



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 05:30 PM UTC

PDB ID : 2LBH / pdb_00002lbh
BMRB ID : 17561
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

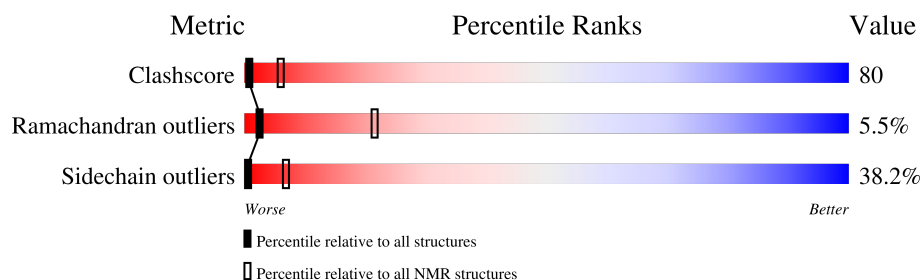
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	92	11% 52% 12% 25%
1	B	92	11% 54% 9% 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)	1.37	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 [i](#)

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.

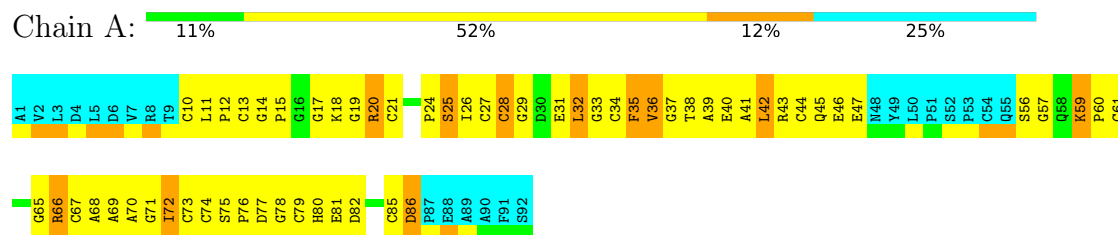
Mol	Chain	Residues	Atoms						Trace
1	A	92	Total	C	H	N	O	S	0
			1217	382	579	112	130	14	
1	B	92	Total	C	H	N	O	S	0
			1217	382	579	112	130	14	

4 Residue-property plots

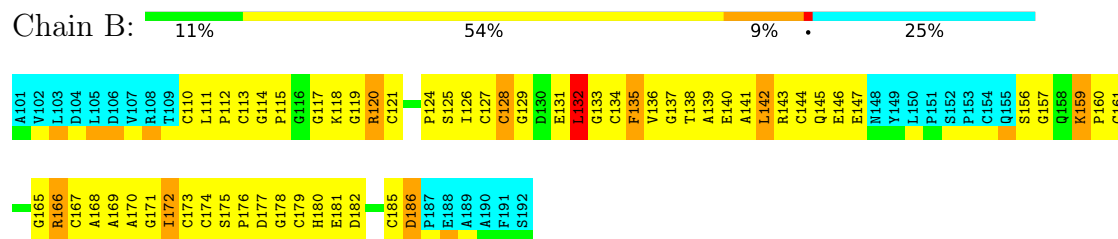
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Neurophysin 1



- Molecule 1: Neurophysin 1

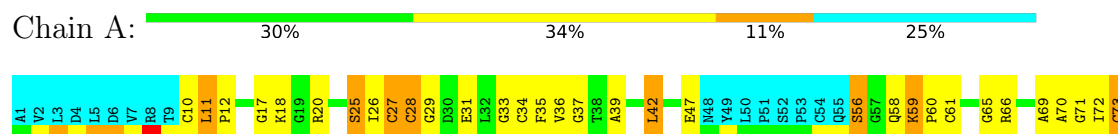


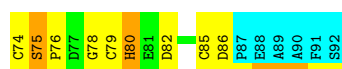
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

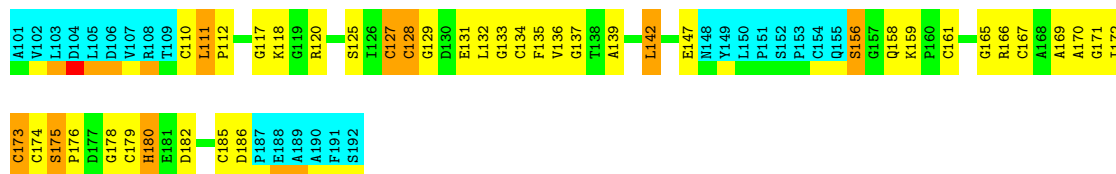
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Neurophysin 1



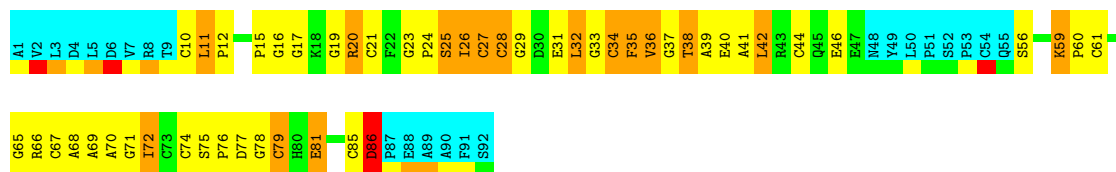
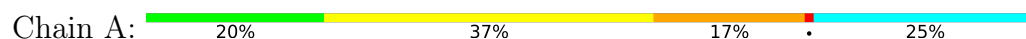


• Molecule 1: Neurophysin 1

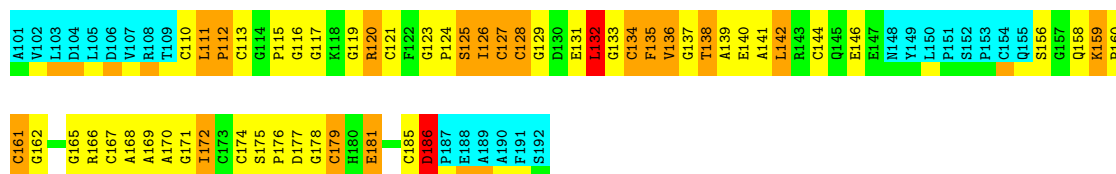


4.2.2 Score per residue for model 2

• Molecule 1: Neurophysin 1

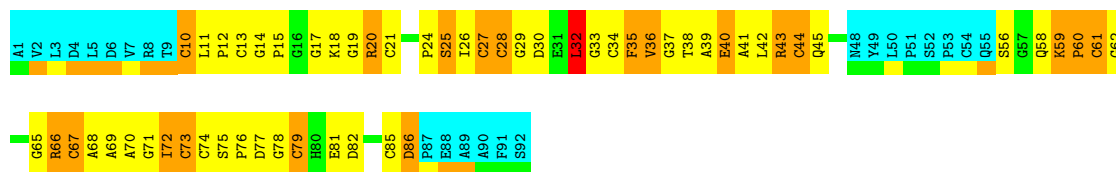


• Molecule 1: Neurophysin 1

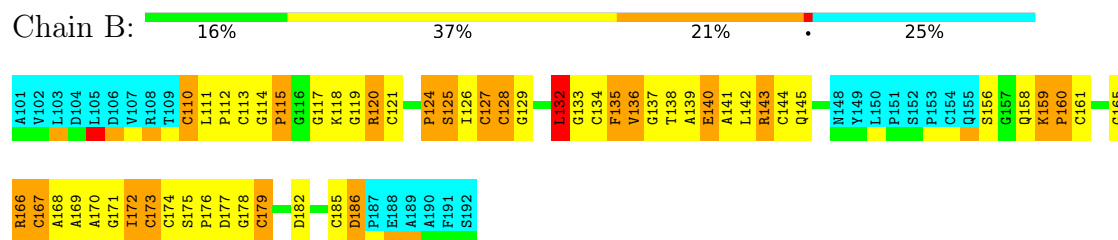


4.2.3 Score per residue for model 3

• Molecule 1: Neurophysin 1

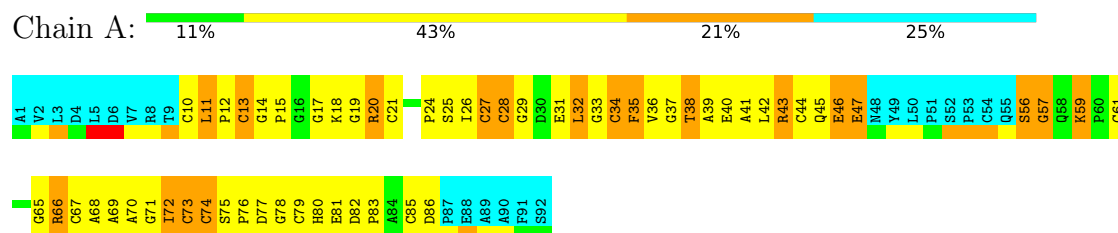


• Molecule 1: Neurophysin 1

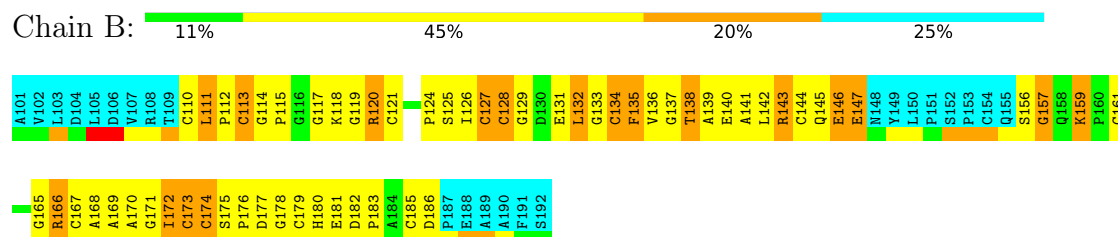


4.2.4 Score per residue for model 4

• Molecule 1: Neurophysin 1

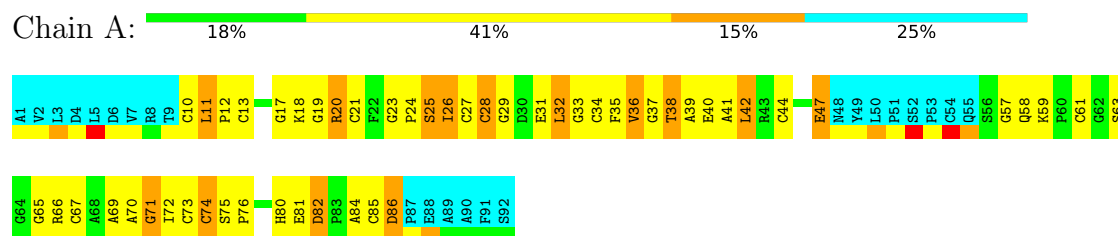


• Molecule 1: Neurophysin 1

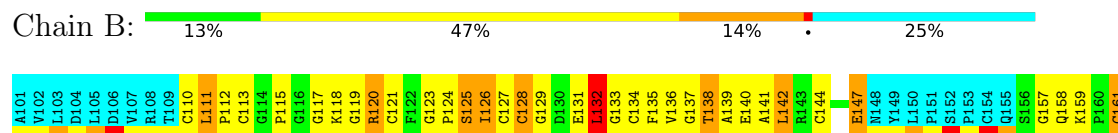


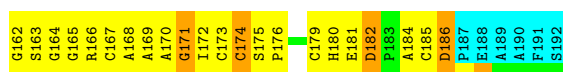
4.2.5 Score per residue for model 5

• Molecule 1: Neurophysin 1



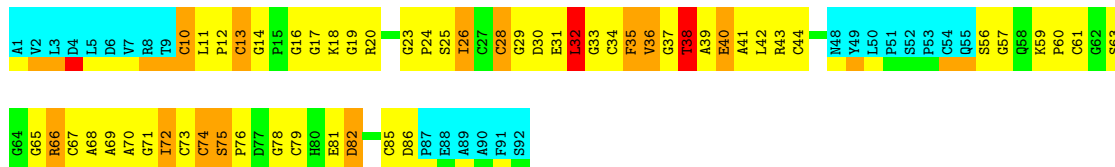
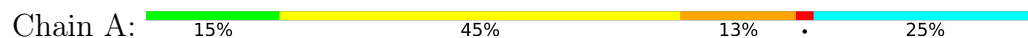
• Molecule 1: Neurophysin 1



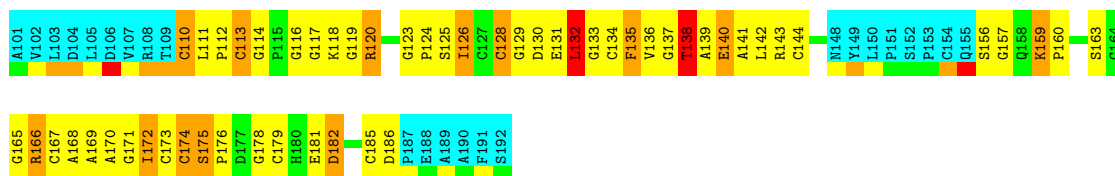


4.2.6 Score per residue for model 6

- Molecule 1: Neurophysin 1

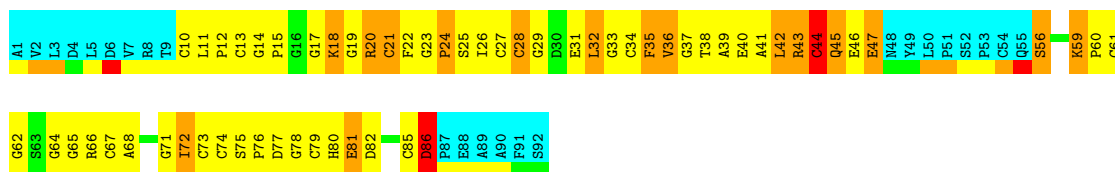


- Molecule 1: Neurophysin 1

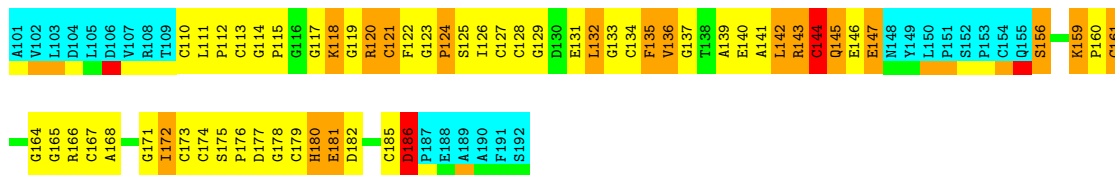


4.2.7 Score per residue for model 7

- Molecule 1: Neurophysin 1

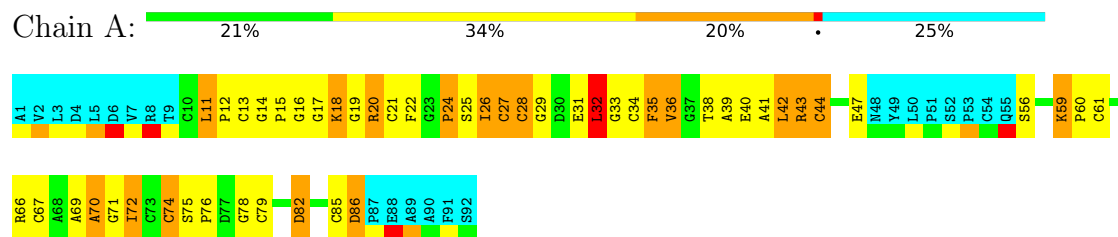


- Molecule 1: Neurophysin 1

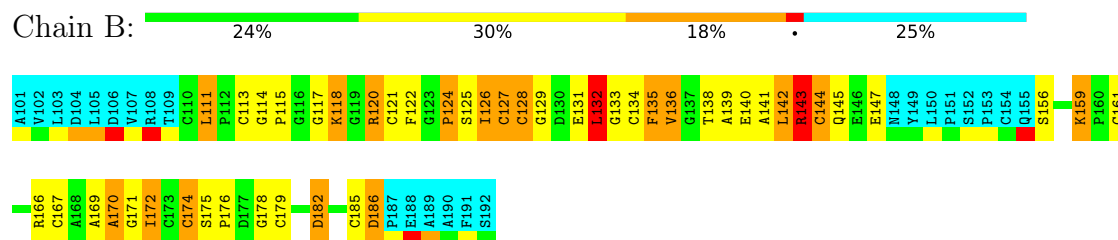


4.2.8 Score per residue for model 8

• Molecule 1: Neurophysin 1

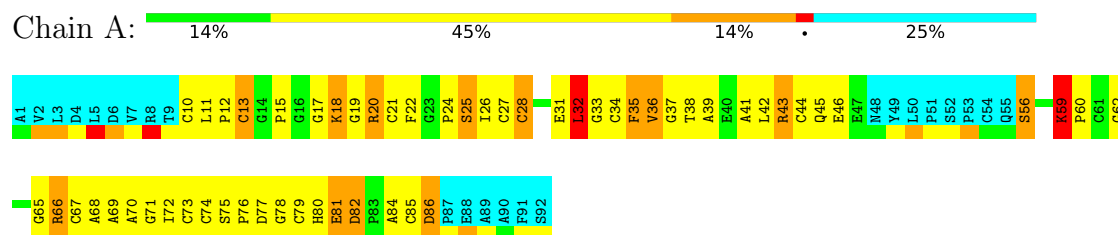


• Molecule 1: Neurophysin 1

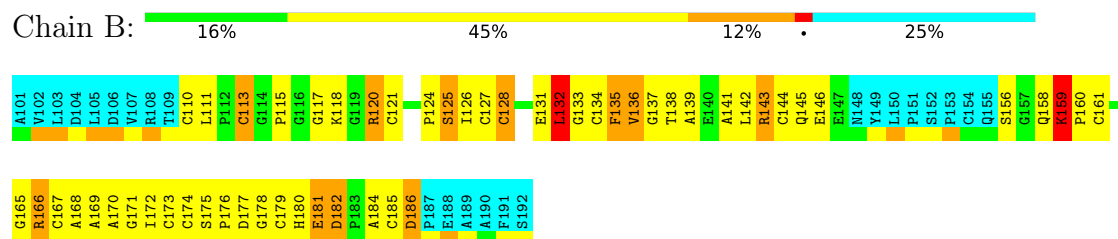


4.2.9 Score per residue for model 9

• Molecule 1: Neurophysin 1

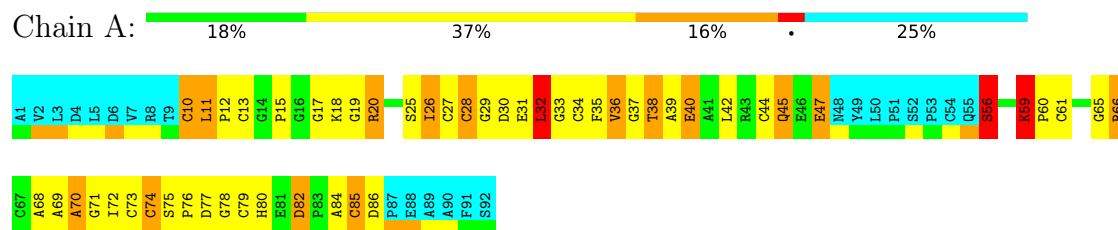


• Molecule 1: Neurophysin 1

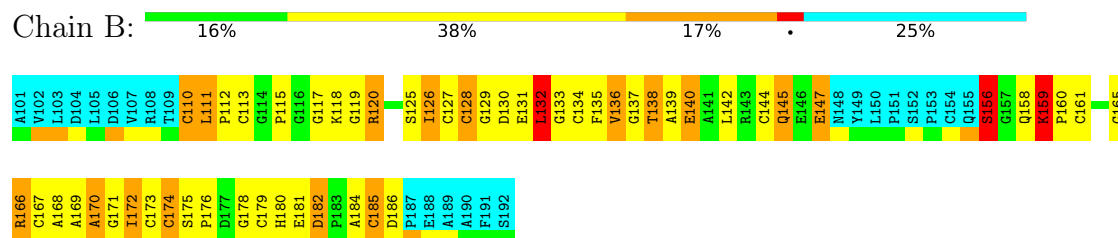


4.2.10 Score per residue for model 10

• Molecule 1: Neurophysin 1

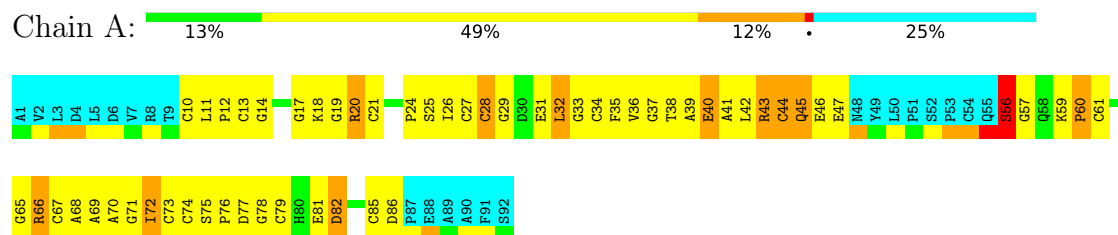


• Molecule 1: Neurophysin 1

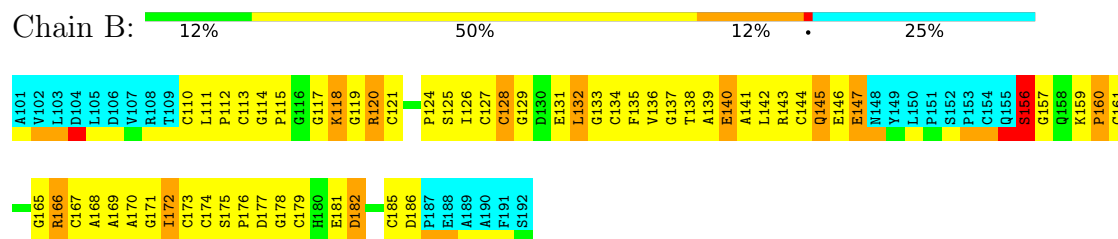


4.2.11 Score per residue for model 11

• Molecule 1: Neurophysin 1

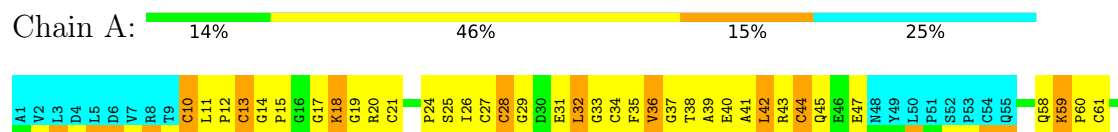


• Molecule 1: Neurophysin 1



4.2.12 Score per residue for model 12

• Molecule 1: Neurophysin 1



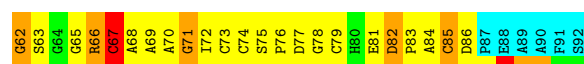
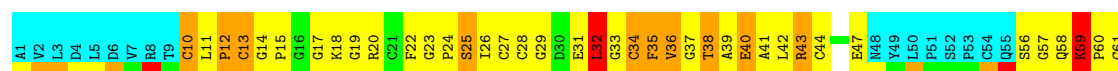


• Molecule 1: Neurophysin 1

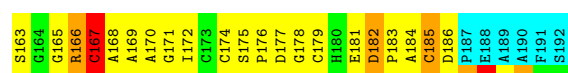


4.2.13 Score per residue for model 13

• Molecule 1: Neurophysin 1



• Molecule 1: Neurophysin 1

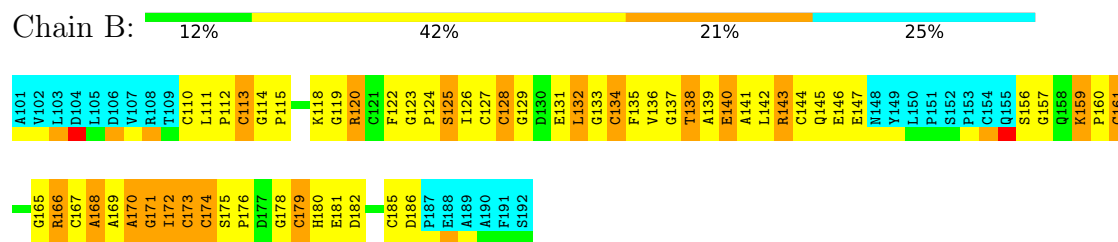


4.2.14 Score per residue for model 14

• Molecule 1: Neurophysin 1

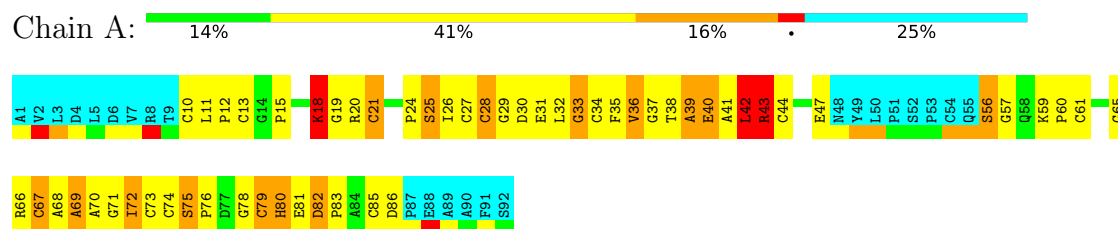


• Molecule 1: Neurophysin 1

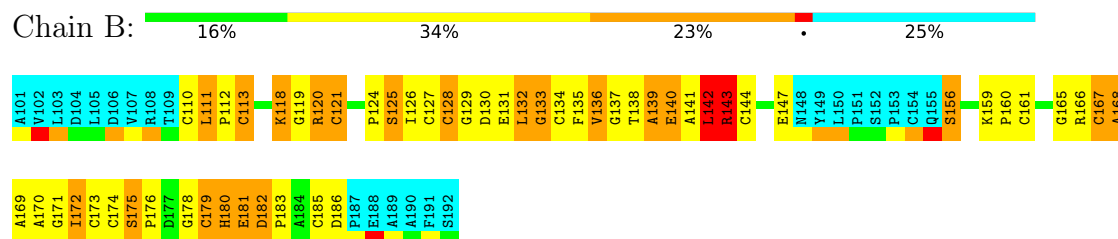


4.2.15 Score per residue for model 15

• Molecule 1: Neurophysin 1

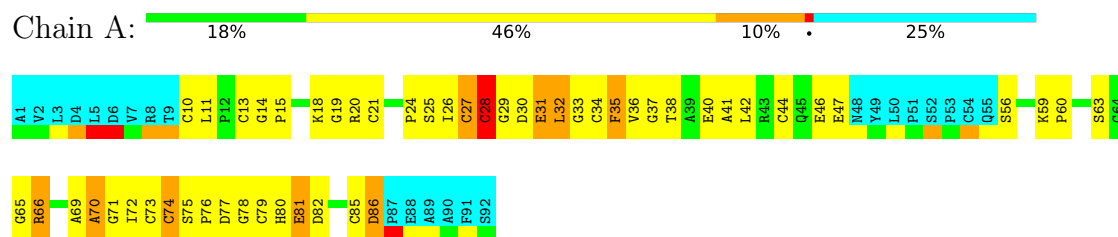


• Molecule 1: Neurophysin 1

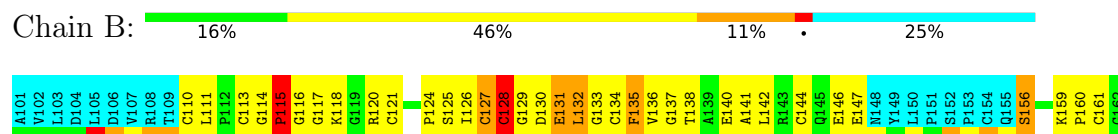


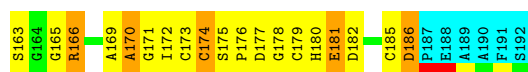
4.2.16 Score per residue for model 16

• Molecule 1: Neurophysin 1



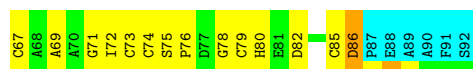
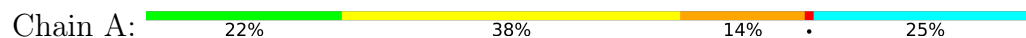
• Molecule 1: Neurophysin 1



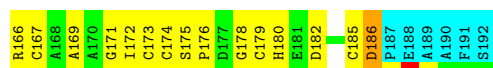
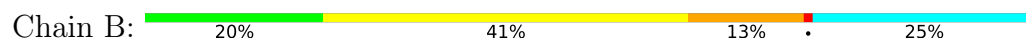


4.2.17 Score per residue for model 17

- Molecule 1: Neurophysin 1



- Molecule 1: Neurophysin 1



4.2.18 Score per residue for model 18

- Molecule 1: Neurophysin 1

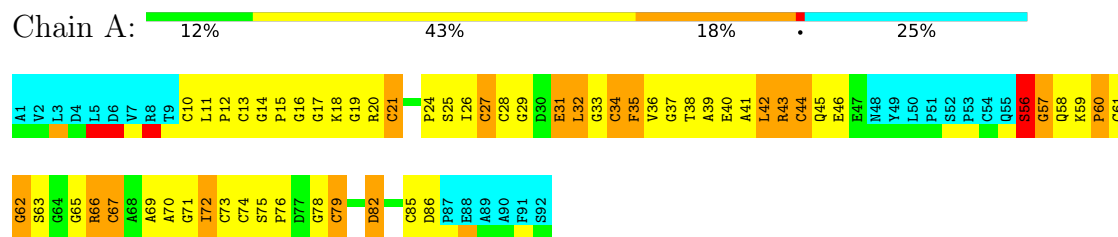


- Molecule 1: Neurophysin 1

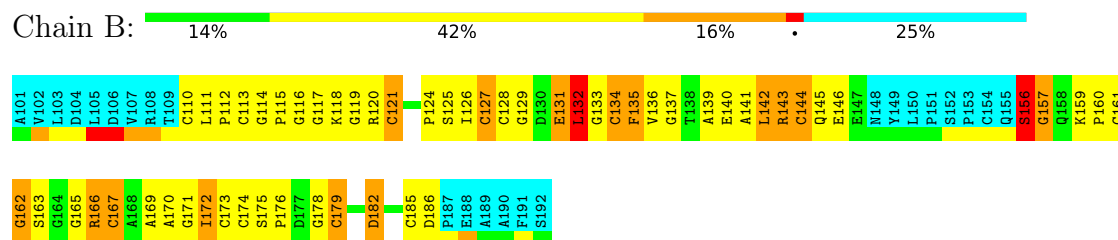


4.2.19 Score per residue for model 19

• Molecule 1: Neurophysin 1

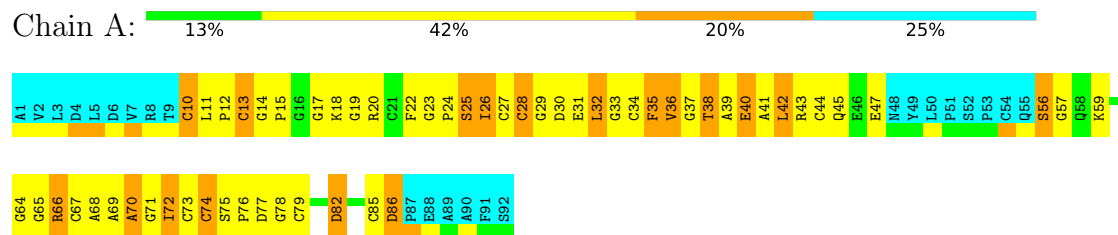


• Molecule 1: Neurophysin 1

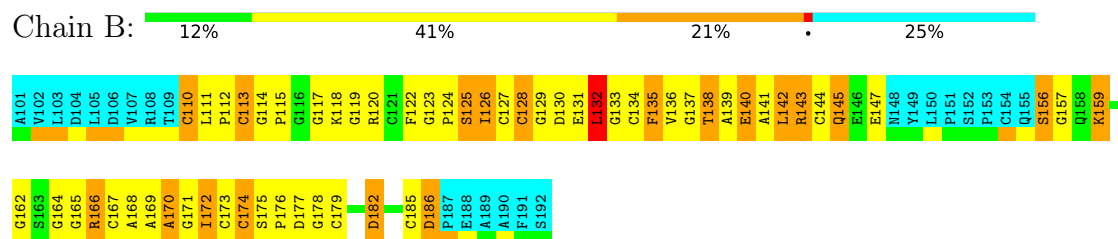


4.2.20 Score per residue for model 20

• Molecule 1: Neurophysin 1

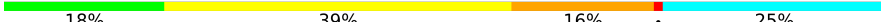


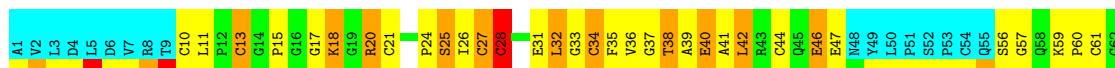
• Molecule 1: Neurophysin 1



4.2.21 Score per residue for model 21

• Molecule 1: Neurophysin 1

Chain A:  18% 39% 16% 25%



● Molecule 1: Neurophysin 1

Chain B:  20% 38% 17% 25%



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)	working_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%

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.83±0.06	0±0/471 (0.0± 0.1%)	1.11±0.05	1±1/635 (0.2± 0.1%)
1	B	0.82±0.05	0±0/471 (0.0± 0.1%)	1.12±0.05	2±1/635 (0.3± 0.2%)
All	All	0.83	5/19782 (0.0%)	1.12	65/26670 (0.2%)

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

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	67	CYS	N-CA	-6.67	1.37	1.46	13	1
1	B	167	CYS	N-CA	-6.62	1.38	1.46	13	1
1	B	132	LEU	N-CA	-5.99	1.39	1.46	15	1
1	A	15	PRO	C-N	-5.06	1.25	1.33	16	1
1	B	115	PRO	C-N	-5.04	1.26	1.33	3	1

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	B	132	LEU	N-CA-C	-8.23	102.68	114.12	10	15
1	A	18	LYS	N-CA-C	-7.04	101.91	112.04	18	3
1	A	32	LEU	N-CA-C	-6.64	104.89	114.12	21	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	74	CYS	N-CA-C	6.60	116.58	107.73	8	4
1	B	174	CYS	N-CA-C	6.57	116.53	107.73	8	4
1	B	168	ALA	N-CA-C	-6.19	104.79	112.90	15	4
1	A	30	ASP	N-CA-C	-5.95	104.42	111.03	3	1
1	A	64	GLY	CA-C-N	-5.83	116.70	122.36	20	2
1	A	64	GLY	C-N-CA	-5.83	116.70	122.36	20	2
1	B	115	PRO	N-CA-C	-5.63	102.36	111.14	16	1
1	A	43	ARG	N-CA-C	-5.47	106.56	113.18	19	2
1	A	28	CYS	N-CA-C	5.46	117.33	108.26	16	2
1	B	118	LYS	N-CA-C	-5.45	106.83	112.93	15	2
1	B	143	ARG	N-CA-C	-5.29	106.77	113.18	19	3
1	B	164	GLY	CA-C-N	-5.29	117.18	122.20	20	2
1	B	164	GLY	C-N-CA	-5.29	117.18	122.20	20	2
1	B	113	CYS	N-CA-C	5.24	115.45	108.38	15	1
1	B	145	GLN	N-CA-C	-5.14	106.52	112.89	11	1
1	A	69	ALA	N-CA-C	5.06	116.53	108.79	15	1
1	B	128	CYS	N-CA-C	5.05	116.64	108.26	16	1
1	A	68	ALA	N-CA-C	-5.05	105.48	111.69	4	1
1	A	35	PHE	N-CA-C	-5.02	99.62	108.20	13	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
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	78±13
1	B	462	410	409	77±12
All	All	19404	17220	17178	2927

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 80.

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:71:GLY:C	1:A:72:ILE:HD13	0.97	1.82	8	3
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:115:PRO:HD2	1:B:132:LEU:HD11	0.91	1.42	10	4
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:72:ILE:HG13	1:A:72:ILE:O	0.91	1.65	15	3
1:A:37:GLY:HA3	1:B:172:ILE:HG21	0.91	1.40	12	8
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	3
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:B:171:GLY:C	1:B:172:ILE:HD13	0.83	1.98	8	4
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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: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:27:CYS:HB2	1:A:41:ALA:HB2	0.76	1.58	8	2
1:A:29:GLY:O	1:A:69:ALA:HB1	0.76	1.80	6	9
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:A:25:SER:C	1:A:26:ILE:HG13	0.73	2.09	18	3
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:B:125:SER:C	1:B:126:ILE:HG13	0.72	2.09	18	4
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	4
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
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:21:CYS:C	1:A:22:PHE:CD1	0.71	2.69	7	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:B:121:CYS:C	1:B:122:PHE:CD1	0.70	2.69	7	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
1:A:36:VAL:N	1:B:134:CYS:O	0.67	2.28	20	15
1:B:111:LEU:HB3	1:B:121:CYS:HB2	0.67	1.66	21	1
1:A:66:ARG:N	1:A:66:ARG:HD2	0.67	2.04	13	2
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: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:A:27:CYS:HB2	1:A:41:ALA:HA	0.66	1.68	13	1
1:B:166:ARG:HD2	1:B:166:ARG:N	0.66	2.05	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:A:59:LYS:C	1:A:66:ARG:HA	0.65	2.17	12	4
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:O	1:A:66:ARG:HD3	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:B:113:CYS:C	1:B:117:GLY:HA2	0.64	2.18	12	6
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:A:13:CYS:C	1:A:17:GLY:HA2	0.64	2.17	12	6
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	3
1:B:159:LYS:C	1:B:166:ARG:HA	0.63	2.19	12	3
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	9
1:A:38:THR:CG2	1:B:135:PHE:HD1	0.62	2.07	4	3
1:B:170:ALA:HA	1:B:185:CYS:CB	0.62	2.17	3	2
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:B:170:ALA:C	1:B:185:CYS:HB3	0.62	2.19	21	1
1:A:70:ALA:C	1:A:85:CYS:HB3	0.62	2.18	21	1
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:110:CYS:O	1:B:111:LEU:C	0.61	2.43	7	13
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:143:ARG:O	1:B:143:ARG:HD3	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:170:ALA:C	1:B:186:ASP:HA	0.61	2.20	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: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:10:CYS:O	1:A:11:LEU:C	0.60	2.43	7	13
1:A:32:LEU:HD23	1:A:35:PHE:CE1	0.60	2.30	11	1
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:70:ALA:C	1:A:86:ASP:HA	0.60	2.20	10	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: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: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:HD22	1:B:111:LEU:H	0.59	1.58	3	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:HD12	1:B:172:ILE:O	0.58	1.97	13	3
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:B:159:LYS:C	1:B:166:ARG:HB3	0.58	2.24	13	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: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: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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:15:PRO:C	1:A:17:GLY:H	0.57	2.06	4	2
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: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:H	1:A:11:LEU:HD22	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:A:32:LEU:O	1:A:33:GLY:C	0.56	2.48	15	1
1:B:111:LEU:HD12	1:B:143:ARG:CZ	0.56	2.29	18	1
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:72:ILE:O	1:A:72:ILE:HD12	0.56	1.99	13	3
1:A:33:GLY:O	1:A:69:ALA:HB3	0.56	2.00	10	1
1:A:68:ALA:HB3	1:A:72:ILE:HB	0.56	1.76	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:H	1:B:166:ARG:HD2	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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:22:PHE:CD1	1:A:22:PHE:N	0.56	2.74	14	1
1:B:118:LYS:HZ1	1:B:132:LEU:CD1	0.56	2.14	17	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:B:115:PRO:C	1:B:117:GLY:H	0.55	2.06	4	3
1:A:66:ARG:H	1:A:66:ARG:HD2	0.55	1.60	18	2
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: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:HD12	1:B:172:ILE:H	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:170:ALA:C	1:B:172:ILE:H	0.55	2.10	21	3
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:A:71:GLY:O	1:A:72:ILE:HD13	0.55	1.99	8	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:A:43:ARG:C	1:A:45:GLN:H	0.54	2.10	3	2
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:A:59:LYS:C	1:A:66:ARG:HB3	0.54	2.28	13	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:O	1:A:72:ILE:CG1	0.54	2.56	14	1
1:B:122:PHE:CD1	1:B:122:PHE:N	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
1:B:169:ALA:O	1:B:170:ALA:C	0.53	2.51	6	7
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:37:GLY:C	1:A:38:THR:HG22	0.53	2.28	21	3
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:N	1:A:66:ARG:CD	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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:O	1:B:172:ILE:CG1	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
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:A:65:GLY:HA3	1:A:75:SER:HA	0.52	1.81	3	2
1:B:159:LYS:CB	1:B:167:CYS:CB	0.52	2.88	2	1
1:A:10:CYS:HB3	1:A:20:ARG:HD3	0.52	1.82	3	1
1:A:69:ALA:O	1:A:70:ALA:C	0.52	2.52	6	6
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:B:172:ILE:O	1:B:172:ILE:HD12	0.52	2.05	21	2
1:A:72:ILE:HD12	1:A:72:ILE:C	0.52	2.29	19	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:A:35:PHE:CE2	1:B:135:PHE:CD2	0.52	2.98	6	1
1:B:165:GLY:HA2	1:B:175:SER:HA	0.52	1.82	9	3
1:B:168:ALA:HB3	1:B:174:CYS:SG	0.52	2.44	9	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:42:LEU:HD13	1:A:42:LEU:C	0.51	2.30	8	2
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:B:142:LEU:HD13	1:B:142:LEU:C	0.51	2.29	8	2
1:A:61:CYS:O	1:A:73:CYS:SG	0.51	2.69	10	1
1:A:18:LYS:HZ1	1:A:32:LEU:CD1	0.51	2.18	17	1
1:B:110:CYS:HB3	1:B:120:ARG:CD	0.51	2.35	11	2
1:A:42:LEU:C	1:A:42:LEU:HD13	0.51	2.31	15	1
1:B:159:LYS:HB3	1:B:167:CYS:H	0.51	1.65	21	1
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:28:CYS:SG	1:A:33:GLY:C	0.51	2.94	7	1
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:135:PHE:N	1:B:135:PHE:CD1	0.50	2.79	6	4
1:A:13:CYS:O	1:A:17:GLY:CA	0.50	2.59	19	2
1:A:33:GLY:HA2	1:A:69:ALA:HB2	0.50	1.83	15	2
1:A:72:ILE:HD12	1:A:72:ILE:O	0.50	2.05	3	3
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: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:28:CYS:SG	1:A:68:ALA:HB3	0.50	2.46	21	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:13:CYS:HA	1:A:43:ARG:NE	0.50	2.19	12	1
1:B:137:GLY:C	1:B:138:THR:HG22	0.50	2.31	20	2
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:A:43:ARG:C	1:A:45:GLN:N	0.50	2.70	3	1
1:B:110:CYS:HB3	1:B:120:ARG:HD3	0.50	1.83	3	1
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:B:139:ALA:C	1:B:141:ALA:N	0.50	2.69	15	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:B:172:ILE:HD12	1:B:172:ILE:C	0.50	2.31	19	1
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: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:B:142:LEU:C	1:B:142:LEU:HD13	0.49	2.31	15	1
1:A:11:LEU:HD22	1:A:11:LEU:H	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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:GLY:H	1:A:85:CYS:C	0.49	2.16	17	2
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:175:SER:C	1:B:177:ASP:H	0.49	2.16	7	6
1:B:161:CYS:O	1:B:165:GLY:O	0.49	2.31	5	3
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:B:171:GLY:H	1:B:185:CYS:C	0.49	2.16	11	2
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:82:ASP:O	1:A:82:ASP:CG	0.48	2.56	20	1
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:69:ALA:C	1:A:72:ILE:HG12	0.48	2.33	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
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:B:128:CYS:C	1:B:133:GLY:O	0.48	2.56	6	4
1:A:70:ALA:O	1:A:72:ILE:HG23	0.48	2.08	15	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:75:SER:C	1:A:77:ASP:H	0.48	2.16	7	6
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:A:75:SER:CB	1:A:76:PRO:HD2	0.48	2.39	6	3
1:A:27:CYS:C	1:A:34:CYS:SG	0.48	2.96	19	2
1:B:115:PRO:O	1:B:115:PRO:HG2	0.48	2.09	3	5
1:A:28:CYS:C	1:A:33:GLY:O	0.48	2.57	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:127:CYS:C	1:B:134:CYS:SG	0.48	2.96	19	2
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:B:137:GLY:O	1:B:138:THR:C	0.48	2.57	6	1
1:A:43:ARG:HB2	1:A:43:ARG:NH1	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:N	1:B:159:LYS:HD2	0.47	2.24	19	1
1:B:175:SER:CB	1:B:176:PRO:HD2	0.47	2.39	6	3
1:A:37:GLY:O	1:A:38:THR:C	0.47	2.57	6	1
1:B:143:ARG:HB2	1:B:143:ARG:NH1	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:B:132:LEU:O	1:B:133:GLY:C	0.47	2.57	15	1
1:B:139:ALA:C	1:B:141:ALA:H	0.47	2.15	15	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
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:182:ASP:O	1:B:182:ASP:CG	0.47	2.56	20	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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:143:ARG:C	1:B:145:GLN:H	0.46	2.17	8	4
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:H	1:B:111:LEU:HD12	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:CD1	0.46	2.89	15	1
1:B:115:PRO:C	1:B:117:GLY:N	0.46	2.74	4	3
1:A:11:LEU:HD12	1:A:11:LEU:H	0.46	1.71	7	1
1:B:112:PRO:CB	1:B:117:GLY:O	0.46	2.64	1	4
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:39:ALA:C	1:A:41:ALA:N	0.46	2.72	15	1
1:A:43:ARG:O	1:A:43:ARG:NE	0.46	2.49	18	1
1:A:66:ARG:HD3	1:A:66:ARG:C	0.46	2.36	18	1
1:B:173:CYS:SG	1:B:182:ASP:CG	0.46	2.99	7	1
1:B:111:LEU:HB3	1:B:143:ARG:NH2	0.46	2.26	18	1
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:169:ALA:C	1:B:172:ILE:HG12	0.45	2.36	8	1
1:B:166:ARG:HD3	1:B:166:ARG:C	0.45	2.36	18	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:142:LEU:C	1:B:142:LEU:CD1	0.45	2.89	15	1
1:A:35:PHE:CD2	1:B:135:PHE:HD2	0.45	2.29	12	1
1:B:143:ARG:O	1:B:143:ARG:NE	0.45	2.49	18	1
1:B:117:GLY:C	1:B:119:GLY:H	0.45	2.18	4	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: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:A:15:PRO:C	1:A:17:GLY:N	0.45	2.73	4	2
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:O	1:B:126:ILE:HG22	0.45	2.11	13	1
1:A:41:ALA:O	1:A:43:ARG:N	0.45	2.50	15	1
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:A:73:CYS:SG	1:A:82:ASP:CG	0.45	2.99	7	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:61:CYS:O	1:A:62:GLY:C	0.44	2.59	13	2
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:37:GLY:C	1:A:38:THR:CG2	0.44	2.90	21	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:A:41:ALA:O	1:A:42:LEU:C	0.44	2.60	7	3
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: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:A:24:PRO:HD2	1:B:181:GLU:CG	0.44	2.42	14	1
1:B:118:LYS:HZ3	1:B:118:LYS:H	0.44	1.55	17	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
1:A:39:ALA:CB	1:A:42:LEU:HD12	0.44	2.43	9	1
1:A:35:PHE:HD2	1:B:135:PHE:HD2	0.44	1.54	12	1
1:A:26:ILE:HG22	1:A:26:ILE:O	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: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:15:PRO:O	1:A:18:LYS:CD	0.44	2.66	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:CYS:CA	1:A:78:GLY:O	0.44	2.66	13	1
1:A:18:LYS:HZ3	1:A:19:GLY:H	0.44	1.53	17	1
1:B:135:PHE:CB	1:B:138:THR:OG1	0.44	2.66	17	1
1:B:166:ARG:H	1:B:166:ARG:CD	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:143:ARG:C	1:B:145:GLN:N	0.44	2.76	8	3
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:141:ALA:O	1:B:142:LEU:C	0.43	2.61	7	3
1:B:125:SER:O	1:B:136:VAL:C	0.43	2.61	7	1
1:B:114:GLY:HA3	1:B:140:GLU:HG2	0.43	1.86	11	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:138:THR:O	1:B:139:ALA:C	0.43	2.61	15	1
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: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
1:A:38:THR:HG21	1:B:135:PHE:CG	0.43	2.49	12	1
1:A:18:LYS:HZ1	1:A:32:LEU:HD11	0.43	1.72	17	1
1:B:127:CYS:CB	1:B:135:PHE:CD2	0.43	3.01	18	1
1:A:17:GLY:C	1:A:19:GLY:H	0.43	2.20	4	1
1:A:36:VAL:CG2	1:B:136:VAL:CB	0.43	2.96	5	1
1:A:70:ALA:C	1:A:85:CYS:O	0.43	2.62	8	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:29:GLY:HA3	1:A:32:LEU:HB2	0.43	1.90	14	2
1:A:68:ALA:HB3	1:A:72:ILE:CD1	0.43	2.41	3	1
1:A:20:ARG:CZ	1:A:20:ARG:HB2	0.43	2.43	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:70:ALA:C	1:A:72:ILE:H	0.43	2.19	21	1
1:B:113:CYS:SG	1:B:120:ARG:C	0.43	3.02	5	2
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:B:170:ALA:C	1:B:172:ILE:N	0.43	2.76	21	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:166:ARG:N	1:B:166:ARG:HD2	0.43	2.29	4	1
1:B:120:ARG:CZ	1:B:120:ARG:HB2	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:A:70:ALA:HA	1:A:85:CYS:C	0.43	2.39	13	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:182:ASP:OD1	1:B:182:ASP:C	0.42	2.62	13	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
1:B:130:ASP:OD1	1:B:130:ASP:N	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:130:ASP:CG	1:B:131:GLU:HG2	0.42	2.39	16	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:82:ASP:OD1	1:A:82:ASP:C	0.42	2.62	13	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:13:CYS:HB3	1:A:19:GLY:C	0.42	2.40	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:GLY:N	1:A:32:LEU:CD1	0.42	2.82	20	1
1:A:20:ARG:C	1:A:27:CYS:SG	0.42	3.03	15	2
1:A:66:ARG:HD2	1:A:66:ARG:N	0.42	2.30	4	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:B:144:CYS:O	1:B:145:GLN:C	0.42	2.62	10	1
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:82:ASP:OD2	1:A:85:CYS:HB2	0.42	2.15	3	2
1:A:25:SER:O	1:A:36:VAL:C	0.42	2.61	7	1
1:A:26:ILE:HD11	1:B:181:GLU:HG3	0.42	1.91	11	1
1:B:161:CYS:O	1:B:162:GLY:C	0.42	2.62	19	2
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: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:H	1:B:111:LEU:CD1	0.42	2.27	7	1
1:B:136:VAL:CG2	1:B:179:CYS:CB	0.42	2.97	7	1
1:A:72:ILE:HG21	1:B:136:VAL:C	0.42	2.39	9	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
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:33:GLY:CA	1:A:69:ALA:HB1	0.42	2.33	18	1
1:B:135:PHE:CD2	1:B:140:GLU:CD	0.42	2.98	19	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:44:CYS:O	1:A:45:GLN:C	0.41	2.62	10	1
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:O	1:A:86:ASP:OD1	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:30:ASP:CG	1:A:31:GLU:HG2	0.41	2.40	16	1
1:A:11:LEU:HB3	1:A:43:ARG:HH22	0.41	1.75	18	1
1:A:35:PHE:CD2	1:A:40:GLU:CD	0.41	2.98	19	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:125:SER:C	1:B:126:ILE:CG1	0.41	2.94	11	1
1:B:144:CYS:SG	1:B:147:GLU:HB2	0.41	2.56	11	1
1:A:21:CYS:C	1:A:22:PHE:CG	0.41	2.98	7	1
1:B:134:CYS:SG	1:B:172:ILE:CD1	0.41	2.93	7	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:13:CYS:SG	1:A:20:ARG:C	0.41	3.03	5	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:128:CYS:SG	1:B:133:GLY:C	0.41	3.04	7	1
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:38:THR:O	1:A:39:ALA:C	0.41	2.63	15	1
1:A:25:SER:HB2	1:B:181:GLU:CG	0.41	2.45	16	1
1:A:68:ALA:N	1:A:72:ILE:O	0.41	2.51	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:120:ARG:C	1:B:127:CYS:SG	0.41	3.04	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:B:158:GLN:C	1:B:160:PRO:HD2	0.41	2.40	2	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:172:ILE:CD1	1:B:174:CYS:SG	0.41	3.09	5	1
1:B:121:CYS:C	1:B:122:PHE:CG	0.41	2.98	7	1
1:B:172:ILE:HG22	1:B:180:HIS:CA	0.41	2.46	7	1
1:B:166:ARG:O	1:B:174:CYS:N	0.41	2.40	10	2
1:A:25:SER:C	1:A:26:ILE:CG1	0.41	2.93	11	1
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: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:A:70:ALA:C	1:A:72:ILE:N	0.41	2.79	21	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
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:B:112:PRO:C	1:B:119:GLY:O	0.41	2.64	17	1
1:A:59:LYS:CB	1:A:67:CYS:CB	0.40	2.98	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:137:GLY:C	1:B:138:THR:CG2	0.40	2.93	21	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:B:170:ALA:C	1:B:185:CYS:O	0.40	2.64	8	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:A:16:GLY:O	1:A:17:GLY:C	0.40	2.63	8	1
1:B:173:CYS:SG	1:B:182:ASP:HB3	0.40	2.57	9	1
1:B:170:ALA:HA	1:B:185:CYS:C	0.40	2.39	13	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:126:ILE:HG23	1:B:136:VAL:CG2	0.40	2.42	18	1
1:A:30:ASP:OD1	1:A:30:ASP:N	0.40	2.53	20	1

6.3 Torsion angles

6.3.1 Protein backbone

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%)	2	21
1	B	69/92 (75%)	50±3 (72±4%)	16±2 (23±3%)	4±2 (5±2%)	2	21
All	All	2898/3864 (75%)	2101 (72%)	637 (22%)	160 (6%)	2	21

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	A	24	PRO	17
1	B	124	PRO	17
1	A	56	SER	11
1	B	156	SER	11
1	A	57	GLY	7
1	B	157	GLY	6
1	A	70	ALA	6
1	B	170	ALA	6
1	A	86	ASP	5
1	B	186	ASP	5
1	A	59	LYS	5
1	A	60	PRO	5
1	B	159	LYS	5
1	B	160	PRO	5
1	A	71	GLY	4
1	B	171	GLY	4
1	A	62	GLY	4
1	B	116	GLY	3
1	A	44	CYS	3
1	B	111	LEU	3
1	B	162	GLY	3
1	A	16	GLY	2
1	A	45	GLN	2
1	B	145	GLN	2
1	A	11	LEU	2
1	A	38	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	B	138	THR	2
1	B	144	CYS	1
1	A	12	PRO	1
1	B	112	PRO	1
1	A	33	GLY	1
1	A	39	ALA	1
1	A	40	GLU	1
1	A	42	LEU	1
1	B	133	GLY	1
1	B	139	ALA	1
1	B	140	GLU	1
1	B	142	LEU	1
1	A	10	CYS	1
1	B	110	CYS	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	49/69 (71%)	30±3 (61±5%)	19±3 (39±5%)	0	6
1	B	49/69 (71%)	30±3 (62±6%)	19±3 (38±6%)	0	7
All	All	2058/2898 (71%)	1271 (62%)	787 (38%)	0	7

All 82 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	A	18	LYS	20
1	A	31	GLU	20
1	B	118	LYS	20
1	B	131	GLU	20
1	A	28	CYS	18
1	B	128	CYS	17
1	A	32	LEU	17
1	B	132	LEU	17

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Mol	Chain	Res	Type	Models (Total)
1	A	25	SER	14
1	A	36	VAL	14
1	B	120	ARG	14
1	A	47	GLU	13
1	A	59	LYS	13
1	B	147	GLU	13
1	B	125	SER	13
1	A	43	ARG	13
1	B	143	ARG	13
1	A	82	ASP	13
1	B	182	ASP	13
1	A	27	CYS	12
1	B	127	CYS	12
1	A	20	ARG	12
1	A	35	PHE	12
1	B	135	PHE	12
1	B	159	LYS	12
1	B	172	ILE	12
1	A	42	LEU	11
1	B	142	LEU	11
1	A	72	ILE	11
1	B	161	CYS	11
1	A	40	GLU	10
1	B	140	GLU	10
1	A	61	CYS	9
1	A	81	GLU	9
1	A	86	ASP	9
1	B	181	GLU	9
1	B	186	ASP	9
1	A	10	CYS	9
1	B	110	CYS	9
1	A	13	CYS	9
1	B	113	CYS	9
1	A	73	CYS	8
1	B	173	CYS	8
1	A	38	THR	8
1	B	138	THR	8
1	A	11	LEU	7
1	B	111	LEU	7
1	A	26	ILE	7
1	A	34	CYS	7
1	A	56	SER	7

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Mol	Chain	Res	Type	Models (Total)
1	B	126	ILE	7
1	B	136	VAL	7
1	A	21	CYS	7
1	B	121	CYS	7
1	A	45	GLN	7
1	B	145	GLN	7
1	A	46	GLU	6
1	A	79	CYS	6
1	B	134	CYS	6
1	B	146	GLU	6
1	B	156	SER	6
1	B	179	CYS	6
1	A	74	CYS	6
1	B	174	CYS	6
1	A	63	SER	6
1	B	163	SER	6
1	A	58	GLN	5
1	B	158	GLN	5
1	A	67	CYS	5
1	B	167	CYS	5
1	A	44	CYS	5
1	B	144	CYS	5
1	A	80	HIS	4
1	B	180	HIS	4
1	A	75	SER	3
1	B	175	SER	3
1	A	85	CYS	2
1	B	185	CYS	2
1	A	77	ASP	2
1	B	177	ASP	2

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 [i](#)

There are no oligosaccharides 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

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: working_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)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	86	0.46 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	154	0.58 ± 0.68	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. 658 atoms were assigned a chemical shift out of a possible 1490. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	452/694 (65%)	264/292 (90%)	70/276 (25%)	118/126 (94%)
Sidechain	204/740 (28%)	204/478 (43%)	0/236 (0%)	0/26 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	2/56 (4%)	2/28 (7%)	0/24 (0%)	0/4 (0%)
Overall	658/1490 (44%)	470/798 (59%)	70/536 (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. 860 atoms were assigned a chemical shift out of a possible 2084. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	578/912 (63%)	338/378 (89%)	86/368 (23%)	154/166 (93%)
Sidechain	280/1078 (26%)	280/700 (40%)	0/342 (0%)	0/36 (0%)
Aromatic	2/94 (2%)	2/46 (4%)	0/44 (0%)	0/4 (0%)
Overall	860/2084 (41%)	620/1124 (55%)	86/754 (11%)	154/206 (75%)

7.1.4 Statistically unusual chemical shifts ⓘ

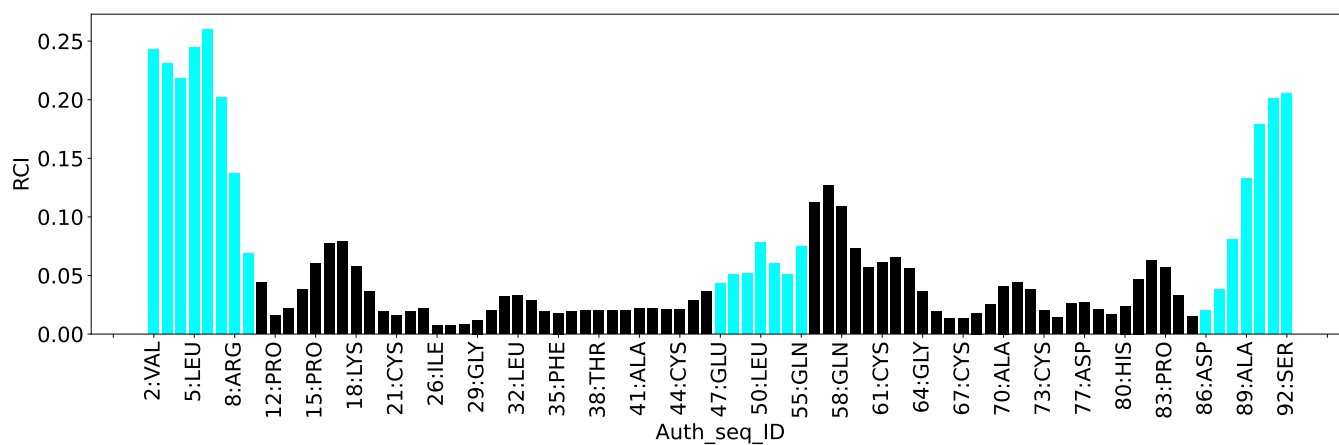
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	38	THR	HG1	4.99	0.08 – 2.19	18.2
1	B	138	THR	HG1	4.99	0.08 – 2.19	18.2

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

