Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 11:00 pm BST

PDB ID	:	2LBH
Title	:	Solution Structure of the Dimeric Form of a Unliganded Bovine Neurophysin, Minimized Average Structure
Authors	:	Lee, H.; Naik, M.; Nguyen, T.; Bracken, C.; Breslow, E.
Deposited on	:	2011-03-31

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

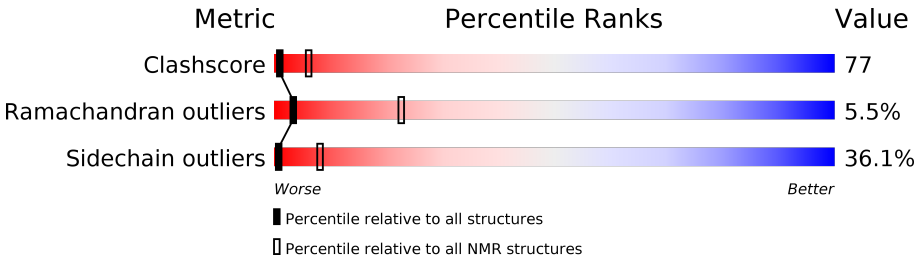
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 44%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	92	13% 52% 10% 25%
1	B	92	13% 52% 10% 25%

2 Ensemble composition and analysis

This entry contains 21 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:10-A:47, A:56-A:86, B:110-B:147, B:156-B:186 (138)	0.79	1

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2434 atoms, of which 1158 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Neurophysin 1.

Mol	Chain	Residues	Atoms						Trace
1	A	92	Total	C	H	N	O	S	0
			1217	382	579	112	130	14	
1	B	92	Total	C	H	N	O	S	0
			1217	382	579	112	130	14	

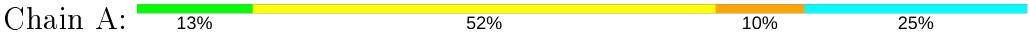
4 Residue-property plots

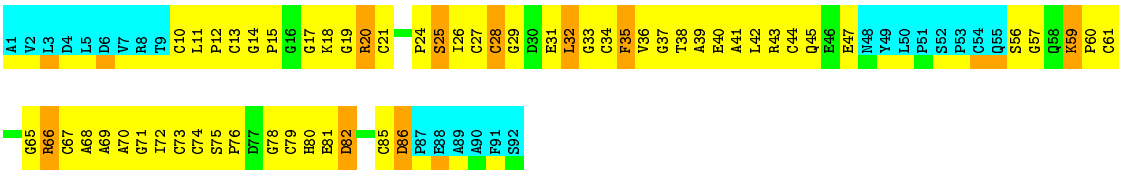
4.1 Average score per residue in the NMR ensemble

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: Neurophysin 1

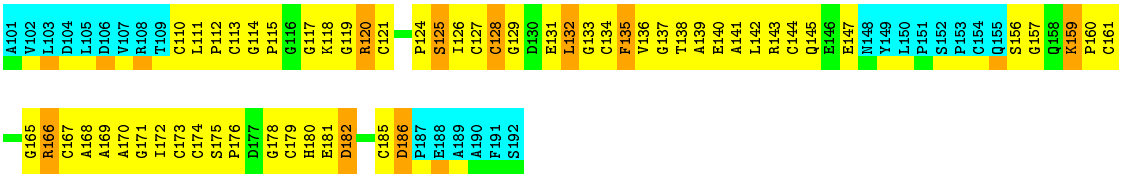
Chain A:





- Molecule 1: Neurophysin 1

Chain B:



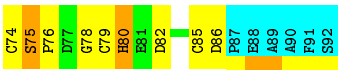
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

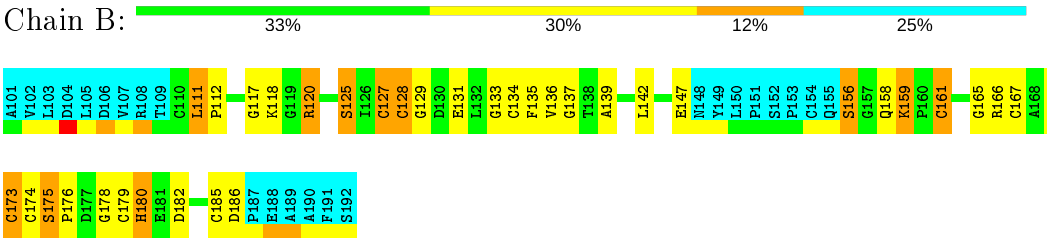
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Neurophysin 1

Chain A:

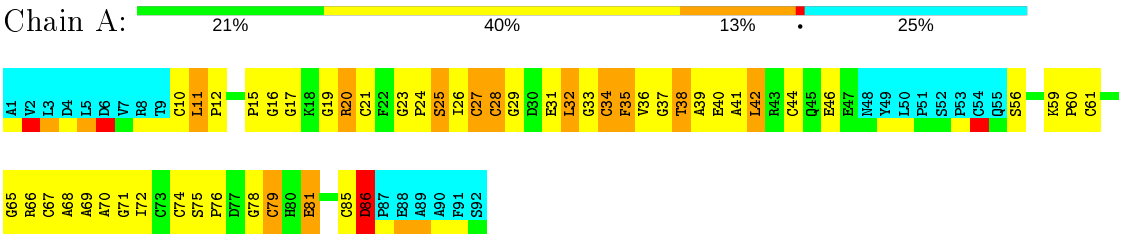


• Molecule 1: Neurophysin 1

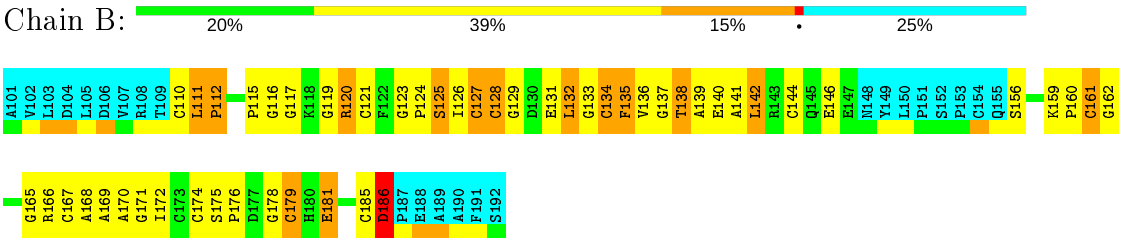


4.2.2 Score per residue for model 2

• Molecule 1: Neurophysin 1

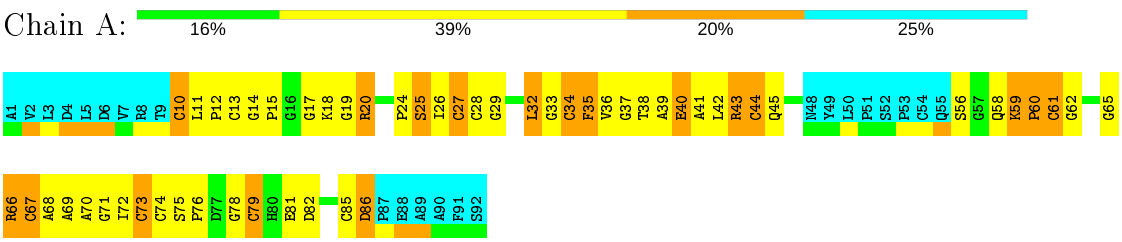


• Molecule 1: Neurophysin 1



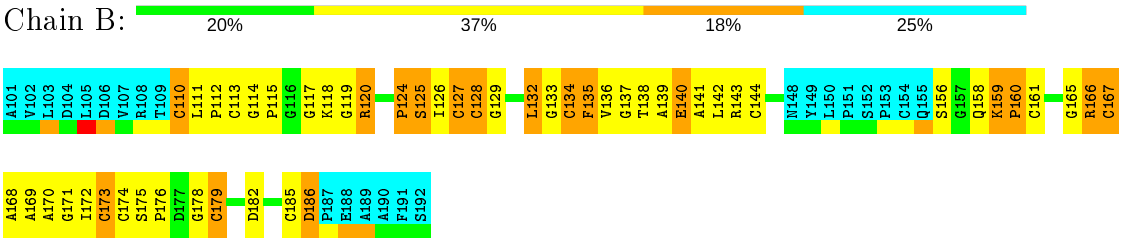
4.2.3 Score per residue for model 3

• Molecule 1: Neurophysin 1



• Molecule 1: Neurophysin 1

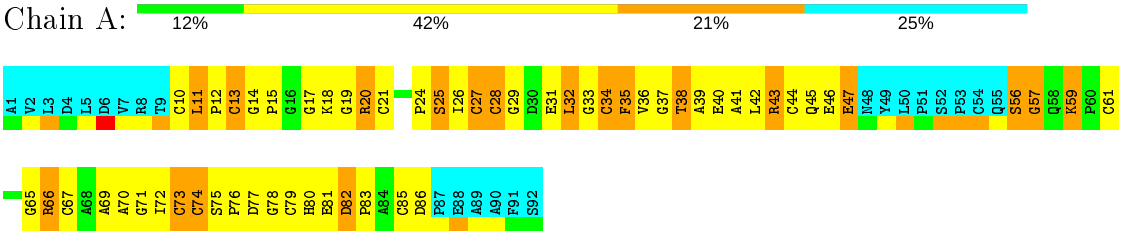
Chain B:



4.2.4 Score per residue for model 4

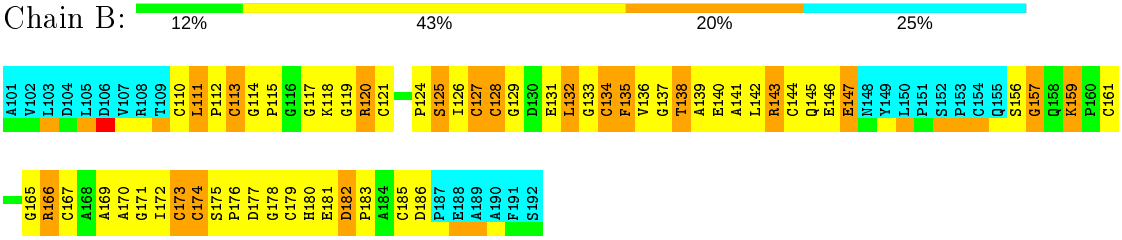
- Molecule 1: Neurophysin 1

Chain A:



- Molecule 1: Neurophysin 1

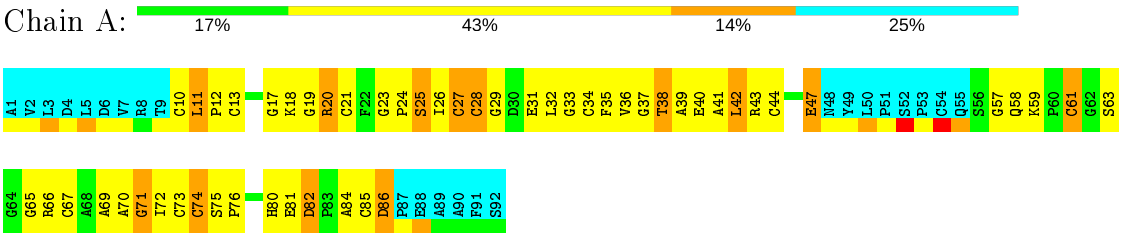
Chain B:



4.2.5 Score per residue for model 5

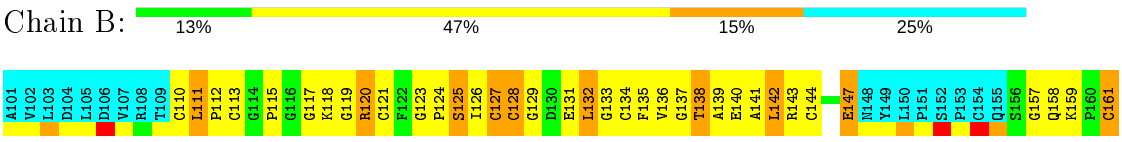
- Molecule 1: Neurophysin 1

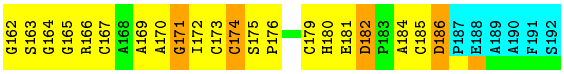
Chain A:



- Molecule 1: Neurophysin 1

Chain B:

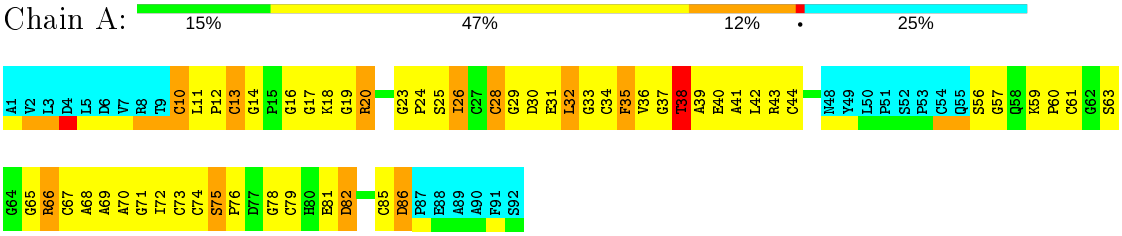




4.2.6 Score per residue for model 6

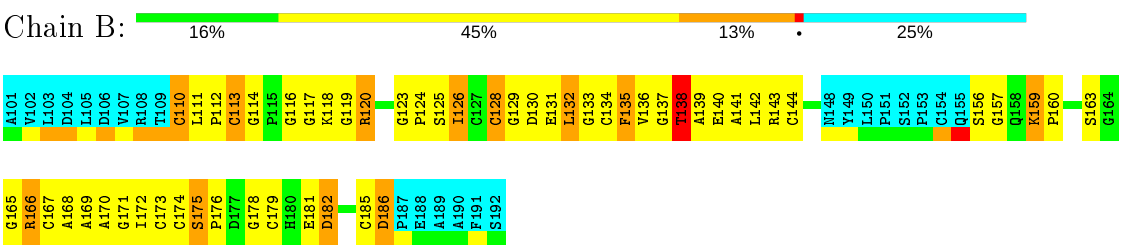
- Molecule 1: Neurophysin 1

Chain A:



- Molecule 1: Neurophysin 1

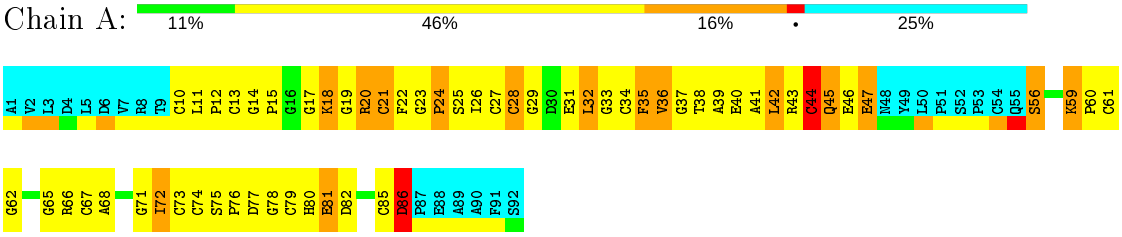
Chain B:



4.2.7 Score per residue for model 7

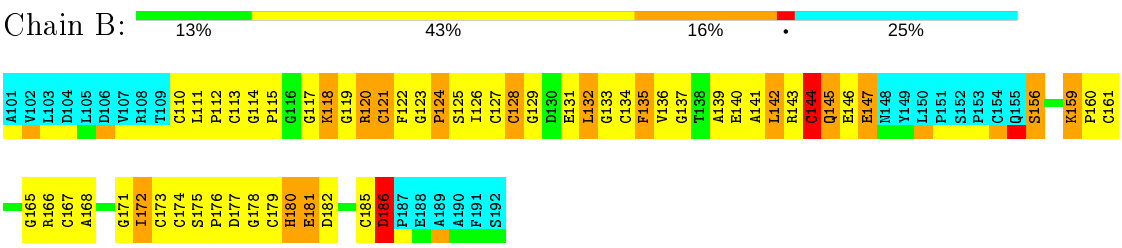
- Molecule 1: Neurophysin 1

Chain A:



- Molecule 1: Neurophysin 1

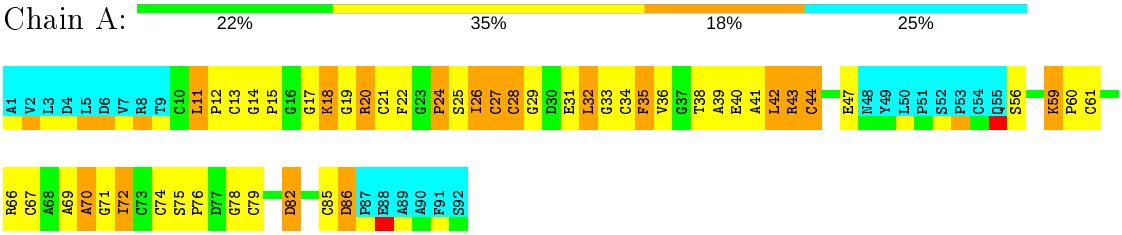
Chain B:



4.2.8 Score per residue for model 8

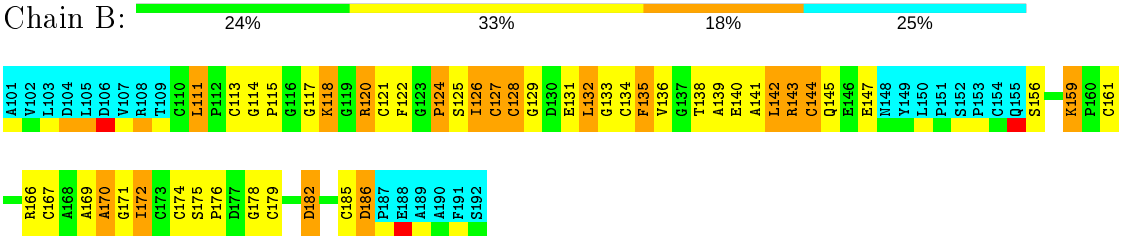
- Molecule 1: Neurophysin 1

Chain A:



- Molecule 1: Neurophysin 1

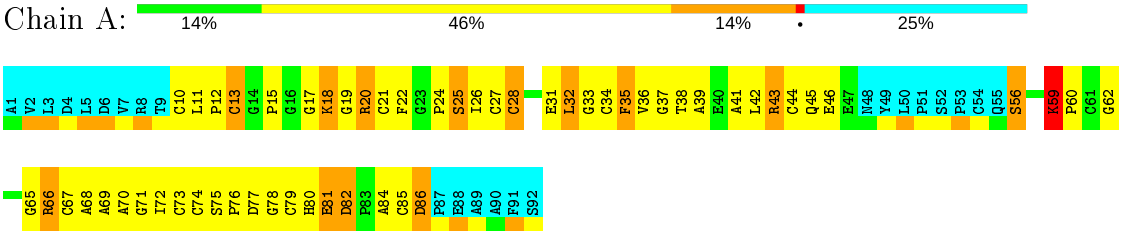
Chain B:



4.2.9 Score per residue for model 9

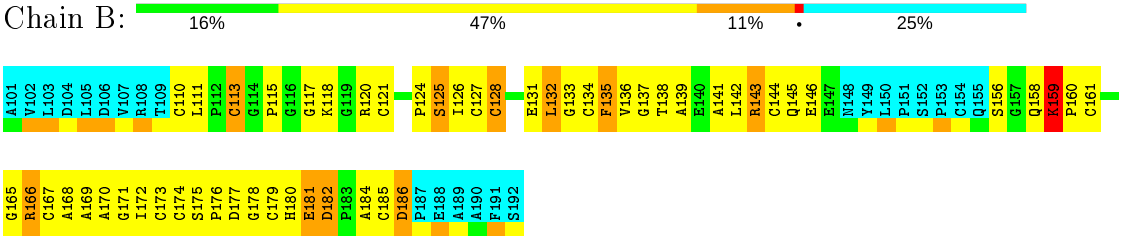
- Molecule 1: Neurophysin 1

Chain A:



- Molecule 1: Neurophysin 1

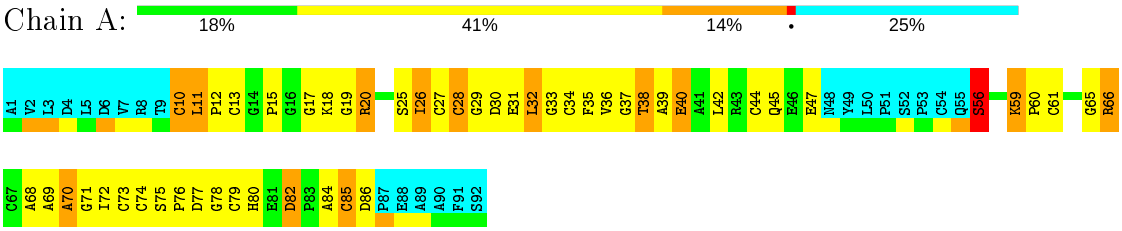
Chain B:



4.2.10 Score per residue for model 10

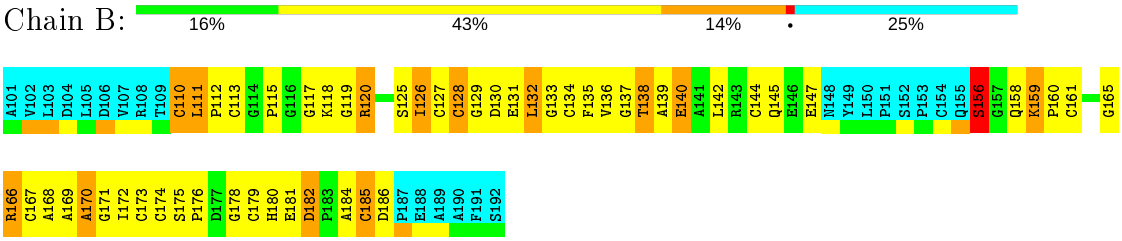
- Molecule 1: Neurophysin 1

Chain A:



• Molecule 1: Neurophysin 1

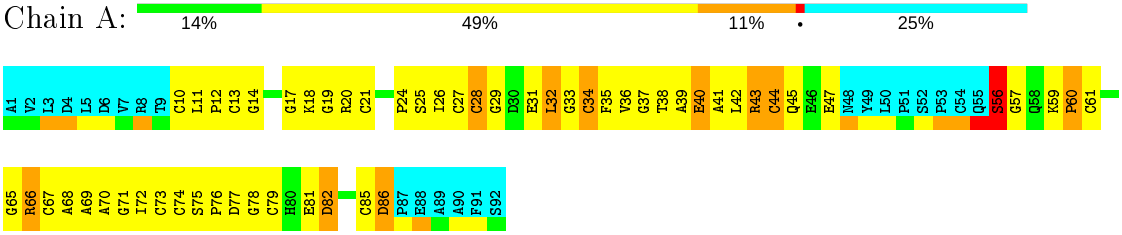
Chain B:



4.2.11 Score per residue for model 11

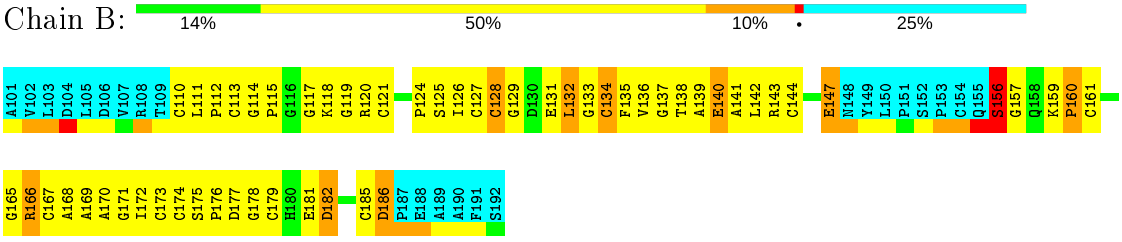
• Molecule 1: Neurophysin 1

Chain A:



• Molecule 1: Neurophysin 1

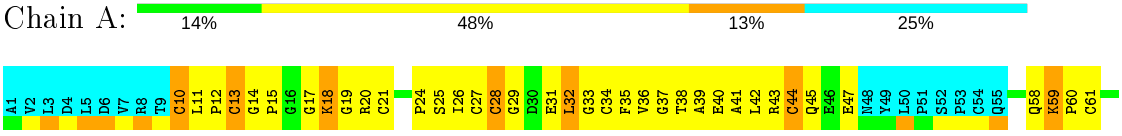
Chain B:

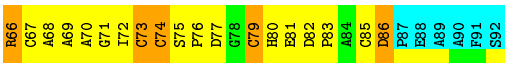


4.2.12 Score per residue for model 12

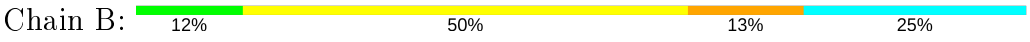
• Molecule 1: Neurophysin 1

Chain A:



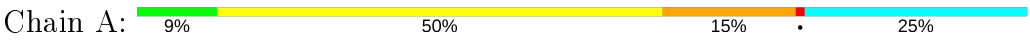


• Molecule 1: Neurophysin 1

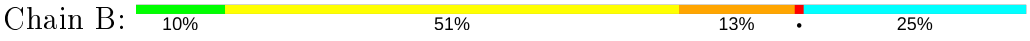


4.2.13 Score per residue for model 13

• Molecule 1: Neurophysin 1

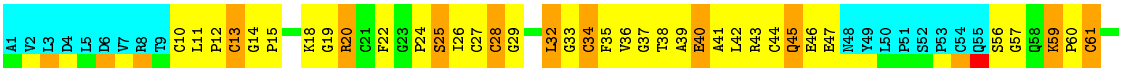


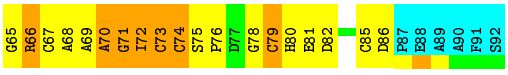
• Molecule 1: Neurophysin 1



4.2.14 Score per residue for model 14

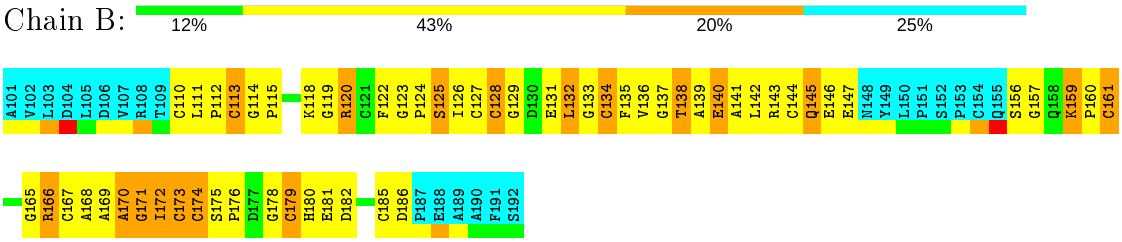
• Molecule 1: Neurophysin 1





• Molecule 1: Neurophysin 1

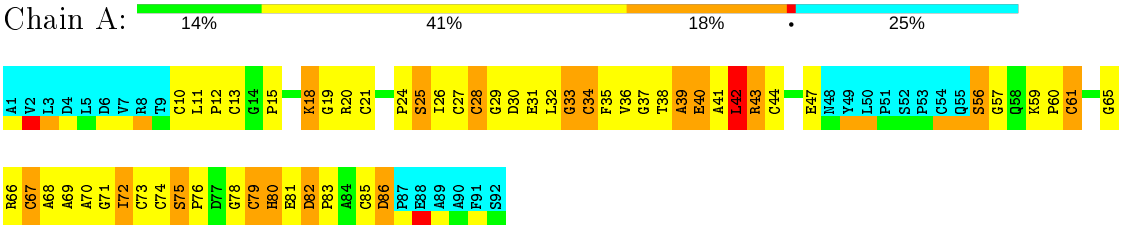
Chain B:



4.2.15 Score per residue for model 15

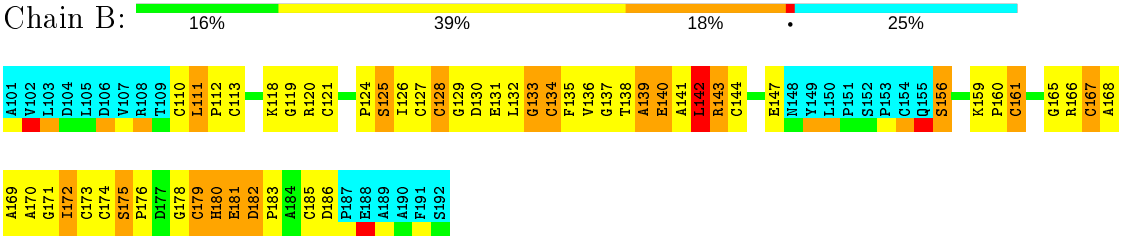
- Molecule 1: Neurophysin 1

Chain A:



- Molecule 1: Neurophysin 1

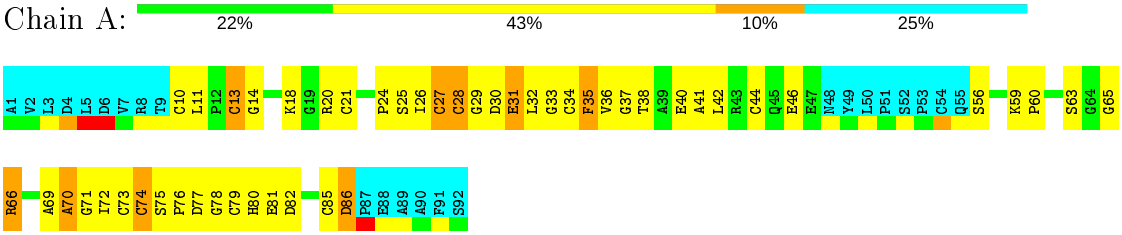
Chain B:



4.2.16 Score per residue for model 16

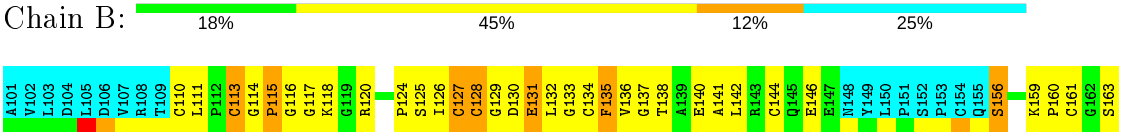
- Molecule 1: Neurophysin 1

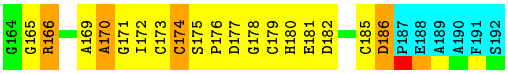
Chain A:



- Molecule 1: Neurophysin 1

Chain B:

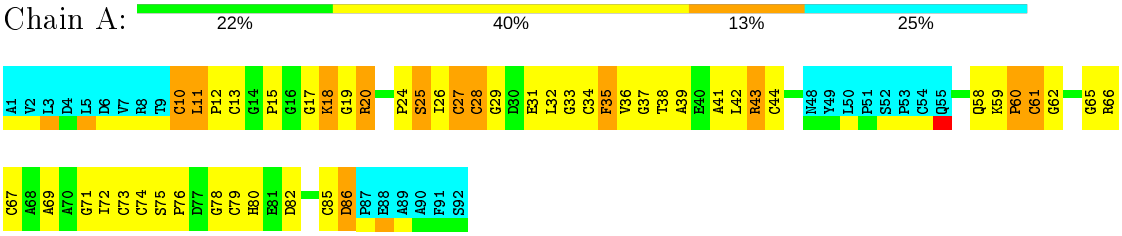




4.2.17 Score per residue for model 17

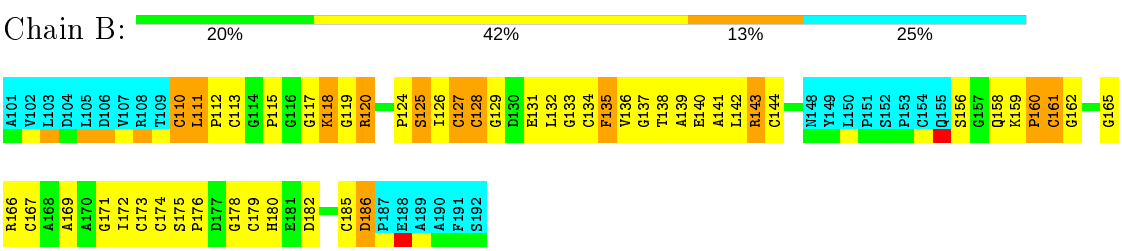
- Molecule 1: Neurophysin 1

Chain A:



- Molecule 1: Neurophysin 1

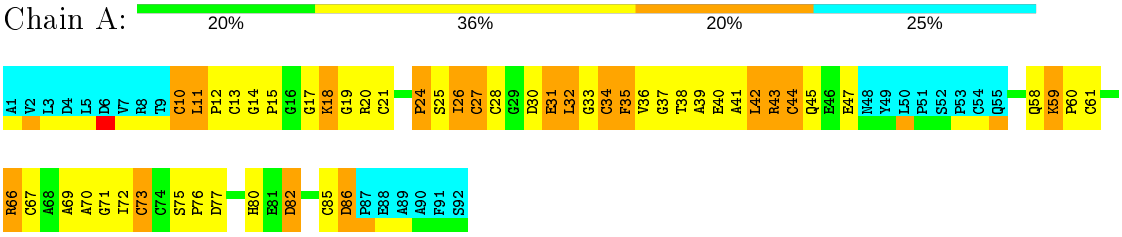
Chain B:



4.2.18 Score per residue for model 18

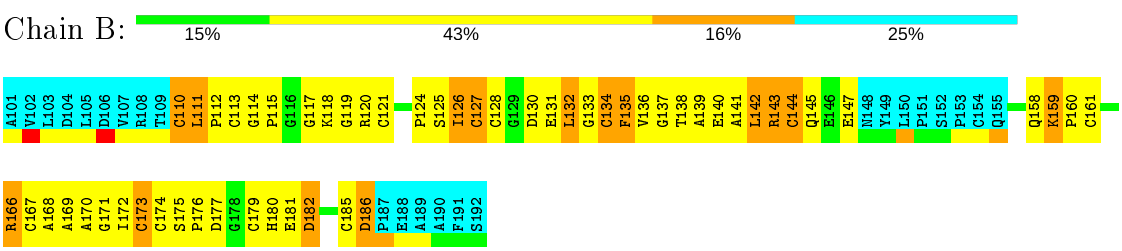
- Molecule 1: Neurophysin 1

Chain A:



- Molecule 1: Neurophysin 1

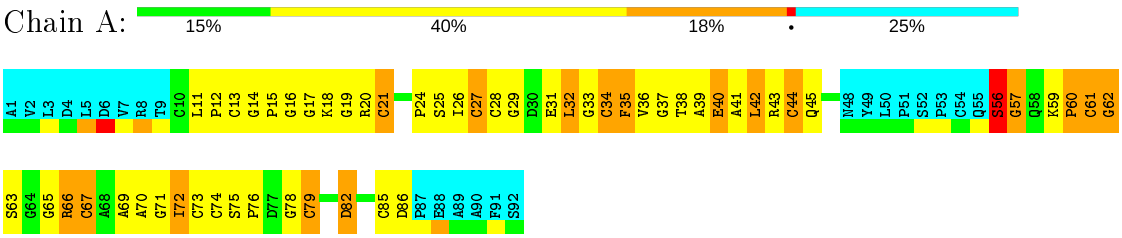
Chain B:



4.2.19 Score per residue for model 19

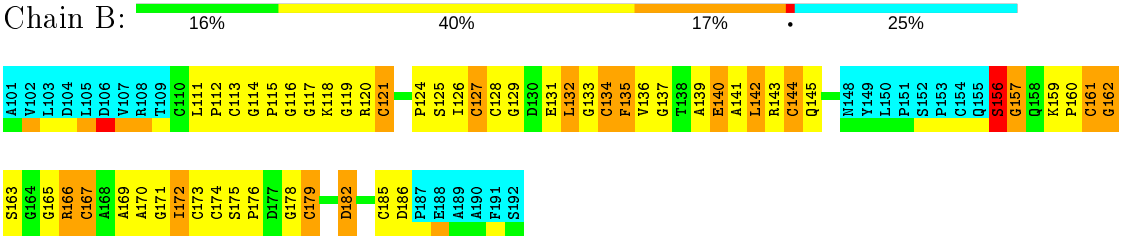
- Molecule 1: Neurophysin 1

Chain A:



- Molecule 1: Neurophysin 1

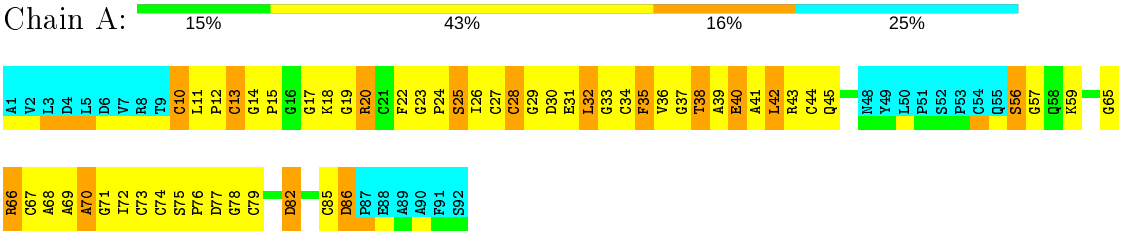
Chain B:



4.2.20 Score per residue for model 20

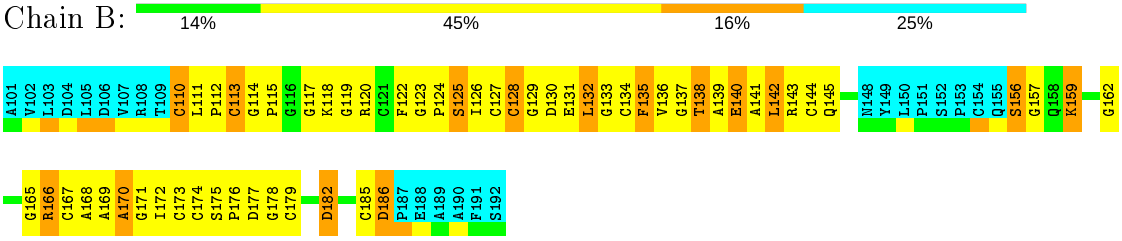
- Molecule 1: Neurophysin 1

Chain A:



- Molecule 1: Neurophysin 1

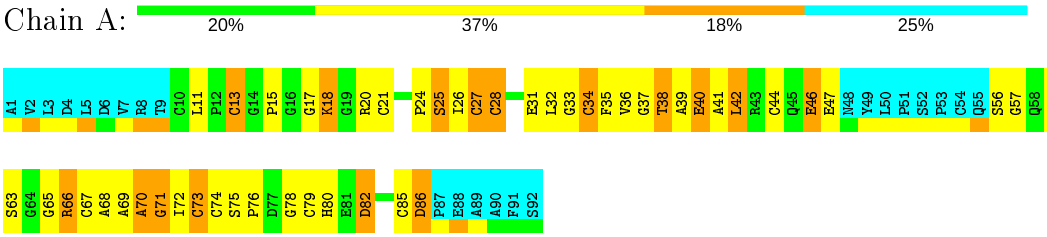
Chain B:



4.2.21 Score per residue for model 21

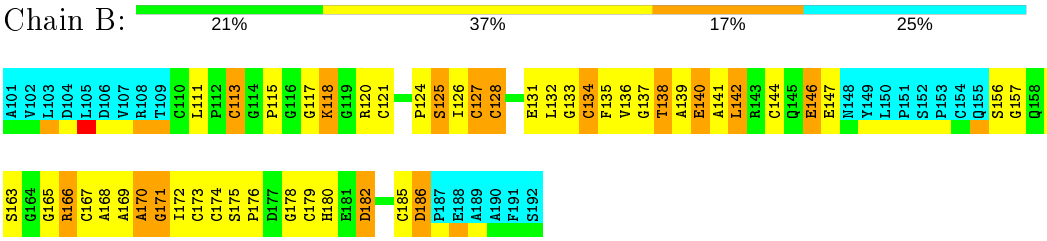
- Molecule 1: Neurophysin 1

Chain A:



- Molecule 1: Neurophysin 1

Chain B:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 21 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CNSSOLVE	refinement	1.0

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

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	862
Number of shifts mapped to atoms	862
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	44%

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

6 Model quality

6.1 Standard geometry

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

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.0±0.2
1	B	0.0±0.0	0.1±0.3
All	All	0	3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	B	112	PRO	Mainchain	1
1	A	71	GLY	Mainchain	1
1	B	115	PRO	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	462	410	409	75±13
1	B	462	410	409	75±12
All	All	19404	17220	17178	2825

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 77.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LYS:O	1:A:66:ARG:HA	1.34	1.18	13	6
1:B:159:LYS:O	1:B:166:ARG:HA	1.26	1.14	13	7
1:B:174:CYS:CB	1:B:179:CYS:HA	1.20	1.66	10	4
1:A:74:CYS:CB	1:A:79:CYS:HA	1.20	1.66	10	4
1:B:128:CYS:HA	1:B:133:GLY:O	1.17	1.39	8	20
1:A:28:CYS:HA	1:A:33:GLY:O	1.16	1.40	20	20
1:A:78:GLY:HA3	1:B:179:CYS:O	1.16	1.41	21	11
1:A:74:CYS:HB3	1:A:79:CYS:HA	1.15	1.17	10	4
1:B:159:LYS:O	1:B:166:ARG:CA	1.15	1.94	13	3
1:A:79:CYS:O	1:B:178:GLY:HA3	1.13	1.42	21	11
1:B:134:CYS:HB2	1:B:172:ILE:HD13	1.10	1.24	4	15
1:B:174:CYS:HB3	1:B:179:CYS:HA	1.10	1.17	10	5
1:A:59:LYS:O	1:A:66:ARG:CA	1.09	2.01	13	3
1:A:34:CYS:HB2	1:A:72:ILE:HD13	1.07	1.22	16	16
1:B:134:CYS:HB2	1:B:172:ILE:HG13	1.06	1.22	10	4
1:A:26:ILE:HG12	1:A:36:VAL:HG13	1.05	1.29	16	20
1:B:126:ILE:HG12	1:B:136:VAL:HG13	1.04	1.29	16	18
1:B:128:CYS:CA	1:B:133:GLY:O	1.02	2.06	8	20
1:A:34:CYS:HB2	1:A:72:ILE:HG13	1.00	1.24	10	4
1:B:110:CYS:HB3	1:B:120:ARG:HG2	1.00	1.34	13	3
1:B:170:ALA:HA	1:B:185:CYS:HB3	0.99	1.30	3	9
1:B:159:LYS:HB3	1:B:166:ARG:HB3	0.99	1.33	12	2
1:A:35:PHE:HA	1:B:135:PHE:HA	0.99	1.32	20	12
1:A:39:ALA:O	1:A:42:LEU:HD12	0.99	1.58	19	3
1:B:139:ALA:O	1:B:142:LEU:HD12	0.99	1.58	19	3
1:A:28:CYS:CA	1:A:33:GLY:O	0.98	2.10	8	20
1:A:70:ALA:HA	1:A:85:CYS:HB3	0.98	1.34	3	9
1:A:59:LYS:HB3	1:A:66:ARG:HB3	0.97	1.36	12	1
1:A:36:VAL:HG11	1:A:78:GLY:HA2	0.96	1.36	7	1
1:B:136:VAL:HG22	1:B:179:CYS:SG	0.96	1.99	7	1
1:A:69:ALA:HB3	1:A:72:ILE:HD11	0.95	1.35	21	9
1:B:134:CYS:SG	1:B:172:ILE:HD13	0.95	2.01	7	1
1:A:10:CYS:HB3	1:A:20:ARG:HG2	0.95	1.34	13	3
1:B:169:ALA:HB3	1:B:172:ILE:HD11	0.95	1.35	21	9
1:A:41:ALA:O	1:A:44:CYS:HB2	0.95	1.61	8	15
1:A:34:CYS:SG	1:A:72:ILE:HD13	0.95	2.02	7	1
1:B:114:GLY:HA2	1:B:140:GLU:HB3	0.94	1.38	3	6
1:B:141:ALA:O	1:B:144:CYS:HB2	0.93	1.63	8	15
1:A:26:ILE:HG13	1:A:36:VAL:HG13	0.93	1.41	4	2
1:A:14:GLY:HA2	1:A:40:GLU:HB3	0.93	1.39	3	6
1:A:71:GLY:C	1:A:72:ILE:HD13	0.93	1.82	8	3
1:B:115:PRO:HD2	1:B:132:LEU:HD11	0.91	1.42	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:VAL:HG22	1:A:79:CYS:SG	0.91	2.05	7	1
1:A:15:PRO:HD2	1:A:32:LEU:HD11	0.91	1.42	10	3
1:A:37:GLY:HA3	1:B:172:ILE:HG21	0.91	1.40	12	8
1:A:72:ILE:O	1:A:72:ILE:HG13	0.91	1.65	15	2
1:A:26:ILE:CG1	1:A:36:VAL:HG13	0.91	1.96	4	14
1:A:18:LYS:HD3	1:A:32:LEU:HD11	0.90	1.42	12	1
1:B:159:LYS:HB3	1:B:167:CYS:HB3	0.90	1.41	4	1
1:A:28:CYS:SG	1:A:68:ALA:HB1	0.89	2.07	2	4
1:B:169:ALA:HB3	1:B:172:ILE:HG12	0.89	1.43	15	5
1:B:174:CYS:HA	1:B:179:CYS:HA	0.89	1.44	11	11
1:B:172:ILE:O	1:B:172:ILE:HG13	0.89	1.67	15	2
1:A:36:VAL:HG23	1:B:136:VAL:HG23	0.89	1.42	7	14
1:A:33:GLY:HA2	1:A:69:ALA:HB1	0.88	1.46	18	9
1:A:74:CYS:HA	1:A:79:CYS:HA	0.88	1.44	11	10
1:B:113:CYS:HB2	1:B:143:ARG:HG3	0.88	1.45	12	1
1:A:21:CYS:HB3	1:A:47:GLU:HG3	0.88	1.45	18	2
1:B:133:GLY:HA2	1:B:169:ALA:HB1	0.88	1.45	18	8
1:B:134:CYS:HB2	1:B:172:ILE:CD1	0.87	1.98	16	14
1:A:34:CYS:HB2	1:A:72:ILE:CD1	0.87	1.98	16	15
1:A:26:ILE:HG12	1:A:36:VAL:CG1	0.87	2.00	12	13
1:B:128:CYS:SG	1:B:168:ALA:HB1	0.87	2.09	2	4
1:A:32:LEU:HD22	1:A:35:PHE:CE1	0.87	2.05	18	11
1:B:112:PRO:HB2	1:B:117:GLY:O	0.87	1.68	18	11
1:A:68:ALA:HB2	1:A:74:CYS:HB2	0.86	1.45	12	3
1:A:72:ILE:HG21	1:B:137:GLY:HA3	0.86	1.44	12	7
1:B:136:VAL:HG11	1:B:178:GLY:HA2	0.86	1.45	7	1
1:A:69:ALA:O	1:A:70:ALA:O	0.86	1.92	14	3
1:A:33:GLY:HA2	1:A:69:ALA:CB	0.86	2.00	11	14
1:B:132:LEU:HD22	1:B:135:PHE:CE1	0.86	2.06	18	11
1:A:65:GLY:HA3	1:A:74:CYS:HA	0.86	1.44	20	2
1:A:59:LYS:HB3	1:A:67:CYS:HB3	0.85	1.48	4	1
1:B:168:ALA:HB2	1:B:174:CYS:HB2	0.85	1.45	12	2
1:A:59:LYS:HB3	1:A:66:ARG:CB	0.85	2.01	12	2
1:A:59:LYS:HA	1:A:66:ARG:HB3	0.85	1.46	13	1
1:B:132:LEU:HD22	1:B:135:PHE:CZ	0.85	2.06	16	11
1:B:171:GLY:N	1:B:185:CYS:O	0.85	2.09	6	11
1:A:69:ALA:HB3	1:A:72:ILE:HG12	0.85	1.46	15	5
1:B:158:GLN:O	1:B:167:CYS:HB3	0.85	1.71	12	3
1:B:121:CYS:HB3	1:B:147:GLU:HG3	0.85	1.44	18	2
1:A:59:LYS:HA	1:A:67:CYS:H	0.85	1.26	12	2
1:B:112:PRO:HA	1:B:119:GLY:O	0.85	1.71	7	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:159:LYS:HB3	1:B:166:ARG:CB	0.85	2.02	12	2
1:A:77:ASP:HB3	1:B:180:HIS:HD2	0.85	1.30	4	1
1:B:159:LYS:HB3	1:B:160:PRO:CD	0.85	2.01	9	2
1:A:74:CYS:HB2	1:A:78:GLY:O	0.84	1.72	8	4
1:B:158:GLN:HB3	1:B:167:CYS:HB3	0.84	1.49	13	1
1:A:71:GLY:N	1:A:85:CYS:O	0.84	2.09	6	11
1:A:13:CYS:HB2	1:A:43:ARG:HG3	0.84	1.49	12	1
1:A:69:ALA:O	1:A:72:ILE:HG13	0.84	1.72	16	3
1:B:118:LYS:HD3	1:B:132:LEU:HD11	0.84	1.45	12	1
1:B:169:ALA:O	1:B:170:ALA:O	0.83	1.94	14	3
1:A:32:LEU:HD22	1:A:35:PHE:CZ	0.83	2.08	16	11
1:B:174:CYS:HB2	1:B:178:GLY:O	0.83	1.72	8	4
1:A:59:LYS:HB3	1:A:60:PRO:CD	0.83	2.03	9	2
1:B:113:CYS:N	1:B:119:GLY:O	0.83	2.12	17	6
1:A:79:CYS:O	1:B:178:GLY:CA	0.83	2.27	21	6
1:A:78:GLY:CA	1:B:179:CYS:O	0.83	2.26	21	8
1:A:72:ILE:CG2	1:B:137:GLY:HA3	0.82	2.04	11	6
1:B:159:LYS:HA	1:B:167:CYS:H	0.82	1.35	12	2
1:B:133:GLY:HA2	1:B:169:ALA:CB	0.82	2.04	9	14
1:B:126:ILE:CG1	1:B:136:VAL:HG13	0.82	2.05	4	12
1:B:173:CYS:HB2	1:B:182:ASP:HB3	0.82	1.52	6	10
1:B:159:LYS:HB2	1:B:167:CYS:HB2	0.82	1.50	11	6
1:B:128:CYS:HB3	1:B:133:GLY:O	0.81	1.75	10	6
1:A:13:CYS:N	1:A:19:GLY:O	0.81	2.13	17	7
1:B:126:ILE:HG12	1:B:136:VAL:CG1	0.81	2.05	12	9
1:B:159:LYS:O	1:B:166:ARG:CB	0.81	2.29	13	2
1:A:12:PRO:HA	1:A:19:GLY:O	0.81	1.75	11	18
1:A:11:LEU:O	1:A:20:ARG:HA	0.80	1.74	7	15
1:B:128:CYS:HB3	1:B:168:ALA:HB1	0.80	1.53	7	1
1:A:59:LYS:CA	1:A:66:ARG:HB3	0.80	2.07	13	1
1:A:10:CYS:HB2	1:A:20:ARG:HG2	0.80	1.52	15	2
1:B:110:CYS:HB2	1:B:120:ARG:HG2	0.80	1.52	15	2
1:A:73:CYS:HB2	1:A:82:ASP:HB3	0.80	1.52	6	10
1:A:58:GLN:O	1:A:67:CYS:HB3	0.79	1.77	12	1
1:B:110:CYS:O	1:B:120:ARG:HG2	0.79	1.77	18	2
1:A:28:CYS:HB3	1:A:33:GLY:O	0.79	1.77	10	5
1:A:34:CYS:SG	1:A:74:CYS:SG	0.79	2.80	7	3
1:A:80:HIS:HD2	1:B:177:ASP:HB3	0.79	1.36	4	1
1:B:113:CYS:HA	1:B:143:ARG:HE	0.79	1.37	12	1
1:B:136:VAL:CG1	1:B:178:GLY:HA2	0.79	2.07	7	1
1:A:12:PRO:HB2	1:A:17:GLY:O	0.79	1.76	18	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:169:ALA:O	1:B:172:ILE:HG13	0.79	1.77	16	3
1:A:75:SER:HB3	1:A:76:PRO:HD2	0.79	1.54	9	4
1:A:28:CYS:HB3	1:A:68:ALA:HB1	0.78	1.53	7	1
1:B:128:CYS:HB2	1:B:169:ALA:HB2	0.78	1.56	10	4
1:B:171:GLY:C	1:B:172:ILE:HD13	0.78	1.98	8	3
1:B:175:SER:HB2	1:B:176:PRO:HD2	0.78	1.56	12	13
1:B:165:GLY:HA3	1:B:174:CYS:HA	0.78	1.54	20	2
1:A:66:ARG:HG2	1:A:74:CYS:O	0.78	1.79	10	1
1:B:111:LEU:O	1:B:120:ARG:HA	0.77	1.78	7	16
1:B:111:LEU:HD22	1:B:147:GLU:HG3	0.77	1.56	4	1
1:A:36:VAL:CG1	1:A:78:GLY:HA2	0.77	2.08	7	1
1:A:38:THR:HG22	1:B:132:LEU:O	0.77	1.80	8	10
1:B:170:ALA:HA	1:B:185:CYS:O	0.77	1.79	13	6
1:B:134:CYS:SG	1:B:174:CYS:SG	0.77	2.82	7	3
1:A:77:ASP:HB3	1:B:180:HIS:CD2	0.77	2.15	4	1
1:B:175:SER:HB3	1:B:176:PRO:HD2	0.77	1.54	9	4
1:A:28:CYS:HB2	1:A:69:ALA:HB2	0.77	1.56	10	4
1:B:126:ILE:HG13	1:B:136:VAL:HG13	0.77	1.54	4	2
1:A:58:GLN:HB3	1:A:67:CYS:HB3	0.77	1.54	13	1
1:A:39:ALA:O	1:A:42:LEU:HB2	0.77	1.80	4	2
1:A:75:SER:HB2	1:A:76:PRO:HD2	0.77	1.57	10	13
1:A:11:LEU:HD22	1:A:47:GLU:HG3	0.76	1.56	4	1
1:A:65:GLY:HA2	1:A:75:SER:HB3	0.76	1.55	4	2
1:A:70:ALA:HA	1:A:85:CYS:O	0.76	1.80	13	6
1:A:69:ALA:HB3	1:A:72:ILE:CG1	0.76	2.10	12	8
1:B:126:ILE:HG22	1:B:134:CYS:SG	0.76	2.20	6	12
1:B:166:ARG:HG2	1:B:174:CYS:O	0.76	1.79	10	1
1:A:11:LEU:HD23	1:A:21:CYS:HB3	0.76	1.57	9	1
1:B:159:LYS:HA	1:B:166:ARG:HB3	0.76	1.57	13	1
1:B:169:ALA:HB3	1:B:172:ILE:CG1	0.76	2.11	11	8
1:A:29:GLY:O	1:A:69:ALA:HB1	0.76	1.80	6	9
1:A:27:CYS:HB2	1:A:41:ALA:HB2	0.76	1.58	8	2
1:B:139:ALA:O	1:B:142:LEU:HB2	0.76	1.80	4	3
1:B:165:GLY:HA2	1:B:175:SER:HB3	0.75	1.55	4	2
1:B:129:GLY:O	1:B:169:ALA:HB1	0.75	1.80	6	9
1:A:27:CYS:O	1:A:34:CYS:HA	0.75	1.81	14	14
1:A:26:ILE:HG22	1:A:34:CYS:SG	0.75	2.21	6	12
1:A:13:CYS:HA	1:A:43:ARG:HE	0.75	1.41	12	1
1:B:165:GLY:CA	1:B:175:SER:HB3	0.75	2.12	4	4
1:A:10:CYS:HB3	1:A:20:ARG:CG	0.74	2.12	11	1
1:A:10:CYS:O	1:A:20:ARG:HG2	0.74	1.81	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:LYS:HD3	1:A:32:LEU:CD1	0.74	2.13	12	1
1:A:11:LEU:HD13	1:A:12:PRO:HD2	0.74	1.57	18	2
1:A:65:GLY:CA	1:A:75:SER:HB3	0.74	2.13	4	5
1:B:170:ALA:CA	1:B:185:CYS:HB3	0.74	2.10	3	2
1:B:159:LYS:HB3	1:B:167:CYS:CB	0.74	2.11	4	2
1:B:139:ALA:HA	1:B:142:LEU:HG	0.74	1.60	15	1
1:B:123:GLY:O	1:B:144:CYS:HB3	0.73	1.83	20	4
1:B:111:LEU:HD13	1:B:112:PRO:HD2	0.73	1.58	18	2
1:B:159:LYS:CB	1:B:167:CYS:HB2	0.73	2.12	11	5
1:B:174:CYS:HB3	1:B:179:CYS:CA	0.73	2.07	10	3
1:A:14:GLY:CA	1:A:40:GLU:HG2	0.73	2.14	11	1
1:B:127:CYS:O	1:B:134:CYS:HA	0.73	1.83	14	14
1:A:35:PHE:CD2	1:B:138:THR:HG21	0.73	2.18	17	2
1:A:26:ILE:HG23	1:A:36:VAL:HG13	0.73	1.60	3	10
1:B:111:LEU:HD23	1:B:121:CYS:HB3	0.73	1.58	9	1
1:B:174:CYS:HB2	1:B:179:CYS:HA	0.73	1.61	10	1
1:B:110:CYS:HB3	1:B:120:ARG:CG	0.73	2.13	11	1
1:B:134:CYS:CB	1:B:172:ILE:HD13	0.72	2.13	12	10
1:A:73:CYS:HB2	1:A:82:ASP:CB	0.72	2.14	10	3
1:A:59:LYS:HB2	1:A:67:CYS:HB2	0.72	1.59	19	3
1:A:15:PRO:HG2	1:A:18:LYS:HD2	0.72	1.61	12	1
1:B:159:LYS:HB3	1:B:160:PRO:HD3	0.72	1.62	10	2
1:B:168:ALA:CB	1:B:174:CYS:HB2	0.72	2.14	12	1
1:B:110:CYS:HB2	1:B:120:ARG:HD2	0.72	1.61	18	1
1:A:26:ILE:HG23	1:A:36:VAL:HG22	0.72	1.62	18	7
1:A:74:CYS:HB3	1:A:79:CYS:CA	0.72	2.07	10	2
1:A:34:CYS:CB	1:A:72:ILE:HD13	0.72	2.14	12	9
1:A:32:LEU:O	1:B:138:THR:HG22	0.72	1.84	8	8
1:A:59:LYS:O	1:A:66:ARG:CB	0.72	2.38	13	2
1:A:38:THR:HG21	1:B:135:PHE:CD2	0.72	2.19	17	2
1:A:37:GLY:O	1:B:133:GLY:HA3	0.72	1.85	10	9
1:B:126:ILE:HG23	1:B:136:VAL:HG22	0.72	1.62	18	9
1:A:69:ALA:HB3	1:A:72:ILE:CD1	0.72	2.15	18	5
1:A:70:ALA:CA	1:A:85:CYS:HB3	0.72	2.13	3	2
1:A:77:ASP:HB2	1:B:180:HIS:ND1	0.72	2.00	9	1
1:B:173:CYS:HB2	1:B:182:ASP:CB	0.71	2.14	10	2
1:B:114:GLY:CA	1:B:140:GLU:HG2	0.71	2.15	11	1
1:A:35:PHE:HB3	1:A:38:THR:CG2	0.71	2.14	13	5
1:B:172:ILE:HD13	1:B:172:ILE:N	0.71	1.99	8	3
1:A:39:ALA:HA	1:A:42:LEU:HG	0.71	1.62	15	1
1:B:110:CYS:HB2	1:B:120:ARG:CD	0.71	2.15	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:159:LYS:HB3	1:B:167:CYS:HB2	0.71	1.61	21	4
1:B:168:ALA:HB3	1:B:172:ILE:HD12	0.71	1.60	3	1
1:A:14:GLY:HA2	1:A:40:GLU:HG2	0.71	1.63	11	2
1:A:10:CYS:HB2	1:A:20:ARG:HD2	0.71	1.63	18	1
1:A:59:LYS:CA	1:A:67:CYS:H	0.70	1.99	3	2
1:A:72:ILE:HG12	1:B:137:GLY:HA3	0.70	1.61	3	1
1:B:126:ILE:CG2	1:B:174:CYS:HB3	0.70	2.15	7	1
1:B:139:ALA:HA	1:B:142:LEU:HD12	0.70	1.62	14	15
1:A:26:ILE:CG2	1:A:74:CYS:HB3	0.70	2.16	7	1
1:A:39:ALA:HA	1:A:42:LEU:HD12	0.70	1.61	14	15
1:A:80:HIS:ND1	1:B:177:ASP:HB2	0.70	2.00	9	1
1:A:23:GLY:O	1:A:44:CYS:HB3	0.70	1.85	20	4
1:B:167:CYS:HA	1:B:172:ILE:O	0.70	1.86	8	3
1:A:10:CYS:HB2	1:A:20:ARG:CD	0.70	2.16	18	1
1:A:80:HIS:CD2	1:B:177:ASP:HB3	0.70	2.21	4	1
1:A:74:CYS:HB2	1:A:79:CYS:HA	0.70	1.61	10	1
1:A:27:CYS:HB2	1:A:41:ALA:CB	0.69	2.16	8	1
1:B:159:LYS:O	1:B:166:ARG:HB3	0.69	1.85	13	1
1:A:36:VAL:CG2	1:B:136:VAL:CG2	0.69	2.69	5	16
1:A:12:PRO:O	1:A:43:ARG:HD2	0.69	1.87	18	1
1:A:41:ALA:O	1:A:44:CYS:N	0.69	2.26	6	13
1:A:67:CYS:HA	1:A:72:ILE:O	0.69	1.87	8	3
1:B:165:GLY:CA	1:B:174:CYS:HA	0.69	2.16	20	2
1:B:118:LYS:HD3	1:B:132:LEU:CD1	0.69	2.18	12	1
1:A:34:CYS:O	1:B:136:VAL:N	0.69	2.26	20	14
1:B:135:PHE:HB3	1:B:138:THR:CG2	0.69	2.18	13	6
1:A:68:ALA:CB	1:A:74:CYS:HB2	0.69	2.16	12	1
1:B:114:GLY:HA2	1:B:140:GLU:HG2	0.69	1.65	11	2
1:B:141:ALA:O	1:B:144:CYS:N	0.68	2.26	6	13
1:A:28:CYS:CB	1:A:68:ALA:HB1	0.68	2.19	13	2
1:B:112:PRO:O	1:B:143:ARG:HD2	0.68	1.88	18	1
1:B:171:GLY:HA2	1:B:182:ASP:O	0.68	1.88	11	7
1:B:169:ALA:HB3	1:B:172:ILE:CD1	0.68	2.18	18	5
1:A:25:SER:C	1:A:26:ILE:HG13	0.68	2.09	18	2
1:B:159:LYS:CA	1:B:166:ARG:HB3	0.68	2.19	13	1
1:A:11:LEU:HB3	1:A:21:CYS:HB2	0.68	1.64	21	1
1:B:127:CYS:HB3	1:B:135:PHE:CE2	0.68	2.24	18	4
1:B:115:PRO:HG2	1:B:118:LYS:HD2	0.68	1.65	12	1
1:A:72:ILE:HD12	1:A:74:CYS:SG	0.67	2.29	1	3
1:B:127:CYS:HB2	1:B:141:ALA:HB2	0.67	1.65	8	2
1:B:172:ILE:HD12	1:B:174:CYS:SG	0.67	2.30	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:VAL:N	1:B:134:CYS:O	0.67	2.28	20	15
1:B:125:SER:C	1:B:126:ILE:HG13	0.67	2.09	18	2
1:B:111:LEU:HB3	1:B:121:CYS:HB2	0.67	1.66	21	1
1:A:66:ARG:HD2	1:A:66:ARG:N	0.67	2.04	13	3
1:A:35:PHE:HD1	1:B:135:PHE:HD1	0.67	1.30	21	1
1:B:139:ALA:CA	1:B:142:LEU:HD22	0.67	2.19	2	1
1:A:56:SER:OG	1:A:59:LYS:HG3	0.67	1.90	9	1
1:A:33:GLY:HA3	1:B:137:GLY:O	0.67	1.89	2	10
1:B:139:ALA:CB	1:B:142:LEU:HD22	0.67	2.20	2	1
1:A:11:LEU:O	1:A:20:ARG:HG3	0.67	1.89	4	3
1:A:68:ALA:HB3	1:A:72:ILE:HD12	0.66	1.67	3	1
1:A:27:CYS:HB3	1:A:35:PHE:CE2	0.66	2.25	18	4
1:B:113:CYS:O	1:B:117:GLY:HA2	0.66	1.90	12	8
1:A:59:LYS:CB	1:A:67:CYS:HB2	0.66	2.20	11	4
1:A:37:GLY:HA3	1:B:172:ILE:HG12	0.66	1.66	3	1
1:B:113:CYS:SG	1:B:114:GLY:N	0.66	2.69	14	6
1:A:42:LEU:HD13	1:A:43:ARG:N	0.66	2.05	19	3
1:A:37:GLY:HA3	1:B:172:ILE:CG2	0.66	2.21	11	6
1:A:21:CYS:C	1:A:22:PHE:CD1	0.66	2.69	7	1
1:A:39:ALA:CA	1:A:42:LEU:HD22	0.66	2.20	2	1
1:A:39:ALA:CB	1:A:42:LEU:HD22	0.66	2.20	2	1
1:A:13:CYS:O	1:A:17:GLY:HA2	0.66	1.89	12	10
1:B:142:LEU:HD13	1:B:143:ARG:N	0.66	2.05	19	3
1:B:114:GLY:CA	1:B:140:GLU:HB3	0.66	2.17	3	1
1:B:121:CYS:C	1:B:122:PHE:CD1	0.66	2.69	7	1
1:B:166:ARG:N	1:B:166:ARG:HD2	0.66	2.05	13	2
1:A:27:CYS:HB2	1:A:41:ALA:HA	0.66	1.68	13	1
1:A:71:GLY:O	1:A:81:GLU:HA	0.66	1.91	13	3
1:B:171:GLY:O	1:B:181:GLU:HA	0.66	1.91	7	4
1:A:25:SER:O	1:A:37:GLY:N	0.65	2.29	17	17
1:B:125:SER:O	1:B:137:GLY:N	0.65	2.28	5	17
1:B:161:CYS:N	1:B:165:GLY:O	0.65	2.29	7	8
1:A:38:THR:HA	1:B:132:LEU:O	0.65	1.91	4	2
1:B:128:CYS:HB3	1:B:168:ALA:CB	0.65	2.20	7	1
1:B:111:LEU:O	1:B:120:ARG:HG3	0.65	1.92	4	4
1:B:132:LEU:HD22	1:B:135:PHE:CE2	0.65	2.27	21	3
1:A:26:ILE:HG23	1:A:36:VAL:HA	0.65	1.67	6	4
1:A:65:GLY:CA	1:A:74:CYS:HA	0.65	2.19	20	2
1:A:59:LYS:HB3	1:A:60:PRO:HD3	0.65	1.69	10	2
1:A:61:CYS:N	1:A:65:GLY:O	0.65	2.30	7	9
1:A:28:CYS:SG	1:A:33:GLY:O	0.65	2.54	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:PHE:CE2	1:B:135:PHE:CE2	0.65	2.85	5	4
1:B:174:CYS:CB	1:B:179:CYS:CA	0.65	2.62	10	1
1:A:13:CYS:SG	1:A:20:ARG:O	0.65	2.55	5	1
1:A:72:ILE:N	1:A:72:ILE:HD13	0.65	2.07	6	2
1:B:113:CYS:SG	1:B:120:ARG:O	0.65	2.55	5	1
1:A:66:ARG:HD3	1:A:66:ARG:O	0.65	1.92	18	1
1:A:59:LYS:N	1:A:60:PRO:CD	0.64	2.60	2	9
1:B:126:ILE:HG23	1:B:136:VAL:HG13	0.64	1.68	3	5
1:A:70:ALA:O	1:A:72:ILE:N	0.64	2.29	21	3
1:A:32:LEU:O	1:B:138:THR:HA	0.64	1.93	4	2
1:A:32:LEU:HD22	1:A:35:PHE:CE2	0.64	2.27	21	3
1:A:59:LYS:HA	1:A:66:ARG:CB	0.64	2.20	13	1
1:B:127:CYS:HB2	1:B:141:ALA:CB	0.64	2.22	8	1
1:A:32:LEU:HD23	1:A:35:PHE:CZ	0.64	2.28	14	1
1:B:141:ALA:O	1:B:144:CYS:CB	0.64	2.45	19	8
1:A:30:ASP:O	1:A:70:ALA:HB3	0.64	1.92	10	2
1:A:13:CYS:SG	1:A:14:GLY:N	0.64	2.70	14	6
1:B:136:VAL:HG11	1:B:178:GLY:CA	0.64	2.23	7	1
1:B:127:CYS:HB2	1:B:141:ALA:HA	0.64	1.70	13	1
1:B:135:PHE:CD1	1:B:135:PHE:N	0.63	2.64	7	5
1:A:71:GLY:HA2	1:A:82:ASP:O	0.63	1.92	18	7
1:A:41:ALA:O	1:A:44:CYS:CB	0.63	2.45	19	8
1:B:132:LEU:HD22	1:B:135:PHE:HZ	0.63	1.52	16	2
1:A:59:LYS:O	1:A:66:ARG:HB3	0.63	1.93	13	1
1:A:14:GLY:CA	1:A:40:GLU:HB3	0.63	2.18	3	1
1:A:40:GLU:O	1:A:43:ARG:HG2	0.63	1.93	4	1
1:B:130:ASP:O	1:B:170:ALA:HB3	0.63	1.93	10	1
1:A:26:ILE:CG2	1:A:36:VAL:HG13	0.63	2.23	10	9
1:A:59:LYS:H	1:A:60:PRO:HD2	0.63	1.52	13	2
1:A:15:PRO:O	1:A:18:LYS:HD3	0.63	1.94	7	2
1:B:111:LEU:HD23	1:B:121:CYS:CB	0.63	2.24	9	1
1:B:166:ARG:O	1:B:166:ARG:HD3	0.63	1.92	18	1
1:B:144:CYS:O	1:B:147:GLU:N	0.63	2.25	10	2
1:B:140:GLU:O	1:B:143:ARG:HG2	0.63	1.92	4	1
1:B:169:ALA:CB	1:B:172:ILE:HG12	0.63	2.21	15	2
1:B:156:SER:OG	1:B:159:LYS:HG3	0.63	1.93	9	1
1:A:69:ALA:CB	1:A:72:ILE:HG12	0.63	2.22	15	1
1:A:59:LYS:HB3	1:A:67:CYS:CB	0.63	2.22	4	1
1:A:72:ILE:HD13	1:A:72:ILE:N	0.63	2.09	8	2
1:A:35:PHE:CD1	1:A:35:PHE:N	0.62	2.64	7	7
1:B:170:ALA:HA	1:B:185:CYS:CB	0.62	2.17	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:THR:CG2	1:B:135:PHE:HD1	0.62	2.07	4	3
1:A:61:CYS:SG	1:A:84:ALA:HB3	0.62	2.34	13	1
1:B:126:ILE:HG23	1:B:134:CYS:SG	0.62	2.34	4	1
1:B:132:LEU:HD23	1:B:135:PHE:CE2	0.62	2.29	14	1
1:A:19:GLY:HA3	1:A:28:CYS:O	0.62	1.94	19	1
1:B:129:GLY:N	1:B:133:GLY:O	0.62	2.31	15	7
1:A:28:CYS:HB3	1:A:68:ALA:CB	0.62	2.23	7	1
1:A:32:LEU:HD22	1:A:35:PHE:HZ	0.62	1.54	16	3
1:B:159:LYS:CA	1:B:167:CYS:H	0.62	2.08	3	2
1:A:36:VAL:HG23	1:B:136:VAL:CG2	0.62	2.25	2	13
1:A:11:LEU:HD23	1:A:21:CYS:CB	0.62	2.24	9	1
1:B:159:LYS:CB	1:B:160:PRO:CD	0.62	2.77	10	3
1:B:113:CYS:HB2	1:B:143:ARG:HB3	0.62	1.71	13	1
1:A:36:VAL:HG11	1:A:78:GLY:CA	0.62	2.18	7	1
1:A:32:LEU:HD23	1:A:35:PHE:CE2	0.62	2.30	14	1
1:B:170:ALA:O	1:B:172:ILE:N	0.62	2.29	21	3
1:B:114:GLY:HA2	1:B:140:GLU:CB	0.62	2.24	16	2
1:A:59:LYS:HB3	1:A:67:CYS:HB2	0.61	1.71	21	2
1:B:115:PRO:CD	1:B:132:LEU:HD11	0.61	2.24	10	1
1:B:173:CYS:N	1:B:180:HIS:O	0.61	2.29	1	1
1:A:60:PRO:HA	1:A:65:GLY:O	0.61	1.95	11	5
1:B:126:ILE:HG23	1:B:136:VAL:HA	0.61	1.73	6	4
1:B:172:ILE:N	1:B:172:ILE:HD13	0.61	2.08	6	1
1:B:143:ARG:HD3	1:B:143:ARG:O	0.61	1.95	9	1
1:B:132:LEU:HD23	1:B:135:PHE:CZ	0.61	2.31	14	1
1:A:14:GLY:HA2	1:A:40:GLU:CB	0.61	2.25	16	2
1:B:132:LEU:HD23	1:B:135:PHE:CE1	0.61	2.30	11	1
1:B:128:CYS:CB	1:B:168:ALA:HB1	0.61	2.25	13	2
1:B:165:GLY:CA	1:B:175:SER:HA	0.61	2.26	9	3
1:B:173:CYS:HB2	1:B:180:HIS:O	0.61	1.96	4	1
1:B:128:CYS:HB2	1:B:168:ALA:HB1	0.61	1.73	13	3
1:B:126:ILE:HD12	1:B:176:PRO:HA	0.61	1.73	20	1
1:A:15:PRO:CD	1:A:32:LEU:HD11	0.61	2.23	10	1
1:A:44:CYS:O	1:A:47:GLU:N	0.61	2.25	10	2
1:A:35:PHE:CE1	1:B:138:THR:HG21	0.61	2.31	21	2
1:A:35:PHE:HD1	1:B:138:THR:CG2	0.60	2.09	4	3
1:A:59:LYS:C	1:A:66:ARG:HA	0.60	2.17	12	3
1:A:38:THR:HG21	1:B:135:PHE:CE2	0.60	2.30	15	2
1:B:139:ALA:HA	1:B:142:LEU:HD22	0.60	1.73	2	1
1:A:37:GLY:CA	1:B:172:ILE:HG21	0.60	2.27	5	2
1:A:32:LEU:HD23	1:A:35:PHE:CE1	0.60	2.30	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LYS:HB2	1:A:60:PRO:CD	0.60	2.26	12	2
1:B:115:PRO:HG2	1:B:132:LEU:HD11	0.60	1.72	4	1
1:A:32:LEU:HD13	1:A:35:PHE:HZ	0.60	1.56	7	1
1:B:128:CYS:CB	1:B:133:GLY:O	0.60	2.50	6	8
1:A:20:ARG:O	1:A:27:CYS:HA	0.60	1.97	4	1
1:A:35:PHE:CE2	1:B:138:THR:HG21	0.60	2.31	15	2
1:A:10:CYS:HB3	1:A:20:ARG:HB3	0.60	1.71	20	2
1:B:125:SER:O	1:B:126:ILE:HG13	0.60	1.96	4	3
1:A:65:GLY:CA	1:A:75:SER:HA	0.60	2.27	9	4
1:B:132:LEU:HD13	1:B:135:PHE:HZ	0.60	1.55	7	1
1:A:74:CYS:HB3	1:A:78:GLY:O	0.60	1.97	9	4
1:A:28:CYS:HB2	1:A:69:ALA:CB	0.60	2.26	10	1
1:A:77:ASP:HB3	1:B:180:HIS:CE1	0.60	2.31	12	1
1:B:161:CYS:SG	1:B:184:ALA:HB3	0.60	2.36	13	1
1:B:171:GLY:CA	1:B:185:CYS:O	0.60	2.50	6	6
1:A:13:CYS:C	1:A:17:GLY:HA2	0.60	2.17	12	5
1:B:120:ARG:O	1:B:127:CYS:HA	0.60	1.97	4	1
1:B:137:GLY:O	1:B:138:THR:O	0.60	2.20	6	1
1:A:28:CYS:HB2	1:A:68:ALA:HB1	0.60	1.74	13	3
1:A:36:VAL:CG2	1:B:136:VAL:HG23	0.59	2.27	3	11
1:B:159:LYS:HB2	1:B:167:CYS:CB	0.59	2.26	17	5
1:B:113:CYS:C	1:B:117:GLY:HA2	0.59	2.18	12	4
1:B:173:CYS:O	1:B:180:HIS:HB2	0.59	1.98	10	1
1:A:39:ALA:HB1	1:A:42:LEU:HD22	0.59	1.74	2	1
1:B:182:ASP:OD1	1:B:185:CYS:HB2	0.59	1.96	7	1
1:B:174:CYS:HB3	1:B:178:GLY:O	0.59	1.97	9	4
1:A:71:GLY:CA	1:A:85:CYS:O	0.59	2.51	17	6
1:B:111:LEU:H	1:B:111:LEU:HD22	0.59	1.58	3	1
1:A:15:PRO:HG2	1:A:32:LEU:HD11	0.59	1.72	4	1
1:A:72:ILE:HG22	1:A:74:CYS:SG	0.59	2.37	20	2
1:A:13:CYS:HB2	1:A:43:ARG:HB3	0.59	1.73	13	1
1:A:37:GLY:O	1:A:38:THR:O	0.59	2.21	6	2
1:A:82:ASP:OD1	1:A:85:CYS:HB2	0.59	1.96	7	2
1:A:73:CYS:O	1:A:80:HIS:HB2	0.59	1.98	10	1
1:B:168:ALA:HB3	1:B:172:ILE:HB	0.59	1.75	10	1
1:A:25:SER:O	1:A:26:ILE:HG13	0.59	1.97	4	3
1:A:83:PRO:HA	1:A:86:ASP:OD2	0.59	1.96	4	1
1:B:127:CYS:SG	1:B:135:PHE:CE2	0.59	2.96	7	1
1:B:172:ILE:HG22	1:B:174:CYS:SG	0.59	2.38	20	3
1:B:172:ILE:O	1:B:172:ILE:HD12	0.58	1.97	13	4
1:B:159:LYS:C	1:B:166:ARG:HA	0.58	2.19	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:CYS:HB2	1:A:80:HIS:O	0.58	1.98	4	1
1:A:72:ILE:HG22	1:B:137:GLY:HA3	0.58	1.75	14	1
1:B:119:GLY:HA3	1:B:128:CYS:O	0.58	1.96	19	1
1:B:183:PRO:HA	1:B:186:ASP:OD2	0.58	1.96	4	1
1:A:59:LYS:HG3	1:A:60:PRO:HD3	0.58	1.74	13	1
1:A:75:SER:HB3	1:A:76:PRO:CD	0.58	2.28	9	3
1:A:29:GLY:N	1:A:33:GLY:O	0.58	2.35	15	9
1:A:39:ALA:HA	1:A:42:LEU:HD22	0.58	1.75	2	1
1:A:72:ILE:HG21	1:B:137:GLY:CA	0.58	2.27	5	2
1:A:27:CYS:O	1:A:35:PHE:N	0.58	2.35	17	6
1:B:175:SER:HB3	1:B:176:PRO:CD	0.58	2.28	9	4
1:A:27:CYS:SG	1:A:35:PHE:CE2	0.58	2.96	7	1
1:B:170:ALA:C	1:B:185:CYS:HB3	0.58	2.19	21	1
1:A:20:ARG:O	1:A:27:CYS:SG	0.58	2.61	1	3
1:A:28:CYS:CB	1:A:33:GLY:O	0.58	2.52	6	8
1:B:126:ILE:CG2	1:B:136:VAL:HG13	0.58	2.27	10	5
1:B:159:LYS:HB2	1:B:160:PRO:CD	0.58	2.28	12	2
1:A:26:ILE:HG23	1:A:34:CYS:SG	0.58	2.38	4	1
1:B:128:CYS:SG	1:B:172:ILE:HD13	0.58	2.39	7	1
1:A:38:THR:HG21	1:B:135:PHE:CE1	0.58	2.34	21	3
1:A:38:THR:HG23	1:A:40:GLU:OE1	0.58	1.99	21	1
1:A:35:PHE:CD2	1:B:135:PHE:CD2	0.58	2.91	6	2
1:B:160:PRO:HA	1:B:165:GLY:O	0.58	1.99	15	5
1:B:115:PRO:O	1:B:118:LYS:HD3	0.58	1.98	17	2
1:B:115:PRO:HG2	1:B:118:LYS:CD	0.57	2.29	12	1
1:A:70:ALA:C	1:A:85:CYS:HB3	0.57	2.18	21	1
1:A:27:CYS:SG	1:A:41:ALA:HA	0.57	2.39	3	1
1:A:35:PHE:CD2	1:B:135:PHE:CE2	0.57	2.93	6	1
1:A:69:ALA:O	1:A:71:GLY:N	0.57	2.38	10	3
1:B:133:GLY:O	1:B:169:ALA:HB3	0.57	1.99	10	1
1:A:57:GLY:HA3	1:A:67:CYS:O	0.57	2.00	14	1
1:A:71:GLY:O	1:A:72:ILE:HD13	0.57	1.99	8	1
1:A:15:PRO:O	1:A:18:LYS:HD2	0.57	1.99	12	1
1:B:127:CYS:HB3	1:B:135:PHE:CD2	0.57	2.35	20	3
1:A:73:CYS:N	1:A:80:HIS:O	0.57	2.30	1	1
1:B:139:ALA:HB1	1:B:142:LEU:HD22	0.57	1.76	2	1
1:B:175:SER:HB2	1:B:176:PRO:CD	0.57	2.28	4	13
1:A:70:ALA:HA	1:A:85:CYS:CB	0.57	2.20	3	2
1:A:26:ILE:HD11	1:A:78:GLY:HA2	0.57	1.75	4	1
1:B:128:CYS:HB2	1:B:169:ALA:CB	0.57	2.27	10	1
1:B:127:CYS:SG	1:B:141:ALA:HA	0.57	2.39	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:169:ALA:O	1:B:171:GLY:N	0.57	2.38	10	4
1:A:26:ILE:CG2	1:A:36:VAL:HG22	0.57	2.29	10	3
1:A:69:ALA:O	1:A:72:ILE:N	0.57	2.32	20	3
1:A:75:SER:HB2	1:A:76:PRO:CD	0.57	2.30	18	14
1:B:110:CYS:O	1:B:111:LEU:C	0.57	2.43	7	8
1:A:11:LEU:HD12	1:A:43:ARG:CZ	0.57	2.30	18	1
1:B:135:PHE:CD2	1:B:140:GLU:HB3	0.56	2.34	2	1
1:A:28:CYS:CB	1:A:68:ALA:CB	0.56	2.83	7	1
1:A:35:PHE:CD2	1:A:40:GLU:HB3	0.56	2.35	2	1
1:A:11:LEU:HD22	1:A:11:LEU:H	0.56	1.59	3	1
1:A:32:LEU:HD22	1:A:35:PHE:HE1	0.56	1.59	3	3
1:A:80:HIS:CE1	1:B:177:ASP:HB3	0.56	2.35	12	1
1:B:111:LEU:HD12	1:B:143:ARG:CZ	0.56	2.29	18	1
1:A:72:ILE:HD12	1:A:72:ILE:O	0.56	1.99	13	3
1:B:126:ILE:CG2	1:B:136:VAL:HG22	0.56	2.30	10	3
1:A:65:GLY:HA2	1:A:75:SER:HA	0.56	1.76	9	3
1:A:68:ALA:HB3	1:A:72:ILE:HB	0.56	1.76	10	1
1:A:33:GLY:O	1:A:69:ALA:HB3	0.56	2.00	10	1
1:A:61:CYS:O	1:A:62:GLY:O	0.56	2.24	13	2
1:A:27:CYS:HB3	1:A:35:PHE:CD2	0.56	2.34	20	3
1:A:26:ILE:HD12	1:A:76:PRO:HA	0.56	1.75	20	1
1:B:127:CYS:O	1:B:135:PHE:N	0.56	2.37	17	6
1:B:128:CYS:CB	1:B:168:ALA:CB	0.56	2.83	7	1
1:B:166:ARG:HD2	1:B:166:ARG:H	0.56	1.60	18	2
1:B:141:ALA:O	1:B:144:CYS:HB3	0.56	2.00	2	1
1:A:59:LYS:CB	1:A:60:PRO:CD	0.56	2.83	10	3
1:B:120:ARG:O	1:B:127:CYS:SG	0.56	2.63	1	3
1:B:171:GLY:H	1:B:185:CYS:CB	0.56	2.13	9	5
1:B:139:ALA:O	1:B:142:LEU:HD23	0.56	2.00	2	1
1:B:170:ALA:C	1:B:186:ASP:HA	0.56	2.20	10	1
1:B:174:CYS:CA	1:B:179:CYS:HA	0.56	2.27	11	1
1:A:18:LYS:CD	1:A:32:LEU:HD11	0.56	2.26	12	1
1:A:28:CYS:CB	1:A:69:ALA:HB2	0.56	2.31	20	2
1:A:12:PRO:CA	1:A:19:GLY:O	0.56	2.54	20	3
1:A:24:PRO:HD2	1:B:181:GLU:OE2	0.56	2.01	11	2
1:B:126:ILE:HD11	1:B:178:GLY:HA2	0.56	1.77	4	1
1:A:10:CYS:O	1:A:11:LEU:C	0.56	2.43	7	8
1:A:22:PHE:N	1:A:22:PHE:CD1	0.56	2.74	14	1
1:A:15:PRO:HG2	1:A:18:LYS:CD	0.56	2.31	12	1
1:A:37:GLY:O	1:B:132:LEU:O	0.56	2.23	20	1
1:A:66:ARG:HD2	1:A:66:ARG:H	0.55	1.60	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LEU:O	1:B:137:GLY:O	0.55	2.23	20	1
1:A:43:ARG:O	1:A:43:ARG:HD3	0.55	2.01	9	1
1:A:70:ALA:C	1:A:86:ASP:HA	0.55	2.20	10	1
1:B:110:CYS:HB3	1:B:120:ARG:HB3	0.55	1.78	20	2
1:B:159:LYS:HB2	1:B:167:CYS:HB3	0.55	1.77	17	2
1:B:172:ILE:H	1:B:172:ILE:HD12	0.55	1.61	7	1
1:A:20:ARG:O	1:A:28:CYS:O	0.55	2.25	20	1
1:A:39:ALA:O	1:A:42:LEU:HD23	0.55	2.02	2	1
1:A:71:GLY:HA2	1:A:85:CYS:O	0.55	2.01	17	4
1:B:126:ILE:CG2	1:B:134:CYS:SG	0.55	2.95	6	4
1:B:165:GLY:HA3	1:B:175:SER:HA	0.55	1.79	3	3
1:A:82:ASP:OD1	1:A:84:ALA:HB3	0.55	2.01	9	2
1:A:57:GLY:O	1:A:66:ARG:HG3	0.55	2.02	11	2
1:B:122:PHE:CE1	1:B:128:CYS:HB2	0.55	2.37	14	1
1:B:124:PRO:HD2	1:B:126:ILE:HD12	0.55	1.79	7	1
1:B:115:PRO:O	1:B:118:LYS:HD2	0.55	2.02	12	1
1:A:37:GLY:HA3	1:B:172:ILE:HG22	0.55	1.77	14	1
1:B:172:ILE:HG13	1:B:172:ILE:O	0.55	2.02	14	1
1:A:72:ILE:H	1:A:72:ILE:HD12	0.54	1.63	7	1
1:A:29:GLY:O	1:A:69:ALA:HB2	0.54	2.02	15	5
1:B:158:GLN:O	1:B:167:CYS:O	0.54	2.25	13	1
1:B:118:LYS:CD	1:B:132:LEU:HD11	0.54	2.29	12	1
1:B:121:CYS:CB	1:B:147:GLU:HG3	0.54	2.28	18	1
1:B:182:ASP:OD1	1:B:184:ALA:HB3	0.54	2.02	9	1
1:B:127:CYS:O	1:B:135:PHE:CD1	0.54	2.60	17	2
1:B:171:GLY:HA2	1:B:185:CYS:O	0.54	2.03	7	5
1:A:35:PHE:CD2	1:A:40:GLU:HB2	0.54	2.38	18	3
1:A:10:CYS:CB	1:A:20:ARG:HD2	0.54	2.33	11	1
1:A:81:GLU:HG3	1:B:126:ILE:HD11	0.54	1.77	11	1
1:A:32:LEU:HD22	1:A:35:PHE:HE2	0.54	1.62	21	1
1:A:28:CYS:SG	1:A:72:ILE:HD13	0.54	2.43	7	1
1:A:72:ILE:HG21	1:B:136:VAL:O	0.54	2.01	17	3
1:A:81:GLU:OE2	1:B:124:PRO:HD2	0.54	2.02	11	1
1:A:36:VAL:O	1:B:172:ILE:HG12	0.54	2.03	7	2
1:A:10:CYS:CB	1:A:20:ARG:HG2	0.54	2.33	6	2
1:A:74:CYS:CA	1:A:79:CYS:HA	0.54	2.27	11	1
1:A:72:ILE:CG1	1:A:72:ILE:O	0.54	2.56	14	1
1:B:122:PHE:N	1:B:122:PHE:CD1	0.54	2.74	14	1
1:B:115:PRO:CG	1:B:132:LEU:HD21	0.54	2.33	20	1
1:B:135:PHE:CD2	1:B:140:GLU:HB2	0.54	2.38	18	3
1:A:79:CYS:N	1:B:179:CYS:O	0.54	2.41	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:172:ILE:HD12	1:B:172:ILE:O	0.53	2.04	9	1
1:B:159:LYS:C	1:B:166:ARG:HB3	0.53	2.24	13	2
1:B:175:SER:N	1:B:178:GLY:O	0.53	2.41	15	1
1:B:125:SER:O	1:B:136:VAL:HA	0.53	2.03	4	1
1:A:38:THR:HB	1:B:132:LEU:O	0.53	2.02	13	3
1:B:157:GLY:O	1:B:166:ARG:HG3	0.53	2.03	11	2
1:A:70:ALA:HB1	1:A:86:ASP:O	0.53	2.03	10	2
1:B:110:CYS:CB	1:B:120:ARG:HD2	0.53	2.34	11	1
1:B:166:ARG:N	1:B:166:ARG:CD	0.53	2.70	13	1
1:B:159:LYS:H	1:B:160:PRO:HD2	0.53	1.64	13	2
1:A:25:SER:O	1:A:36:VAL:HA	0.53	2.03	4	1
1:A:66:ARG:CD	1:A:66:ARG:N	0.53	2.70	13	1
1:A:75:SER:N	1:A:78:GLY:O	0.53	2.41	15	1
1:A:15:PRO:O	1:A:15:PRO:HG2	0.53	2.02	9	5
1:B:139:ALA:HA	1:B:142:LEU:HB3	0.53	1.80	2	1
1:B:171:GLY:O	1:B:182:ASP:N	0.53	2.42	6	1
1:B:112:PRO:CA	1:B:119:GLY:O	0.53	2.54	7	4
1:A:59:LYS:H	1:A:60:PRO:CD	0.53	2.17	13	1
1:B:130:ASP:OD2	1:B:131:GLU:HG2	0.53	2.04	18	2
1:A:59:LYS:HA	1:A:67:CYS:HB2	0.53	1.79	3	1
1:B:111:LEU:CD2	1:B:147:GLU:HG3	0.53	2.32	4	1
1:A:13:CYS:SG	1:A:40:GLU:O	0.53	2.66	13	1
1:B:129:GLY:HA3	1:B:132:LEU:HB2	0.53	1.80	14	1
1:B:138:THR:HG23	1:B:140:GLU:OE1	0.53	2.02	21	1
1:B:113:CYS:SG	1:B:140:GLU:O	0.53	2.66	13	1
1:A:77:ASP:HB2	1:B:180:HIS:CE1	0.53	2.39	18	1
1:A:74:CYS:HA	1:A:78:GLY:O	0.53	2.04	13	3
1:B:174:CYS:HA	1:B:178:GLY:O	0.53	2.04	13	3
1:A:15:PRO:C	1:A:17:GLY:H	0.52	2.06	4	1
1:A:71:GLY:O	1:A:82:ASP:N	0.52	2.42	6	1
1:A:72:ILE:HD12	1:B:136:VAL:O	0.52	2.03	8	1
1:A:34:CYS:SG	1:A:72:ILE:HG21	0.52	2.44	10	1
1:A:38:THR:O	1:A:40:GLU:N	0.52	2.42	15	1
1:A:26:ILE:CG2	1:A:34:CYS:SG	0.52	2.96	6	4
1:A:24:PRO:HD2	1:A:26:ILE:HD12	0.52	1.79	7	1
1:B:123:GLY:O	1:B:144:CYS:SG	0.52	2.67	7	1
1:B:143:ARG:CZ	1:B:143:ARG:HB2	0.52	2.34	8	1
1:B:172:ILE:CG1	1:B:172:ILE:O	0.52	2.58	14	1
1:B:138:THR:O	1:B:140:GLU:N	0.52	2.42	15	1
1:A:27:CYS:O	1:A:35:PHE:CD1	0.52	2.62	17	2
1:A:44:CYS:O	1:A:47:GLU:HG2	0.52	2.04	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:132:LEU:HD22	1:B:135:PHE:HE2	0.52	1.62	21	1
1:A:11:LEU:CD2	1:A:47:GLU:HG3	0.52	2.32	4	1
1:A:74:CYS:CB	1:A:79:CYS:CA	0.52	2.62	10	1
1:A:35:PHE:HB3	1:A:38:THR:OG1	0.52	2.04	12	2
1:A:30:ASP:OD2	1:A:31:GLU:HG2	0.52	2.03	18	2
1:B:159:LYS:CB	1:B:167:CYS:CB	0.52	2.88	2	1
1:A:65:GLY:HA3	1:A:75:SER:HA	0.52	1.81	3	2
1:A:10:CYS:HB3	1:A:20:ARG:HD3	0.52	1.82	3	1
1:A:22:PHE:CE1	1:A:28:CYS:HB2	0.52	2.38	14	2
1:B:127:CYS:HB2	1:B:144:CYS:SG	0.52	2.44	5	1
1:A:39:ALA:O	1:A:42:LEU:N	0.52	2.41	6	1
1:A:26:ILE:HD13	1:A:75:SER:O	0.52	2.03	7	1
1:A:43:ARG:CZ	1:A:43:ARG:HB2	0.52	2.34	8	1
1:A:71:GLY:HA3	1:A:86:ASP:OD1	0.52	2.03	21	1
1:A:71:GLY:H	1:A:85:CYS:CB	0.52	2.16	9	6
1:A:23:GLY:O	1:A:44:CYS:SG	0.52	2.68	7	1
1:B:157:GLY:HA3	1:B:167:CYS:O	0.52	2.05	14	1
1:B:128:CYS:HB2	1:B:168:ALA:CB	0.52	2.35	15	1
1:B:132:LEU:HD22	1:B:135:PHE:HE1	0.52	1.58	3	4
1:A:32:LEU:O	1:A:33:GLY:C	0.52	2.48	15	1
1:B:129:GLY:O	1:B:169:ALA:CB	0.52	2.57	19	6
1:A:27:CYS:HB2	1:A:44:CYS:SG	0.52	2.45	5	1
1:A:29:GLY:O	1:A:69:ALA:CB	0.52	2.58	19	7
1:B:115:PRO:C	1:B:117:GLY:H	0.52	2.06	4	2
1:A:35:PHE:CE2	1:B:135:PHE:CD2	0.52	2.98	6	1
1:B:168:ALA:HB3	1:B:174:CYS:SG	0.52	2.44	9	1
1:B:165:GLY:HA2	1:B:175:SER:HA	0.52	1.82	9	3
1:B:121:CYS:HB2	1:B:147:GLU:HG2	0.51	1.82	5	1
1:A:39:ALA:HA	1:A:42:LEU:HB3	0.51	1.82	2	1
1:A:72:ILE:HG12	1:B:136:VAL:O	0.51	2.05	3	2
1:A:39:ALA:HA	1:A:42:LEU:CD1	0.51	2.35	9	1
1:B:170:ALA:HB1	1:B:186:ASP:O	0.51	2.03	10	2
1:A:21:CYS:O	1:A:22:PHE:CD1	0.51	2.63	7	1
1:B:110:CYS:CB	1:B:120:ARG:HG2	0.51	2.34	6	2
1:B:144:CYS:O	1:B:147:GLU:HG2	0.51	2.05	21	1
1:B:115:PRO:O	1:B:117:GLY:N	0.51	2.44	2	2
1:A:21:CYS:HB2	1:A:47:GLU:HG2	0.51	1.82	5	1
1:A:61:CYS:O	1:A:73:CYS:SG	0.51	2.69	10	1
1:B:110:CYS:HB3	1:B:120:ARG:CD	0.51	2.35	11	2
1:A:18:LYS:HZ1	1:A:32:LEU:CD1	0.51	2.19	17	1
1:B:159:LYS:HB3	1:B:167:CYS:H	0.51	1.65	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:134:CYS:SG	1:B:172:ILE:HG21	0.51	2.45	10	1
1:A:36:VAL:CG2	1:B:136:VAL:HB	0.51	2.36	5	2
1:A:77:ASP:O	1:B:181:GLU:HG3	0.51	2.06	9	1
1:B:135:PHE:HB3	1:B:138:THR:OG1	0.51	2.04	12	2
1:A:28:CYS:SG	1:A:72:ILE:CD1	0.51	2.99	21	1
1:B:121:CYS:O	1:B:122:PHE:CD1	0.51	2.63	7	1
1:A:15:PRO:HG2	1:A:15:PRO:O	0.51	2.06	12	1
1:B:161:CYS:O	1:B:162:GLY:O	0.51	2.28	13	2
1:B:127:CYS:HB3	1:B:135:PHE:CD1	0.51	2.41	17	2
1:A:10:CYS:HB3	1:A:20:ARG:CD	0.51	2.35	11	2
1:B:170:ALA:O	1:B:185:CYS:HB2	0.51	2.05	14	2
1:B:111:LEU:HD22	1:B:111:LEU:H	0.51	1.66	16	1
1:A:13:CYS:O	1:A:17:GLY:CA	0.50	2.59	19	2
1:A:43:ARG:C	1:A:45:GLN:H	0.50	2.10	3	2
1:A:33:GLY:HA2	1:A:69:ALA:HB2	0.50	1.83	15	2
1:B:132:LEU:CD2	1:B:135:PHE:CZ	0.50	2.94	12	2
1:A:65:GLY:N	1:A:75:SER:HB3	0.50	2.22	7	1
1:B:170:ALA:C	1:B:172:ILE:H	0.50	2.10	21	2
1:A:80:HIS:CE1	1:B:177:ASP:HB2	0.50	2.41	18	1
1:B:159:LYS:CB	1:B:167:CYS:HB3	0.50	2.27	4	2
1:A:61:CYS:SG	1:A:84:ALA:HB2	0.50	2.46	5	1
1:A:32:LEU:CD2	1:A:35:PHE:CZ	0.50	2.95	6	2
1:A:36:VAL:O	1:B:172:ILE:HG21	0.50	2.06	17	2
1:B:132:LEU:HD22	1:B:140:GLU:OE2	0.50	2.06	10	1
1:B:128:CYS:SG	1:B:172:ILE:CD1	0.50	2.99	21	1
1:B:129:GLY:O	1:B:169:ALA:HB2	0.50	2.06	15	4
1:A:58:GLN:HB3	1:A:67:CYS:O	0.50	2.05	13	1
1:A:42:LEU:O	1:A:45:GLN:HB2	0.50	2.07	14	1
1:B:128:CYS:SG	1:B:168:ALA:HB3	0.50	2.46	21	3
1:A:28:CYS:SG	1:A:68:ALA:HB3	0.50	2.46	21	2
1:A:13:CYS:HA	1:A:43:ARG:NE	0.50	2.19	12	1
1:A:36:VAL:O	1:B:172:ILE:HD13	0.50	2.06	2	1
1:A:35:PHE:HB3	1:A:38:THR:HG21	0.50	1.83	5	1
1:B:110:CYS:O	1:B:111:LEU:O	0.50	2.30	10	2
1:A:15:PRO:CG	1:A:32:LEU:HD21	0.50	2.37	20	1
1:B:135:PHE:HB3	1:B:138:THR:HG21	0.50	1.83	5	1
1:B:139:ALA:O	1:B:142:LEU:N	0.50	2.41	6	1
1:A:70:ALA:CA	1:A:85:CYS:O	0.50	2.59	11	3
1:B:170:ALA:CA	1:B:185:CYS:O	0.50	2.60	11	2
1:A:35:PHE:HD1	1:B:135:PHE:CD1	0.50	2.19	21	1
1:B:110:CYS:HB3	1:B:120:ARG:HD3	0.50	1.83	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:113:CYS:O	1:B:117:GLY:CA	0.50	2.60	19	3
1:B:115:PRO:HD2	1:B:132:LEU:HD21	0.50	1.82	14	1
1:A:38:THR:HG21	1:B:135:PHE:HD1	0.50	1.67	4	2
1:B:115:PRO:O	1:B:118:LYS:HG3	0.50	2.07	8	1
1:A:66:ARG:O	1:A:74:CYS:N	0.50	2.39	10	2
1:A:72:ILE:O	1:A:72:ILE:HD12	0.49	2.06	9	3
1:B:113:CYS:HA	1:B:143:ARG:NE	0.49	2.16	12	1
1:B:139:ALA:O	1:B:141:ALA:N	0.49	2.45	15	1
1:B:161:CYS:SG	1:B:184:ALA:HB2	0.49	2.47	5	1
1:A:59:LYS:C	1:A:66:ARG:HB3	0.49	2.28	13	2
1:B:156:SER:HA	1:B:159:LYS:HE3	0.49	1.83	13	1
1:A:27:CYS:HB3	1:A:35:PHE:CD1	0.49	2.41	17	2
1:B:168:ALA:HB3	1:B:172:ILE:CD1	0.49	2.36	3	1
1:A:61:CYS:O	1:A:65:GLY:O	0.49	2.30	14	3
1:A:68:ALA:HB3	1:A:74:CYS:SG	0.49	2.48	9	1
1:A:32:LEU:HD22	1:A:40:GLU:OE2	0.49	2.06	10	1
1:A:28:CYS:SG	1:A:72:ILE:HD11	0.49	2.47	14	3
1:A:11:LEU:H	1:A:11:LEU:HD22	0.49	1.67	16	1
1:A:36:VAL:O	1:B:172:ILE:HD12	0.49	2.06	8	1
1:B:139:ALA:HA	1:B:142:LEU:CD1	0.49	2.37	9	1
1:B:135:PHE:HB2	1:B:138:THR:OG1	0.49	2.08	3	3
1:B:161:CYS:O	1:B:173:CYS:SG	0.49	2.70	10	1
1:A:35:PHE:N	1:A:35:PHE:CD1	0.49	2.80	6	2
1:A:15:PRO:O	1:A:18:LYS:HG3	0.49	2.08	8	1
1:A:41:ALA:O	1:A:44:CYS:HB3	0.49	2.06	2	1
1:B:127:CYS:HB3	1:B:141:ALA:HB2	0.49	1.84	5	1
1:A:15:PRO:HD2	1:A:32:LEU:HD21	0.49	1.82	14	1
1:A:72:ILE:HD13	1:B:136:VAL:O	0.49	2.08	2	1
1:B:161:CYS:O	1:B:165:GLY:O	0.49	2.31	5	3
1:B:169:ALA:O	1:B:170:ALA:C	0.49	2.51	6	5
1:A:74:CYS:CB	1:A:78:GLY:O	0.49	2.57	8	2
1:A:35:PHE:HB2	1:A:38:THR:OG1	0.49	2.08	3	2
1:B:172:ILE:N	1:B:172:ILE:CD1	0.49	2.73	8	1
1:A:57:GLY:O	1:A:66:ARG:HB2	0.48	2.08	21	3
1:B:111:LEU:HD23	1:B:121:CYS:HB2	0.48	1.85	11	1
1:A:37:GLY:C	1:A:38:THR:HG22	0.48	2.28	21	2
1:A:14:GLY:HA2	1:A:40:GLU:OE1	0.48	2.08	4	1
1:B:169:ALA:O	1:B:172:ILE:N	0.48	2.30	6	3
1:A:14:GLY:HA2	1:A:40:GLU:HG3	0.48	1.85	8	1
1:A:56:SER:HA	1:A:59:LYS:HE3	0.48	1.84	13	1
1:B:157:GLY:O	1:B:166:ARG:HB2	0.48	2.08	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LYS:HB3	1:A:60:PRO:HD2	0.48	1.79	9	1
1:A:81:GLU:HG3	1:B:177:ASP:O	0.48	2.07	9	1
1:B:142:LEU:O	1:B:145:GLN:HB2	0.48	2.08	14	1
1:A:59:LYS:O	1:A:61:CYS:SG	0.48	2.71	7	1
1:A:82:ASP:O	1:A:86:ASP:HB2	0.48	2.09	17	1
1:A:70:ALA:O	1:A:72:ILE:HG23	0.48	2.08	15	1
1:B:118:LYS:HZ1	1:B:132:LEU:HD11	0.48	1.69	17	1
1:A:26:ILE:HA	1:A:36:VAL:HA	0.48	1.85	18	1
1:B:114:GLY:HA2	1:B:140:GLU:OE1	0.48	2.08	4	1
1:A:79:CYS:O	1:B:179:CYS:N	0.48	2.46	13	2
1:A:70:ALA:O	1:A:85:CYS:HB2	0.48	2.08	14	2
1:A:36:VAL:HG23	1:B:136:VAL:HB	0.48	1.83	21	2
1:B:126:ILE:HG23	1:B:136:VAL:CA	0.48	2.39	10	2
1:B:159:LYS:HA	1:B:166:ARG:CB	0.48	2.36	13	1
1:A:15:PRO:HD2	1:A:35:PHE:CZ	0.48	2.44	3	1
1:A:35:PHE:CD1	1:B:138:THR:HG21	0.48	2.44	11	2
1:A:26:ILE:HG23	1:A:36:VAL:CA	0.48	2.38	10	3
1:B:127:CYS:SG	1:B:135:PHE:HD2	0.48	2.32	21	1
1:B:135:PHE:N	1:B:135:PHE:CD1	0.48	2.82	18	2
1:A:75:SER:CB	1:A:76:PRO:HD2	0.48	2.39	6	3
1:B:115:PRO:O	1:B:115:PRO:HG2	0.48	2.09	3	2
1:A:36:VAL:HG23	1:B:136:VAL:CB	0.48	2.38	5	1
1:A:71:GLY:N	1:A:86:ASP:HA	0.48	2.23	11	1
1:B:159:LYS:HG3	1:B:160:PRO:HD3	0.48	1.85	13	1
1:A:27:CYS:SG	1:A:35:PHE:HD2	0.48	2.32	21	1
1:B:159:LYS:HB3	1:B:166:ARG:HB2	0.48	1.85	3	1
1:A:35:PHE:HD1	1:B:138:THR:HG21	0.48	1.68	4	2
1:A:43:ARG:NH1	1:A:43:ARG:HB2	0.48	2.24	8	1
1:B:159:LYS:HB3	1:B:160:PRO:HD2	0.48	1.78	9	1
1:A:11:LEU:HB3	1:A:43:ARG:NH2	0.48	2.24	18	1
1:B:126:ILE:HD13	1:B:175:SER:O	0.47	2.08	7	1
1:B:159:LYS:HD2	1:B:159:LYS:N	0.47	2.24	19	1
1:B:175:SER:CB	1:B:176:PRO:HD2	0.47	2.39	6	3
1:A:69:ALA:O	1:A:70:ALA:C	0.47	2.52	6	5
1:B:143:ARG:NH1	1:B:143:ARG:HB2	0.47	2.24	8	1
1:A:73:CYS:O	1:A:80:HIS:N	0.47	2.47	14	3
1:A:10:CYS:HB3	1:A:20:ARG:NE	0.47	2.24	4	1
1:A:14:GLY:HA3	1:A:40:GLU:OE2	0.47	2.09	11	1
1:A:12:PRO:CB	1:A:17:GLY:O	0.47	2.62	1	3
1:B:133:GLY:HA2	1:B:169:ALA:HB3	0.47	1.85	2	1
1:B:126:ILE:HA	1:B:136:VAL:HA	0.47	1.86	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:173:CYS:O	1:B:180:HIS:N	0.47	2.47	14	3
1:A:71:GLY:N	1:A:85:CYS:HB3	0.47	2.25	13	2
1:A:10:CYS:O	1:A:11:LEU:O	0.47	2.32	10	2
1:B:128:CYS:CB	1:B:169:ALA:HB2	0.47	2.38	20	2
1:A:11:LEU:HD23	1:A:21:CYS:HB2	0.47	1.85	11	1
1:B:182:ASP:O	1:B:186:ASP:HB2	0.47	2.09	17	1
1:A:69:ALA:CB	1:A:72:ILE:HD11	0.47	2.36	18	1
1:B:110:CYS:HB3	1:B:120:ARG:NE	0.47	2.24	4	1
1:A:34:CYS:HB2	1:A:72:ILE:CG1	0.47	2.18	10	1
1:A:59:LYS:HB2	1:A:60:PRO:HD3	0.47	1.86	12	1
1:B:128:CYS:SG	1:B:172:ILE:HD11	0.47	2.49	14	4
1:B:114:GLY:HA2	1:B:140:GLU:CG	0.47	2.40	16	1
1:A:72:ILE:HD12	1:A:72:ILE:C	0.47	2.29	19	1
1:A:36:VAL:HB	1:B:136:VAL:CG2	0.47	2.40	5	2
1:A:61:CYS:SG	1:A:65:GLY:O	0.47	2.72	10	1
1:B:158:GLN:HB3	1:B:167:CYS:O	0.47	2.09	13	1
1:A:59:LYS:HB2	1:A:67:CYS:CB	0.47	2.40	17	1
1:B:161:CYS:SG	1:B:162:GLY:N	0.47	2.87	2	2
1:B:133:GLY:HA2	1:B:169:ALA:HB2	0.47	1.86	15	2
1:A:32:LEU:O	1:B:138:THR:HB	0.47	2.10	20	2
1:B:113:CYS:HB3	1:B:120:ARG:N	0.47	2.24	16	1
1:A:81:GLU:CG	1:B:125:SER:HB2	0.47	2.40	16	1
1:B:114:GLY:HA3	1:B:140:GLU:OE2	0.46	2.10	11	1
1:B:128:CYS:HA	1:B:134:CYS:HA	0.46	1.87	17	1
1:B:111:LEU:HD12	1:B:111:LEU:H	0.46	1.69	7	1
1:A:34:CYS:SG	1:A:68:ALA:CB	0.46	3.03	13	1
1:A:42:LEU:C	1:A:42:LEU:HD13	0.46	2.30	8	1
1:B:142:LEU:C	1:B:142:LEU:HD13	0.46	2.29	8	2
1:A:11:LEU:H	1:A:11:LEU:HD12	0.46	1.71	7	1
1:B:112:PRO:CB	1:B:117:GLY:O	0.46	2.64	1	4
1:A:28:CYS:SG	1:A:33:GLY:C	0.46	2.94	7	1
1:A:35:PHE:HB3	1:B:135:PHE:HB3	0.46	1.87	7	1
1:A:78:GLY:HA2	1:B:179:CYS:O	0.46	2.10	10	1
1:B:135:PHE:CD1	1:B:140:GLU:OE1	0.46	2.69	2	1
1:A:39:ALA:CA	1:A:42:LEU:HD12	0.46	2.41	9	2
1:B:161:CYS:SG	1:B:165:GLY:O	0.46	2.74	10	1
1:B:171:GLY:N	1:B:186:ASP:HA	0.46	2.25	11	1
1:B:171:GLY:N	1:B:185:CYS:HB3	0.46	2.25	13	1
1:A:43:ARG:O	1:A:43:ARG:NE	0.46	2.49	18	1
1:A:42:LEU:HD13	1:A:42:LEU:C	0.46	2.31	15	1
1:B:111:LEU:HB3	1:B:143:ARG:NH2	0.46	2.26	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:165:GLY:O	1:B:173:CYS:SG	0.46	2.74	20	1
1:B:121:CYS:SG	1:B:123:GLY:O	0.46	2.74	2	1
1:A:81:GLU:CG	1:B:124:PRO:HD2	0.46	2.41	14	1
1:A:78:GLY:HA3	1:B:180:HIS:HB3	0.46	1.88	15	1
1:B:115:PRO:HD2	1:B:135:PHE:CZ	0.46	2.46	3	1
1:A:66:ARG:H	1:A:66:ARG:HD2	0.46	1.71	9	1
1:B:170:ALA:O	1:B:172:ILE:HG23	0.46	2.11	15	1
1:A:18:LYS:CE	1:A:32:LEU:CD1	0.46	2.94	17	1
1:A:60:PRO:HA	1:A:66:ARG:HA	0.46	1.88	6	3
1:B:159:LYS:O	1:B:161:CYS:SG	0.46	2.74	7	1
1:A:77:ASP:HA	1:B:181:GLU:OE1	0.46	2.11	10	1
1:B:159:LYS:HB2	1:B:160:PRO:HD3	0.46	1.87	12	1
1:B:119:GLY:N	1:B:132:LEU:CD1	0.46	2.79	20	1
1:B:159:LYS:N	1:B:160:PRO:CD	0.45	2.79	2	2
1:A:11:LEU:H	1:A:11:LEU:CD2	0.45	2.24	3	1
1:B:136:VAL:HG22	1:B:179:CYS:CB	0.45	2.41	7	1
1:A:15:PRO:HG3	1:A:32:LEU:HD21	0.45	1.87	20	1
1:B:115:PRO:HG3	1:B:132:LEU:HD21	0.45	1.87	20	1
1:A:35:PHE:CD1	1:A:40:GLU:OE1	0.45	2.69	2	1
1:A:38:THR:HG21	1:B:135:PHE:CD1	0.45	2.45	4	3
1:A:30:ASP:O	1:A:70:ALA:HB2	0.45	2.10	6	1
1:B:160:PRO:HA	1:B:166:ARG:HA	0.45	1.88	6	3
1:B:137:GLY:C	1:B:138:THR:HG22	0.45	2.31	20	2
1:A:35:PHE:CD2	1:B:135:PHE:HD2	0.45	2.29	12	1
1:B:139:ALA:C	1:B:141:ALA:N	0.45	2.69	15	1
1:B:143:ARG:NE	1:B:143:ARG:O	0.45	2.49	18	1
1:A:19:GLY:HA2	1:A:29:GLY:HA3	0.45	1.88	6	1
1:B:143:ARG:O	1:B:145:GLN:N	0.45	2.49	7	1
1:A:34:CYS:CB	1:A:72:ILE:HG21	0.45	2.41	10	3
1:B:135:PHE:HB2	1:B:138:THR:CG2	0.45	2.42	20	1
1:A:43:ARG:C	1:A:45:GLN:N	0.45	2.70	3	1
1:A:59:LYS:HB3	1:A:66:ARG:HB2	0.45	1.87	3	1
1:B:114:GLY:HA2	1:B:140:GLU:HG3	0.45	1.87	8	1
1:A:80:HIS:HB3	1:B:178:GLY:HA3	0.45	1.88	15	1
1:A:15:PRO:CG	1:A:32:LEU:HD11	0.45	2.41	19	1
1:B:172:ILE:HD12	1:B:172:ILE:C	0.45	2.31	19	1
1:A:43:ARG:O	1:A:45:GLN:N	0.45	2.49	7	2
1:A:21:CYS:O	1:A:22:PHE:CG	0.45	2.70	7	1
1:A:14:GLY:HA3	1:A:40:GLU:HG2	0.45	1.87	11	1
1:B:126:ILE:HG22	1:B:126:ILE:O	0.45	2.11	13	1
1:A:41:ALA:O	1:A:43:ARG:N	0.45	2.50	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:174:CYS:SG	1:B:178:GLY:O	0.45	2.75	15	1
1:A:81:GLU:OE2	1:B:124:PRO:HG2	0.45	2.12	3	1
1:A:36:VAL:CB	1:B:136:VAL:HG23	0.45	2.42	5	1
1:B:130:ASP:O	1:B:170:ALA:HB2	0.45	2.12	6	1
1:B:139:ALA:CA	1:B:142:LEU:HD12	0.45	2.42	9	2
1:A:27:CYS:O	1:A:34:CYS:CA	0.45	2.59	14	1
1:A:15:PRO:O	1:A:18:LYS:HG2	0.45	2.11	15	1
1:A:74:CYS:SG	1:A:78:GLY:O	0.45	2.75	15	1
1:B:115:PRO:CG	1:B:132:LEU:HD11	0.45	2.42	19	1
1:A:77:ASP:OD1	1:A:78:GLY:N	0.45	2.50	20	1
1:A:35:PHE:CD1	1:B:135:PHE:HD1	0.45	2.19	21	1
1:B:111:LEU:H	1:B:111:LEU:CD2	0.45	2.23	3	1
1:A:59:LYS:CG	1:A:60:PRO:HD3	0.45	2.42	13	1
1:A:72:ILE:N	1:A:82:ASP:OD1	0.45	2.49	15	1
1:B:168:ALA:HB3	1:B:172:ILE:HD11	0.45	1.88	15	1
1:A:10:CYS:HB3	1:A:20:ARG:CZ	0.45	2.42	4	1
1:A:39:ALA:O	1:A:41:ALA:N	0.45	2.50	15	1
1:B:118:LYS:CE	1:B:132:LEU:CD1	0.45	2.95	17	1
1:A:36:VAL:HG22	1:A:79:CYS:CB	0.44	2.42	7	1
1:B:113:CYS:CA	1:B:117:GLY:HA2	0.44	2.43	12	1
1:B:174:CYS:HA	1:B:179:CYS:CA	0.44	2.41	15	1
1:A:35:PHE:HB2	1:A:38:THR:CG2	0.44	2.42	20	1
1:A:72:ILE:HG13	1:A:72:ILE:O	0.44	2.12	1	1
1:A:15:PRO:HD3	1:A:40:GLU:OE1	0.44	2.12	4	1
1:B:121:CYS:O	1:B:122:PHE:CG	0.44	2.70	7	1
1:B:134:CYS:CB	1:B:172:ILE:HG21	0.44	2.42	20	2
1:A:59:LYS:HB2	1:A:67:CYS:HB3	0.44	1.88	17	1
1:B:115:PRO:HD2	1:B:132:LEU:CD1	0.44	2.43	19	1
1:B:132:LEU:CD2	1:B:135:PHE:HZ	0.44	2.26	12	2
1:B:139:ALA:CB	1:B:142:LEU:HD12	0.44	2.43	9	1
1:A:66:ARG:HD3	1:A:75:SER:HB3	0.44	1.90	10	1
1:A:18:LYS:HZ3	1:A:19:GLY:H	0.44	1.53	17	1
1:A:44:CYS:O	1:A:46:GLU:N	0.44	2.50	4	1
1:A:36:VAL:HB	1:B:136:VAL:HG23	0.44	1.88	21	2
1:B:144:CYS:O	1:B:146:GLU:N	0.44	2.50	4	1
1:B:162:GLY:O	1:B:164:GLY:N	0.44	2.50	5	1
1:B:175:SER:C	1:B:177:ASP:H	0.44	2.16	7	1
1:A:24:PRO:HD2	1:B:181:GLU:CG	0.44	2.42	14	1
1:A:15:PRO:O	1:A:18:LYS:HE3	0.44	2.13	18	1
1:B:121:CYS:SG	1:B:127:CYS:SG	0.44	3.16	19	1
1:B:110:CYS:HB3	1:B:120:ARG:CZ	0.44	2.43	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ALA:CB	1:A:42:LEU:HD12	0.44	2.43	9	1
1:B:171:GLY:H	1:B:185:CYS:C	0.44	2.16	11	1
1:A:35:PHE:HD2	1:B:135:PHE:HD2	0.44	1.54	12	1
1:A:26:ILE:O	1:A:26:ILE:HG22	0.44	2.12	13	1
1:A:15:PRO:CD	1:A:32:LEU:HD21	0.44	2.43	14	1
1:B:115:PRO:CD	1:B:132:LEU:HD21	0.44	2.43	14	1
1:A:21:CYS:SG	1:A:23:GLY:O	0.44	2.75	2	1
1:A:34:CYS:CB	1:A:72:ILE:CD1	0.44	2.96	2	1
1:B:159:LYS:O	1:B:167:CYS:N	0.44	2.46	9	3
1:B:120:ARG:HB2	1:B:128:CYS:O	0.44	2.12	11	1
1:B:141:ALA:O	1:B:143:ARG:N	0.44	2.50	15	1
1:A:82:ASP:CG	1:A:82:ASP:O	0.44	2.56	20	1
1:A:22:PHE:CE1	1:A:28:CYS:O	0.44	2.71	8	1
1:A:24:PRO:O	1:A:44:CYS:HB3	0.44	2.13	8	1
1:A:69:ALA:C	1:A:72:ILE:HG12	0.44	2.33	8	1
1:A:15:PRO:O	1:A:18:LYS:CD	0.44	2.66	12	1
1:A:74:CYS:CA	1:A:78:GLY:O	0.44	2.66	13	1
1:B:135:PHE:CB	1:B:138:THR:OG1	0.44	2.66	17	1
1:B:166:ARG:CD	1:B:166:ARG:H	0.44	2.26	18	1
1:B:110:CYS:O	1:B:120:ARG:HB3	0.44	2.12	20	1
1:B:177:ASP:OD1	1:B:178:GLY:N	0.44	2.50	20	1
1:B:128:CYS:HB2	1:B:174:CYS:SG	0.44	2.52	7	1
1:A:58:GLN:CB	1:A:67:CYS:HB3	0.44	2.38	13	1
1:A:78:GLY:CA	1:B:180:HIS:HB3	0.44	2.43	15	1
1:B:115:PRO:HD3	1:B:140:GLU:OE1	0.43	2.13	4	1
1:A:15:PRO:O	1:A:18:LYS:CG	0.43	2.66	8	4
1:A:59:LYS:N	1:A:60:PRO:HD2	0.43	2.28	2	1
1:B:128:CYS:C	1:B:133:GLY:O	0.43	2.56	6	1
1:B:115:PRO:HG2	1:B:115:PRO:O	0.43	2.13	21	3
1:B:114:GLY:HA3	1:B:140:GLU:HG2	0.43	1.86	11	1
1:A:18:LYS:HZ1	1:A:32:LEU:HD11	0.43	1.72	17	1
1:B:166:ARG:HD3	1:B:175:SER:HB3	0.43	1.90	10	1
1:B:122:PHE:HE1	1:B:128:CYS:O	0.43	1.96	13	2
1:B:168:ALA:N	1:B:172:ILE:O	0.43	2.51	6	1
1:A:15:PRO:HD2	1:A:32:LEU:CD1	0.43	2.43	19	2
1:B:174:CYS:CA	1:B:178:GLY:O	0.43	2.66	13	1
1:B:139:ALA:C	1:B:141:ALA:H	0.43	2.15	15	1
1:B:143:ARG:O	1:B:143:ARG:HD2	0.43	2.13	15	1
1:A:65:GLY:O	1:A:73:CYS:SG	0.43	2.77	20	1
1:B:173:CYS:HB3	1:B:182:ASP:HB3	0.43	1.90	21	1
1:A:36:VAL:HG21	1:A:79:CYS:HB2	0.43	1.91	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:SER:C	1:A:77:ASP:H	0.43	2.16	7	1
1:A:38:THR:HG21	1:B:135:PHE:CG	0.43	2.49	12	1
1:B:127:CYS:CB	1:B:135:PHE:CD2	0.43	3.01	18	1
1:A:36:VAL:CG2	1:B:136:VAL:CB	0.43	2.96	5	1
1:B:159:LYS:HB3	1:B:167:CYS:SG	0.43	2.54	18	2
1:B:174:CYS:CB	1:B:178:GLY:O	0.43	2.57	20	2
1:A:59:LYS:O	1:A:67:CYS:N	0.43	2.51	9	1
1:B:168:ALA:HB2	1:B:174:CYS:SG	0.43	2.53	10	1
1:A:21:CYS:SG	1:A:27:CYS:SG	0.43	3.16	19	1
1:B:119:GLY:HA2	1:B:129:GLY:HA3	0.43	1.90	20	1
1:A:68:ALA:HB3	1:A:72:ILE:CD1	0.43	2.41	3	1
1:A:29:GLY:HA3	1:A:32:LEU:HB2	0.43	1.90	14	2
1:A:20:ARG:HB2	1:A:20:ARG:CZ	0.43	2.43	5	1
1:A:28:CYS:C	1:A:33:GLY:O	0.43	2.57	6	1
1:B:137:GLY:O	1:B:138:THR:C	0.43	2.57	6	1
1:A:14:GLY:HA2	1:A:40:GLU:CG	0.43	2.44	16	2
1:B:161:CYS:HB3	1:B:173:CYS:HB3	0.43	1.64	9	1
1:A:35:PHE:CG	1:B:138:THR:HG21	0.43	2.48	12	1
1:B:127:CYS:C	1:B:134:CYS:SG	0.43	2.96	19	1
1:B:182:ASP:O	1:B:182:ASP:CG	0.43	2.56	20	1
1:A:32:LEU:CD2	1:A:35:PHE:CE1	0.43	3.01	9	1
1:A:26:ILE:HG23	1:A:36:VAL:CG1	0.43	2.43	10	2
1:A:68:ALA:HB2	1:A:74:CYS:SG	0.43	2.54	10	1
1:A:10:CYS:HB2	1:A:20:ARG:CG	0.43	2.44	14	1
1:A:27:CYS:C	1:A:34:CYS:SG	0.43	2.96	19	1
1:A:37:GLY:O	1:A:38:THR:C	0.43	2.57	6	1
1:A:38:THR:OG1	1:A:39:ALA:N	0.43	2.51	13	1
1:A:80:HIS:HB3	1:B:178:GLY:CA	0.43	2.44	15	1
1:A:21:CYS:CB	1:A:47:GLU:HG3	0.43	2.29	18	1
1:A:73:CYS:HB3	1:A:82:ASP:HB3	0.43	1.90	21	1
1:B:120:ARG:HB2	1:B:120:ARG:CZ	0.43	2.43	5	1
1:A:70:ALA:HB1	1:A:85:CYS:O	0.43	2.14	9	1
1:A:13:CYS:CA	1:A:17:GLY:HA2	0.43	2.44	12	1
1:B:159:LYS:CG	1:B:160:PRO:HD3	0.43	2.44	13	1
1:A:62:GLY:HA3	1:A:80:HIS:CE1	0.43	2.49	17	1
1:A:27:CYS:CB	1:A:35:PHE:CD2	0.43	3.02	18	1
1:A:28:CYS:HA	1:A:34:CYS:HA	0.42	1.91	17	2
1:B:138:THR:OG1	1:B:139:ALA:N	0.42	2.52	13	1
1:B:132:LEU:O	1:B:133:GLY:C	0.42	2.57	15	1
1:A:14:GLY:HA2	1:A:40:GLU:HA	0.42	1.90	11	1
1:A:44:CYS:O	1:A:47:GLU:HB2	0.42	2.14	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:130:ASP:N	1:B:130:ASP:OD1	0.42	2.53	20	1
1:A:75:SER:CB	1:A:76:PRO:CD	0.42	2.97	1	3
1:A:36:VAL:CG2	1:A:79:CYS:HB2	0.42	2.44	7	1
1:B:115:PRO:HD3	1:B:140:GLU:CG	0.42	2.45	13	1
1:B:162:GLY:HA3	1:B:180:HIS:CE1	0.42	2.49	17	1
1:A:26:ILE:HG23	1:A:36:VAL:CG2	0.42	2.40	18	1
1:B:134:CYS:HB2	1:B:172:ILE:HD11	0.42	1.92	2	1
1:A:11:LEU:H	1:A:11:LEU:CD1	0.42	2.28	7	1
1:A:69:ALA:O	1:A:72:ILE:HG12	0.42	2.15	8	1
1:A:57:GLY:CA	1:A:67:CYS:O	0.42	2.67	14	1
1:B:110:CYS:HB2	1:B:120:ARG:CG	0.42	2.45	14	1
1:A:19:GLY:N	1:A:32:LEU:CD1	0.42	2.82	20	1
1:A:15:PRO:HG2	1:A:18:LYS:HD3	0.42	1.91	7	1
1:A:65:GLY:CA	1:A:74:CYS:O	0.42	2.67	21	2
1:A:66:ARG:H	1:A:66:ARG:CD	0.42	2.26	18	1
1:A:65:GLY:HA3	1:A:75:SER:HB3	0.42	1.91	21	1
1:A:37:GLY:O	1:B:133:GLY:CA	0.42	2.66	2	1
1:B:136:VAL:CG2	1:B:179:CYS:HB2	0.42	2.44	7	1
1:B:170:ALA:HB1	1:B:185:CYS:O	0.42	2.14	9	1
1:B:127:CYS:HB3	1:B:135:PHE:HD2	0.42	1.74	16	1
1:A:59:LYS:HD3	1:A:67:CYS:HB2	0.42	1.92	19	1
1:A:30:ASP:N	1:A:30:ASP:OD1	0.42	2.53	20	1
1:A:82:ASP:OD2	1:A:85:CYS:HB2	0.42	2.15	3	2
1:A:26:ILE:HD11	1:B:181:GLU:HG3	0.42	1.91	11	1
1:A:28:CYS:HB2	1:A:68:ALA:CB	0.42	2.44	15	1
1:A:27:CYS:HB3	1:A:35:PHE:HD2	0.42	1.75	16	1
1:B:118:LYS:HZ3	1:B:119:GLY:H	0.42	1.58	17	1
1:B:115:PRO:C	1:B:117:GLY:N	0.42	2.73	2	2
1:B:136:VAL:HG21	1:B:179:CYS:HB2	0.42	1.91	3	1
1:A:26:ILE:HG23	1:A:79:CYS:SG	0.42	2.55	7	1
1:B:111:LEU:CD1	1:B:111:LEU:H	0.42	2.27	7	1
1:B:136:VAL:CG2	1:B:179:CYS:CB	0.42	2.97	7	1
1:B:143:ARG:C	1:B:145:GLN:H	0.42	2.17	8	1
1:B:134:CYS:SG	1:B:168:ALA:CB	0.42	3.08	13	1
1:B:140:GLU:HA	1:B:143:ARG:HD3	0.42	1.92	17	1
1:B:186:ASP:O	1:B:186:ASP:OD1	0.42	2.38	17	1
1:B:170:ALA:O	1:B:185:CYS:HB3	0.42	2.15	21	1
1:B:134:CYS:CB	1:B:172:ILE:CD1	0.42	2.97	2	1
1:A:61:CYS:SG	1:A:62:GLY:N	0.42	2.93	3	2
1:B:159:LYS:CB	1:B:160:PRO:HD2	0.42	2.44	9	1
1:B:126:ILE:HG23	1:B:136:VAL:CG1	0.42	2.45	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:GLY:O	1:A:16:GLY:N	0.42	2.53	19	1
1:B:166:ARG:N	1:B:174:CYS:O	0.42	2.52	21	1
1:B:126:ILE:HG23	1:B:179:CYS:SG	0.42	2.55	7	1
1:A:22:PHE:HE1	1:A:28:CYS:O	0.42	1.98	9	1
1:A:42:LEU:CD1	1:A:42:LEU:C	0.42	2.89	15	1
1:A:33:GLY:CA	1:A:69:ALA:HB1	0.42	2.33	18	1
1:B:135:PHE:CD2	1:B:140:GLU:OE2	0.42	2.73	19	1
1:B:165:GLY:CA	1:B:174:CYS:O	0.42	2.68	21	1
1:A:34:CYS:SG	1:A:72:ILE:CD1	0.41	2.94	7	1
1:B:172:ILE:HG22	1:B:180:HIS:N	0.41	2.30	7	1
1:B:115:PRO:O	1:B:118:LYS:CG	0.41	2.68	8	2
1:A:66:ARG:O	1:A:74:CYS:O	0.41	2.38	10	1
1:A:36:VAL:O	1:B:134:CYS:HB2	0.41	2.14	13	1
1:A:86:ASP:OD1	1:A:86:ASP:O	0.41	2.38	17	1
1:B:165:GLY:HA3	1:B:175:SER:HB3	0.41	1.91	21	1
1:B:175:SER:CB	1:B:176:PRO:CD	0.41	2.97	1	3
1:A:15:PRO:O	1:A:17:GLY:N	0.41	2.53	2	1
1:A:36:VAL:CB	1:B:136:VAL:CG2	0.41	2.98	5	1
1:A:36:VAL:CG2	1:A:79:CYS:SG	0.41	2.95	7	1
1:B:114:GLY:O	1:B:116:GLY:N	0.41	2.53	19	2
1:A:81:GLU:HG2	1:B:124:PRO:HD2	0.41	1.91	14	1
1:A:39:ALA:C	1:A:41:ALA:N	0.41	2.72	15	1
1:A:11:LEU:HB3	1:A:43:ARG:HH22	0.41	1.75	18	1
1:A:22:PHE:CZ	1:A:68:ALA:O	0.41	2.73	20	1
1:B:126:ILE:CD1	1:B:176:PRO:HA	0.41	2.45	20	1
1:A:66:ARG:N	1:A:74:CYS:O	0.41	2.53	21	1
1:B:115:PRO:N	1:B:140:GLU:HG2	0.41	2.30	3	1
1:A:26:ILE:HG23	1:A:36:VAL:CB	0.41	2.45	10	1
1:B:166:ARG:O	1:B:174:CYS:O	0.41	2.38	10	1
1:A:20:ARG:HB2	1:A:28:CYS:O	0.41	2.14	11	1
1:B:144:CYS:SG	1:B:147:GLU:HB2	0.41	2.56	11	1
1:B:134:CYS:SG	1:B:172:ILE:CD1	0.41	2.93	7	1
1:A:71:GLY:H	1:A:85:CYS:C	0.41	2.17	11	1
1:B:114:GLY:HA2	1:B:140:GLU:HA	0.41	1.90	11	1
1:A:83:PRO:HA	1:A:86:ASP:HB2	0.41	1.92	12	1
1:A:39:ALA:O	1:A:43:ARG:HD3	0.41	2.15	17	1
1:A:35:PHE:CD2	1:A:40:GLU:OE2	0.41	2.73	19	1
1:B:171:GLY:HA3	1:B:186:ASP:OD1	0.41	2.16	21	1
1:A:32:LEU:CD2	1:A:35:PHE:HZ	0.41	2.28	6	1
1:B:115:PRO:HG2	1:B:118:LYS:HD3	0.41	1.92	7	1
1:B:173:CYS:SG	1:B:182:ASP:CG	0.41	2.99	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:124:PRO:O	1:B:144:CYS:HB3	0.41	2.15	8	1
1:A:28:CYS:CB	1:A:69:ALA:CB	0.41	2.99	20	2
1:A:25:SER:HB2	1:B:181:GLU:CG	0.41	2.45	16	1
1:A:66:ARG:HD3	1:A:66:ARG:C	0.41	2.36	18	1
1:A:68:ALA:N	1:A:72:ILE:O	0.41	2.51	6	1
1:B:126:ILE:HG23	1:B:128:CYS:SG	0.41	2.56	13	1
1:B:110:CYS:SG	1:B:120:ARG:HG2	0.41	2.56	6	1
1:A:28:CYS:HB2	1:A:74:CYS:SG	0.41	2.56	7	1
1:A:74:CYS:HA	1:A:79:CYS:CA	0.41	2.41	15	1
1:B:142:LEU:CD1	1:B:143:ARG:N	0.41	2.84	15	1
1:A:59:LYS:HB3	1:A:67:CYS:SG	0.41	2.55	18	1
1:A:10:CYS:SG	1:A:20:ARG:HD3	0.41	2.56	3	1
1:A:27:CYS:HB3	1:A:41:ALA:HB2	0.41	1.91	5	1
1:A:61:CYS:HB2	1:A:73:CYS:HB2	0.41	1.78	7	1
1:A:73:CYS:SG	1:A:82:ASP:HB3	0.41	2.56	9	1
1:B:169:ALA:CB	1:B:172:ILE:HD11	0.41	2.39	18	2
1:B:182:ASP:OD2	1:B:185:CYS:HB2	0.41	2.16	17	1
1:A:37:GLY:O	1:A:38:THR:HG22	0.41	2.15	21	1
1:A:34:CYS:HB2	1:A:72:ILE:HD11	0.41	1.91	2	1
1:A:13:CYS:O	1:A:19:GLY:HA3	0.41	2.16	4	1
1:B:117:GLY:C	1:B:119:GLY:H	0.41	2.18	4	1
1:B:172:ILE:CD1	1:B:174:CYS:SG	0.41	3.09	5	1
1:A:73:CYS:SG	1:A:82:ASP:CG	0.41	2.99	7	1
1:B:172:ILE:HG22	1:B:180:HIS:CA	0.41	2.46	7	1
1:B:169:ALA:C	1:B:172:ILE:HG12	0.41	2.36	8	1
1:B:166:ARG:O	1:B:174:CYS:N	0.41	2.40	10	2
1:B:123:GLY:HA2	1:B:147:GLU:OE1	0.41	2.16	12	1
1:B:183:PRO:HA	1:B:186:ASP:HB2	0.41	1.92	12	1
1:A:68:ALA:HB3	1:A:72:ILE:HD11	0.41	1.92	15	1
1:B:121:CYS:HA	1:B:127:CYS:HA	0.41	1.93	15	1
1:B:142:LEU:C	1:B:142:LEU:CD1	0.41	2.89	15	1
1:B:118:LYS:CE	1:B:132:LEU:HD11	0.41	2.46	17	1
1:B:159:LYS:O	1:B:161:CYS:N	0.41	2.54	17	1
1:B:166:ARG:C	1:B:166:ARG:HD3	0.41	2.36	18	1
1:A:68:ALA:HB2	1:A:74:CYS:CB	0.41	2.46	2	1
1:B:135:PHE:CB	1:B:138:THR:CG2	0.41	2.99	2	1
1:B:172:ILE:HB	1:B:179:CYS:SG	0.41	2.56	5	1
1:A:36:VAL:CG2	1:A:79:CYS:CB	0.41	2.99	7	1
1:A:69:ALA:HB3	1:A:72:ILE:HG13	0.41	1.91	8	1
1:B:122:PHE:CE1	1:B:128:CYS:O	0.41	2.75	8	1
1:B:144:CYS:O	1:B:147:GLU:HB2	0.41	2.16	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ILE:HG23	1:A:28:CYS:SG	0.41	2.55	13	1
1:A:61:CYS:SG	1:A:82:ASP:HB2	0.41	2.55	15	1
1:B:183:PRO:O	1:B:186:ASP:HB2	0.41	2.16	15	1
1:A:59:LYS:CB	1:A:67:CYS:CB	0.40	2.98	2	1
1:B:172:ILE:HD12	1:B:172:ILE:N	0.40	2.30	7	1
1:A:69:ALA:CA	1:A:72:ILE:HG12	0.40	2.47	8	1
1:A:21:CYS:HA	1:A:27:CYS:HA	0.40	1.93	15	1
1:A:42:LEU:CD1	1:A:43:ARG:N	0.40	2.84	15	1
1:B:172:ILE:N	1:B:182:ASP:OD1	0.40	2.54	15	1
1:A:35:PHE:CB	1:A:38:THR:OG1	0.40	2.69	17	1
1:A:28:CYS:HB3	1:A:69:ALA:HB2	0.40	1.93	19	1
1:B:159:LYS:HD3	1:B:167:CYS:HB2	0.40	1.92	19	1
1:B:182:ASP:OD1	1:B:184:ALA:N	0.40	2.54	5	1
1:A:81:GLU:CG	1:B:126:ILE:HD11	0.40	2.45	11	1
1:A:35:PHE:HD2	1:B:135:PHE:CD2	0.40	2.34	12	1
1:A:15:PRO:HD3	1:A:40:GLU:CG	0.40	2.45	13	1
1:B:170:ALA:O	1:B:185:CYS:CB	0.40	2.70	21	1
1:B:110:CYS:SG	1:B:120:ARG:HD3	0.40	2.57	3	1
1:B:128:CYS:HB3	1:B:134:CYS:HB2	0.40	1.82	6	1
1:B:128:CYS:CB	1:B:169:ALA:CB	0.40	2.99	10	1
1:B:115:PRO:HD3	1:B:140:GLU:HG2	0.40	1.93	13	1
1:A:83:PRO:O	1:A:86:ASP:HB2	0.40	2.16	15	1
1:B:161:CYS:SG	1:B:182:ASP:HB2	0.40	2.56	15	1
1:B:111:LEU:CG	1:B:143:ARG:NH2	0.40	2.84	18	1
1:A:35:PHE:CB	1:A:38:THR:CG2	0.40	2.99	2	1
1:A:82:ASP:OD1	1:A:84:ALA:N	0.40	2.55	5	1
1:A:10:CYS:SG	1:A:20:ARG:HG2	0.40	2.56	6	1
1:A:61:CYS:HB3	1:A:73:CYS:HB3	0.40	1.70	13	1
1:B:119:GLY:N	1:B:132:LEU:HD12	0.40	2.31	20	1
1:B:122:PHE:CZ	1:B:168:ALA:O	0.40	2.75	20	1
1:B:165:GLY:N	1:B:175:SER:HB3	0.40	2.31	7	1
1:B:173:CYS:SG	1:B:182:ASP:HB3	0.40	2.57	9	1
1:A:81:GLU:OE2	1:B:123:GLY:HA3	0.40	2.16	14	1
1:A:71:GLY:CA	1:A:82:ASP:OD1	0.40	2.69	15	1
1:A:13:CYS:HB3	1:A:20:ARG:N	0.40	2.32	16	1
1:B:118:LYS:NZ	1:B:132:LEU:CD1	0.40	2.85	17	1
1:B:126:ILE:HG23	1:B:136:VAL:CG2	0.40	2.42	18	1
1:A:37:GLY:C	1:A:38:THR:CG2	0.40	2.90	21	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	69/92 (75%)	50±3 (73±4%)	15±2 (21±4%)	4±2 (6±2%)	3	22
1	B	69/92 (75%)	50±3 (72±4%)	16±2 (23±3%)	4±2 (5±2%)	3	23
All	All	2898/3864 (75%)	2101 (72%)	637 (22%)	160 (6%)	3	23

All 40 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	124	PRO	17
1	A	24	PRO	17
1	A	56	SER	11
1	B	156	SER	11
1	A	57	GLY	7
1	B	157	GLY	6
1	B	170	ALA	6
1	A	70	ALA	6
1	B	160	PRO	5
1	A	60	PRO	5
1	B	159	LYS	5
1	A	59	LYS	5
1	B	186	ASP	5
1	A	86	ASP	5
1	B	171	GLY	4
1	A	62	GLY	4
1	A	71	GLY	4
1	B	116	GLY	3
1	A	44	CYS	3
1	B	111	LEU	3
1	B	162	GLY	3
1	B	145	GLN	2
1	A	11	LEU	2
1	B	138	THR	2
1	A	38	THR	2
1	A	45	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	16	GLY	2
1	A	33	GLY	1
1	A	42	LEU	1
1	B	144	CYS	1
1	B	139	ALA	1
1	A	10	CYS	1
1	B	110	CYS	1
1	B	112	PRO	1
1	A	40	GLU	1
1	B	142	LEU	1
1	B	140	GLU	1
1	B	133	GLY	1
1	A	12	PRO	1
1	A	39	ALA	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	49/69 (71%)	31±3 (64±5%)	18±3 (36±5%)	1 8
1	B	49/69 (71%)	31±3 (64±6%)	18±3 (36±6%)	1 8
All	All	2058/2898 (71%)	1315 (64%)	743 (36%)	1 8

All 81 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	66	ARG	21
1	B	166	ARG	21
1	B	118	LYS	20
1	A	18	LYS	20
1	B	128	CYS	18
1	B	131	GLU	18
1	A	31	GLU	18
1	A	28	CYS	17
1	A	32	LEU	16
1	B	132	LEU	16

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Mol	Chain	Res	Type	Models (Total)
1	B	125	SER	15
1	A	25	SER	15
1	A	82	ASP	15
1	B	182	ASP	15
1	A	20	ARG	14
1	B	161	CYS	14
1	A	61	CYS	14
1	B	127	CYS	13
1	A	27	CYS	13
1	A	43	ARG	13
1	B	143	ARG	13
1	A	35	PHE	12
1	B	120	ARG	12
1	A	86	ASP	12
1	B	135	PHE	12
1	B	159	LYS	11
1	A	59	LYS	11
1	B	186	ASP	11
1	A	34	CYS	10
1	B	113	CYS	10
1	A	13	CYS	10
1	B	142	LEU	9
1	A	40	GLU	9
1	B	134	CYS	9
1	A	47	GLU	9
1	A	42	LEU	9
1	A	10	CYS	9
1	B	147	GLU	9
1	B	110	CYS	9
1	A	73	CYS	9
1	B	140	GLU	9
1	A	81	GLU	8
1	B	181	GLU	8
1	A	38	THR	8
1	B	173	CYS	8
1	B	138	THR	8
1	B	145	GLN	7
1	A	56	SER	7
1	A	11	LEU	7
1	B	111	LEU	7
1	A	45	GLN	7
1	B	174	CYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	63	SER	6
1	A	79	CYS	6
1	B	163	SER	6
1	B	156	SER	6
1	A	74	CYS	6
1	B	179	CYS	6
1	B	167	CYS	5
1	B	144	CYS	5
1	A	67	CYS	5
1	A	21	CYS	5
1	A	44	CYS	5
1	A	58	GLN	5
1	B	172	ILE	5
1	B	158	GLN	5
1	A	72	ILE	5
1	A	26	ILE	4
1	B	180	HIS	4
1	A	80	HIS	4
1	B	126	ILE	4
1	B	121	CYS	4
1	B	146	GLU	3
1	B	175	SER	3
1	A	46	GLU	3
1	A	75	SER	3
1	A	77	ASP	2
1	B	177	ASP	2
1	B	185	CYS	2
1	A	85	CYS	2
1	A	36	VAL	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 44% for the well-defined parts and 41% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	862
Number of shifts mapped to atoms	862
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	86	0.45 ± 0.15	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	154	0.52 ± 0.38	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 44%, i.e. 602 atoms were assigned a chemical shift out of a possible 1382. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	426/666 (64%)	238/264 (90%)	70/276 (25%)	118/126 (94%)
Sidechain	174/664 (26%)	174/402 (43%)	0/236 (0%)	0/26 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	2/52 (4%)	2/28 (7%)	0/20 (0%)	0/4 (0%)
Overall	602/1382 (44%)	414/694 (60%)	70/532 (13%)	118/156 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 41%, i.e. 782 atoms were assigned a chemical shift out of a possible 1916. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	552/884 (62%)	312/350 (89%)	86/368 (23%)	154/166 (93%)
Sidechain	228/946 (24%)	228/568 (40%)	0/342 (0%)	0/36 (0%)
Aromatic	2/86 (2%)	2/46 (4%)	0/36 (0%)	0/4 (0%)
Overall	782/1916 (41%)	542/964 (56%)	86/746 (12%)	154/206 (75%)

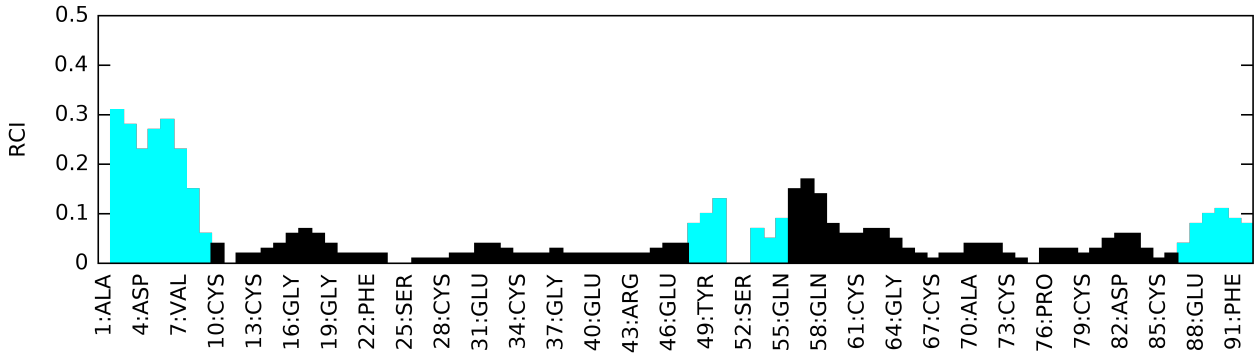
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

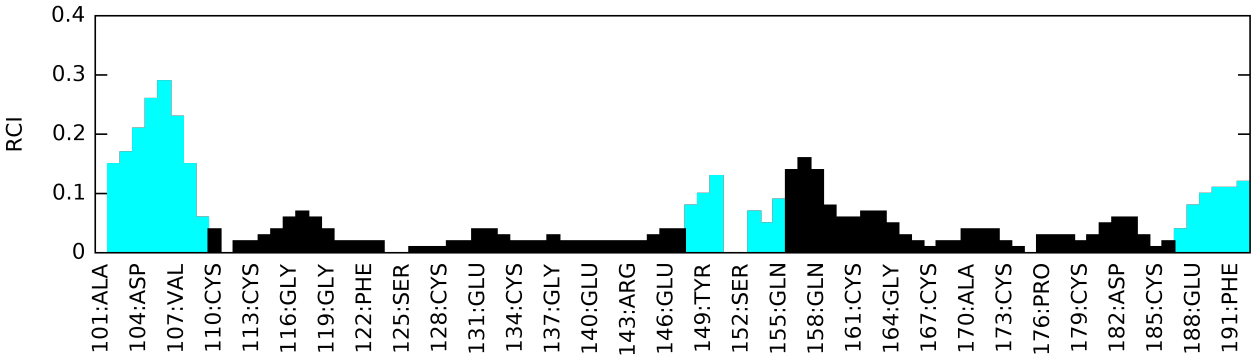
7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:


RCI
0.4
0.3
0.2
0.1
0
101:ALA
104:ASP
107:VAL
110:CYS
113:CYS
116:GLY
119:GLY
122:PHE
125:SER
128:CYS
131:GLU
134:CYS
137:GLY
140:GLU
143:ARG
146:GLU
149:TYR
152:SER
155:GLN
158:GLN
161:CYS
164:GLY
167:CYS
170:ALA
173:CYS
176:PRO
179:CYS
182:ASP
185:CYS
188:GLU
191:PHE