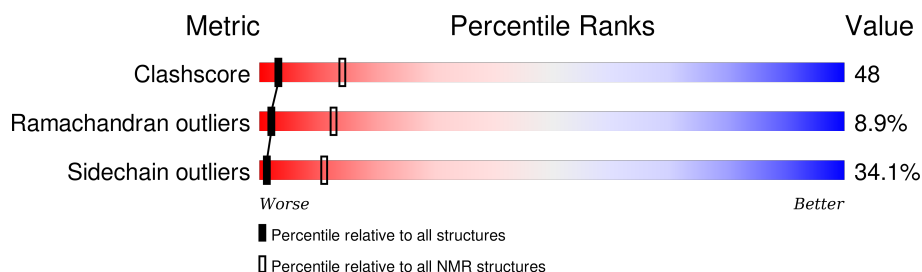
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment 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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	209	
1	B	209	

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:209, B:8-B:209 (404)	0.64	3

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 6704 atoms, of which 3404 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CATABOLITE GENE ACTIVATOR.

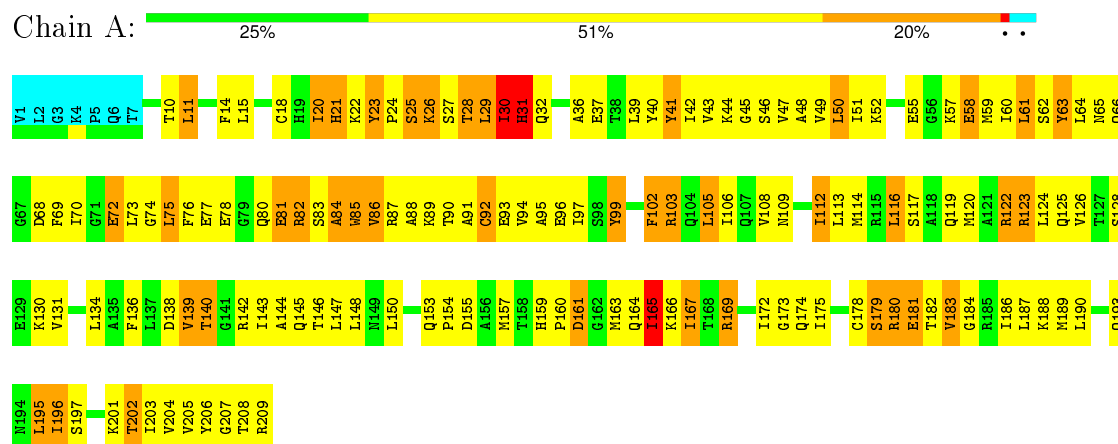
Mol	Chain	Residues	Atoms						Trace
1	A	209	Total	C	H	N	O	S	0
			3352	1044	1702	290	307	9	
1	B	209	Total	C	H	N	O	S	0
			3352	1044	1702	290	307	9	

## 4 Residue-property plots

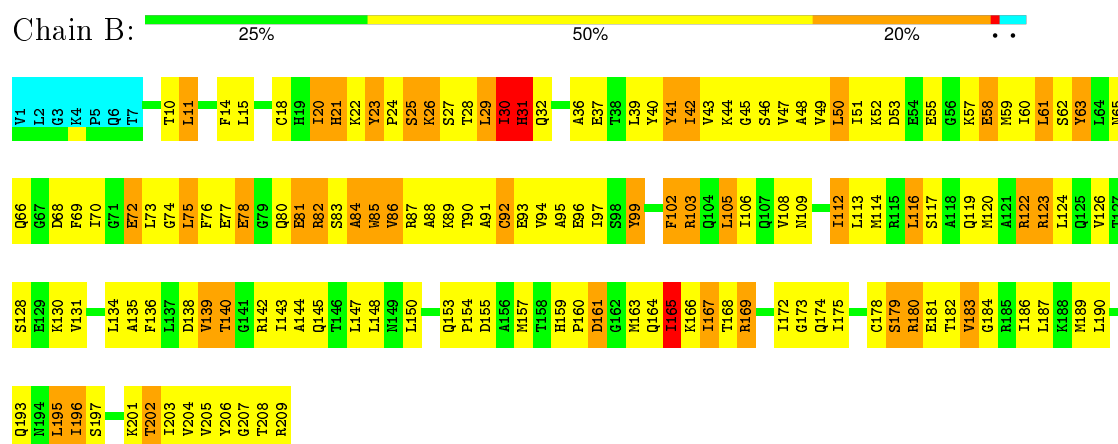
### 4.1 Average score per residue in the NMR ensemble

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

#### • Molecule 1: CATABOLITE GENE ACTIVATOR



#### • Molecule 1: CATABOLITE GENE ACTIVATOR

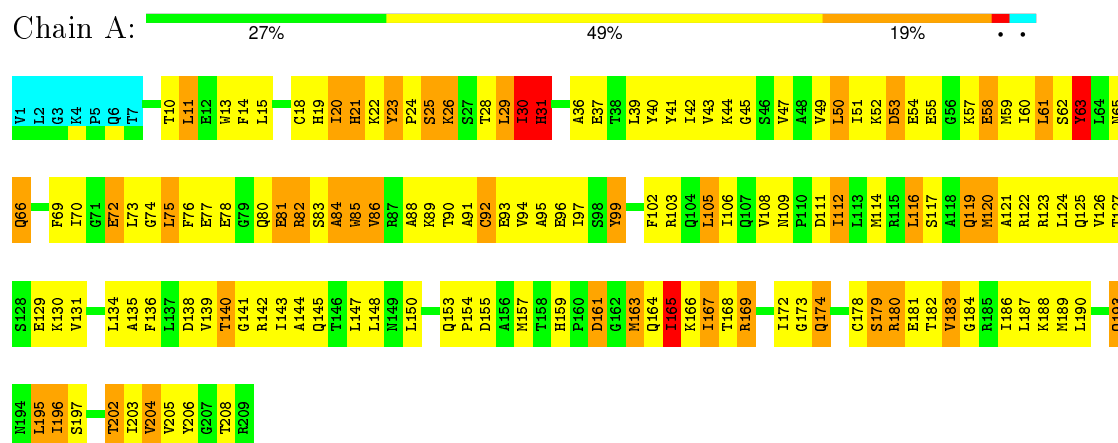


### 4.2 Scores per residue for each member of the ensemble

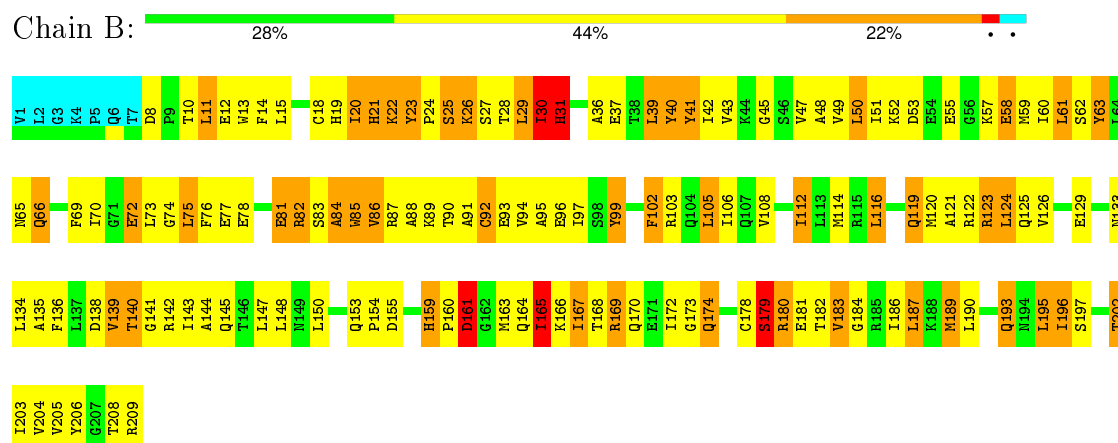
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

• Molecule 1: CATABOLITE GENE ACTIVATOR



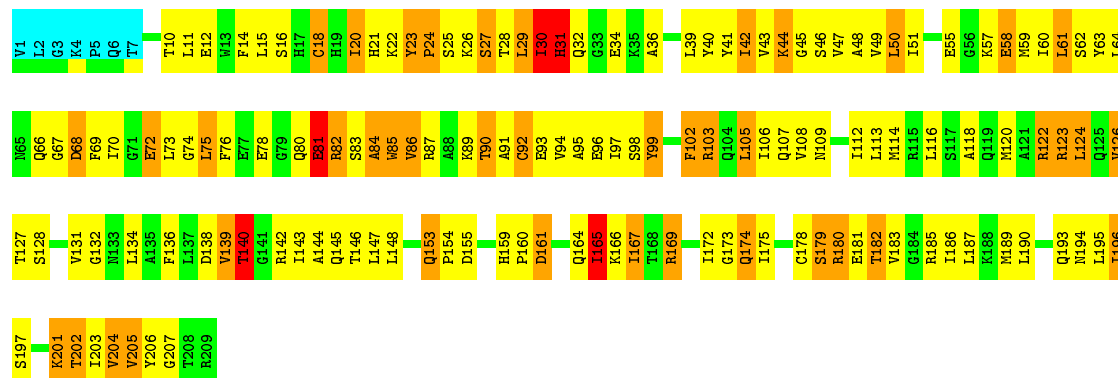
- Molecule 1: CATABOLITE GENE ACTIVATOR



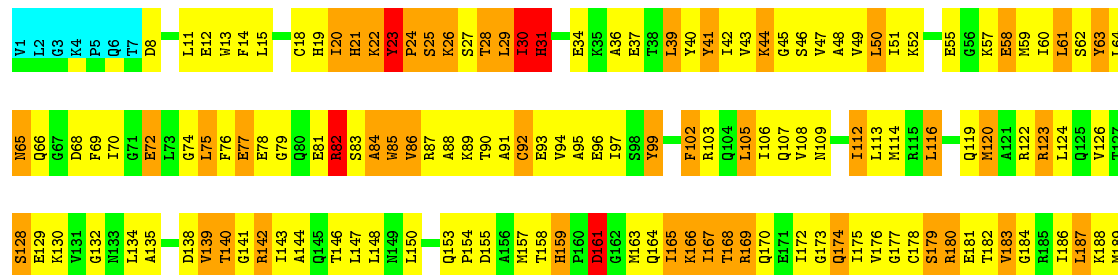
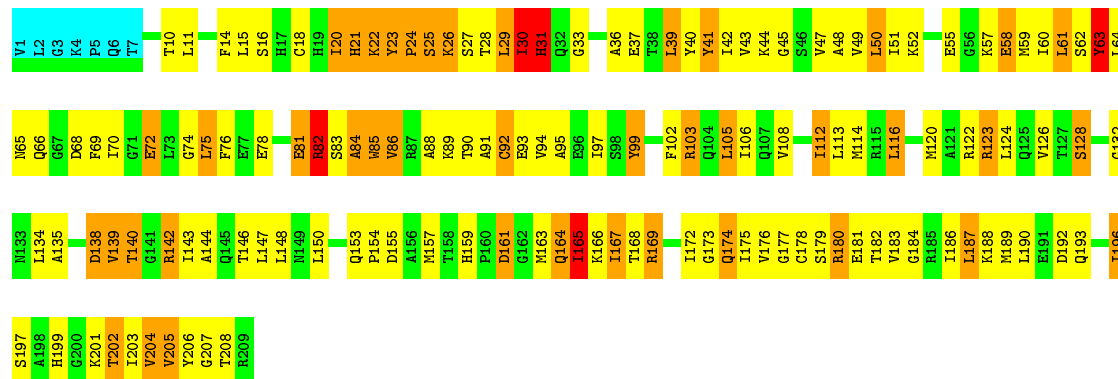
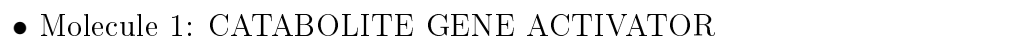
#### 4.2.2 Score per residue for model 2

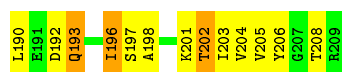
- Molecule 1: CATABOLITE GENE ACTIVATOR





### 4.2.3 Score per residue for model 3 (medoid)

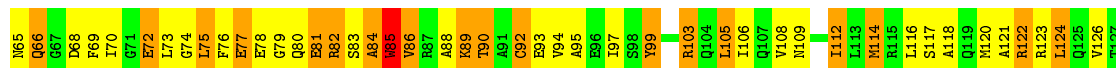
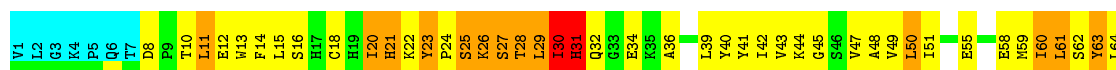




#### 4.2.4 Score per residue for model 4

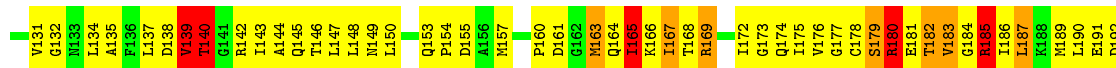
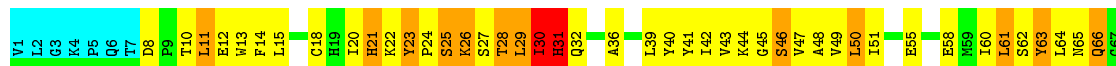
- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 26% 47% 21% . .



- Molecule 1: CATABOLITE GENE ACTIVATOR

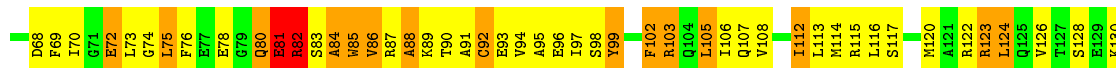
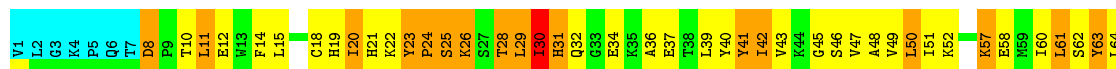
Chain B: 25% 49% 19% . .



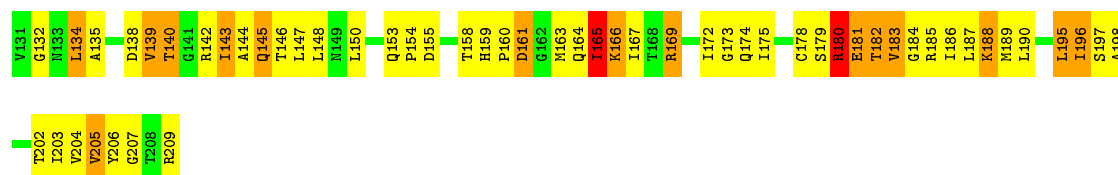
#### 4.2.5 Score per residue for model 5

- Molecule 1: CATABOLITE GENE ACTIVATOR

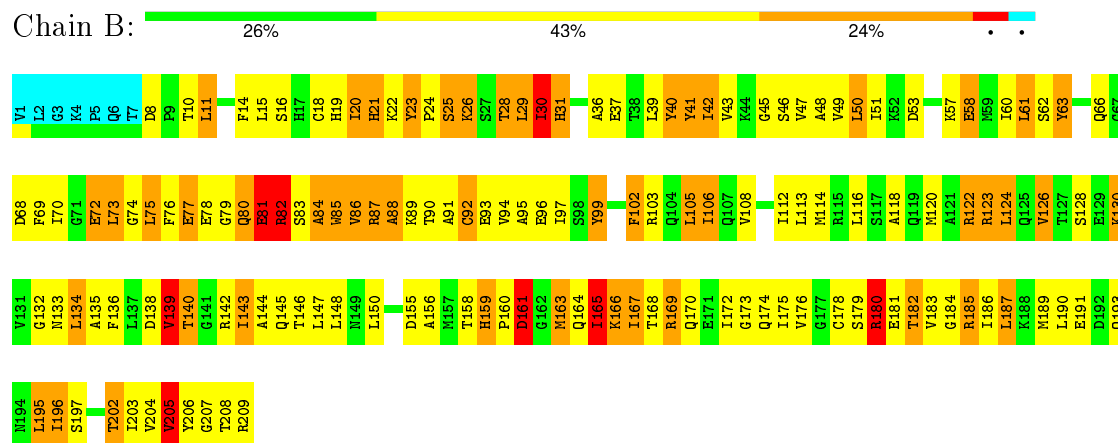
Chain A: 27% 45% 22% . .





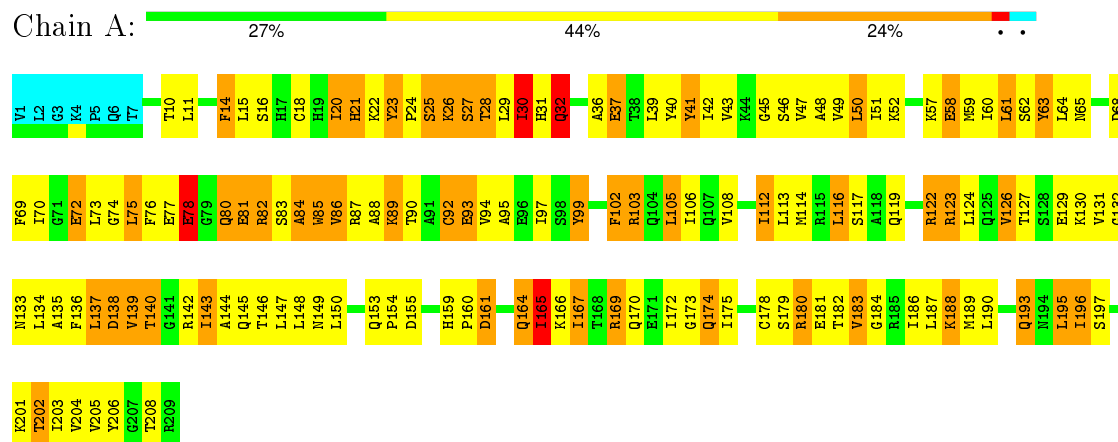


- Molecule 1: CATABOLITE GENE ACTIVATOR

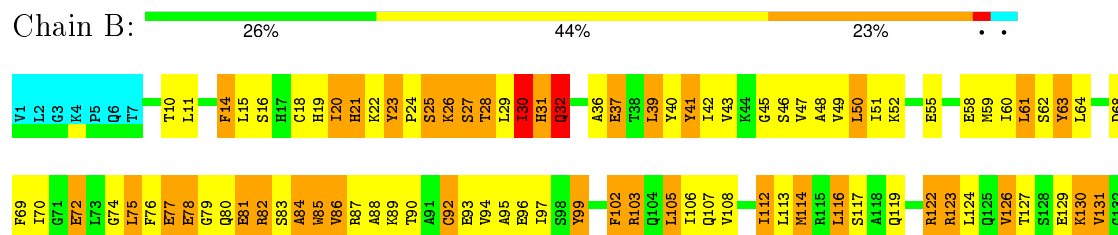


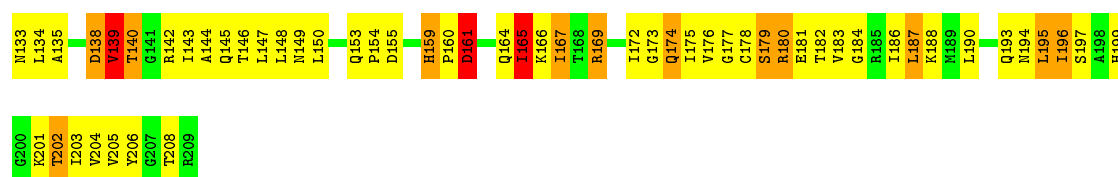
#### 4.2.6 Score per residue for model 6

- Molecule 1: CATABOLITE GENE ACTIVATOR



- Molecule 1: CATABOLITE GENE ACTIVATOR

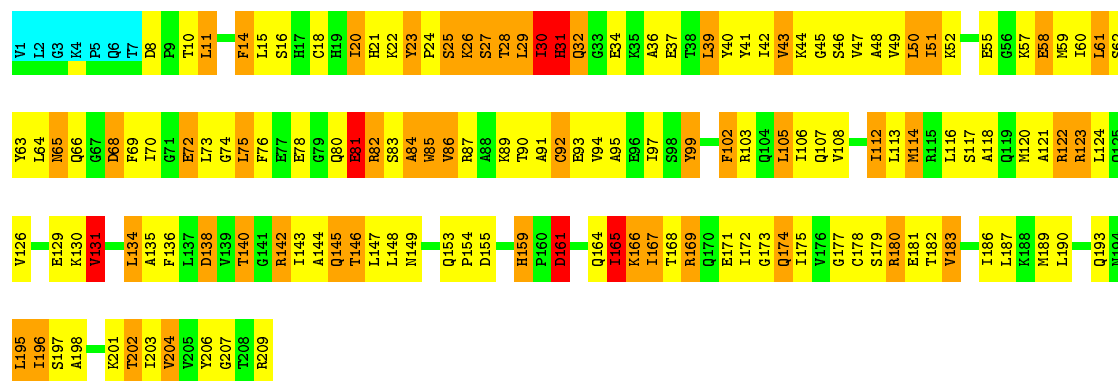




#### 4.2.7 Score per residue for model 7

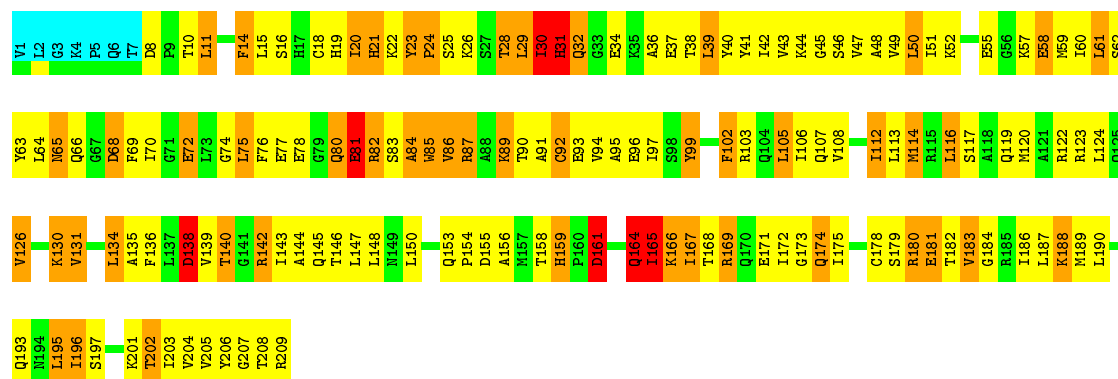
- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 26% 44% 23%



- Molecule 1: CATABOLITE GENE ACTIVATOR

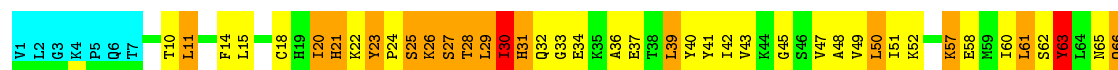
Chain B: 24% 46% 23%

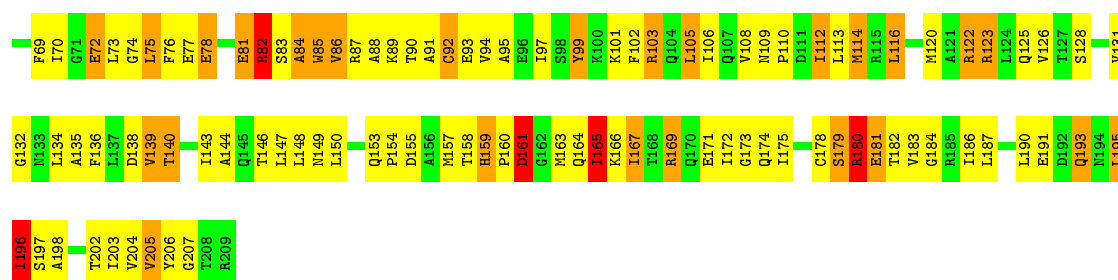


#### 4.2.8 Score per residue for model 8

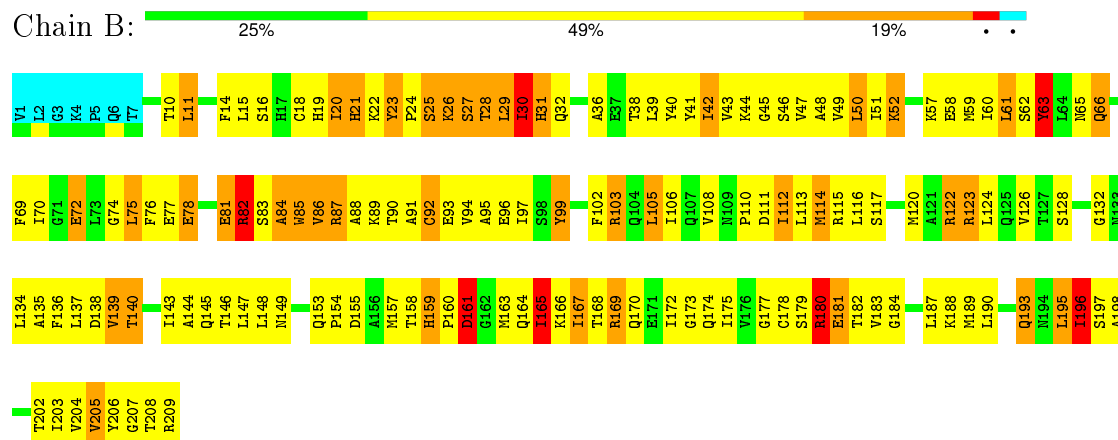
- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 29% 45% 20%



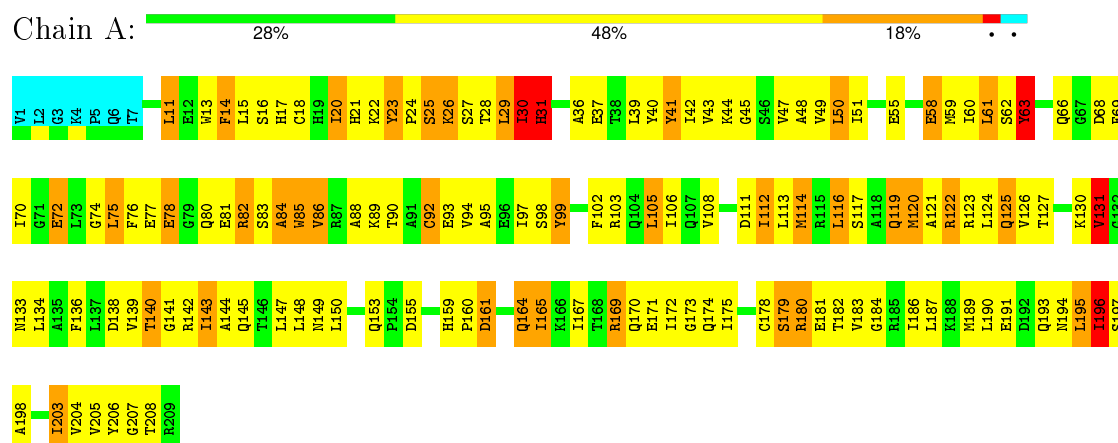


• Molecule 1: CATABOLITE GENE ACTIVATOR

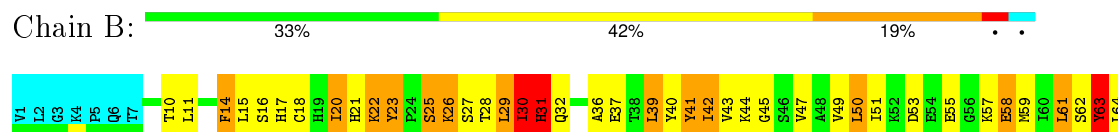


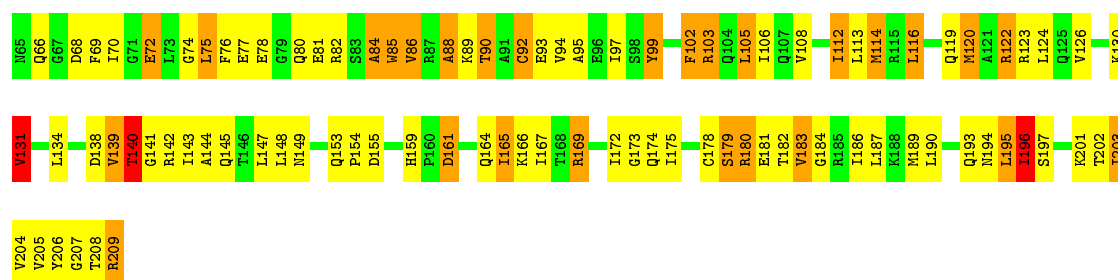
#### 4.2.9 Score per residue for model 9

• Molecule 1: CATABOLITE GENE ACTIVATOR



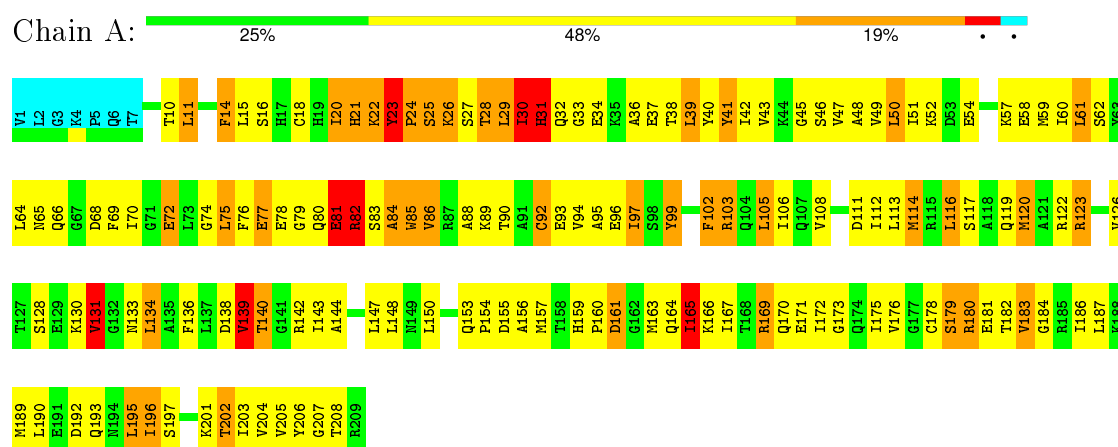
• Molecule 1: CATABOLITE GENE ACTIVATOR



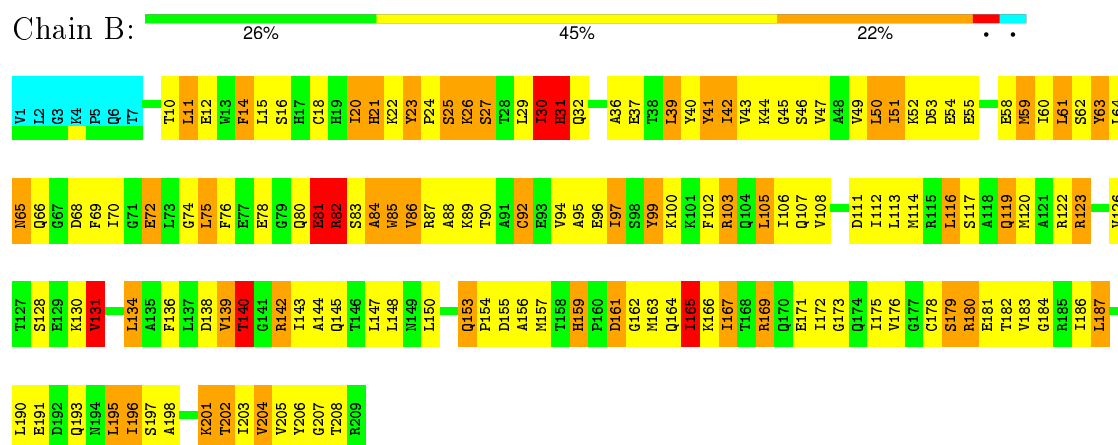


#### 4.2.10 Score per residue for model 10

- Molecule 1: CATABOLITE GENE ACTIVATOR



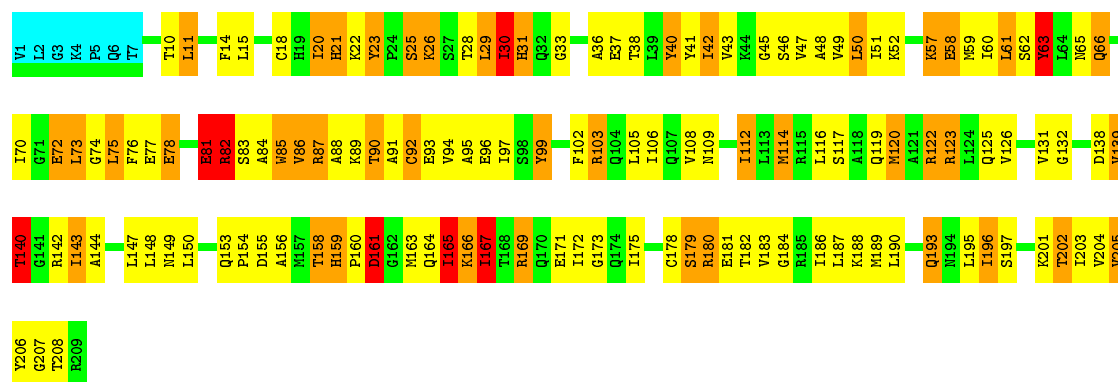
- Molecule 1: CATABOLITE GENE ACTIVATOR



#### 4.2.11 Score per residue for model 11

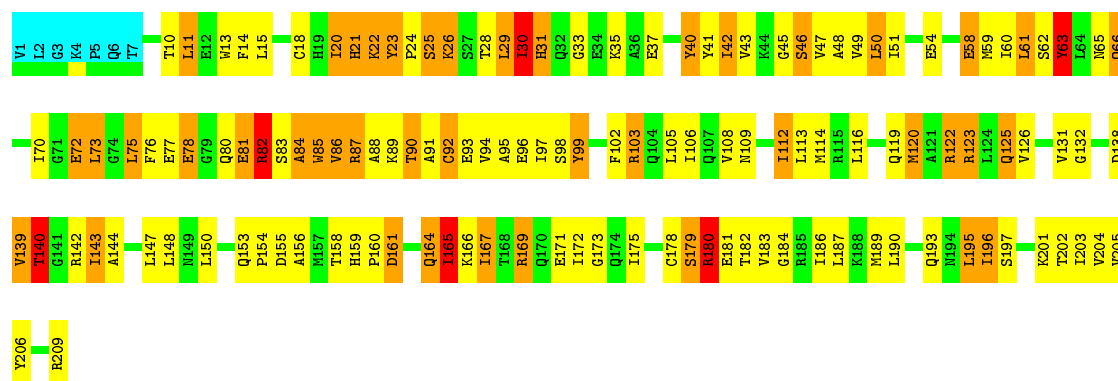
- Molecule 1: CATABOLITE GENE ACTIVATOR





• Molecule 1: CATABOLITE GENE ACTIVATOR

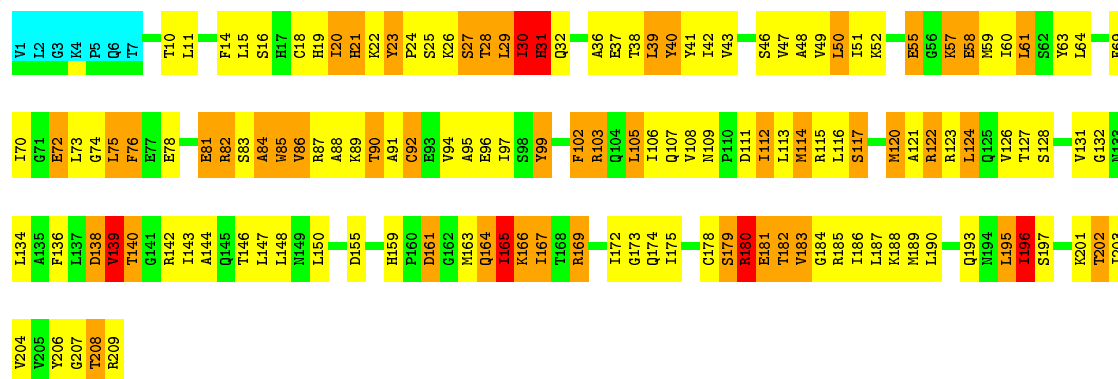
Chain B: 33% 40% 21%



#### 4.2.12 Score per residue for model 12

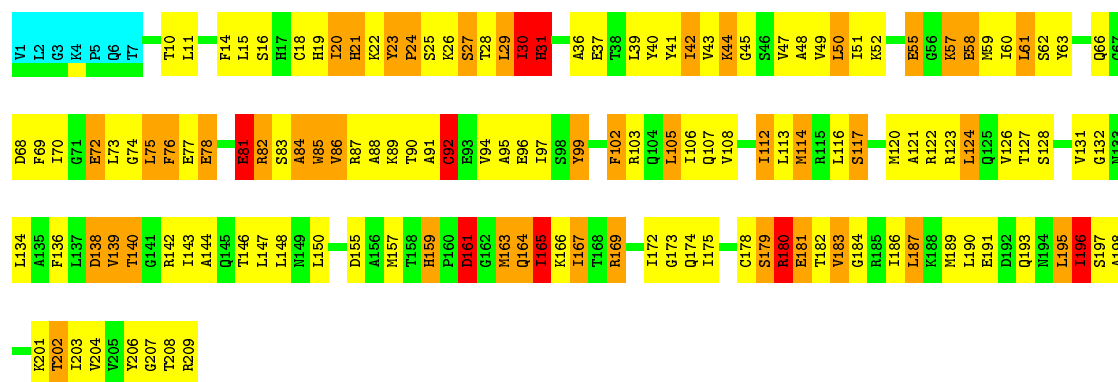
• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 29% 43% 22%



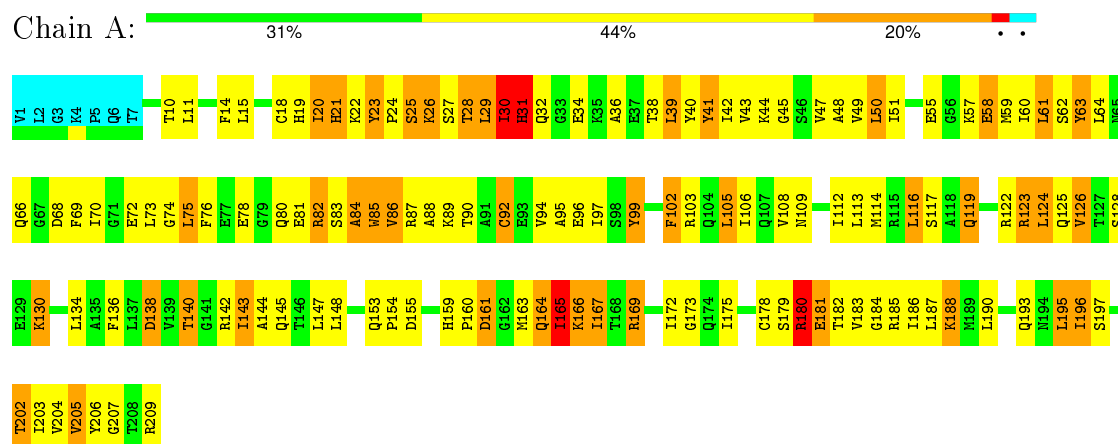
• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain B: 29% 44% 20%

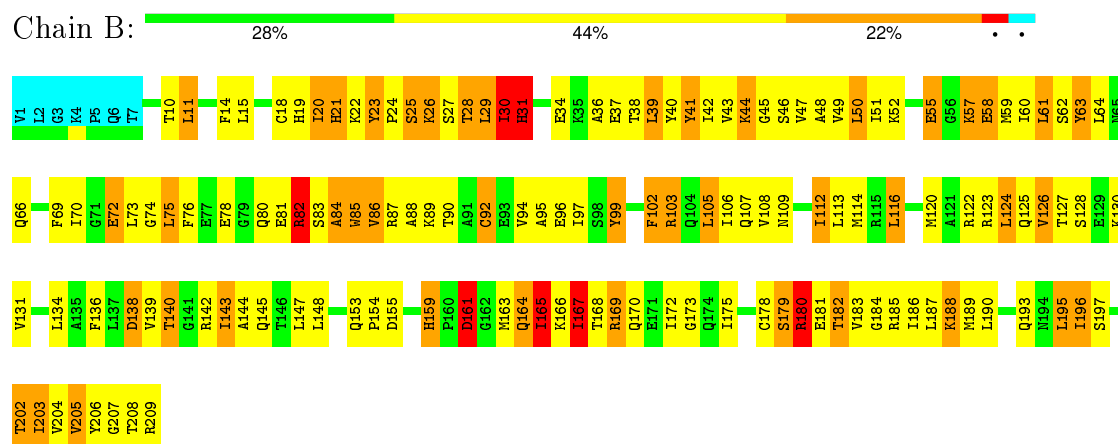


#### 4.2.13 Score per residue for model 13

- Molecule 1: CATABOLITE GENE ACTIVATOR



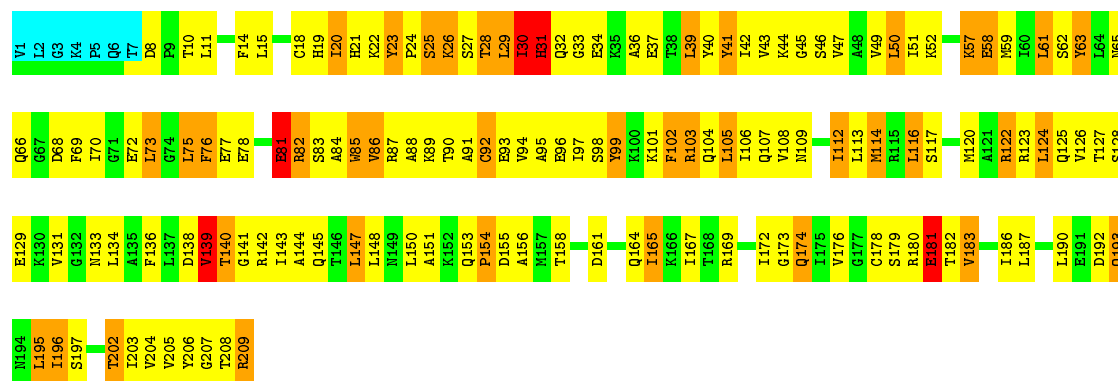
- Molecule 1: CATABOLITE GENE ACTIVATOR



#### 4.2.14 Score per residue for model 14

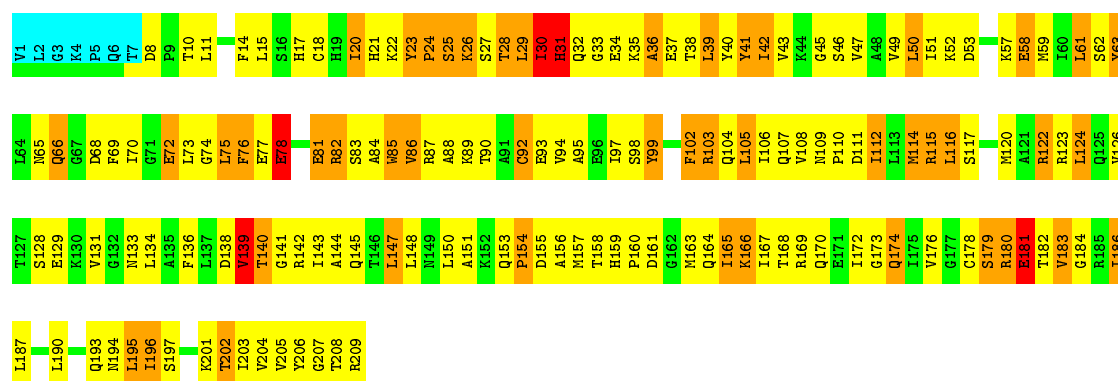
- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 



• Molecule 1: CATABOLITE GENE ACTIVATOR

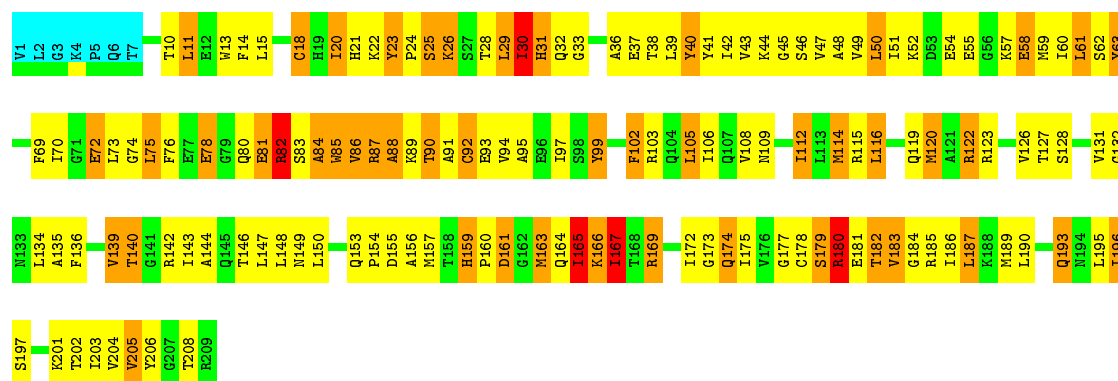
Chain B: 



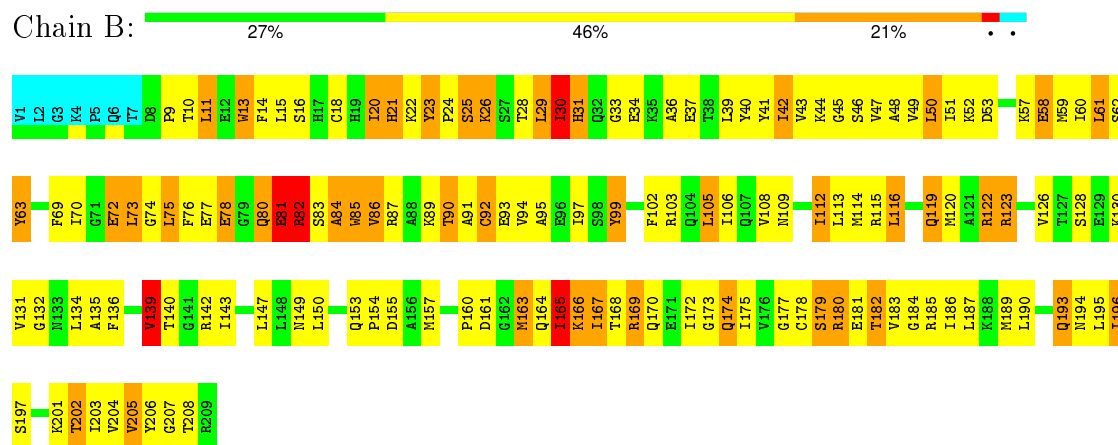
#### 4.2.15 Score per residue for model 15

• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A: 

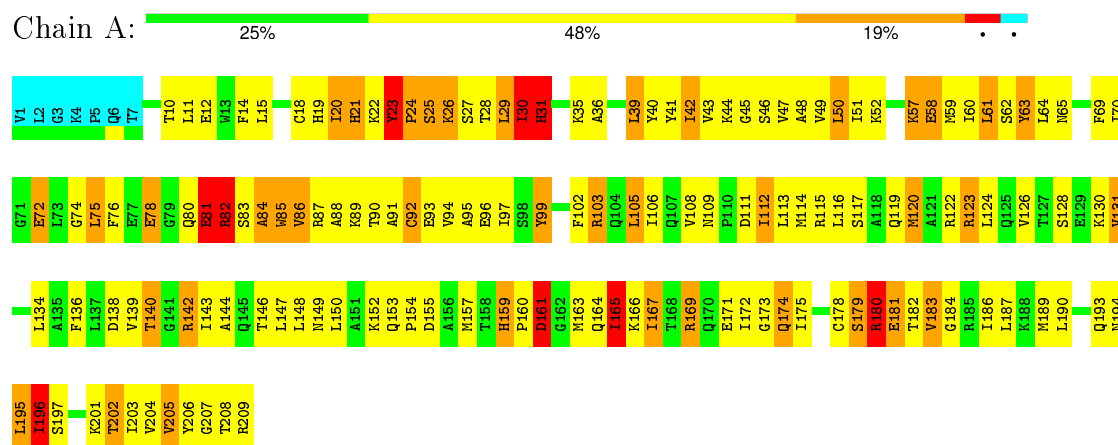


• Molecule 1: CATABOLITE GENE ACTIVATOR

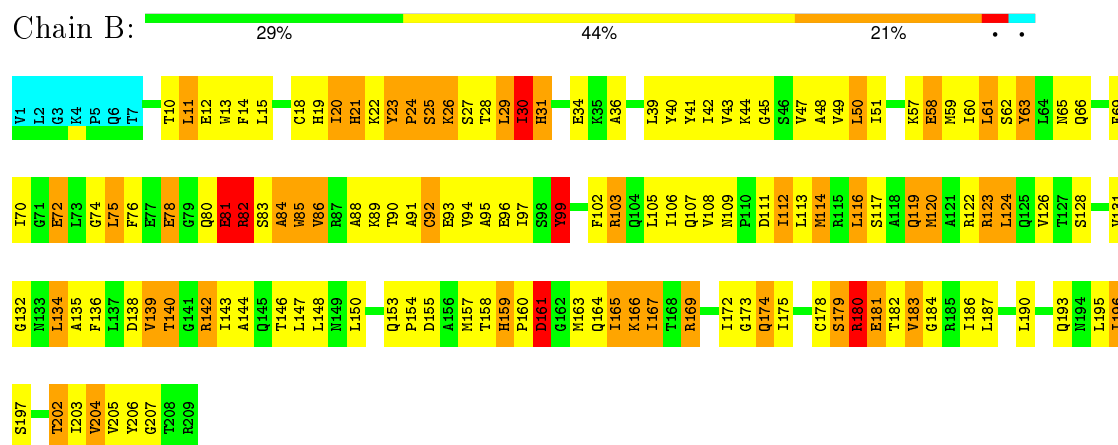


#### 4.2.16 Score per residue for model 16

- Molecule 1: CATABOLITE GENE ACTIVATOR



- Molecule 1: CATABOLITE GENE ACTIVATOR

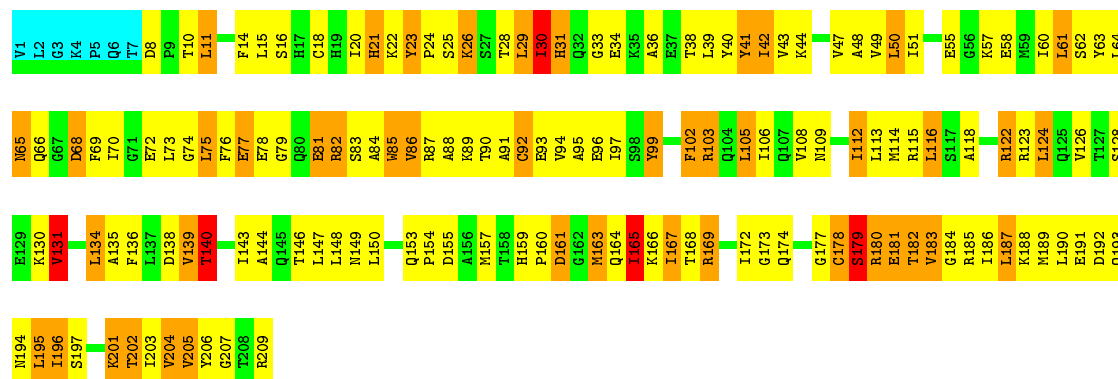




#### 4.2.17 Score per residue for model 17

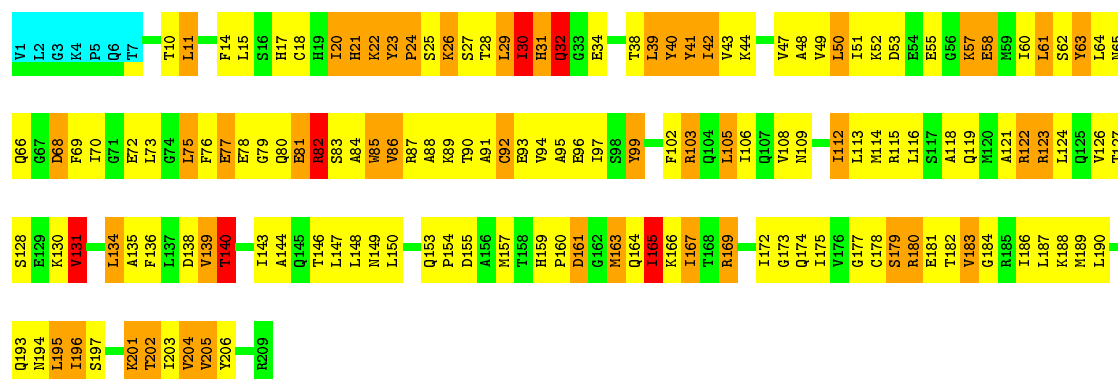
• Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A:  25% 48% 22% • •



- Molecule 1: CATABOLITE GENE ACTIVATOR

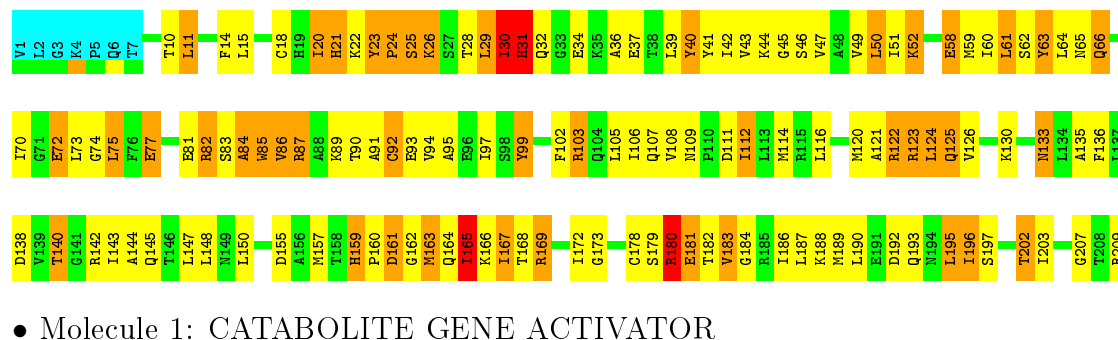
Chain B:  25% 46% 22% . .



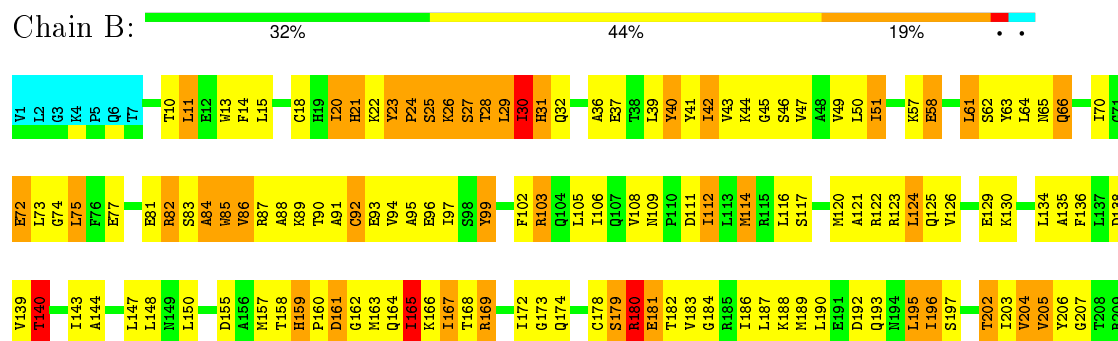
#### 4.2.18 Score per residue for model 18

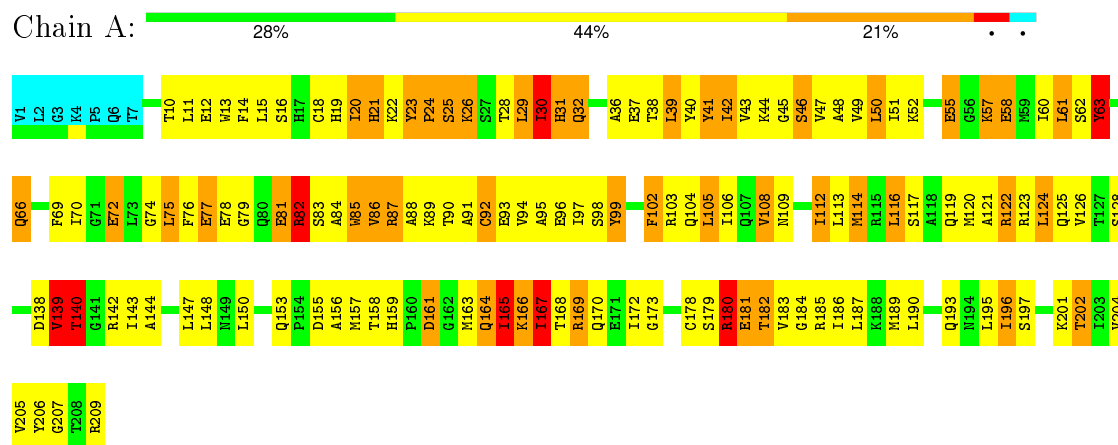
- Molecule 1: CATABOLITE GENE ACTIVATOR

Chain A:  34% 40% 21% . .

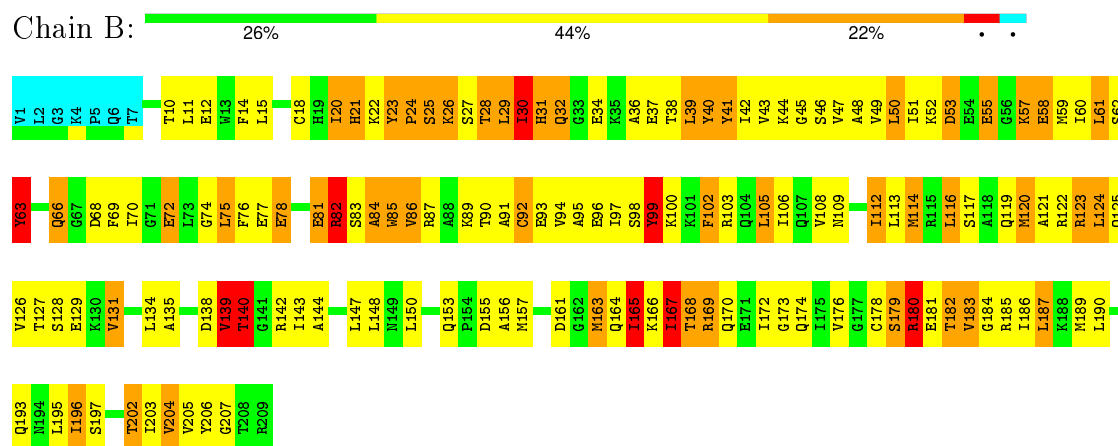


- Molecule 1: CATABOLITE GENE ACTIVATOR





• Molecule 1: CATABOLITE GENE ACTIVATOR



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
HADDOCK-CNS	refinement	
NMRVIEW	structure solution	
ARIA	structure solution	
HADDOCK	structure solution	
CNS	structure solution	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

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	0.61±0.02	0±0/1624 (0.0±0.0%)	0.98±0.02	2±1/2186 (0.1±0.0%)
1	B	0.61±0.01	0±0/1624 (0.0±0.0%)	0.98±0.02	3±1/2186 (0.1±0.0%)
All	All	0.61	0/64960 (0.0%)	0.98	97/87440 (0.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.7±0.6
1	B	0.0±0.0	0.7±0.7
All	All	0	28

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	205	VAL	N-CA-C	-8.55	87.91	111.00	11	15
1	B	205	VAL	N-CA-C	-7.64	90.37	111.00	4	19
1	B	24	PRO	CA-C-N	-6.58	102.71	117.20	12	8
1	A	28	THR	CA-C-N	-6.44	103.04	117.20	4	4
1	A	24	PRO	CA-C-N	-6.39	103.15	117.20	5	6
1	B	63	TYR	CA-C-N	-6.16	103.66	117.20	19	7
1	A	63	TYR	CA-C-N	-6.07	103.85	117.20	19	9
1	B	28	THR	CA-C-N	-6.01	103.98	117.20	4	3
1	B	187	LEU	CB-CA-C	5.63	120.91	110.20	6	8
1	B	138	ASP	N-CA-C	5.54	125.97	111.00	12	3
1	A	187	LEU	CB-CA-C	5.42	120.49	110.20	3	4
1	B	23	TYR	CB-CG-CD1	5.39	124.23	121.00	3	1
1	A	179	SER	CA-C-N	-5.29	105.56	117.20	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	164	GLN	CA-C-N	-5.25	105.64	117.20	7	1
1	A	138	ASP	N-CA-C	5.22	125.08	111.00	12	2
1	B	30	ILE	CA-C-N	-5.15	105.86	117.20	17	1
1	A	31	HIS	N-CA-CB	-5.15	101.33	110.60	7	1
1	A	30	ILE	CA-C-N	-5.13	105.91	117.20	17	1
1	A	30	ILE	N-CA-CB	5.13	122.60	110.80	20	1
1	A	23	TYR	CB-CG-CD1	5.11	124.06	121.00	10	2

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	31	HIS	Mainchain	13
1	B	31	HIS	Mainchain	11
1	B	92	CYS	Mainchain	1
1	B	179	SER	Mainchain	1
1	B	138	ASP	Mainchain	1
1	A	138	ASP	Mainchain	1

## 6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1599	1642	1636	157±10
1	B	1599	1642	1636	157±11
All	All	63960	65680	65439	6157

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 48.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:VAL:O	1:A:66:GLN:CG	1.08	2.02	17	2
1:A:43:VAL:O	1:A:66:GLN:HG3	1.06	1.47	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:43:VAL:O	1:B:66:GLN:CG	1.01	2.08	17	2
1:B:18:CYS:SG	1:B:95:ALA:HB1	0.97	2.00	4	20
1:A:190:LEU:HD22	1:A:196:ILE:HG12	0.97	1.32	13	3
1:B:169:ARG:HB3	1:B:187:LEU:HD12	0.96	1.37	20	19
1:A:18:CYS:SG	1:A:95:ALA:HB1	0.96	2.01	18	20
1:B:44:LYS:HA	1:B:66:GLN:HG3	0.94	1.39	17	6
1:A:169:ARG:HB3	1:A:187:LEU:HD12	0.93	1.39	15	20
1:A:153:GLN:OE1	1:A:155:ASP:OD2	0.93	1.87	14	1
1:B:43:VAL:O	1:B:66:GLN:HG3	0.92	1.62	17	2
1:B:153:GLN:OE1	1:B:155:ASP:OD2	0.90	1.89	14	1
1:A:49:VAL:HB	1:A:62:SER:O	0.90	1.65	16	4
1:B:173:GLY:HA2	1:B:178:CYS:O	0.89	1.66	17	19
1:B:49:VAL:HB	1:B:62:SER:O	0.88	1.68	6	3
1:B:51:ILE:O	1:B:58:GLU:HA	0.87	1.68	20	20
1:A:42:ILE:HD11	1:A:46:SER:HA	0.87	1.47	11	8
1:A:135:ALA:HB3	1:B:135:ALA:HB3	0.87	1.45	3	7
1:A:15:LEU:HA	1:A:18:CYS:SG	0.86	2.10	20	20
1:B:22:LYS:HB3	1:B:92:CYS:O	0.86	1.70	12	19
1:A:70:ILE:HG23	1:A:86:VAL:HG21	0.85	1.46	10	15
1:B:40:TYR:O	1:B:70:ILE:HB	0.85	1.71	2	20
1:B:45:GLY:H	1:B:66:GLN:HG2	0.84	1.29	8	8
1:B:42:ILE:HD11	1:B:46:SER:HA	0.84	1.48	11	10
1:A:45:GLY:H	1:A:66:GLN:HG2	0.84	1.33	19	7
1:A:40:TYR:O	1:A:70:ILE:HB	0.84	1.73	12	20
1:A:15:LEU:HB3	1:A:20:ILE:HD11	0.84	1.50	1	14
1:A:190:LEU:HD22	1:A:196:ILE:CG1	0.84	2.03	16	16
1:A:124:LEU:HD21	1:B:124:LEU:HD21	0.83	1.48	18	1
1:A:173:GLY:HA2	1:A:178:CYS:O	0.83	1.72	17	19
1:A:51:ILE:O	1:A:58:GLU:HA	0.83	1.74	14	20
1:A:42:ILE:HA	1:A:94:VAL:HG12	0.83	1.50	6	18
1:B:72:GLU:HB3	1:B:116:LEU:HD11	0.82	1.49	7	16
1:B:44:LYS:HA	1:B:66:GLN:CG	0.82	2.05	17	1
1:B:18:CYS:HA	1:B:97:ILE:HG21	0.82	1.51	11	20
1:A:187:LEU:HD22	1:A:190:LEU:HD11	0.81	1.51	13	14
1:B:42:ILE:HA	1:B:94:VAL:HG12	0.81	1.51	11	18
1:B:42:ILE:HD12	1:B:47:VAL:HG13	0.81	1.50	14	10
1:A:41:TYR:HB3	1:A:95:ALA:HB3	0.81	1.52	8	16
1:B:193:GLN:HA	1:B:196:ILE:O	0.81	1.74	8	20
1:B:147:LEU:HD22	1:B:167:ILE:HD13	0.81	1.52	11	5
1:B:41:TYR:HB3	1:B:95:ALA:HB3	0.81	1.52	13	16
1:A:143:ILE:HG12	1:A:183:VAL:HG22	0.80	1.52	20	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LYS:HA	1:A:66:GLN:HG3	0.80	1.51	17	5
1:A:18:CYS:HA	1:A:97:ILE:HG21	0.80	1.54	8	20
1:B:15:LEU:HB3	1:B:20:ILE:HD11	0.80	1.52	20	11
1:B:164:GLN:HB3	1:B:204:VAL:HG23	0.80	1.51	18	12
1:B:47:VAL:HB	1:B:87:ARG:O	0.80	1.77	15	6
1:B:22:LYS:HG2	1:B:23:TYR:CD1	0.80	2.12	12	19
1:B:37:GLU:HA	1:B:99:TYR:CE2	0.79	2.12	15	14
1:A:20:ILE:HD13	1:A:95:ALA:HB2	0.79	1.52	18	10
1:B:45:GLY:N	1:B:66:GLN:HG2	0.79	1.93	11	8
1:B:196:ILE:HG22	1:B:197:SER:H	0.79	1.38	11	14
1:B:15:LEU:HD22	1:B:20:ILE:HD11	0.78	1.55	17	5
1:B:22:LYS:HG3	1:B:94:VAL:HG22	0.78	1.54	1	17
1:B:20:ILE:HD13	1:B:95:ALA:HB2	0.78	1.55	18	9
1:B:75:LEU:HB2	1:B:99:TYR:CD2	0.78	2.14	17	18
1:A:20:ILE:HG13	1:A:43:VAL:HG21	0.78	1.55	2	1
1:B:146:THR:HG21	1:B:175:ILE:HG21	0.77	1.55	6	9
1:B:43:VAL:O	1:B:66:GLN:HG2	0.77	1.77	17	1
1:A:196:ILE:HG22	1:A:197:SER:H	0.77	1.38	2	13
1:B:44:LYS:CA	1:B:66:GLN:HG3	0.77	2.09	17	1
1:A:128:SER:HB3	1:B:51:ILE:HG21	0.77	1.57	15	11
1:A:51:ILE:HG21	1:B:128:SER:HB3	0.77	1.57	15	9
1:A:193:GLN:HA	1:A:196:ILE:O	0.77	1.80	1	19
1:A:26:LYS:H	1:A:88:ALA:HB3	0.76	1.40	6	7
1:A:48:ALA:HB1	1:A:60:ILE:HD12	0.76	1.55	8	6
1:B:15:LEU:HA	1:B:18:CYS:SG	0.76	2.20	4	20
1:A:190:LEU:HD22	1:A:196:ILE:HG13	0.76	1.56	8	11
1:B:49:VAL:HA	1:B:85:TRP:O	0.76	1.81	4	7
1:A:44:LYS:HG2	1:A:66:GLN:NE2	0.76	1.96	17	2
1:B:22:LYS:HG2	1:B:23:TYR:CE1	0.76	2.15	12	18
1:B:26:LYS:H	1:B:88:ALA:HB3	0.75	1.42	10	8
1:A:47:VAL:HB	1:A:87:ARG:O	0.75	1.81	12	4
1:A:75:LEU:HB2	1:A:99:TYR:CD2	0.75	2.17	2	19
1:A:72:GLU:HB3	1:A:116:LEU:HD11	0.75	1.56	3	15
1:B:167:ILE:HD11	1:B:203:ILE:HD12	0.74	1.59	9	2
1:A:49:VAL:HA	1:A:85:TRP:O	0.74	1.82	7	9
1:B:172:ILE:HG13	1:B:187:LEU:HD11	0.74	1.59	19	7
1:A:147:LEU:HA	1:A:150:LEU:HD12	0.74	1.58	16	13
1:A:77:GLU:HA	1:B:121:ALA:HB1	0.74	1.58	18	3
1:A:164:GLN:HB3	1:A:204:VAL:HG23	0.74	1.57	5	10
1:B:139:VAL:HG23	1:B:176:VAL:HG11	0.74	1.60	20	4
1:A:22:LYS:HG2	1:A:23:TYR:CD1	0.74	2.18	6	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:53:ASP:HB3	1:B:55:GLU:OE2	0.73	1.83	19	1
1:B:49:VAL:HG12	1:B:61:LEU:HD11	0.73	1.59	19	17
1:A:123:ARG:O	1:A:126:VAL:HG12	0.73	1.83	14	16
1:A:106:ILE:HD13	1:A:113:LEU:HD13	0.73	1.60	3	11
1:B:47:VAL:HG22	1:B:64:LEU:HD12	0.73	1.60	6	8
1:B:14:PHE:CD2	1:B:105:LEU:HD21	0.73	2.17	2	13
1:A:45:GLY:N	1:A:66:GLN:HG2	0.73	1.98	11	6
1:A:37:GLU:HA	1:A:99:TYR:CE2	0.73	2.17	1	14
1:A:14:PHE:CD2	1:A:105:LEU:HD21	0.73	2.19	7	12
1:A:11:LEU:O	1:A:15:LEU:HG	0.73	1.83	2	20
1:A:42:ILE:HD12	1:A:47:VAL:HG13	0.73	1.60	14	11
1:A:43:VAL:O	1:A:66:GLN:HG2	0.73	1.82	17	1
1:B:20:ILE:HG12	1:B:43:VAL:HG21	0.72	1.61	4	3
1:B:155:ASP:HB3	1:B:165:ILE:CG2	0.72	2.15	9	7
1:B:14:PHE:HD2	1:B:105:LEU:HD21	0.72	1.44	15	4
1:A:123:ARG:HA	1:A:126:VAL:HG12	0.72	1.61	3	5
1:B:75:LEU:HG	1:B:76:PHE:N	0.72	1.98	6	18
1:B:138:ASP:O	1:B:142:ARG:HB2	0.72	1.85	13	8
1:B:44:LYS:HE2	1:B:66:GLN:OE1	0.71	1.85	19	2
1:B:99:TYR:O	1:B:103:ARG:HB3	0.71	1.84	14	16
1:A:138:ASP:O	1:A:142:ARG:HB2	0.71	1.85	13	8
1:B:11:LEU:O	1:B:15:LEU:HG	0.71	1.84	9	20
1:B:169:ARG:CB	1:B:187:LEU:HD12	0.71	2.15	11	18
1:B:36:ALA:HB3	1:B:74:GLY:HA3	0.71	1.61	4	16
1:A:24:PRO:HA	1:A:91:ALA:HB2	0.71	1.60	5	12
1:A:75:LEU:HG	1:A:76:PHE:N	0.71	1.99	6	19
1:A:76:PHE:CZ	1:B:121:ALA:HB2	0.71	2.20	12	1
1:B:31:HIS:CE1	1:B:50:LEU:HG	0.71	2.21	8	15
1:B:28:THR:HG23	1:B:86:VAL:O	0.71	1.86	19	1
1:A:190:LEU:HD13	1:A:196:ILE:HD11	0.71	1.62	13	2
1:B:155:ASP:HB3	1:B:165:ILE:HG22	0.71	1.63	6	20
1:A:172:ILE:HG13	1:A:187:LEU:HD11	0.71	1.63	9	7
1:A:22:LYS:C	1:A:23:TYR:HD1	0.70	1.89	19	13
1:A:44:LYS:HA	1:A:66:GLN:CG	0.70	2.16	17	2
1:B:84:ALA:O	1:B:85:TRP:HB2	0.70	1.87	9	20
1:B:190:LEU:HD22	1:B:196:ILE:CG1	0.70	2.16	12	16
1:A:22:LYS:HB3	1:A:92:CYS:O	0.70	1.86	14	19
1:A:29:LEU:N	1:A:29:LEU:HD23	0.70	2.01	17	7
1:B:29:LEU:N	1:B:29:LEU:HD23	0.70	2.01	17	7
1:B:69:PHE:CD1	1:B:116:LEU:HD12	0.70	2.22	6	8
1:A:20:ILE:HD13	1:A:43:VAL:HG21	0.70	1.62	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:GLY:O	1:A:145:GLN:HB2	0.70	1.87	1	4
1:B:48:ALA:HB1	1:B:60:ILE:HD12	0.69	1.63	8	4
1:B:46:SER:O	1:B:89:LYS:HB3	0.69	1.87	18	9
1:B:157:MET:O	1:B:163:MET:HA	0.69	1.87	8	12
1:A:169:ARG:CB	1:A:187:LEU:HD12	0.69	2.17	13	17
1:B:187:LEU:HD22	1:B:190:LEU:HD11	0.69	1.62	9	13
1:B:22:LYS:C	1:B:23:TYR:HD1	0.69	1.90	20	15
1:A:144:ALA:O	1:A:148:LEU:HG	0.69	1.87	19	20
1:B:144:ALA:O	1:B:148:LEU:HG	0.69	1.88	1	19
1:A:47:VAL:HG22	1:A:64:LEU:HD12	0.69	1.62	6	10
1:B:72:GLU:HB2	1:B:120:MET:SD	0.69	2.28	12	7
1:A:29:LEU:HD23	1:A:29:LEU:N	0.69	2.03	19	10
1:A:36:ALA:HB3	1:A:74:GLY:HA3	0.69	1.63	10	18
1:A:22:LYS:HD2	1:A:92:CYS:SG	0.69	2.28	12	9
1:B:29:LEU:HD23	1:B:29:LEU:N	0.68	2.03	20	10
1:A:72:GLU:HA	1:A:75:LEU:HD23	0.68	1.65	1	4
1:A:172:ILE:HG22	1:A:183:VAL:HG21	0.68	1.66	10	20
1:A:69:PHE:CD1	1:A:116:LEU:HD12	0.68	2.24	6	5
1:A:31:HIS:CD2	1:A:31:HIS:O	0.68	2.46	12	10
1:A:186:ILE:O	1:A:189:MET:HG2	0.68	1.89	11	14
1:A:46:SER:O	1:A:89:LYS:HB3	0.68	1.88	18	10
1:B:11:LEU:HD11	1:B:41:TYR:CE2	0.68	2.24	13	9
1:A:76:PHE:CZ	1:B:117:SER:HB3	0.68	2.24	14	1
1:A:106:ILE:HG22	1:A:112:ILE:CG2	0.67	2.20	3	16
1:A:164:GLN:HA	1:A:203:ILE:O	0.67	1.89	9	15
1:A:122:ARG:HD2	1:B:77:GLU:OE2	0.67	1.89	7	4
1:B:141:GLY:O	1:B:145:GLN:HB2	0.67	1.89	1	4
1:A:103:ARG:O	1:A:106:ILE:HG12	0.67	1.89	19	1
1:A:84:ALA:O	1:A:85:TRP:HB2	0.67	1.88	17	20
1:B:187:LEU:HD23	1:B:190:LEU:HD12	0.67	1.64	10	1
1:A:147:LEU:HD22	1:A:167:ILE:HD13	0.67	1.67	11	5
1:A:18:CYS:HA	1:A:97:ILE:CG2	0.67	2.20	14	20
1:B:28:THR:CA	1:B:29:LEU:HD23	0.67	2.20	4	16
1:A:53:ASP:HB3	1:A:55:GLU:OE2	0.67	1.90	19	1
1:A:106:ILE:HG22	1:A:112:ILE:HG22	0.67	1.65	3	7
1:A:22:LYS:HG3	1:A:94:VAL:HG22	0.67	1.64	1	18
1:A:157:MET:O	1:A:163:MET:HA	0.67	1.88	8	11
1:B:172:ILE:HG22	1:B:183:VAL:HG21	0.67	1.65	20	20
1:A:29:LEU:O	1:A:30:ILE:HG13	0.67	1.90	20	3
1:A:155:ASP:HB3	1:A:165:ILE:HG22	0.66	1.66	10	20
1:A:103:ARG:O	1:A:107:GLN:HB3	0.66	1.90	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:THR:HA	1:A:29:LEU:HD23	0.66	1.66	16	9
1:B:29:LEU:CB	1:B:86:VAL:HB	0.66	2.20	10	2
1:B:44:LYS:HD3	1:B:66:GLN:NE2	0.66	2.05	12	1
1:A:186:ILE:HG22	1:A:187:LEU:HD23	0.66	1.67	16	14
1:A:33:GLY:N	1:A:82:ARG:HD3	0.66	2.05	17	5
1:A:117:SER:HA	1:A:120:MET:SD	0.66	2.31	12	1
1:A:69:PHE:CG	1:A:116:LEU:HD12	0.66	2.25	17	15
1:A:121:ALA:HB2	1:B:76:PHE:CZ	0.66	2.26	12	1
1:B:31:HIS:CD2	1:B:31:HIS:O	0.66	2.49	12	8
1:B:31:HIS:O	1:B:31:HIS:CD2	0.66	2.49	14	9
1:B:24:PRO:HA	1:B:91:ALA:CB	0.66	2.21	3	8
1:A:11:LEU:HD12	1:A:15:LEU:HG	0.66	1.67	5	3
1:A:22:LYS:HG2	1:A:23:TYR:CE1	0.66	2.26	9	18
1:B:44:LYS:HG2	1:B:66:GLN:NE2	0.66	2.05	17	2
1:A:171:GLU:HA	1:A:174:GLN:NE2	0.66	2.06	7	1
1:A:124:LEU:O	1:A:128:SER:HB2	0.66	1.91	14	1
1:B:186:ILE:O	1:B:190:LEU:HG	0.66	1.91	10	13
1:A:41:TYR:HB2	1:A:95:ALA:HB3	0.65	1.68	7	1
1:B:196:ILE:HG22	1:B:204:VAL:O	0.65	1.91	4	10
1:B:123:ARG:O	1:B:126:VAL:HG12	0.65	1.90	9	16
1:B:143:ILE:HG12	1:B:183:VAL:HG22	0.65	1.68	10	5
1:A:196:ILE:HG22	1:A:204:VAL:O	0.65	1.92	15	4
1:A:11:LEU:HD21	1:A:41:TYR:CE2	0.65	2.26	19	6
1:A:197:SER:O	1:A:204:VAL:HB	0.65	1.91	9	4
1:A:44:LYS:CG	1:A:66:GLN:NE2	0.65	2.59	17	1
1:B:164:GLN:HA	1:B:203:ILE:O	0.65	1.90	9	15
1:A:28:THR:CA	1:A:29:LEU:HD23	0.65	2.22	4	16
1:B:179:SER:C	1:B:181:GLU:H	0.65	1.93	19	20
1:A:47:VAL:HA	1:A:89:LYS:H	0.65	1.51	14	6
1:B:143:ILE:O	1:B:147:LEU:HG	0.65	1.91	5	18
1:B:103:ARG:O	1:B:106:ILE:HG12	0.65	1.91	19	1
1:B:186:ILE:HG22	1:B:187:LEU:HD23	0.65	1.69	18	10
1:A:30:ILE:HD12	1:A:86:VAL:HG21	0.65	1.69	2	3
1:B:42:ILE:HD11	1:B:47:VAL:HG13	0.65	1.69	9	1
1:A:77:GLU:OE2	1:B:122:ARG:HD2	0.65	1.92	9	1
1:A:31:HIS:CE1	1:A:50:LEU:HG	0.65	2.27	17	15
1:A:39:LEU:HD13	1:A:102:PHE:CZ	0.65	2.27	20	2
1:B:11:LEU:HD21	1:B:41:TYR:CE2	0.65	2.26	2	8
1:A:31:HIS:O	1:A:31:HIS:CD2	0.65	2.50	14	7
1:B:18:CYS:HA	1:B:97:ILE:CG2	0.65	2.23	2	20
1:A:14:PHE:HD2	1:A:105:LEU:HD21	0.65	1.50	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:ALA:HB2	1:A:195:LEU:HD21	0.65	1.66	13	6
1:B:44:LYS:CG	1:B:66:GLN:NE2	0.64	2.60	17	1
1:B:103:ARG:O	1:B:107:GLN:HB3	0.64	1.92	14	3
1:B:23:TYR:N	1:B:23:TYR:CD1	0.64	2.64	1	9
1:A:20:ILE:O	1:A:21:HIS:HB2	0.64	1.91	20	14
1:A:24:PRO:HA	1:A:91:ALA:CB	0.64	2.22	20	10
1:B:24:PRO:HA	1:B:91:ALA:HB2	0.64	1.68	3	12
1:B:47:VAL:HA	1:B:89:LYS:H	0.64	1.52	9	7
1:B:20:ILE:O	1:B:21:HIS:HB2	0.64	1.93	1	15
1:A:179:SER:C	1:A:181:GLU:H	0.64	1.94	8	19
1:A:187:LEU:HD22	1:A:190:LEU:CD1	0.64	2.23	13	16
1:B:20:ILE:HG23	1:B:43:VAL:HG21	0.64	1.68	2	6
1:B:190:LEU:HD13	1:B:196:ILE:HD11	0.64	1.69	9	3
1:B:69:PHE:CG	1:B:116:LEU:HD12	0.64	2.28	13	16
1:A:69:PHE:CE2	1:A:116:LEU:HA	0.64	2.28	16	7
1:A:30:ILE:HD12	1:A:86:VAL:CG2	0.64	2.22	2	8
1:A:166:LYS:HB3	1:A:202:THR:HG22	0.64	1.67	5	1
1:B:31:HIS:CE1	1:B:58:GLU:HB3	0.64	2.27	8	3
1:A:179:SER:HB3	1:A:181:GLU:OE2	0.64	1.93	14	1
1:A:42:ILE:HD11	1:A:47:VAL:HG13	0.64	1.70	12	3
1:A:146:THR:HG21	1:A:175:ILE:HG21	0.64	1.67	6	9
1:B:47:VAL:O	1:B:63:TYR:HB3	0.63	1.93	9	15
1:A:150:LEU:HD13	1:A:167:ILE:HG12	0.63	1.68	4	8
1:B:197:SER:HB2	1:B:206:TYR:CE1	0.63	2.28	17	13
1:A:48:ALA:HB1	1:A:60:ILE:HD13	0.63	1.69	16	9
1:A:20:ILE:HG12	1:A:43:VAL:HG21	0.63	1.69	10	1
1:B:123:ARG:HA	1:B:126:VAL:HG12	0.63	1.70	14	5
1:B:106:ILE:HD13	1:B:113:LEU:HD13	0.63	1.70	7	11
1:A:190:LEU:HD13	1:A:196:ILE:HD12	0.63	1.69	14	15
1:B:49:VAL:HG22	1:B:85:TRP:O	0.63	1.93	13	17
1:B:23:TYR:N	1:B:23:TYR:HD1	0.63	1.91	1	2
1:B:44:LYS:HD2	1:B:66:GLN:CD	0.63	2.14	20	1
1:A:18:CYS:CB	1:A:97:ILE:HG12	0.63	2.24	14	12
1:A:23:TYR:CD1	1:A:23:TYR:N	0.63	2.67	3	15
1:B:48:ALA:HB1	1:B:60:ILE:HD13	0.63	1.70	15	11
1:B:70:ILE:HG23	1:B:86:VAL:HG21	0.63	1.68	15	12
1:B:182:THR:O	1:B:185:ARG:HB2	0.63	1.94	5	5
1:A:143:ILE:O	1:A:147:LEU:HG	0.63	1.93	18	17
1:B:134:LEU:HD22	1:B:174:GLN:O	0.63	1.94	1	12
1:B:69:PHE:CE2	1:B:116:LEU:HA	0.63	2.28	13	6
1:A:44:LYS:CA	1:A:66:GLN:HG3	0.63	2.23	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LEU:HD11	1:A:41:TYR:CE2	0.63	2.28	11	11
1:A:187:LEU:HA	1:A:190:LEU:HG	0.63	1.68	8	19
1:A:44:LYS:O	1:A:92:CYS:HB3	0.63	1.94	16	5
1:A:82:ARG:HG2	1:A:83:SER:N	0.63	2.09	17	17
1:B:41:TYR:HB2	1:B:95:ALA:HB3	0.63	1.70	7	1
1:B:42:ILE:HD11	1:B:46:SER:CA	0.63	2.24	18	8
1:B:20:ILE:CG1	1:B:43:VAL:HG21	0.62	2.24	4	4
1:A:87:ARG:HD3	1:A:88:ALA:O	0.62	1.94	11	1
1:A:49:VAL:HG22	1:A:85:TRP:O	0.62	1.94	6	15
1:B:82:ARG:HG2	1:B:83:SER:N	0.62	2.08	12	13
1:A:99:TYR:O	1:A:103:ARG:HB3	0.62	1.94	2	17
1:B:187:LEU:HA	1:B:190:LEU:HG	0.62	1.69	9	19
1:A:47:VAL:O	1:A:63:TYR:HB3	0.62	1.94	9	14
1:B:103:ARG:O	1:B:106:ILE:HG13	0.62	1.95	18	6
1:B:61:LEU:HD12	1:B:62:SER:N	0.62	2.10	19	1
1:A:72:GLU:HB2	1:A:120:MET:SD	0.62	2.35	1	8
1:B:33:GLY:N	1:B:82:ARG:HD3	0.62	2.10	11	2
1:B:166:LYS:HG2	1:B:202:THR:HG22	0.62	1.70	9	1
1:A:155:ASP:HB3	1:A:165:ILE:CG2	0.62	2.24	9	9
1:A:134:LEU:HD22	1:A:174:GLN:O	0.62	1.94	16	11
1:B:31:HIS:CG	1:B:31:HIS:O	0.62	2.53	2	13
1:A:29:LEU:C	1:A:30:ILE:HG13	0.62	2.15	2	18
1:B:180:ARG:HA	1:B:183:VAL:HG12	0.62	1.72	8	7
1:B:30:ILE:HD12	1:B:86:VAL:CG2	0.61	2.25	1	11
1:B:190:LEU:HD22	1:B:196:ILE:HG13	0.61	1.73	17	13
1:A:197:SER:HB2	1:A:206:TYR:CE1	0.61	2.30	17	13
1:B:39:LEU:HD11	1:B:41:TYR:CE1	0.61	2.31	7	1
1:A:49:VAL:HG12	1:A:61:LEU:HD11	0.61	1.72	10	15
1:A:42:ILE:CA	1:A:94:VAL:HG12	0.61	2.23	20	15
1:B:29:LEU:C	1:B:30:ILE:HG13	0.61	2.15	1	16
1:A:29:LEU:CB	1:A:86:VAL:HB	0.61	2.25	6	1
1:B:190:LEU:HD13	1:B:196:ILE:CD1	0.61	2.26	13	3
1:B:186:ILE:O	1:B:189:MET:HG2	0.61	1.94	11	12
1:A:42:ILE:HD11	1:A:46:SER:CA	0.61	2.25	20	7
1:A:117:SER:HB3	1:B:76:PHE:CZ	0.61	2.30	14	1
1:B:11:LEU:HD12	1:B:15:LEU:HG	0.61	1.72	5	4
1:B:49:VAL:CG1	1:B:61:LEU:HD11	0.61	2.26	19	1
1:B:87:ARG:HD3	1:B:88:ALA:O	0.61	1.96	11	1
1:A:103:ARG:HA	1:A:106:ILE:CG1	0.61	2.26	17	17
1:A:31:HIS:O	1:A:31:HIS:CG	0.61	2.54	2	11
1:B:52:LYS:HA	1:B:57:LYS:O	0.61	1.96	7	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:147:LEU:CD2	1:B:203:ILE:HG21	0.61	2.26	19	1
1:B:25:SER:O	1:B:26:LYS:HG3	0.61	1.96	10	2
1:A:134:LEU:O	1:A:177:GLY:HA3	0.61	1.96	4	5
1:B:42:ILE:CA	1:B:94:VAL:HG12	0.60	2.26	20	16
1:B:150:LEU:HD13	1:B:167:ILE:HG12	0.60	1.73	3	10
1:B:190:LEU:HD13	1:B:196:ILE:HD12	0.60	1.73	20	15
1:B:166:LYS:HG3	1:B:202:THR:HG23	0.60	1.73	15	1
1:B:147:LEU:HD22	1:B:167:ILE:CD1	0.60	2.26	11	4
1:A:49:VAL:HG12	1:A:61:LEU:CD1	0.60	2.27	10	20
1:A:117:SER:HB2	1:B:76:PHE:CE1	0.60	2.31	4	3
1:A:147:LEU:HD22	1:A:167:ILE:CD1	0.60	2.26	7	5
1:A:77:GLU:HG3	1:A:79:GLY:N	0.60	2.11	20	4
1:A:131:VAL:HG12	1:B:131:VAL:HG12	0.60	1.73	9	4
1:B:44:LYS:HA	1:B:66:GLN:CD	0.60	2.16	17	1
1:B:49:VAL:HG12	1:B:61:LEU:CD1	0.60	2.27	9	19
1:A:20:ILE:HA	1:A:94:VAL:O	0.60	1.97	12	14
1:B:31:HIS:O	1:B:31:HIS:CG	0.60	2.54	10	5
1:B:103:ARG:HA	1:B:106:ILE:CG1	0.60	2.26	18	19
1:B:20:ILE:HD13	1:B:43:VAL:HG21	0.60	1.72	20	2
1:B:150:LEU:HB3	1:B:165:ILE:HG21	0.60	1.73	11	4
1:A:143:ILE:CD1	1:A:186:ILE:HD13	0.60	2.27	1	3
1:B:50:LEU:CB	1:B:60:ILE:HA	0.60	2.26	10	12
1:B:147:LEU:HA	1:B:150:LEU:HD12	0.60	1.74	5	12
1:A:23:TYR:N	1:A:23:TYR:CD1	0.60	2.70	17	3
1:B:28:THR:HA	1:B:29:LEU:HD23	0.60	1.72	1	7
1:A:196:ILE:HG22	1:A:197:SER:N	0.60	2.11	19	12
1:A:72:GLU:HG3	1:A:120:MET:HE2	0.60	1.73	14	1
1:A:44:LYS:HE2	1:A:66:GLN:OE1	0.60	1.95	19	1
1:B:41:TYR:O	1:B:43:VAL:HG23	0.60	1.97	11	11
1:A:41:TYR:CB	1:A:95:ALA:HB3	0.60	2.26	7	6
1:A:19:HIS:HB3	1:A:96:GLU:O	0.60	1.97	1	7
1:B:42:ILE:HD11	1:B:64:LEU:HD12	0.60	1.72	10	2
1:B:89:LYS:CE	1:B:155:ASP:OD1	0.60	2.50	10	1
1:A:37:GLU:HA	1:A:99:TYR:CZ	0.60	2.31	11	4
1:B:28:THR:HA	1:B:87:ARG:HA	0.60	1.71	15	4
1:B:59:MET:HE3	1:B:174:GLN:HB2	0.60	1.74	3	3
1:A:48:ALA:CB	1:A:60:ILE:HD12	0.60	2.27	3	4
1:A:143:ILE:HD13	1:A:186:ILE:HG21	0.59	1.72	8	2
1:A:173:GLY:CA	1:A:178:CYS:O	0.59	2.50	14	3
1:A:180:ARG:O	1:A:184:GLY:HA3	0.59	1.97	19	14
1:B:196:ILE:HG22	1:B:209:ARG:OXT	0.59	1.96	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:44:LYS:O	1:B:92:CYS:HB3	0.59	1.96	16	6
1:A:31:HIS:CG	1:A:31:HIS:O	0.59	2.55	10	7
1:B:23:TYR:CD1	1:B:23:TYR:N	0.59	2.70	18	10
1:A:63:TYR:CD2	1:A:89:LYS:HD2	0.59	2.32	18	2
1:B:159:HIS:CE1	1:B:161:ASP:HB3	0.59	2.33	18	5
1:A:51:ILE:HD12	1:A:61:LEU:HB3	0.59	1.74	7	1
1:A:63:TYR:O	1:A:64:LEU:HD23	0.59	1.97	12	1
1:A:28:THR:HA	1:A:87:ARG:HA	0.59	1.73	11	4
1:B:179:SER:HB2	1:B:181:GLU:OE2	0.59	1.98	14	1
1:B:106:ILE:HG22	1:B:112:ILE:CG2	0.59	2.27	17	14
1:B:31:HIS:CE1	1:B:58:GLU:HB2	0.59	2.32	1	5
1:A:122:ARG:NH2	1:B:78:GLU:HB3	0.59	2.13	19	6
1:A:31:HIS:CE1	1:A:58:GLU:HB3	0.59	2.31	8	4
1:A:53:ASP:HB2	1:A:57:LYS:HG2	0.59	1.74	1	2
1:A:103:ARG:O	1:A:106:ILE:HG13	0.59	1.97	1	9
1:B:196:ILE:HG22	1:B:197:SER:N	0.59	2.12	19	10
1:A:76:PHE:CE2	1:A:120:MET:HG3	0.59	2.33	12	1
1:B:27:SER:O	1:B:88:ALA:N	0.59	2.32	13	3
1:A:195:LEU:O	1:A:209:ARG:HB3	0.59	1.98	20	1
1:B:180:ARG:O	1:B:184:GLY:HA3	0.59	1.98	12	13
1:B:134:LEU:O	1:B:177:GLY:HA3	0.59	1.97	4	6
1:A:24:PRO:HA	1:A:91:ALA:CA	0.59	2.28	12	10
1:B:50:LEU:HB3	1:B:60:ILE:HG22	0.59	1.75	10	1
1:A:77:GLU:OE2	1:B:122:ARG:HA	0.59	1.97	9	1
1:B:22:LYS:HD2	1:B:92:CYS:SG	0.58	2.38	15	13
1:A:22:LYS:C	1:A:23:TYR:CD1	0.58	2.77	2	19
1:B:47:VAL:HA	1:B:89:LYS:N	0.58	2.12	12	15
1:A:182:THR:O	1:A:185:ARG:HB2	0.58	1.97	4	6
1:B:102:PHE:CE1	1:B:106:ILE:HG21	0.58	2.33	12	9
1:A:27:SER:O	1:A:88:ALA:N	0.58	2.34	13	3
1:A:102:PHE:CE1	1:A:106:ILE:HG21	0.58	2.32	12	9
1:B:169:ARG:CB	1:B:187:LEU:HD13	0.58	2.28	10	1
1:B:51:ILE:HD12	1:B:61:LEU:HB3	0.58	1.72	18	1
1:A:23:TYR:N	1:A:23:TYR:HD1	0.58	1.96	3	4
1:B:42:ILE:HG21	1:B:45:GLY:O	0.58	1.98	2	1
1:B:196:ILE:HG13	1:B:197:SER:N	0.58	2.14	13	1
1:B:99:TYR:HA	1:B:102:PHE:HB3	0.58	1.76	20	14
1:B:69:PHE:CG	1:B:116:LEU:HD13	0.58	2.34	2	1
1:B:172:ILE:CG2	1:B:183:VAL:HG21	0.58	2.28	14	8
1:A:28:THR:C	1:A:29:LEU:HD23	0.58	2.19	12	14
1:A:11:LEU:HD11	1:A:41:TYR:HE2	0.58	1.59	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:ARG:CA	1:A:126:VAL:HG12	0.58	2.28	3	2
1:A:72:GLU:CB	1:A:116:LEU:HD11	0.58	2.28	7	5
1:A:102:PHE:CE2	1:A:106:ILE:HG23	0.58	2.33	3	1
1:A:30:ILE:HG22	1:A:34:GLU:HB2	0.58	1.74	10	3
1:A:143:ILE:HG21	1:A:187:LEU:HD21	0.58	1.75	10	4
1:A:20:ILE:CG1	1:A:43:VAL:HG21	0.58	2.29	2	1
1:B:139:VAL:HA	1:B:176:VAL:CG1	0.58	2.29	3	1
1:A:123:ARG:HA	1:A:126:VAL:CG1	0.57	2.29	14	2
1:A:41:TYR:O	1:A:43:VAL:HG23	0.57	1.98	11	9
1:A:23:TYR:HD1	1:A:23:TYR:N	0.57	1.97	18	4
1:A:186:ILE:O	1:A:190:LEU:HG	0.57	2.00	17	13
1:A:70:ILE:HD13	1:A:86:VAL:HG11	0.57	1.76	13	14
1:A:52:LYS:HA	1:A:57:LYS:O	0.57	1.98	7	12
1:B:70:ILE:HD13	1:B:86:VAL:HG11	0.57	1.76	20	14
1:B:28:THR:HA	1:B:29:LEU:HD22	0.57	1.77	13	1
1:A:117:SER:HB2	1:B:76:PHE:CZ	0.57	2.34	4	5
1:B:117:SER:HA	1:B:120:MET:CE	0.57	2.29	4	1
1:B:190:LEU:CD1	1:B:196:ILE:HD12	0.57	2.29	18	12
1:B:61:LEU:HD22	1:B:62:SER:HB2	0.57	1.75	10	9
1:A:15:LEU:HD22	1:A:20:ILE:HD11	0.57	1.76	17	3
1:B:169:ARG:CG	1:B:187:LEU:HD12	0.57	2.30	2	2
1:B:174:GLN:HG2	1:B:175:ILE:N	0.57	2.14	6	3
1:A:28:THR:HB	1:A:87:ARG:HA	0.57	1.76	2	4
1:B:104:GLN:O	1:B:107:GLN:HG2	0.57	2.00	19	1
1:A:72:GLU:CB	1:A:120:MET:HE1	0.56	2.30	4	2
1:B:187:LEU:HD22	1:B:190:LEU:CD1	0.56	2.30	1	15
1:A:41:TYR:O	1:A:43:VAL:HG13	0.56	2.00	19	4
1:B:169:ARG:HB3	1:B:187:LEU:HD13	0.56	1.75	10	1
1:A:53:ASP:HB2	1:A:57:LYS:CG	0.56	2.30	1	1
1:B:197:SER:HB3	1:B:206:TYR:CE1	0.56	2.35	15	6
1:A:172:ILE:CG2	1:A:183:VAL:HG21	0.56	2.30	14	8
1:A:60:ILE:HB	1:A:174:GLN:CD	0.56	2.19	3	4
1:B:22:LYS:C	1:B:23:TYR:CD1	0.56	2.78	5	19
1:B:167:ILE:CD1	1:B:203:ILE:HD12	0.56	2.30	10	10
1:A:22:LYS:H	1:A:93:GLU:HA	0.56	1.59	17	17
1:B:166:LYS:HA	1:B:201:LYS:O	0.56	2.01	10	6
1:B:11:LEU:HD11	1:B:41:TYR:HE2	0.56	1.61	5	1
1:B:114:MET:HA	1:B:117:SER:OG	0.56	2.00	7	7
1:B:190:LEU:HD22	1:B:196:ILE:HG12	0.56	1.77	13	3
1:B:144:ALA:HB2	1:B:195:LEU:HD21	0.56	1.77	9	5
1:B:18:CYS:CB	1:B:97:ILE:HG12	0.56	2.31	6	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:37:GLU:HA	1:B:99:TYR:CZ	0.56	2.36	11	3
1:B:119:GLN:O	1:B:123:ARG:HD3	0.56	2.00	7	9
1:A:113:LEU:HD12	1:A:116:LEU:HD23	0.56	1.76	2	1
1:B:39:LEU:HD11	1:B:41:TYR:HE1	0.56	1.61	7	1
1:A:147:LEU:CD2	1:A:203:ILE:HG21	0.56	2.30	19	2
1:B:23:TYR:HD1	1:B:23:TYR:N	0.56	1.98	3	5
1:A:118:ALA:O	1:A:122:ARG:HB2	0.56	2.01	2	4
1:A:49:VAL:N	1:A:62:SER:O	0.56	2.39	14	13
1:B:173:GLY:CA	1:B:178:CYS:O	0.56	2.54	14	3
1:B:20:ILE:HG13	1:B:95:ALA:HB2	0.56	1.76	4	1
1:A:89:LYS:CE	1:A:155:ASP:OD1	0.56	2.53	10	1
1:B:65:ASN:O	1:B:68:ASP:HB2	0.56	2.01	7	4
1:B:42:ILE:HG22	1:B:68:ASP:H	0.56	1.59	12	2
1:B:49:VAL:N	1:B:62:SER:O	0.56	2.39	14	14
1:B:149:ASN:O	1:B:153:GLN:HG3	0.56	2.00	8	2
1:B:22:LYS:CG	1:B:94:VAL:HG22	0.56	2.30	1	1
1:A:187:LEU:CD2	1:A:190:LEU:HD11	0.56	2.31	8	4
1:B:197:SER:O	1:B:204:VAL:HB	0.56	2.01	9	3
1:A:43:VAL:C	1:A:66:GLN:HG3	0.56	2.19	17	1
1:B:208:THR:O	1:B:209:ARG:HB2	0.56	2.01	14	1
1:B:167:ILE:HD12	1:B:203:ILE:HD12	0.56	1.76	11	2
1:B:53:ASP:HB2	1:B:57:LYS:CG	0.56	2.31	1	1
1:B:166:LYS:HG2	1:B:202:THR:HG23	0.56	1.77	13	1
1:A:29:LEU:HD12	1:A:40:TYR:CD1	0.55	2.36	10	1
1:B:183:VAL:HG13	1:B:187:LEU:HD12	0.55	1.77	10	1
1:A:149:ASN:O	1:A:153:GLN:HG3	0.55	2.01	8	2
1:B:63:TYR:CD2	1:B:89:LYS:HD2	0.55	2.35	8	2
1:B:20:ILE:HA	1:B:94:VAL:O	0.55	2.01	1	16
1:B:167:ILE:HD11	1:B:203:ILE:CD1	0.55	2.29	9	1
1:B:53:ASP:OD1	1:B:57:LYS:HB3	0.55	2.02	14	1
1:B:18:CYS:HB3	1:B:97:ILE:HG12	0.55	1.78	14	14
1:A:169:ARG:HB2	1:A:180:ARG:HB3	0.55	1.78	2	14
1:B:169:ARG:HB2	1:B:180:ARG:HB3	0.55	1.78	7	11
1:A:51:ILE:HA	1:A:84:ALA:HB1	0.55	1.76	15	3
1:B:198:ALA:HB2	1:B:203:ILE:HG12	0.55	1.78	12	4
1:A:60:ILE:O	1:A:174:GLN:HG3	0.55	2.01	3	3
1:B:180:ARG:O	1:B:184:GLY:CA	0.55	2.55	13	16
1:A:29:LEU:HD12	1:A:70:ILE:HG21	0.55	1.78	11	8
1:A:8:ASP:O	1:A:12:GLU:HB2	0.55	2.01	4	1
1:B:45:GLY:HA3	1:B:92:CYS:CB	0.55	2.31	16	5
1:B:28:THR:C	1:B:29:LEU:HD23	0.55	2.22	12	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:41:TYR:CB	1:B:95:ALA:HB3	0.55	2.31	15	8
1:A:47:VAL:HA	1:A:89:LYS:N	0.55	2.16	17	14
1:A:114:MET:HA	1:A:117:SER:OG	0.55	2.02	12	6
1:B:190:LEU:CD2	1:B:195:LEU:HB3	0.55	2.31	13	10
1:B:29:LEU:O	1:B:30:ILE:HG13	0.55	2.01	6	5
1:A:121:ALA:HB1	1:B:77:GLU:HA	0.55	1.76	18	4
1:B:124:LEU:HA	1:B:128:SER:HB2	0.55	1.79	14	1
1:B:143:ILE:HG23	1:B:172:ILE:HG21	0.55	1.77	16	13
1:B:143:ILE:HD13	1:B:186:ILE:HG12	0.55	1.79	10	2
1:A:171:GLU:O	1:A:175:ILE:HG13	0.55	2.02	10	4
1:A:164:GLN:HB3	1:A:204:VAL:CG2	0.55	2.32	20	7
1:B:189:MET:SD	1:B:195:LEU:HD13	0.55	2.42	7	3
1:A:76:PHE:HD2	1:A:120:MET:SD	0.55	2.25	16	7
1:B:143:ILE:HD12	1:B:143:ILE:H	0.54	1.62	10	1
1:B:11:LEU:O	1:B:14:PHE:HB3	0.54	2.02	7	5
1:A:139:VAL:HG23	1:A:176:VAL:HG11	0.54	1.78	14	3
1:A:42:ILE:CD1	1:A:47:VAL:HG13	0.54	2.32	8	6
1:B:20:ILE:HD13	1:B:95:ALA:CB	0.54	2.32	13	6
1:A:24:PRO:HA	1:A:91:ALA:HA	0.54	1.78	12	7
1:A:39:LEU:HB2	1:A:75:LEU:HD22	0.54	1.78	13	1
1:A:20:ILE:HD13	1:A:95:ALA:CB	0.54	2.31	16	8
1:A:99:TYR:HA	1:A:102:PHE:HB3	0.54	1.79	20	11
1:A:159:HIS:CE1	1:A:161:ASP:HB3	0.54	2.37	18	4
1:A:105:LEU:HG	1:A:106:ILE:N	0.54	2.17	14	8
1:A:42:ILE:HD13	1:A:46:SER:HA	0.54	1.79	2	1
1:B:14:PHE:CD2	1:B:102:PHE:CE2	0.54	2.95	8	8
1:B:80:GLN:O	1:B:81:GLU:HB2	0.54	2.03	7	8
1:A:28:THR:HA	1:A:29:LEU:HD22	0.54	1.79	10	2
1:A:52:LYS:O	1:B:129:GLU:HA	0.54	2.03	6	3
1:B:72:GLU:O	1:B:76:PHE:HB3	0.54	2.03	4	4
1:A:61:LEU:HD13	1:A:62:SER:N	0.54	2.18	14	8
1:A:20:ILE:HG23	1:A:43:VAL:HG21	0.54	1.80	6	9
1:B:8:ASP:O	1:B:12:GLU:HB2	0.54	2.03	3	2
1:A:142:ARG:O	1:A:145:GLN:HB3	0.54	2.03	5	4
1:B:105:LEU:HG	1:B:106:ILE:N	0.54	2.17	14	7
1:B:132:GLY:HA2	1:B:135:ALA:HB3	0.54	1.79	5	1
1:A:81:GLU:O	1:A:82:ARG:HD2	0.54	2.02	14	1
1:B:151:ALA:HA	1:B:156:ALA:HB2	0.54	1.78	19	2
1:B:150:LEU:CD1	1:B:167:ILE:HG12	0.54	2.33	15	4
1:A:138:ASP:OD2	1:A:142:ARG:HD3	0.54	2.03	11	1
1:B:19:HIS:HB3	1:B:96:GLU:O	0.54	2.02	1	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:113:LEU:HD12	1:B:116:LEU:HD23	0.54	1.78	2	1
1:B:39:LEU:HD22	1:B:102:PHE:CD1	0.54	2.38	13	7
1:A:195:LEU:O	1:A:209:ARG:HG3	0.54	2.02	12	4
1:B:134:LEU:HD13	1:B:174:GLN:O	0.54	2.03	7	1
1:B:29:LEU:HB3	1:B:40:TYR:CZ	0.54	2.38	13	1
1:B:41:TYR:O	1:B:94:VAL:HA	0.53	2.02	11	7
1:A:197:SER:CB	1:A:206:TYR:CE1	0.53	2.91	1	17
1:A:180:ARG:O	1:A:184:GLY:CA	0.53	2.56	10	17
1:B:197:SER:CB	1:B:206:TYR:CE1	0.53	2.91	1	16
1:B:22:LYS:H	1:B:93:GLU:HA	0.53	1.62	17	17
1:B:45:GLY:HA3	1:B:92:CYS:HB3	0.53	1.80	10	15
1:B:123:ARG:HA	1:B:126:VAL:CG1	0.53	2.34	14	2
1:B:77:GLU:HG3	1:B:79:GLY:N	0.53	2.19	5	5
1:B:72:GLU:CB	1:B:116:LEU:HD11	0.53	2.33	18	4
1:B:20:ILE:HG13	1:B:43:VAL:HG21	0.53	1.79	15	1
1:A:167:ILE:HD11	1:A:203:ILE:CD1	0.53	2.33	9	1
1:A:11:LEU:O	1:A:14:PHE:HB3	0.53	2.03	7	3
1:A:183:VAL:O	1:A:187:LEU:HG	0.53	2.04	4	3
1:B:24:PRO:HA	1:B:91:ALA:CA	0.53	2.33	20	9
1:A:59:MET:HE3	1:A:174:GLN:HB2	0.53	1.79	3	4
1:A:18:CYS:HB3	1:A:97:ILE:HG12	0.53	1.80	17	14
1:A:190:LEU:CD1	1:A:196:ILE:HD12	0.53	2.34	18	14
1:B:156:ALA:HA	1:B:164:GLN:O	0.53	2.02	20	4
1:A:129:GLU:HA	1:B:52:LYS:O	0.53	2.03	6	2
1:A:29:LEU:HD23	1:A:86:VAL:HB	0.53	1.79	13	1
1:A:45:GLY:HA3	1:A:92:CYS:HB3	0.53	1.81	10	15
1:B:143:ILE:HG21	1:B:187:LEU:HD21	0.53	1.79	20	4
1:B:24:PRO:HA	1:B:91:ALA:HA	0.53	1.80	12	9
1:B:49:VAL:HG13	1:B:85:TRP:HA	0.53	1.80	19	5
1:A:174:GLN:HG2	1:A:175:ILE:N	0.53	2.18	6	2
1:B:164:GLN:HG3	1:B:202:THR:HG22	0.53	1.81	19	2
1:A:143:ILE:HG23	1:A:172:ILE:HG21	0.53	1.80	4	14
1:A:80:GLN:O	1:A:81:GLU:HB2	0.53	2.03	5	8
1:A:198:ALA:HB2	1:A:203:ILE:HG12	0.53	1.80	8	3
1:A:180:ARG:HA	1:A:183:VAL:HG12	0.53	1.80	20	6
1:B:171:GLU:HB3	1:B:175:ILE:HD12	0.53	1.79	7	1
1:B:42:ILE:O	1:B:42:ILE:HG12	0.53	2.02	5	1
1:A:106:ILE:HG22	1:A:112:ILE:HG21	0.53	1.81	7	7
1:A:31:HIS:HA	1:A:82:ARG:HG3	0.53	1.80	17	6
1:A:134:LEU:HB3	1:A:175:ILE:O	0.53	2.04	9	1
1:B:41:TYR:O	1:B:43:VAL:HG13	0.53	2.04	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:LEU:HD22	1:A:29:LEU:N	0.53	2.19	10	2
1:A:45:GLY:HA3	1:A:92:CYS:CB	0.53	2.34	16	7
1:A:41:TYR:O	1:A:94:VAL:HA	0.53	2.03	11	6
1:B:42:ILE:O	1:B:67:GLY:HA2	0.53	2.03	2	1
1:B:123:ARG:HD3	1:B:123:ARG:N	0.53	2.19	20	1
1:B:32:GLN:H	1:B:82:ARG:HG3	0.53	1.64	6	2
1:A:119:GLN:O	1:A:123:ARG:HD3	0.52	2.05	2	8
1:B:183:VAL:HG13	1:B:187:LEU:CD1	0.52	2.34	10	1
1:B:11:LEU:HD11	1:B:41:TYR:OH	0.52	2.04	19	1
1:B:126:VAL:O	1:B:130:LYS:HB2	0.52	2.04	13	1
1:A:48:ALA:HB1	1:A:60:ILE:HG21	0.52	1.81	4	1
1:B:23:TYR:O	1:B:91:ALA:HA	0.52	2.05	1	8
1:B:165:ILE:HD12	1:B:165:ILE:O	0.52	2.04	20	1
1:B:22:LYS:CB	1:B:92:CYS:O	0.52	2.51	12	1
1:B:179:SER:C	1:B:181:GLU:N	0.52	2.61	14	19
1:B:139:VAL:HG22	1:B:143:ILE:HD11	0.52	1.81	20	1
1:A:196:ILE:CD1	1:A:203:ILE:HG23	0.52	2.35	13	1
1:A:39:LEU:HD11	1:A:41:TYR:CE1	0.52	2.39	7	1
1:A:100:LYS:O	1:A:103:ARG:HG2	0.52	2.04	19	1
1:B:138:ASP:CG	1:B:138:ASP:O	0.52	2.48	12	1
1:A:73:LEU:HD23	1:A:120:MET:SD	0.52	2.44	11	1
1:A:22:LYS:N	1:A:93:GLU:HA	0.52	2.19	2	10
1:A:121:ALA:CB	1:B:77:GLU:HA	0.52	2.35	18	1
1:A:29:LEU:CD1	1:A:70:ILE:HG21	0.52	2.34	19	6
1:B:30:ILE:O	1:B:86:VAL:HG23	0.52	2.05	2	1
1:B:20:ILE:HD12	1:B:43:VAL:HG21	0.52	1.81	9	2
1:A:138:ASP:CG	1:A:138:ASP:O	0.52	2.48	20	1
1:B:23:TYR:CB	1:B:24:PRO:HD2	0.52	2.34	10	7
1:B:25:SER:HB3	1:B:90:THR:N	0.52	2.20	4	2
1:B:106:ILE:HG22	1:B:112:ILE:HG22	0.52	1.80	17	6
1:B:32:GLN:N	1:B:82:ARG:HG3	0.52	2.19	17	3
1:A:166:LYS:HG3	1:A:201:LYS:HB3	0.52	1.82	4	1
1:A:29:LEU:CD2	1:A:29:LEU:N	0.52	2.73	18	9
1:A:14:PHE:C	1:A:14:PHE:CD1	0.52	2.83	10	3
1:B:134:LEU:HD22	1:B:176:VAL:HA	0.52	1.80	10	1
1:B:60:ILE:HB	1:B:174:GLN:CD	0.52	2.25	7	5
1:B:76:PHE:HD2	1:B:120:MET:SD	0.52	2.28	11	6
1:B:76:PHE:CD2	1:B:120:MET:SD	0.52	3.03	12	3
1:A:124:LEU:HA	1:A:128:SER:HB2	0.52	1.82	14	1
1:B:173:GLY:HA3	1:B:178:CYS:O	0.52	2.05	14	1
1:B:196:ILE:CD1	1:B:203:ILE:HG23	0.52	2.34	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:TYR:HD2	1:A:27:SER:CB	0.52	2.17	14	5
1:A:138:ASP:O	1:A:140:THR:N	0.52	2.43	8	10
1:A:15:LEU:HD21	1:A:41:TYR:CE2	0.52	2.40	10	2
1:A:49:VAL:HG13	1:A:85:TRP:HA	0.52	1.81	19	5
1:A:65:ASN:O	1:A:68:ASP:HB2	0.52	2.05	7	3
1:A:124:LEU:HG	1:B:124:LEU:HD23	0.52	1.81	20	1
1:A:142:ARG:O	1:A:145:GLN:HB2	0.52	2.04	13	1
1:B:138:ASP:O	1:B:140:THR:N	0.51	2.44	10	11
1:A:135:ALA:HA	1:B:135:ALA:HA	0.51	1.83	5	1
1:B:48:ALA:O	1:B:87:ARG:HB3	0.51	2.05	15	2
1:B:102:PHE:CE2	1:B:106:ILE:HG23	0.51	2.40	17	2
1:A:44:LYS:HA	1:A:66:GLN:CD	0.51	2.24	17	1
1:B:29:LEU:N	1:B:29:LEU:CD2	0.51	2.72	1	6
1:A:162:GLY:HA3	1:A:204:VAL:CG2	0.51	2.35	2	1
1:A:197:SER:HB3	1:A:206:TYR:CE1	0.51	2.40	13	3
1:A:178:CYS:SG	1:A:183:VAL:HB	0.51	2.44	17	1
1:A:51:ILE:HD12	1:B:128:SER:HA	0.51	1.81	4	1
1:A:42:ILE:HG12	1:A:42:ILE:O	0.51	2.05	5	1
1:A:47:VAL:HA	1:A:89:LYS:CB	0.51	2.35	12	4
1:B:36:ALA:CB	1:B:74:GLY:HA3	0.51	2.34	7	10
1:A:14:PHE:CD2	1:A:102:PHE:CE2	0.51	2.97	3	7
1:B:50:LEU:HB2	1:B:59:MET:O	0.51	2.05	11	6
1:A:96:GLU:O	1:A:96:GLU:HG3	0.51	2.05	17	1
1:A:33:GLY:HA2	1:A:82:ARG:HB3	0.51	1.82	19	2
1:B:22:LYS:NZ	1:B:29:LEU:HD11	0.51	2.21	13	1
1:A:36:ALA:CB	1:A:74:GLY:HA3	0.51	2.35	7	12
1:B:51:ILE:HA	1:B:84:ALA:HB1	0.51	1.81	2	5
1:B:47:VAL:HA	1:B:89:LYS:CB	0.51	2.35	12	3
1:B:179:SER:O	1:B:181:GLU:N	0.51	2.32	1	10
1:B:43:VAL:C	1:B:66:GLN:HG3	0.51	2.23	17	1
1:B:193:GLN:HG2	1:B:197:SER:OG	0.51	2.05	19	1
1:B:30:ILE:HD12	1:B:86:VAL:HG23	0.51	1.81	4	4
1:B:106:ILE:HG22	1:B:112:ILE:HG21	0.51	1.82	2	8
1:A:165:ILE:O	1:A:165:ILE:HD12	0.51	2.05	20	2
1:B:183:VAL:O	1:B:187:LEU:HG	0.51	2.05	4	4
1:A:50:LEU:CB	1:A:60:ILE:HA	0.51	2.36	15	9
1:B:139:VAL:CG2	1:B:183:VAL:HG23	0.51	2.36	20	2
1:B:63:TYR:OH	1:B:175:ILE:HD11	0.51	2.05	13	1
1:B:47:VAL:CG2	1:B:64:LEU:HD12	0.51	2.35	6	3
1:B:25:SER:O	1:B:26:LYS:CB	0.51	2.59	19	15
1:B:146:THR:O	1:B:149:ASN:HB3	0.51	2.06	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:167:ILE:HG13	1:B:203:ILE:HD12	0.51	1.81	14	1
1:A:72:GLU:HB2	1:A:120:MET:CE	0.51	2.36	5	2
1:A:22:LYS:HE2	1:A:27:SER:OG	0.51	2.06	10	1
1:B:187:LEU:N	1:B:187:LEU:HD23	0.51	2.20	1	6
1:A:22:LYS:HB3	1:A:92:CYS:C	0.51	2.26	2	4
1:B:30:ILE:HG22	1:B:34:GLU:HB2	0.51	1.83	13	2
1:B:14:PHE:CE1	1:B:41:TYR:CD2	0.51	2.99	17	3
1:A:47:VAL:CG2	1:A:64:LEU:HD12	0.51	2.35	6	1
1:A:208:THR:O	1:A:209:ARG:HB2	0.51	2.05	19	2
1:A:11:LEU:HD11	1:A:41:TYR:OH	0.51	2.06	19	1
1:A:153:GLN:HB3	1:A:154:PRO:HD2	0.51	1.83	15	15
1:A:102:PHE:CZ	1:A:106:ILE:HG21	0.51	2.41	15	7
1:B:45:GLY:HA3	1:B:92:CYS:HA	0.51	1.83	20	8
1:A:78:GLU:HB3	1:B:122:ARG:NH2	0.51	2.21	19	4
1:B:109:ASN:CG	1:B:112:ILE:HG13	0.51	2.25	14	1
1:A:109:ASN:OD1	1:A:112:ILE:HG13	0.51	2.06	19	2
1:A:139:VAL:CG2	1:A:183:VAL:HG23	0.51	2.36	4	4
1:A:61:LEU:HD22	1:A:62:SER:HB2	0.51	1.81	10	6
1:B:14:PHE:C	1:B:14:PHE:CD1	0.51	2.85	7	2
1:B:31:HIS:HA	1:B:82:ARG:HG3	0.51	1.83	15	5
1:B:14:PHE:CD1	1:B:15:LEU:HD23	0.50	2.42	19	6
1:B:82:ARG:CG	1:B:83:SER:N	0.50	2.73	12	17
1:B:164:GLN:HB3	1:B:204:VAL:CG2	0.50	2.36	1	6
1:B:166:LYS:CA	1:B:202:THR:HA	0.50	2.36	4	7
1:B:29:LEU:HB2	1:B:86:VAL:HB	0.50	1.83	10	2
1:A:169:ARG:HG3	1:A:180:ARG:HB3	0.50	1.83	20	1
1:B:60:ILE:HG21	1:B:63:TYR:CE2	0.50	2.41	1	9
1:A:150:LEU:CD1	1:A:167:ILE:HG12	0.50	2.35	4	7
1:A:179:SER:C	1:A:181:GLU:N	0.50	2.65	13	19
1:A:60:ILE:HD11	1:A:87:ARG:NH1	0.50	2.21	2	1
1:A:166:LYS:O	1:A:166:LYS:HD3	0.50	2.06	7	1
1:B:29:LEU:HD22	1:B:29:LEU:N	0.50	2.20	13	1
1:A:29:LEU:N	1:A:29:LEU:CD2	0.50	2.74	10	6
1:A:82:ARG:CG	1:A:83:SER:N	0.50	2.74	5	18
1:A:205:VAL:HG12	1:A:209:ARG:OXT	0.50	2.07	5	2
1:B:123:ARG:CA	1:B:126:VAL:HG12	0.50	2.36	3	4
1:A:191:GLU:HG2	1:A:198:ALA:O	0.50	2.06	9	1
1:A:166:LYS:HG2	1:A:202:THR:HG23	0.50	1.83	20	2
1:A:106:ILE:CD1	1:A:113:LEU:HD22	0.50	2.36	19	1
1:A:29:LEU:HB3	1:A:40:TYR:CZ	0.50	2.41	13	1
1:A:50:LEU:HB2	1:A:59:MET:C	0.50	2.27	15	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:GLU:HA	1:B:121:ALA:CB	0.50	2.34	18	1
1:B:121:ALA:O	1:B:124:LEU:HB2	0.50	2.06	18	3
1:B:73:LEU:HD23	1:B:120:MET:SD	0.50	2.46	11	1
1:A:103:ARG:HA	1:A:106:ILE:HG12	0.50	1.83	4	7
1:A:14:PHE:CD1	1:A:14:PHE:C	0.50	2.85	13	3
1:A:69:PHE:CD1	1:A:116:LEU:HD13	0.50	2.41	2	1
1:B:60:ILE:O	1:B:174:GLN:HG3	0.50	2.07	15	4
1:B:18:CYS:HB3	1:B:97:ILE:CD1	0.50	2.37	20	8
1:A:146:THR:HG21	1:A:175:ILE:HG23	0.50	1.84	7	1
1:B:143:ILE:HG12	1:B:183:VAL:CG2	0.50	2.36	11	1
1:B:42:ILE:CD1	1:B:46:SER:HA	0.50	2.35	4	3
1:A:23:TYR:CB	1:A:24:PRO:HD2	0.50	2.36	10	7
1:B:72:GLU:HA	1:B:75:LEU:HD23	0.50	1.82	8	6
1:A:11:LEU:HD23	1:A:14:PHE:HB3	0.50	1.84	9	4
1:B:50:LEU:HB2	1:B:59:MET:C	0.50	2.27	20	14
1:A:166:LYS:HB3	1:A:202:THR:HA	0.50	1.82	20	2
1:B:146:THR:HG21	1:B:175:ILE:HG23	0.50	1.81	7	1
1:B:81:GLU:O	1:B:82:ARG:HD2	0.50	2.06	14	1
1:A:164:GLN:HB2	1:A:202:THR:HG22	0.50	1.84	12	1
1:A:196:ILE:CG2	1:A:197:SER:H	0.50	2.17	18	7
1:A:75:LEU:CB	1:A:99:TYR:CD2	0.50	2.95	11	9
1:B:187:LEU:CD2	1:B:190:LEU:HD11	0.50	2.35	9	4
1:B:23:TYR:CD2	1:B:27:SER:HB3	0.50	2.42	6	2
1:A:143:ILE:H	1:A:143:ILE:HD12	0.50	1.64	10	1
1:A:42:ILE:HG12	1:A:94:VAL:HG12	0.50	1.84	2	1
1:B:11:LEU:HD23	1:B:14:PHE:HB3	0.50	1.84	19	2
1:A:124:LEU:HG	1:B:124:LEU:CD2	0.50	2.37	20	3
1:A:129:GLU:O	1:A:130:LYS:HG2	0.50	2.07	6	1
1:A:187:LEU:HA	1:A:190:LEU:CG	0.50	2.37	8	1
1:B:33:GLY:HA2	1:B:82:ARG:HB3	0.50	1.83	19	1
1:A:104:GLN:O	1:A:107:GLN:HG2	0.50	2.06	19	1
1:A:42:ILE:CD1	1:A:46:SER:HA	0.50	2.36	5	3
1:B:14:PHE:CD1	1:B:14:PHE:C	0.50	2.84	9	3
1:A:89:LYS:HE2	1:A:155:ASP:OD1	0.50	2.07	10	1
1:B:50:LEU:HB3	1:B:60:ILE:HA	0.50	1.83	10	2
1:B:55:GLU:OE1	1:B:57:LYS:HB2	0.50	2.06	20	3
1:A:186:ILE:HA	1:A:189:MET:HG2	0.50	1.84	17	1
1:B:103:ARG:HA	1:B:106:ILE:HG12	0.49	1.83	4	7
1:B:166:LYS:HA	1:B:202:THR:HA	0.49	1.84	6	13
1:A:169:ARG:HB2	1:A:180:ARG:CB	0.49	2.37	11	7
1:A:11:LEU:HD12	1:A:15:LEU:CG	0.49	2.38	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:171:GLU:O	1:B:175:ILE:HG13	0.49	2.07	10	2
1:A:196:ILE:HG12	1:A:209:ARG:OXT	0.49	2.07	7	2
1:A:11:LEU:C	1:A:13:TRP:H	0.49	2.10	20	1
1:A:31:HIS:CE1	1:A:58:GLU:HB2	0.49	2.42	4	4
1:A:128:SER:HB3	1:B:51:ILE:CG2	0.49	2.35	5	5
1:B:196:ILE:CG2	1:B:197:SER:H	0.49	2.16	6	6
1:B:47:VAL:HG21	1:B:86:VAL:HG12	0.49	1.83	2	2
1:A:50:LEU:HB2	1:A:59:MET:O	0.49	2.08	11	5
1:B:109:ASN:OD1	1:B:112:ILE:HG13	0.49	2.07	19	2
1:A:15:LEU:HA	1:A:18:CYS:HG	0.49	1.66	5	2
1:B:29:LEU:CD2	1:B:29:LEU:N	0.49	2.73	17	6
1:B:61:LEU:HD13	1:B:62:SER:N	0.49	2.22	15	6
1:B:147:LEU:O	1:B:150:LEU:HB2	0.49	2.07	20	3
1:A:60:ILE:HG21	1:A:63:TYR:CE2	0.49	2.43	16	4
1:B:50:LEU:HA	1:B:61:LEU:HD12	0.49	1.84	11	1
1:B:143:ILE:HD12	1:B:186:ILE:HB	0.49	1.84	18	2
1:B:29:LEU:HD12	1:B:70:ILE:HG21	0.49	1.84	11	10
1:A:166:LYS:HA	1:A:202:THR:HA	0.49	1.83	12	11
1:A:25:SER:O	1:A:26:LYS:CB	0.49	2.60	19	17
1:A:24:PRO:CA	1:A:91:ALA:HB2	0.49	2.34	5	1
1:B:102:PHE:CZ	1:B:106:ILE:HG21	0.49	2.43	9	7
1:A:164:GLN:HG3	1:A:202:THR:HG22	0.49	1.83	14	3
1:B:50:LEU:HB3	1:B:60:ILE:HD13	0.49	1.84	17	3
1:B:117:SER:HA	1:B:120:MET:HE3	0.49	1.85	4	1
1:A:164:GLN:C	1:A:165:ILE:HG13	0.49	2.28	12	10
1:A:144:ALA:HB2	1:A:195:LEU:CD2	0.49	2.37	18	4
1:B:22:LYS:HB3	1:B:92:CYS:C	0.49	2.28	14	4
1:B:23:TYR:HD2	1:B:27:SER:CB	0.49	2.20	14	3
1:B:42:ILE:CD1	1:B:47:VAL:HG13	0.49	2.37	13	5
1:A:120:MET:O	1:A:123:ARG:HB2	0.49	2.07	16	2
1:A:49:VAL:CA	1:A:85:TRP:O	0.49	2.59	16	2
1:A:41:TYR:HD1	1:A:68:ASP:O	0.49	1.91	10	2
1:B:169:ARG:HG3	1:B:180:ARG:HB2	0.49	1.85	10	1
1:A:50:LEU:HB3	1:A:60:ILE:HD13	0.49	1.84	6	3
1:A:190:LEU:HD13	1:A:196:ILE:CD1	0.49	2.37	13	2
1:B:22:LYS:NZ	1:B:88:ALA:HB2	0.49	2.23	18	2
1:B:103:ARG:HA	1:B:106:ILE:HG13	0.49	1.85	13	9
1:B:64:LEU:HB3	1:B:68:ASP:CB	0.49	2.37	2	2
1:A:146:THR:HG21	1:A:175:ILE:CG2	0.49	2.37	7	1
1:A:117:SER:HB3	1:B:76:PHE:CE2	0.49	2.43	14	1
1:B:101:LYS:O	1:B:104:GLN:HG2	0.49	2.08	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:75:LEU:CB	1:B:99:TYR:CD2	0.49	2.95	6	11
1:B:143:ILE:CD1	1:B:183:VAL:HA	0.49	2.37	18	1
1:A:135:ALA:HB1	1:B:135:ALA:HB1	0.49	1.84	1	2
1:A:41:TYR:CD1	1:A:41:TYR:C	0.49	2.85	13	3
1:A:40:TYR:HB2	1:A:70:ILE:HB	0.49	1.83	20	1
1:B:138:ASP:O	1:B:142:ARG:CB	0.49	2.60	7	1
1:A:14:PHE:O	1:A:17:HIS:HB2	0.49	2.08	9	1
1:A:135:ALA:CB	1:B:135:ALA:HB3	0.49	2.36	6	2
1:A:41:TYR:CE1	1:A:69:PHE:HD1	0.49	2.26	7	1
1:A:69:PHE:CG	1:A:116:LEU:HD13	0.48	2.43	2	1
1:A:167:ILE:HG22	1:A:171:GLU:HG3	0.48	1.84	8	1
1:B:22:LYS:CG	1:B:23:TYR:CD1	0.48	2.96	16	1
1:B:22:LYS:N	1:B:93:GLU:HA	0.48	2.23	2	11
1:A:184:GLY:O	1:A:188:LYS:HB2	0.48	2.08	6	5
1:B:15:LEU:HD21	1:B:41:TYR:HE2	0.48	1.68	10	1
1:A:81:GLU:O	1:A:82:ARG:HD3	0.48	2.09	2	3
1:B:99:TYR:CD1	1:B:99:TYR:C	0.48	2.86	20	8
1:A:32:GLN:N	1:A:82:ARG:HG3	0.48	2.23	6	3
1:A:166:LYS:C	1:A:167:ILE:HG13	0.48	2.28	15	2
1:A:37:GLU:O	1:A:99:TYR:CD1	0.48	2.66	19	1
1:B:143:ILE:CG2	1:B:187:LEU:HD21	0.48	2.38	5	4
1:A:102:PHE:CE2	1:A:106:ILE:CG2	0.48	2.96	3	4
1:B:96:GLU:HG3	1:B:96:GLU:O	0.48	2.09	17	2
1:A:157:MET:O	1:A:163:MET:HB3	0.48	2.08	3	1
1:A:14:PHE:CD1	1:A:15:LEU:HD23	0.48	2.43	19	7
1:B:31:HIS:HB2	1:B:84:ALA:HA	0.48	1.84	14	1
1:A:47:VAL:CG1	1:A:88:ALA:HA	0.48	2.38	12	1
1:B:180:ARG:HD2	1:B:181:GLU:OE2	0.48	2.07	12	1
1:A:39:LEU:HD22	1:A:102:PHE:CD1	0.48	2.43	20	6
1:B:18:CYS:HA	1:B:97:ILE:HG23	0.48	1.84	10	1
1:A:33:GLY:N	1:A:82:ARG:HD2	0.48	2.24	10	1
1:B:11:LEU:HD23	1:B:14:PHE:CG	0.48	2.44	9	1
1:A:51:ILE:HG21	1:B:128:SER:HB2	0.48	1.85	3	1
1:B:140:THR:O	1:B:142:ARG:N	0.48	2.46	3	1
1:B:143:ILE:HD13	1:B:186:ILE:CG1	0.48	2.38	20	1
1:B:76:PHE:CD1	1:B:120:MET:HE1	0.48	2.44	14	1
1:A:54:GLU:HB2	1:B:133:ASN:OD1	0.48	2.07	1	1
1:B:156:ALA:HA	1:B:165:ILE:HG23	0.48	1.84	20	2
1:A:121:ALA:O	1:A:124:LEU:HB2	0.48	2.07	18	2
1:B:143:ILE:HD13	1:B:183:VAL:HA	0.48	1.85	18	2
1:A:130:LYS:HG3	1:A:133:ASN:OD1	0.48	2.08	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:143:ILE:HD13	1:B:186:ILE:HG13	0.48	1.85	1	1
1:B:169:ARG:CA	1:B:187:LEU:HD12	0.48	2.38	11	1
1:A:103:ARG:HA	1:A:106:ILE:HG13	0.48	1.85	17	8
1:A:18:CYS:HA	1:A:97:ILE:HG23	0.48	1.84	10	3
1:A:103:ARG:O	1:A:107:GLN:HG2	0.48	2.09	18	1
1:A:34:GLU:OE2	1:A:82:ARG:HB2	0.48	2.08	17	5
1:B:164:GLN:C	1:B:165:ILE:HG13	0.48	2.29	12	9
1:B:118:ALA:O	1:B:122:ARG:HB2	0.48	2.08	2	4
1:A:23:TYR:O	1:A:91:ALA:HA	0.48	2.08	5	7
1:A:156:ALA:HA	1:A:165:ILE:HG23	0.48	1.85	20	4
1:B:39:LEU:HG	1:B:40:TYR:N	0.48	2.24	3	3
1:A:166:LYS:HB3	1:A:202:THR:HG23	0.48	1.86	10	1
1:A:169:ARG:HG3	1:A:180:ARG:CB	0.48	2.39	20	1
1:B:48:ALA:CB	1:B:60:ILE:HD12	0.48	2.37	8	3
1:A:147:LEU:CD2	1:A:167:ILE:HD11	0.48	2.39	19	2
1:A:124:LEU:HA	1:A:128:SER:CB	0.48	2.38	14	1
1:A:190:LEU:CD2	1:A:195:LEU:HB3	0.48	2.39	14	6
1:A:143:ILE:CG2	1:A:187:LEU:HD21	0.48	2.38	8	2
1:A:122:ARG:CZ	1:B:78:GLU:HB3	0.48	2.38	20	3
1:B:77:GLU:O	1:B:78:GLU:HB2	0.48	2.09	14	1
1:A:124:LEU:HG	1:B:124:LEU:HG	0.48	1.86	13	4
1:A:99:TYR:C	1:A:99:TYR:CD1	0.48	2.87	3	7
1:B:106:ILE:HD13	1:B:113:LEU:HD22	0.48	1.85	15	3
1:A:173:GLY:HA3	1:A:178:CYS:O	0.48	2.09	14	1
1:A:109:ASN:CB	1:A:112:ILE:HG13	0.48	2.39	11	2
1:A:166:LYS:HA	1:A:201:LYS:O	0.47	2.10	10	4
1:A:11:LEU:HD23	1:A:14:PHE:CG	0.47	2.44	14	4
1:B:143:ILE:CG1	1:B:183:VAL:HG22	0.47	2.38	10	1
1:B:51:ILE:CD1	1:B:61:LEU:HB3	0.47	2.39	18	1
1:A:42:ILE:HB	1:A:68:ASP:O	0.47	2.09	2	1
1:A:54:GLU:OE1	1:B:130:LYS:HE3	0.47	2.09	15	1
1:A:109:ASN:CG	1:A:112:ILE:HG13	0.47	2.29	14	1
1:B:117:SER:HA	1:B:120:MET:HE2	0.47	1.86	12	1
1:A:45:GLY:HA3	1:A:92:CYS:HA	0.47	1.85	20	6
1:A:147:LEU:O	1:A:150:LEU:HB2	0.47	2.09	20	4
1:B:143:ILE:HD12	1:B:186:ILE:CB	0.47	2.39	18	2
1:B:33:GLY:H	1:B:82:ARG:HB2	0.47	1.68	14	1
1:B:28:THR:HB	1:B:87:ARG:HA	0.47	1.86	7	4
1:B:69:PHE:CB	1:B:116:LEU:HD12	0.47	2.39	9	3
1:B:14:PHE:CE1	1:B:41:TYR:HD2	0.47	2.27	2	1
1:B:187:LEU:HD23	1:B:187:LEU:N	0.47	2.25	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:TYR:CD2	1:A:27:SER:HB3	0.47	2.44	6	1
1:A:51:ILE:HD13	1:A:51:ILE:H	0.47	1.69	7	1
1:B:8:ASP:O	1:B:12:GLU:HG2	0.47	2.09	1	1
1:B:138:ASP:OD2	1:B:142:ARG:HD3	0.47	2.09	11	1
1:A:109:ASN:HB2	1:A:112:ILE:HG13	0.47	1.86	13	11
1:A:27:SER:N	1:A:88:ALA:HB3	0.47	2.25	14	4
1:B:166:LYS:HB3	1:B:202:THR:HG23	0.47	1.87	5	1
1:A:76:PHE:CE1	1:B:117:SER:HB2	0.47	2.45	10	1
1:B:134:LEU:HB3	1:B:175:ILE:O	0.47	2.09	9	1
1:B:75:LEU:CB	1:B:99:TYR:HD2	0.47	2.22	20	2
1:B:33:GLY:HA2	1:B:82:ARG:CB	0.47	2.39	14	1
1:B:102:PHE:O	1:B:106:ILE:HG23	0.47	2.08	19	1
1:B:153:GLN:HB3	1:B:154:PRO:HD2	0.47	1.85	17	15
1:B:99:TYR:C	1:B:99:TYR:CD1	0.47	2.87	5	5
1:A:123:ARG:N	1:A:123:ARG:HD3	0.47	2.23	7	1
1:A:190:LEU:HD23	1:A:195:LEU:HB3	0.47	1.85	19	2
1:B:147:LEU:HD21	1:B:203:ILE:HG21	0.47	1.86	14	1
1:A:179:SER:O	1:A:181:GLU:N	0.47	2.48	13	8
1:A:27:SER:H	1:A:88:ALA:HB3	0.47	1.70	14	3
1:B:169:ARG:HB2	1:B:180:ARG:CB	0.47	2.39	11	5
1:A:99:TYR:CD1	1:A:99:TYR:C	0.47	2.88	5	5
1:A:64:LEU:HD13	1:A:68:ASP:HB3	0.47	1.84	10	1
1:A:76:PHE:CD2	1:A:120:MET:SD	0.47	3.08	16	5
1:A:14:PHE:CE1	1:A:41:TYR:HD2	0.47	2.27	2	3
1:B:69:PHE:CD1	1:B:116:LEU:HD13	0.47	2.45	2	1
1:A:150:LEU:HB3	1:A:165:ILE:HG21	0.47	1.86	9	3
1:A:157:MET:O	1:A:163:MET:CA	0.47	2.63	8	1
1:A:141:GLY:O	1:A:145:GLN:CB	0.47	2.63	14	1
1:B:147:LEU:CD2	1:B:167:ILE:HD11	0.47	2.40	14	1
1:A:46:SER:HB2	1:A:64:LEU:O	0.47	2.09	12	1
1:B:122:ARG:O	1:B:125:GLN:HG2	0.47	2.08	11	1
1:A:20:ILE:HD12	1:A:43:VAL:HG21	0.47	1.86	11	3
1:B:76:PHE:CE2	1:B:120:MET:HE3	0.47	2.45	2	1
1:A:22:LYS:NZ	1:A:88:ALA:HB2	0.47	2.25	9	3
1:A:167:ILE:HD11	1:A:203:ILE:HD12	0.47	1.86	9	1
1:A:164:GLN:OE1	1:A:202:THR:HB	0.47	2.10	19	1
1:A:180:ARG:HD2	1:A:181:GLU:OE1	0.47	2.10	4	3
1:A:60:ILE:HB	1:A:174:GLN:NE2	0.47	2.25	3	2
1:B:15:LEU:HA	1:B:18:CYS:HG	0.47	1.69	8	4
1:A:61:LEU:HD22	1:A:61:LEU:C	0.47	2.30	12	5
1:B:47:VAL:HB	1:B:88:ALA:HA	0.47	1.85	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:130:LYS:HA	1:B:133:ASN:OD1	0.47	2.09	5	3
1:A:128:SER:O	1:B:51:ILE:HG13	0.47	2.10	10	1
1:A:14:PHE:CE1	1:A:41:TYR:CD2	0.47	3.03	1	6
1:B:60:ILE:HB	1:B:174:GLN:NE2	0.47	2.25	6	4
1:B:157:MET:O	1:B:163:MET:HB3	0.47	2.09	3	1
1:B:45:GLY:HA3	1:B:92:CYS:CA	0.47	2.39	16	3
1:B:124:LEU:O	1:B:128:SER:HB2	0.47	2.10	14	1
1:B:33:GLY:N	1:B:82:ARG:HB2	0.47	2.25	14	1
1:A:51:ILE:CG2	1:B:128:SER:HB3	0.46	2.38	5	4
1:A:11:LEU:HD13	1:A:41:TYR:OH	0.46	2.11	10	3
1:A:143:ILE:CD1	1:A:183:VAL:HG22	0.46	2.41	16	2
1:B:109:ASN:CB	1:B:112:ILE:HG13	0.46	2.40	11	3
1:A:77:GLU:OE1	1:B:122:ARG:HD2	0.46	2.10	14	1
1:B:102:PHE:CE2	1:B:106:ILE:HG22	0.46	2.45	19	1
1:A:166:LYS:CA	1:A:202:THR:HA	0.46	2.40	4	4
1:B:178:CYS:SG	1:B:182:THR:HB	0.46	2.50	5	1
1:B:64:LEU:HA	1:B:123:ARG:NH2	0.46	2.24	17	2
1:B:76:PHE:CE2	1:B:116:LEU:HG	0.46	2.45	2	1
1:B:102:PHE:CE2	1:B:106:ILE:CG2	0.46	2.99	15	3
1:B:99:TYR:HD1	1:B:100:LYS:N	0.46	2.08	20	1
1:B:23:TYR:HB3	1:B:24:PRO:HD2	0.46	1.86	13	1
1:A:25:SER:HB3	1:A:90:THR:N	0.46	2.24	19	2
1:B:61:LEU:HD22	1:B:61:LEU:C	0.46	2.30	12	5
1:A:28:THR:CA	1:A:29:LEU:HD22	0.46	2.40	10	1
1:B:25:SER:O	1:B:26:LYS:CG	0.46	2.63	10	1
1:A:39:LEU:HD22	1:A:102:PHE:CE1	0.46	2.45	20	1
1:B:41:TYR:CE1	1:B:69:PHE:HD1	0.46	2.29	7	1
1:A:76:PHE:CE1	1:A:113:LEU:HD21	0.46	2.45	17	1
1:A:143:ILE:HG23	1:A:172:ILE:CG2	0.46	2.40	8	1
1:A:72:GLU:O	1:A:76:PHE:HB3	0.46	2.10	12	1
1:B:142:ARG:O	1:B:145:GLN:HB3	0.46	2.10	4	4
1:A:32:GLN:OE1	1:A:32:GLN:HA	0.46	2.09	4	2
1:A:18:CYS:HB3	1:A:97:ILE:CD1	0.46	2.41	13	5
1:B:96:GLU:O	1:B:96:GLU:HG3	0.46	2.11	10	1
1:B:103:ARG:C	1:B:106:ILE:HG13	0.46	2.31	18	1
1:B:22:LYS:HG3	1:B:94:VAL:CG2	0.46	2.39	19	2
1:B:30:ILE:HD12	1:B:86:VAL:HG21	0.46	1.86	1	1
1:A:64:LEU:HA	1:A:123:ARG:NH2	0.46	2.26	10	3
1:A:14:PHE:CE2	1:A:102:PHE:CE1	0.46	3.04	10	2
1:A:28:THR:CB	1:A:87:ARG:HA	0.46	2.41	17	2
1:A:133:ASN:HD21	1:A:142:ARG:NH2	0.46	2.09	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:167:ILE:CD1	1:A:203:ILE:HD12	0.46	2.40	6	6
1:A:155:ASP:CB	1:A:165:ILE:HG22	0.46	2.41	15	2
1:A:15:LEU:HD22	1:A:20:ILE:CD1	0.46	2.40	11	2
1:A:96:GLU:O	1:A:97:ILE:HG23	0.46	2.11	11	2
1:B:27:SER:N	1:B:88:ALA:HB3	0.46	2.26	9	5
1:B:50:LEU:O	1:B:50:LEU:HD23	0.46	2.11	5	1
1:B:196:ILE:CG2	1:B:197:SER:N	0.46	2.78	19	3
1:B:187:LEU:HA	1:B:190:LEU:CG	0.46	2.41	9	1
1:A:78:GLU:HB3	1:B:122:ARG:CZ	0.46	2.40	9	1
1:A:34:GLU:O	1:A:82:ARG:HA	0.46	2.11	14	1
1:B:44:LYS:CE	1:B:66:GLN:OE1	0.46	2.59	19	1
1:A:41:TYR:CE2	1:A:69:PHE:CE1	0.46	3.04	16	4
1:B:109:ASN:HB2	1:B:112:ILE:HG13	0.46	1.87	18	9
1:A:122:ARG:HA	1:B:77:GLU:OE2	0.46	2.11	8	1
1:B:143:ILE:O	1:B:147:LEU:HD12	0.46	2.11	19	1
1:A:61:LEU:C	1:A:61:LEU:HD22	0.46	2.32	6	8
1:A:70:ILE:CG2	1:A:86:VAL:HG21	0.46	2.32	10	1
1:B:155:ASP:CB	1:B:165:ILE:HG22	0.46	2.41	20	1
1:B:96:GLU:O	1:B:97:ILE:HG23	0.46	2.11	11	2
1:A:146:THR:O	1:A:149:ASN:HB2	0.46	2.11	16	1
1:A:64:LEU:HB3	1:A:68:ASP:CB	0.46	2.41	2	2
1:A:113:LEU:HD21	1:B:114:MET:HG2	0.46	1.88	9	1
1:A:138:ASP:O	1:A:138:ASP:CG	0.46	2.54	6	2
1:A:127:THR:O	1:A:131:VAL:HG23	0.46	2.11	6	2
1:B:22:LYS:HZ3	1:B:88:ALA:HB2	0.46	1.71	19	1
1:B:60:ILE:HD11	1:B:87:ARG:NH1	0.46	2.26	2	1
1:A:76:PHE:CE2	1:A:116:LEU:HG	0.46	2.46	2	1
1:B:29:LEU:CD1	1:B:70:ILE:HG21	0.46	2.41	9	3
1:A:76:PHE:HD2	1:A:120:MET:CE	0.46	2.24	7	1
1:B:150:LEU:HD13	1:B:165:ILE:HD13	0.45	1.88	5	1
1:A:96:GLU:HG3	1:A:96:GLU:O	0.45	2.10	10	3
1:A:139:VAL:HG21	1:A:183:VAL:HG23	0.45	1.88	10	1
1:A:187:LEU:N	1:A:187:LEU:HD23	0.45	2.26	13	6
1:A:30:ILE:O	1:A:86:VAL:HG23	0.45	2.11	2	1
1:A:128:SER:HB3	1:B:128:SER:HB3	0.45	1.87	14	1
1:B:89:LYS:NZ	1:B:155:ASP:OD2	0.45	2.48	10	1
1:B:47:VAL:HA	1:B:89:LYS:HB3	0.45	1.87	18	1
1:A:116:LEU:HG	1:A:120:MET:CE	0.45	2.41	18	1
1:B:90:THR:O	1:B:91:ALA:C	0.45	2.55	11	2
1:A:11:LEU:HD21	1:A:41:TYR:CZ	0.45	2.46	16	2
1:B:184:GLY:O	1:B:188:LYS:HB2	0.45	2.11	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ASP:CB	1:A:57:LYS:HG2	0.45	2.42	19	2
1:A:31:HIS:CE1	1:A:58:GLU:CB	0.45	3.00	20	5
1:A:114:MET:HG2	1:B:113:LEU:HD21	0.45	1.88	9	2
1:A:125:GLN:O	1:A:125:GLN:HG3	0.45	2.10	9	1
1:A:22:LYS:HZ1	1:A:29:LEU:HD22	0.45	1.71	12	1
1:B:117:SER:HA	1:B:120:MET:SD	0.45	2.51	4	1
1:B:147:LEU:HD13	1:B:203:ILE:HG21	0.45	1.87	18	1
1:A:76:PHE:CE2	1:A:120:MET:HE3	0.45	2.46	2	1
1:B:193:GLN:CA	1:B:196:ILE:O	0.45	2.59	12	1
1:A:46:SER:HB2	1:A:64:LEU:C	0.45	2.32	12	1
1:B:76:PHE:CE2	1:B:120:MET:SD	0.45	3.10	4	1
1:A:147:LEU:HD22	1:A:167:ILE:HD11	0.45	1.89	13	1
1:A:164:GLN:CB	1:A:204:VAL:HG23	0.45	2.42	4	1
1:A:124:LEU:CD2	1:B:124:LEU:HG	0.45	2.42	4	1
1:A:169:ARG:CG	1:A:187:LEU:HD12	0.45	2.42	5	3
1:A:97:ILE:HD12	1:A:102:PHE:HB2	0.45	1.89	10	2
1:B:209:ARG:HG3	1:B:209:ARG:OXT	0.45	2.12	8	1
1:A:123:ARG:C	1:A:126:VAL:HG12	0.45	2.30	14	1
1:A:124:LEU:CA	1:A:128:SER:HB2	0.45	2.42	14	1
1:B:33:GLY:CA	1:B:82:ARG:HB2	0.45	2.41	14	1
1:B:196:ILE:CG1	1:B:197:SER:N	0.45	2.79	13	1
1:B:142:ARG:O	1:B:145:GLN:HB2	0.45	2.12	13	1
1:A:47:VAL:HB	1:A:88:ALA:HA	0.45	1.87	5	2
1:B:27:SER:H	1:B:88:ALA:HB3	0.45	1.70	14	2
1:A:131:VAL:HG12	1:A:132:GLY:N	0.45	2.26	6	1
1:B:53:ASP:CB	1:B:57:LYS:HG2	0.45	2.41	1	1
1:A:81:GLU:O	1:A:83:SER:N	0.45	2.50	11	2
1:B:14:PHE:CE2	1:B:102:PHE:CE1	0.45	3.05	10	1
1:A:48:ALA:CB	1:A:60:ILE:HD13	0.45	2.40	15	2
1:A:14:PHE:HD1	1:A:15:LEU:HD23	0.45	1.72	14	3
1:B:40:TYR:N	1:B:40:TYR:CD2	0.45	2.84	20	1
1:A:119:GLN:OE1	1:A:119:GLN:HA	0.45	2.12	6	1
1:A:103:ARG:O	1:A:107:GLN:HB2	0.45	2.12	12	2
1:A:180:ARG:NH1	1:A:181:GLU:HA	0.45	2.27	17	1
1:B:15:LEU:HD21	1:B:41:TYR:CE2	0.45	2.46	10	1
1:B:144:ALA:HB2	1:B:195:LEU:CD2	0.45	2.42	18	2
1:A:47:VAL:HG21	1:A:86:VAL:HG12	0.45	1.89	17	2
1:B:39:LEU:HD13	1:B:102:PHE:CZ	0.45	2.46	9	1
1:B:195:LEU:O	1:B:209:ARG:HG3	0.45	2.12	7	3
1:A:196:ILE:CG2	1:A:197:SER:N	0.45	2.80	19	2
1:A:23:TYR:HB3	1:A:24:PRO:HD2	0.45	1.87	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:39:LEU:HB2	1:B:75:LEU:HD22	0.45	1.89	13	1
1:A:11:LEU:O	1:A:15:LEU:N	0.45	2.50	5	8
1:B:139:VAL:HG23	1:B:176:VAL:CG1	0.45	2.42	5	1
1:A:41:TYR:C	1:A:41:TYR:CD1	0.45	2.91	6	3
1:A:51:ILE:HG21	1:B:128:SER:CB	0.45	2.41	10	1
1:B:47:VAL:HG21	1:B:70:ILE:HD11	0.45	1.88	12	1
1:A:63:TYR:OH	1:A:175:ILE:HD11	0.45	2.12	13	1
1:B:20:ILE:HG21	1:B:43:VAL:HG21	0.44	1.89	10	1
1:A:143:ILE:CG1	1:A:183:VAL:HG22	0.44	2.38	10	1
1:B:27:SER:O	1:B:88:ALA:HB2	0.44	2.12	18	1
1:A:190:LEU:CD1	1:A:203:ILE:HD13	0.44	2.42	14	2
1:B:157:MET:O	1:B:163:MET:CA	0.44	2.62	8	1
1:A:134:LEU:HD21	1:A:174:GLN:O	0.44	2.12	14	2
1:A:20:ILE:CD1	1:A:95:ALA:HB2	0.44	2.40	16	1
1:B:190:LEU:CD1	1:B:203:ILE:HD13	0.44	2.41	16	1
1:A:143:ILE:HD12	1:A:186:ILE:HB	0.44	1.89	4	2
1:A:32:GLN:O	1:A:34:GLU:HG3	0.44	2.12	7	2
1:B:106:ILE:HD12	1:B:113:LEU:HB2	0.44	1.87	5	2
1:B:51:ILE:HD13	1:B:51:ILE:H	0.44	1.72	18	1
1:A:52:LYS:O	1:B:129:GLU:HG2	0.44	2.12	18	1
1:B:14:PHE:HD1	1:B:15:LEU:HD23	0.44	1.72	20	3
1:A:172:ILE:HB	1:A:183:VAL:HG11	0.44	1.88	3	1
1:A:135:ALA:HB3	1:B:135:ALA:CB	0.44	2.40	6	1
1:B:41:TYR:CE2	1:B:69:PHE:CE1	0.44	3.04	17	3
1:A:147:LEU:HD21	1:A:203:ILE:HG21	0.44	1.89	14	1
1:A:31:HIS:HB2	1:A:84:ALA:HA	0.44	1.87	14	1
1:A:102:PHE:CE2	1:A:106:ILE:HG22	0.44	2.47	19	1
1:A:49:VAL:CB	1:A:62:SER:O	0.44	2.54	16	1
1:B:120:MET:O	1:B:123:ARG:HB2	0.44	2.11	11	1
1:A:76:PHE:CZ	1:B:117:SER:HB2	0.44	2.46	7	4
1:A:196:ILE:HD12	1:A:203:ILE:HG23	0.44	1.88	13	2
1:A:128:SER:HA	1:B:51:ILE:HD12	0.44	1.90	4	1
1:A:20:ILE:O	1:A:21:HIS:CB	0.44	2.65	16	8
1:A:23:TYR:CD2	1:A:27:SER:CB	0.44	3.00	2	2
1:B:189:MET:CG	1:B:195:LEU:HB2	0.44	2.42	1	1
1:B:72:GLU:HB2	1:B:120:MET:CE	0.44	2.43	7	3
1:B:42:ILE:HD11	1:B:64:LEU:CD1	0.44	2.43	10	1
1:A:143:ILE:CD1	1:A:186:ILE:HG13	0.44	2.41	10	1
1:A:143:ILE:HD13	1:A:183:VAL:HG22	0.44	1.90	13	2
1:B:103:ARG:O	1:B:107:GLN:HB2	0.44	2.13	12	4
1:A:204:VAL:HG12	1:A:204:VAL:O	0.44	2.12	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:GLN:O	1:A:108:VAL:HB	0.44	2.13	20	1
1:A:47:VAL:HG21	1:A:70:ILE:HD11	0.44	1.90	7	1
1:A:149:ASN:O	1:A:153:GLN:HG2	0.44	2.12	4	1
1:A:166:LYS:HB3	1:A:202:THR:CG2	0.44	2.40	5	1
1:B:106:ILE:HB	1:B:113:LEU:HB2	0.44	1.89	15	1
1:A:90:THR:O	1:A:91:ALA:C	0.44	2.56	11	3
1:A:128:SER:HB2	1:B:51:ILE:HG21	0.44	1.90	3	1
1:B:20:ILE:CD1	1:B:43:VAL:HG21	0.44	2.43	11	1
1:B:159:HIS:O	1:B:161:ASP:N	0.44	2.49	8	5
1:A:189:MET:SD	1:A:195:LEU:HD13	0.44	2.53	18	1
1:B:39:LEU:O	1:B:96:GLU:HA	0.44	2.13	20	3
1:B:11:LEU:HD21	1:B:41:TYR:CZ	0.44	2.47	20	2
1:B:76:PHE:HD2	1:B:120:MET:CE	0.44	2.25	7	1
1:A:110:PRO:HB3	1:B:110:PRO:HB3	0.44	1.90	19	2
1:A:195:LEU:HA	1:A:209:ARG:NH2	0.44	2.27	16	1
1:A:51:ILE:HG23	1:A:61:LEU:CD1	0.44	2.42	7	1
1:A:134:LEU:HD13	1:A:174:GLN:O	0.44	2.12	7	1
1:A:72:GLU:CG	1:A:120:MET:HE2	0.44	2.41	14	1
1:B:138:ASP:O	1:B:138:ASP:CG	0.44	2.56	20	2
1:B:169:ARG:HG3	1:B:180:ARG:CB	0.44	2.43	15	1
1:B:11:LEU:O	1:B:15:LEU:N	0.44	2.48	11	5
1:A:40:TYR:O	1:A:70:ILE:N	0.44	2.51	20	1
1:B:41:TYR:C	1:B:41:TYR:CD1	0.44	2.91	6	2
1:A:138:ASP:O	1:A:142:ARG:CB	0.44	2.65	7	1
1:B:169:ARG:HD3	1:B:180:ARG:HB3	0.44	1.90	17	1
1:B:100:LYS:O	1:B:103:ARG:HG2	0.44	2.13	19	1
1:B:106:ILE:HD12	1:B:113:LEU:HD22	0.44	1.88	19	1
1:A:105:LEU:HD11	1:A:112:ILE:HD12	0.44	1.89	19	1
1:A:40:TYR:N	1:A:40:TYR:CD2	0.44	2.85	12	1
1:A:47:VAL:H	1:A:64:LEU:HB2	0.44	1.72	12	1
1:B:169:ARG:HA	1:B:187:LEU:HD12	0.44	1.88	11	1
1:A:187:LEU:HD23	1:A:187:LEU:N	0.43	2.28	4	5
1:A:30:ILE:HD12	1:A:86:VAL:HG23	0.43	1.90	4	4
1:B:159:HIS:HD2	1:B:162:GLY:O	0.43	1.96	18	2
1:B:166:LYS:HB2	1:B:202:THR:HA	0.43	1.90	18	1
1:B:9:PRO:O	1:B:13:TRP:HB2	0.43	2.13	15	1
1:A:191:GLU:O	1:A:191:GLU:HG2	0.43	2.13	17	1
1:B:111:ASP:O	1:B:115:ARG:HB3	0.43	2.13	14	1
1:B:106:ILE:CD1	1:B:113:LEU:HD22	0.43	2.44	19	1
1:A:113:LEU:O	1:A:116:LEU:HB3	0.43	2.12	12	1
1:A:143:ILE:HG12	1:A:183:VAL:CG2	0.43	2.40	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:156:ALA:HB1	1:B:163:MET:SD	0.43	2.52	5	1
1:B:61:LEU:C	1:B:61:LEU:HD22	0.43	2.34	13	6
1:A:18:CYS:HG	1:A:95:ALA:HB1	0.43	1.73	3	2
1:A:55:GLU:OE1	1:A:57:LYS:HB2	0.43	2.13	20	2
1:B:196:ILE:HG12	1:B:209:ARG:OXT	0.43	2.12	7	1
1:A:18:CYS:SG	1:A:19:HIS:N	0.43	2.92	19	1
1:B:99:TYR:HD1	1:B:99:TYR:C	0.43	2.17	5	3
1:A:39:LEU:HG	1:A:40:TYR:N	0.43	2.27	3	4
1:A:143:ILE:HD12	1:A:186:ILE:CB	0.43	2.43	18	1
1:A:42:ILE:HG12	1:A:94:VAL:CG1	0.43	2.42	2	1
1:B:46:SER:O	1:B:90:THR:HG23	0.43	2.14	2	1
1:A:146:THR:O	1:A:149:ASN:HB3	0.43	2.13	6	3
1:A:139:VAL:HA	1:A:176:VAL:CG1	0.43	2.43	3	1
1:B:142:ARG:HB3	1:B:176:VAL:HG13	0.43	1.90	19	1
1:B:99:TYR:C	1:B:99:TYR:HD1	0.43	2.16	6	3
1:B:23:TYR:CD2	1:B:27:SER:CB	0.43	3.01	2	1
1:A:143:ILE:HD13	1:A:183:VAL:HA	0.43	1.90	17	2
1:B:34:GLU:OE2	1:B:82:ARG:HB2	0.43	2.13	3	3
1:B:11:LEU:HD13	1:B:41:TYR:OH	0.43	2.13	9	1
1:A:30:ILE:HG21	1:A:36:ALA:HA	0.43	1.90	14	1
1:A:151:ALA:HA	1:A:156:ALA:HB2	0.43	1.90	14	1
1:A:126:VAL:O	1:A:130:LYS:HB2	0.43	2.14	13	1
1:A:99:TYR:C	1:A:99:TYR:HD1	0.43	2.17	3	2
1:B:180:ARG:HD2	1:B:181:GLU:OE1	0.43	2.14	7	2
1:B:35:LYS:HA	1:B:81:GLU:HA	0.43	1.89	19	3
1:B:25:SER:O	1:B:26:LYS:HB2	0.43	2.14	11	2
1:A:132:GLY:HA2	1:A:135:ALA:HB3	0.43	1.89	5	1
1:A:69:PHE:CB	1:A:116:LEU:HD12	0.43	2.44	9	3
1:B:27:SER:O	1:B:29:LEU:CD2	0.43	2.65	18	2
1:B:153:GLN:CB	1:B:154:PRO:HD2	0.43	2.44	3	2
1:B:48:ALA:CB	1:B:60:ILE:HD13	0.43	2.42	15	1
1:B:53:ASP:HB2	1:B:57:LYS:HB2	0.43	1.91	15	1
1:A:187:LEU:O	1:A:190:LEU:HG	0.43	2.13	9	1
1:A:11:LEU:HA	1:A:14:PHE:HB3	0.43	1.90	6	3
1:A:190:LEU:O	1:A:197:SER:HA	0.43	2.12	19	2
1:A:143:ILE:HD12	1:A:186:ILE:HD13	0.43	1.90	17	1
1:B:159:HIS:CG	1:B:160:PRO:HD2	0.43	2.49	14	1
1:A:127:THR:HG22	1:A:127:THR:O	0.43	2.14	14	1
1:A:191:GLU:HG2	1:A:191:GLU:O	0.43	2.13	8	1
1:A:33:GLY:H	1:A:82:ARG:HB2	0.43	1.73	14	1
1:A:156:ALA:HA	1:A:164:GLN:O	0.43	2.13	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:143:ILE:HD13	1:B:183:VAL:HG22	0.43	1.90	7	2
1:B:49:VAL:HG13	1:B:85:TRP:O	0.43	2.14	15	1
1:B:18:CYS:HB3	1:B:97:ILE:CG1	0.43	2.42	14	3
1:B:166:LYS:CB	1:B:202:THR:HA	0.43	2.43	20	1
1:B:32:GLN:O	1:B:34:GLU:HG3	0.43	2.14	7	1
1:A:130:LYS:HG2	1:A:130:LYS:O	0.43	2.14	19	1
1:B:53:ASP:HB2	1:B:57:LYS:HG2	0.43	1.89	1	1
1:B:22:LYS:HB2	1:B:94:VAL:HG22	0.43	1.89	12	1
1:B:137:LEU:HG	1:B:178:CYS:SG	0.43	2.53	4	1
1:A:158:THR:HA	1:A:163:MET:HB3	0.43	1.91	5	2
1:A:30:ILE:CG2	1:A:34:GLU:HB2	0.43	2.44	2	1
1:B:23:TYR:CD2	1:B:27:SER:HB2	0.43	2.49	2	1
1:A:50:LEU:HA	1:A:61:LEU:HD12	0.43	1.91	11	2
1:B:30:ILE:CG2	1:B:34:GLU:HB2	0.43	2.43	17	2
1:B:178:CYS:SG	1:B:183:VAL:HB	0.43	2.54	17	1
1:A:147:LEU:CG	1:A:167:ILE:HD11	0.43	2.44	14	1
1:A:169:ARG:HB3	1:A:187:LEU:CD1	0.43	2.40	16	1
1:A:47:VAL:HG12	1:A:88:ALA:HA	0.43	1.91	12	1
1:A:196:ILE:HG22	1:A:209:ARG:O	0.43	2.13	13	1
1:B:20:ILE:O	1:B:21:HIS:CB	0.43	2.67	15	1
1:B:14:PHE:O	1:B:17:HIS:HB2	0.43	2.13	9	1
1:A:139:VAL:HG22	1:A:143:ILE:HD11	0.43	1.91	20	1
1:B:11:LEU:HA	1:B:14:PHE:HB3	0.43	1.91	20	2
1:A:153:GLN:C	1:A:155:ASP:H	0.43	2.16	8	1
1:A:33:GLY:HA2	1:A:82:ARG:NH1	0.43	2.29	11	1
1:B:165:ILE:O	1:B:165:ILE:HD12	0.42	2.14	5	1
1:B:70:ILE:CD1	1:B:86:VAL:HG11	0.42	2.44	5	1
1:B:51:ILE:HD12	1:B:61:LEU:CB	0.42	2.43	18	1
1:A:159:HIS:O	1:A:161:ASP:N	0.42	2.51	16	4
1:A:137:LEU:HG	1:A:178:CYS:SG	0.42	2.54	6	1
1:B:34:GLU:O	1:B:82:ARG:HA	0.42	2.14	14	1
1:B:31:HIS:CA	1:B:82:ARG:HG3	0.42	2.44	8	1
1:A:114:MET:O	1:A:117:SER:HB2	0.42	2.14	14	1
1:B:44:LYS:HD3	1:B:66:GLN:HB3	0.42	1.91	18	1
1:A:25:SER:O	1:A:26:LYS:HG3	0.42	2.13	6	1
1:A:102:PHE:CD2	1:A:103:ARG:N	0.42	2.87	17	2
1:B:114:MET:O	1:B:117:SER:HB2	0.42	2.13	14	1
1:A:190:LEU:CD2	1:A:196:ILE:HG12	0.42	2.23	13	1
1:A:103:ARG:C	1:A:106:ILE:HG13	0.42	2.34	18	3
1:B:41:TYR:O	1:B:95:ALA:N	0.42	2.49	14	2
1:B:168:THR:HB	1:B:170:GLN:OE1	0.42	2.14	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ILE:HG23	1:A:43:VAL:CG2	0.42	2.45	7	2
1:A:52:LYS:HG3	1:A:58:GLU:HB3	0.42	1.90	1	1
1:A:150:LEU:C	1:A:152:LYS:N	0.42	2.73	16	1
1:A:42:ILE:CB	1:A:94:VAL:HG12	0.42	2.45	5	1
1:A:122:ARG:O	1:A:125:GLN:HG2	0.42	2.14	18	1
1:A:114:MET:CE	1:B:113:LEU:HD21	0.42	2.44	15	2
1:B:169:ARG:HA	1:B:172:ILE:HG12	0.42	1.92	15	1
1:A:11:LEU:HD22	1:A:41:TYR:HE2	0.42	1.74	13	2
1:A:150:LEU:HD13	1:A:165:ILE:HD13	0.42	1.92	14	2
1:A:31:HIS:CA	1:A:82:ARG:HG3	0.42	2.45	3	1
1:A:99:TYR:HA	1:A:102:PHE:CD2	0.42	2.50	20	1
1:A:166:LYS:CB	1:A:202:THR:HA	0.42	2.45	16	2
1:B:42:ILE:HG23	1:B:42:ILE:O	0.42	2.14	8	1
1:B:60:ILE:HD11	1:B:87:ARG:HD3	0.42	1.91	8	1
1:B:153:GLN:C	1:B:155:ASP:H	0.42	2.17	8	1
1:B:37:GLU:O	1:B:99:TYR:CD1	0.42	2.72	19	1
1:A:18:CYS:HB2	1:A:97:ILE:HG12	0.42	1.90	19	1
1:A:48:ALA:HB1	1:A:60:ILE:HG23	0.42	1.90	19	1
1:B:42:ILE:O	1:B:42:ILE:HG23	0.42	2.14	16	1
1:A:121:ALA:HA	1:A:124:LEU:HB2	0.42	1.91	4	1
1:B:81:GLU:O	1:B:83:SER:N	0.42	2.52	10	3
1:A:169:ARG:HD3	1:A:180:ARG:HB3	0.42	1.92	17	2
1:A:75:LEU:CG	1:A:76:PHE:N	0.42	2.81	14	1
1:B:143:ILE:HD12	1:B:186:ILE:HD12	0.42	1.91	14	1
1:A:172:ILE:O	1:A:176:VAL:HG23	0.42	2.14	14	1
1:A:196:ILE:HD12	1:A:203:ILE:CG2	0.42	2.45	16	1
1:B:143:ILE:CD1	1:B:186:ILE:HD13	0.42	2.44	11	1
1:B:21:HIS:HA	1:B:93:GLU:OE1	0.42	2.14	5	1
1:B:14:PHE:HE2	1:B:102:PHE:CE1	0.42	2.32	10	2
1:B:167:ILE:HD12	1:B:167:ILE:O	0.42	2.14	9	1
1:B:59:MET:HB3	1:B:174:GLN:HG2	0.42	1.91	20	1
1:B:179:SER:HB3	1:B:180:ARG:H	0.42	1.46	14	1
1:B:77:GLU:O	1:B:78:GLU:CB	0.42	2.68	4	2
1:B:139:VAL:HG21	1:B:178:CYS:SG	0.42	2.55	5	1
1:B:81:GLU:O	1:B:82:ARG:HD3	0.42	2.15	12	4
1:B:41:TYR:HD1	1:B:68:ASP:O	0.42	1.98	10	2
1:B:31:HIS:CE1	1:B:58:GLU:CB	0.42	3.03	2	4
1:A:14:PHE:CE2	1:A:102:PHE:CD1	0.42	3.08	7	2
1:B:76:PHE:CD1	1:B:113:LEU:HD11	0.42	2.50	6	1
1:A:51:ILE:CD1	1:A:61:LEU:HB3	0.42	2.45	7	1
1:A:42:ILE:HD11	1:A:64:LEU:CD1	0.42	2.44	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:LEU:HG	1:A:167:ILE:HD11	0.42	1.90	14	1
1:A:47:VAL:C	1:A:89:LYS:HB2	0.42	2.34	14	1
1:A:57:LYS:HG3	1:A:57:LYS:O	0.42	2.14	19	1
1:B:189:MET:SD	1:B:195:LEU:HB2	0.42	2.55	13	1
1:A:41:TYR:CD1	1:A:68:ASP:O	0.42	2.73	13	1
1:B:113:LEU:HG	1:B:113:LEU:O	0.42	2.14	5	1
1:B:172:ILE:HG22	1:B:183:VAL:CG2	0.42	2.44	10	1
1:A:39:LEU:O	1:A:96:GLU:HA	0.42	2.15	20	1
1:B:143:ILE:CD1	1:B:186:ILE:HG13	0.42	2.45	1	1
1:B:190:LEU:HD22	1:B:196:ILE:CB	0.42	2.45	16	1
1:B:166:LYS:O	1:B:167:ILE:HG23	0.42	2.15	13	1
1:A:22:LYS:HB2	1:A:94:VAL:N	0.42	2.30	2	2
1:B:116:LEU:HG	1:B:120:MET:CE	0.42	2.44	18	1
1:B:119:GLN:HA	1:B:119:GLN:OE1	0.42	2.14	20	1
1:B:14:PHE:CE2	1:B:102:PHE:CD1	0.42	3.08	7	1
1:A:129:GLU:O	1:A:130:LYS:HG3	0.42	2.15	7	1
1:B:42:ILE:HD11	1:B:64:LEU:CB	0.42	2.45	17	1
1:A:40:TYR:HB2	1:A:70:ILE:CG2	0.42	2.45	16	1
1:B:143:ILE:CD1	1:B:183:VAL:HG22	0.42	2.45	16	1
1:B:147:LEU:HD22	1:B:167:ILE:HD11	0.42	1.92	13	1
1:B:22:LYS:HB2	1:B:94:VAL:N	0.41	2.30	2	1
1:A:73:LEU:HD21	1:B:124:LEU:CD1	0.41	2.45	2	1
1:B:15:LEU:HB3	1:B:20:ILE:CD1	0.41	2.45	15	1
1:B:25:SER:HB3	1:B:90:THR:CA	0.41	2.44	9	2
1:B:31:HIS:O	1:B:32:GLN:HB2	0.41	2.14	17	1
1:B:169:ARG:HD2	1:B:170:GLN:N	0.41	2.31	14	1
1:A:180:ARG:HD2	1:A:181:GLU:OE2	0.41	2.15	12	1
1:A:196:ILE:HG21	1:A:203:ILE:HG23	0.41	1.91	11	1
1:A:124:LEU:CD1	1:B:73:LEU:HD21	0.41	2.45	4	2
1:A:99:TYR:HD1	1:A:99:TYR:C	0.41	2.18	5	4
1:A:50:LEU:HD23	1:A:50:LEU:O	0.41	2.15	5	1
1:A:8:ASP:CG	1:A:115:ARG:HH12	0.41	2.19	5	1
1:B:205:VAL:HG12	1:B:209:ARG:O	0.41	2.15	5	1
1:A:134:LEU:HD22	1:A:176:VAL:HA	0.41	1.92	10	1
1:B:103:ARG:O	1:B:107:GLN:HG3	0.41	2.15	13	2
1:A:159:HIS:HD2	1:A:162:GLY:O	0.41	1.98	18	1
1:A:73:LEU:HA	1:A:77:GLU:HB2	0.41	1.92	8	1
1:A:11:LEU:HD23	1:A:14:PHE:CB	0.41	2.45	13	2
1:B:123:ARG:C	1:B:126:VAL:HG12	0.41	2.35	14	1
1:A:85:TRP:CZ2	1:A:123:ARG:HG2	0.41	2.51	16	1
1:B:196:ILE:HG21	1:B:203:ILE:HG23	0.41	1.92	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:GLU:O	1:A:78:GLU:CB	0.41	2.68	11	1
1:A:72:GLU:HG2	1:A:116:LEU:HD11	0.41	1.91	4	1
1:A:15:LEU:HD21	1:A:41:TYR:HE2	0.41	1.74	10	1
1:A:45:GLY:HA3	1:A:92:CYS:CA	0.41	2.46	18	1
1:B:166:LYS:C	1:B:167:ILE:HG13	0.41	2.35	20	1
1:B:40:TYR:CD2	1:B:40:TYR:N	0.41	2.88	17	2
1:A:41:TYR:HB3	1:A:95:ALA:CB	0.41	2.37	8	1
1:A:106:ILE:HD12	1:A:113:LEU:HD22	0.41	1.90	19	1
1:A:14:PHE:HE2	1:A:102:PHE:CE1	0.41	2.34	13	2
1:B:23:TYR:CB	1:B:24:PRO:CD	0.41	2.99	10	1
1:B:52:LYS:HG2	1:B:58:GLU:HB3	0.41	1.91	10	1
1:B:164:GLN:CB	1:B:204:VAL:HG23	0.41	2.41	10	1
1:B:127:THR:O	1:B:131:VAL:HG22	0.41	2.15	6	1
1:A:14:PHE:HE2	1:A:97:ILE:HD11	0.41	1.75	8	1
1:B:134:LEU:HD21	1:B:174:GLN:O	0.41	2.15	14	1
1:B:147:LEU:HD22	1:B:196:ILE:HD13	0.41	1.91	19	1
1:B:149:ASN:O	1:B:153:GLN:HG2	0.41	2.16	4	1
1:A:8:ASP:O	1:A:12:GLU:HG3	0.41	2.15	5	1
1:B:73:LEU:HG	1:B:85:TRP:CD2	0.41	2.51	2	2
1:A:184:GLY:O	1:A:185:ARG:C	0.41	2.59	15	1
1:A:102:PHE:O	1:A:106:ILE:HG23	0.41	2.15	19	2
1:A:198:ALA:CB	1:A:203:ILE:HG12	0.41	2.46	8	1
1:B:190:LEU:HD23	1:B:195:LEU:HB3	0.41	1.91	14	1
1:A:72:GLU:HG2	1:A:73:LEU:N	0.41	2.31	14	1
1:B:47:VAL:CG1	1:B:88:ALA:HA	0.41	2.46	12	1
1:B:15:LEU:HD22	1:B:20:ILE:CD1	0.41	2.46	11	1
1:B:166:LYS:HB3	1:B:202:THR:HA	0.41	1.92	16	2
1:A:70:ILE:CD1	1:A:86:VAL:HG11	0.41	2.46	20	3
1:A:147:LEU:HD13	1:A:203:ILE:HG21	0.41	1.92	18	1
1:B:139:VAL:HG21	1:B:183:VAL:HG23	0.41	1.91	20	1
1:A:75:LEU:HB3	1:A:99:TYR:CD2	0.41	2.51	20	1
1:A:189:MET:SD	1:A:195:LEU:HB2	0.41	2.56	6	1
1:A:41:TYR:CE1	1:A:69:PHE:CD1	0.41	3.08	7	1
1:B:42:ILE:CG2	1:B:94:VAL:HG12	0.41	2.46	17	1
1:B:180:ARG:HA	1:B:183:VAL:CG1	0.41	2.45	1	1
1:A:27:SER:O	1:A:29:LEU:CD2	0.41	2.69	16	2
1:B:42:ILE:HG22	1:B:68:ASP:N	0.41	2.29	12	1
1:A:82:ARG:NE	1:A:83:SER:H	0.41	2.13	11	1
1:B:172:ILE:HB	1:B:183:VAL:HG11	0.41	1.92	3	1
1:B:127:THR:HG22	1:B:131:VAL:HG13	0.41	1.92	20	1
1:A:50:LEU:HB3	1:A:60:ILE:HA	0.41	1.93	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:169:ARG:HA	1:A:172:ILE:CG1	0.41	2.46	17	1
1:B:205:VAL:HG23	1:B:205:VAL:O	0.41	2.16	19	1
1:A:179:SER:O	1:A:183:VAL:HB	0.41	2.16	16	1
1:B:113:LEU:O	1:B:116:LEU:HB3	0.41	2.15	12	1
1:A:196:ILE:HG13	1:A:197:SER:N	0.41	2.30	13	1
1:B:186:ILE:HA	1:B:189:MET:HG2	0.41	1.93	4	3
1:A:167:ILE:O	1:A:167:ILE:HD12	0.41	2.15	10	2
1:A:59:MET:CE	1:A:175:ILE:HA	0.41	2.46	10	1
1:A:138:ASP:OD1	1:A:142:ARG:HD3	0.41	2.16	18	1
1:A:61:LEU:HD22	1:A:62:SER:HB3	0.41	1.92	2	1
1:A:164:GLN:HB3	1:A:204:VAL:HB	0.41	1.93	2	1
1:B:23:TYR:CE2	1:B:27:SER:HB2	0.41	2.51	2	1
1:A:25:SER:O	1:A:26:LYS:HB2	0.41	2.15	15	2
1:B:140:THR:C	1:B:142:ARG:N	0.41	2.74	3	1
1:B:102:PHE:CD2	1:B:103:ARG:N	0.41	2.89	13	3
1:A:77:GLU:O	1:A:78:GLU:HB2	0.41	2.15	6	1
1:B:179:SER:OG	1:B:181:GLU:HB2	0.41	2.15	17	1
1:B:170:GLN:O	1:B:174:GLN:HB2	0.41	2.16	14	1
1:A:124:LEU:HB2	1:B:124:LEU:HG	0.41	1.92	19	1
1:B:183:VAL:HG13	1:B:187:LEU:HG	0.41	1.92	1	1
1:B:186:ILE:HG23	1:B:195:LEU:HD13	0.41	1.92	12	1
1:A:22:LYS:HE2	1:A:88:ALA:HB2	0.41	1.93	13	1
1:A:23:TYR:CD2	1:A:27:SER:HB2	0.41	2.51	2	3
1:A:42:ILE:HG23	1:A:42:ILE:O	0.41	2.16	15	1
1:B:166:LYS:CG	1:B:202:THR:HG23	0.41	2.44	15	1
1:B:73:LEU:HD13	1:B:77:GLU:HB2	0.41	1.93	15	1
1:A:18:CYS:CA	1:A:97:ILE:CG2	0.41	2.98	16	2
1:B:198:ALA:CB	1:B:203:ILE:HG12	0.41	2.46	8	1
1:B:35:LYS:HA	1:B:81:GLU:CA	0.41	2.46	19	1
1:B:198:ALA:HA	1:B:203:ILE:HA	0.40	1.91	10	1
1:A:124:LEU:CD2	1:B:124:LEU:HD21	0.40	2.33	18	1
1:A:78:GLU:HB3	1:B:122:ARG:NH1	0.40	2.31	2	1
1:B:169:ARG:HG3	1:B:180:ARG:HB3	0.40	1.92	20	1
1:A:14:PHE:HE2	1:A:102:PHE:CD1	0.40	2.34	7	1
1:A:73:LEU:HD13	1:A:77:GLU:HG3	0.40	1.93	8	1
1:B:147:LEU:HD21	1:B:167:ILE:HD11	0.40	1.93	14	1
1:B:186:ILE:O	1:B:189:MET:HB2	0.40	2.16	19	1
1:B:182:THR:O	1:B:186:ILE:HD12	0.40	2.16	13	1
1:B:32:GLN:HA	1:B:32:GLN:OE1	0.40	2.16	4	1
1:B:59:MET:O	1:B:59:MET:HG2	0.40	2.16	10	1
1:A:42:ILE:O	1:A:67:GLY:HA2	0.40	2.16	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:SER:O	1:A:84:ALA:HB3	0.40	2.16	6	2
1:B:53:ASP:HB2	1:B:57:LYS:HB3	0.40	1.94	9	1
1:B:34:GLU:O	1:B:82:ARG:N	0.40	2.54	20	1
1:A:22:LYS:HZ1	1:A:29:LEU:HD21	0.40	1.75	6	1
1:B:14:PHE:HE2	1:B:102:PHE:CD1	0.40	2.33	7	1
1:B:11:LEU:HD21	1:B:41:TYR:OH	0.40	2.16	17	1
1:A:169:ARG:HA	1:A:172:ILE:HG12	0.40	1.92	17	1
1:B:153:GLN:HB2	1:B:154:PRO:HD2	0.40	1.92	14	1
1:B:14:PHE:CE2	1:B:97:ILE:HD11	0.40	2.52	19	1
1:A:205:VAL:O	1:A:205:VAL:HG23	0.40	2.15	19	1
1:A:31:HIS:HE2	1:A:58:GLU:HB2	0.40	1.76	11	1
1:B:83:SER:O	1:B:84:ALA:HB3	0.40	2.16	4	1
1:A:34:GLU:O	1:A:82:ARG:N	0.40	2.53	5	1
1:B:158:THR:HA	1:B:163:MET:HB3	0.40	1.93	18	1
1:B:147:LEU:HD12	1:B:196:ILE:CD1	0.40	2.47	6	1
1:A:42:ILE:O	1:A:42:ILE:HG23	0.40	2.16	8	1
1:B:72:GLU:CB	1:B:120:MET:SD	0.40	3.07	12	1
1:B:42:ILE:CB	1:B:94:VAL:HG12	0.40	2.47	5	1
1:A:189:MET:CG	1:A:195:LEU:HB2	0.40	2.46	5	1
1:B:187:LEU:HD23	1:B:203:ILE:HD11	0.40	1.92	10	1
1:B:179:SER:O	1:B:183:VAL:HB	0.40	2.16	18	1
1:B:73:LEU:HG	1:B:85:TRP:CE3	0.40	2.51	2	1
1:B:129:GLU:O	1:B:130:LYS:HG3	0.40	2.15	3	1
1:A:171:GLU:HB3	1:A:175:ILE:HD12	0.40	1.92	7	1
1:B:110:PRO:O	1:B:114:MET:HB2	0.40	2.17	14	1
1:B:172:ILE:HG21	1:B:183:VAL:CG2	0.40	2.46	14	1
1:A:18:CYS:HB3	1:A:97:ILE:CG1	0.40	2.46	13	1
1:B:31:HIS:NE2	1:B:58:GLU:HB2	0.40	2.32	11	1
1:A:49:VAL:O	1:A:61:LEU:HD13	0.40	2.15	4	1
1:B:72:GLU:OE2	1:B:72:GLU:N	0.40	2.53	10	1
1:A:143:ILE:CD1	1:A:183:VAL:HA	0.40	2.46	18	1
1:B:184:GLY:O	1:B:185:ARG:C	0.40	2.59	15	1
1:B:22:LYS:HZ1	1:B:29:LEU:CD1	0.40	2.29	9	1
1:B:138:ASP:C	1:B:138:ASP:OD2	0.40	2.60	6	1
1:A:41:TYR:CZ	1:A:69:PHE:CE1	0.40	3.09	7	1
1:B:53:ASP:N	1:B:57:LYS:O	0.40	2.54	17	1
1:A:72:GLU:N	1:A:72:GLU:OE2	0.40	2.54	17	1
1:A:153:GLN:HB2	1:A:154:PRO:HD2	0.40	1.93	14	1
1:A:147:LEU:HD21	1:A:167:ILE:HD11	0.40	1.93	14	1
1:B:141:GLY:O	1:B:145:GLN:CB	0.40	2.67	14	1
1:B:49:VAL:HG13	1:B:85:TRP:CA	0.40	2.46	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:143:ILE:HG23	1:B:172:ILE:CG2	0.40	2.46	1	1
1:A:124:LEU:HD23	1:B:124:LEU:HD23	0.40	1.91	12	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	201/209 (96%)	157±4 (78±2%)	26±4 (13±2%)	18±2 (9±1%)	2	13
1	B	201/209 (96%)	158±3 (79±2%)	25±3 (13±2%)	18±2 (9±1%)	2	13
All	All	8040/8360 (96%)	6296 (78%)	1032 (13%)	712 (9%)	2	13

All 81 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	161	ASP	20
1	A	81	GLU	20
1	A	85	TRP	20
1	B	21	HIS	20
1	A	30	ILE	20
1	B	81	GLU	20
1	B	31	HIS	20
1	A	196	ILE	20
1	A	161	ASP	20
1	A	21	HIS	20
1	B	30	ILE	20
1	B	85	TRP	20
1	A	31	HIS	20
1	B	26	LYS	20
1	A	26	LYS	20
1	A	78	GLU	19
1	B	196	ILE	19
1	B	78	GLU	19
1	B	180	ARG	18

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Mol	Chain	Res	Type	Models (Total)
1	B	139	VAL	17
1	A	180	ARG	17
1	B	84	ALA	17
1	A	165	ILE	17
1	A	139	VAL	16
1	A	207	GLY	16
1	B	165	ILE	15
1	A	84	ALA	15
1	B	140	THR	15
1	A	140	THR	14
1	B	207	GLY	14
1	A	160	PRO	13
1	B	66	GLN	11
1	B	160	PRO	11
1	B	82	ARG	10
1	A	66	GLN	9
1	B	132	GLY	8
1	A	82	ARG	8
1	A	132	GLY	7
1	B	42	ILE	7
1	A	131	VAL	5
1	A	42	ILE	4
1	B	32	GLN	4
1	A	32	GLN	4
1	A	143	ILE	4
1	B	131	VAL	4
1	A	201	LYS	3
1	A	167	ILE	3
1	B	143	ILE	3
1	B	130	LYS	3
1	B	36	ALA	2
1	B	99	TYR	2
1	A	88	ALA	2
1	B	135	ALA	2
1	A	179	SER	2
1	B	128	SER	2
1	B	167	ILE	2
1	A	130	LYS	2
1	B	88	ALA	2
1	B	185	ARG	2
1	A	181	GLU	2
1	A	83	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	36	ALA	1
1	A	208	THR	1
1	A	136	PHE	1
1	B	136	PHE	1
1	B	208	THR	1
1	B	179	SER	1
1	B	137	LEU	1
1	A	133	ASN	1
1	A	45	GLY	1
1	A	28	THR	1
1	B	141	GLY	1
1	A	138	ASP	1
1	B	53	ASP	1
1	A	128	SER	1
1	A	154	PRO	1
1	B	181	GLU	1
1	B	28	THR	1
1	B	201	LYS	1
1	A	185	ARG	1
1	B	154	PRO	1

### 6.3.2 Protein sidechains ⓘ

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	174/180 (97%)	115±4 (66±2%)	59±4 (34±2%)	1	11
1	B	174/180 (97%)	114±4 (66±2%)	60±4 (34±2%)	1	10
All	All	6960/7200 (97%)	4589 (66%)	2371 (34%)	1	11

All 270 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	25	SER	20
1	A	30	ILE	20
1	B	25	SER	20
1	B	92	CYS	20

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Mol	Chain	Res	Type	Models (Total)
1	A	82	ARG	20
1	A	122	ARG	20
1	A	105	LEU	20
1	B	82	ARG	20
1	A	61	LEU	20
1	B	99	TYR	20
1	A	92	CYS	20
1	B	108	VAL	20
1	B	86	VAL	20
1	A	75	LEU	20
1	A	108	VAL	20
1	B	50	LEU	20
1	A	182	THR	20
1	B	105	LEU	20
1	B	122	ARG	20
1	B	61	LEU	20
1	A	165	ILE	20
1	B	165	ILE	20
1	B	23	TYR	20
1	B	30	ILE	20
1	B	182	THR	20
1	A	50	LEU	20
1	A	86	VAL	20
1	A	99	TYR	20
1	B	75	LEU	20
1	A	23	TYR	20
1	B	114	MET	19
1	A	29	LEU	19
1	B	139	VAL	19
1	A	10	THR	19
1	A	114	MET	19
1	B	140	THR	19
1	A	140	THR	19
1	A	90	THR	19
1	B	169	ARG	19
1	A	39	LEU	19
1	B	90	THR	19
1	B	39	LEU	19
1	B	10	THR	19
1	A	169	ARG	19
1	B	202	THR	19
1	B	20	ILE	19

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Mol	Chain	Res	Type	Models (Total)
1	B	112	ILE	18
1	B	29	LEU	18
1	B	195	LEU	18
1	B	72	GLU	18
1	A	159	HIS	18
1	B	167	ILE	18
1	A	20	ILE	18
1	A	202	THR	18
1	B	63	TYR	17
1	A	112	ILE	17
1	A	195	LEU	17
1	A	72	GLU	17
1	B	179	SER	16
1	B	159	HIS	16
1	A	167	ILE	16
1	B	124	LEU	16
1	B	58	GLU	15
1	A	58	GLU	15
1	A	63	TYR	15
1	A	161	ASP	15
1	B	123	ARG	15
1	A	183	VAL	14
1	A	73	LEU	14
1	A	123	ARG	14
1	B	161	ASP	14
1	A	65	ASN	14
1	B	55	GLU	13
1	B	131	VAL	13
1	A	136	PHE	13
1	A	124	LEU	13
1	A	180	ARG	13
1	A	103	ARG	13
1	A	139	VAL	13
1	B	11	LEU	13
1	A	11	LEU	13
1	B	136	PHE	12
1	A	131	VAL	12
1	B	103	ARG	12
1	B	81	GLU	12
1	A	116	LEU	12
1	B	116	LEU	12
1	A	55	GLU	11

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Mol	Chain	Res	Type	Models (Total)
1	A	81	GLU	11
1	A	208	THR	11
1	B	183	VAL	11
1	A	102	PHE	11
1	B	208	THR	11
1	A	87	ARG	11
1	B	102	PHE	11
1	B	41	TYR	11
1	B	65	ASN	11
1	B	180	ARG	11
1	A	57	LYS	11
1	B	27	SER	11
1	A	41	TYR	10
1	A	142	ARG	10
1	A	179	SER	10
1	B	142	ARG	10
1	B	73	LEU	10
1	A	125	GLN	10
1	A	16	SER	10
1	B	57	LYS	9
1	B	126	VAL	9
1	B	16	SER	9
1	A	181	GLU	9
1	B	163	MET	9
1	A	166	LYS	9
1	B	68	ASP	9
1	B	174	GLN	9
1	A	201	LYS	9
1	B	201	LYS	9
1	B	168	THR	9
1	B	87	ARG	9
1	A	204	VAL	8
1	B	205	VAL	8
1	B	188	LYS	8
1	B	204	VAL	8
1	A	32	GLN	8
1	B	120	MET	8
1	A	174	GLN	8
1	B	166	LYS	8
1	A	188	LYS	8
1	B	32	GLN	8
1	A	120	MET	7

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Mol	Chain	Res	Type	Models (Total)
1	A	126	VAL	7
1	A	168	THR	7
1	A	130	LYS	7
1	A	164	GLN	7
1	B	158	THR	7
1	A	27	SER	7
1	A	38	THR	7
1	A	28	THR	7
1	A	68	ASP	7
1	B	13	TRP	7
1	B	80	GLN	7
1	B	28	THR	7
1	B	134	LEU	7
1	A	163	MET	6
1	A	133	ASN	6
1	B	130	LYS	6
1	B	38	THR	6
1	B	194	ASN	6
1	B	44	LYS	6
1	B	31	HIS	6
1	B	40	TYR	6
1	A	111	ASP	6
1	A	77	GLU	6
1	A	193	GLN	6
1	B	181	GLU	6
1	A	205	VAL	6
1	B	125	GLN	6
1	A	31	HIS	6
1	A	44	LYS	5
1	B	164	GLN	5
1	B	22	LYS	5
1	A	134	LEU	5
1	B	77	GLU	5
1	B	119	GLN	5
1	B	111	ASP	5
1	A	98	SER	5
1	B	12	GLU	5
1	B	42	ILE	5
1	A	115	ARG	5
1	A	119	GLN	5
1	A	192	ASP	5
1	A	13	TRP	4

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Mol	Chain	Res	Type	Models (Total)
1	A	194	ASN	4
1	A	117	SER	4
1	A	14	PHE	4
1	B	127	THR	4
1	A	40	TYR	4
1	A	158	THR	4
1	A	196	ILE	4
1	A	80	GLN	4
1	B	191	GLU	4
1	A	170	GLN	4
1	A	12	GLU	4
1	B	193	GLN	4
1	B	14	PHE	4
1	A	8	ASP	4
1	B	98	SER	4
1	B	115	ARG	4
1	A	127	THR	3
1	B	203	ILE	3
1	B	145	GLN	3
1	B	209	ARG	3
1	B	78	GLU	3
1	B	8	ASP	3
1	B	192	ASP	3
1	A	101	LYS	3
1	B	170	GLN	3
1	B	76	PHE	3
1	A	78	GLU	3
1	A	145	GLN	3
1	B	153	GLN	3
1	B	53	ASP	3
1	A	76	PHE	3
1	B	196	ILE	3
1	B	106	ILE	2
1	A	138	ASP	2
1	A	42	ILE	2
1	A	104	GLN	2
1	A	18	CYS	2
1	B	147	LEU	2
1	A	149	ASN	2
1	B	104	GLN	2
1	B	17	HIS	2
1	A	22	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	52	LYS	2
1	A	89	LYS	2
1	B	189	MET	2
1	B	52	LYS	2
1	B	46	SER	2
1	B	185	ARG	2
1	A	147	LEU	2
1	B	138	ASP	2
1	B	51	ILE	2
1	B	54	GLU	2
1	A	209	ARG	2
1	A	199	HIS	1
1	B	83	SER	1
1	A	43	VAL	1
1	B	18	CYS	1
1	B	186	ILE	1
1	B	129	GLU	1
1	A	143	ILE	1
1	B	199	HIS	1
1	B	37	GLU	1
1	A	171	GLU	1
1	A	17	HIS	1
1	A	37	GLU	1
1	B	117	SER	1
1	A	96	GLU	1
1	A	60	ILE	1
1	A	46	SER	1
1	A	137	LEU	1
1	A	97	ILE	1
1	B	24	PRO	1
1	B	107	GLN	1
1	A	178	CYS	1
1	B	133	ASN	1
1	A	203	ILE	1
1	B	59	MET	1
1	A	107	GLN	1
1	A	129	GLU	1
1	B	97	ILE	1
1	B	89	LYS	1
1	B	85	TRP	1
1	A	85	TRP	1
1	A	53	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	186	ILE	1
1	A	35	LYS	1
1	B	93	GLU	1
1	A	54	GLU	1
1	A	185	ARG	1
1	A	24	PRO	1
1	A	153	GLN	1
1	B	96	GLU	1
1	B	149	ASN	1
1	A	93	GLU	1
1	B	34	GLU	1
1	B	100	LYS	1
1	A	146	THR	1
1	A	51	ILE	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided