



Full wwPDB NMR Structure Validation Report ⓘ

Jun 11, 2024 – 08:20 PM EDT

PDB ID : 1JAJ
BMRB ID : 5010
Title : Solution Structure of DNA Polymerase X from the African Swine Fever Virus
Authors : Maciejewski, M.W.; Shin, R.; Pan, B.; Mullen, G.P.
Deposited on : 2001-05-30

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

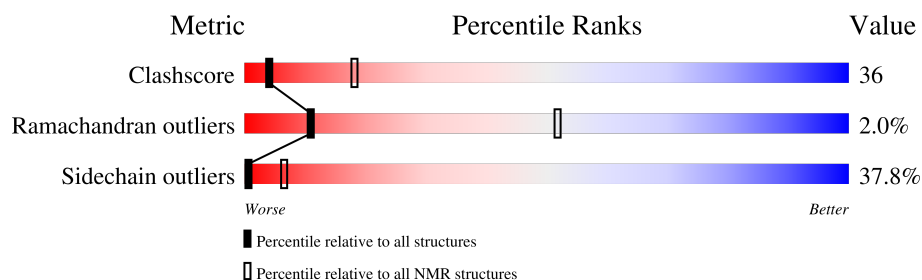
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	174	

2 Ensemble composition and analysis

This entry contains 25 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:2-A:174 (173)	0.59	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 3 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3003 atoms, of which 1570 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA POLYMERASE BETA-LIKE PROTEIN.

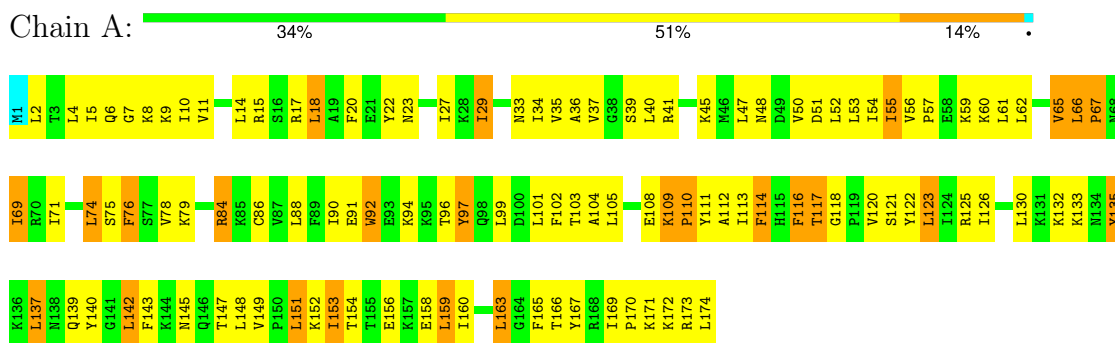
Mol	Chain	Residues	Atoms						Trace
1	A	174	Total	C	H	N	O	S	0
			3003	943	1570	248	238	4	

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: DNA POLYMERASE BETA-LIKE PROTEIN

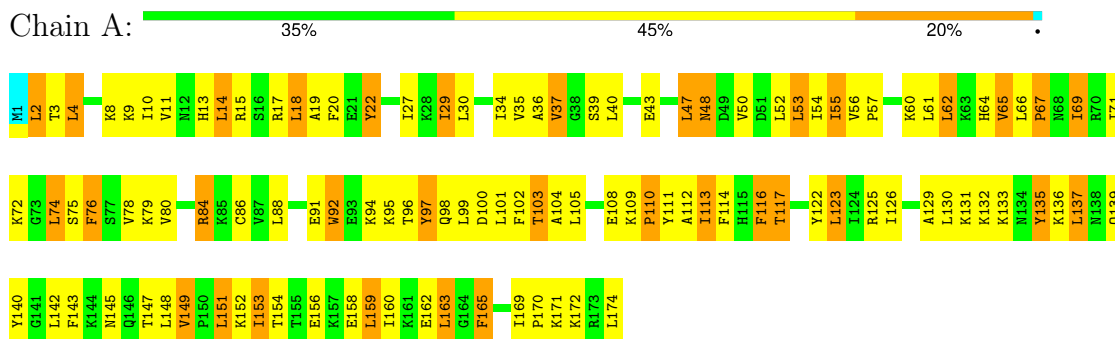


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

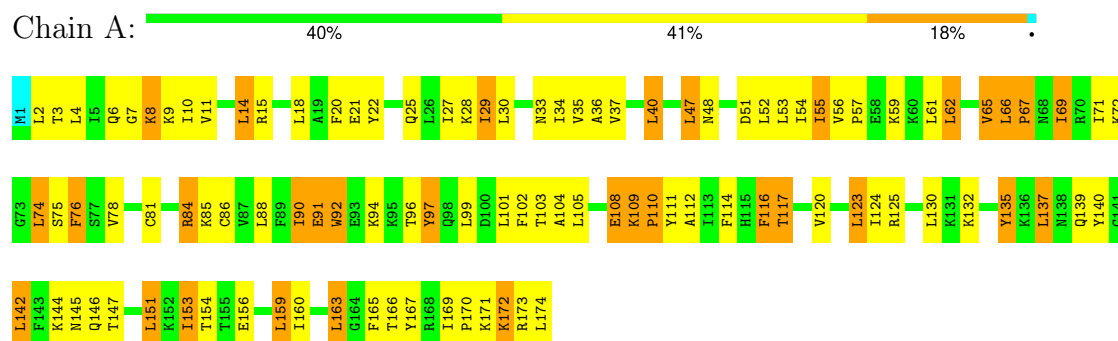
4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



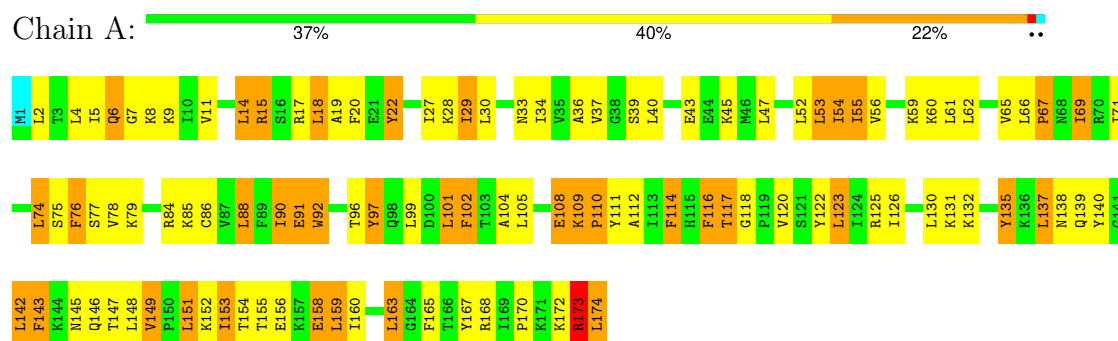
4.2.2 Score per residue for model 2

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



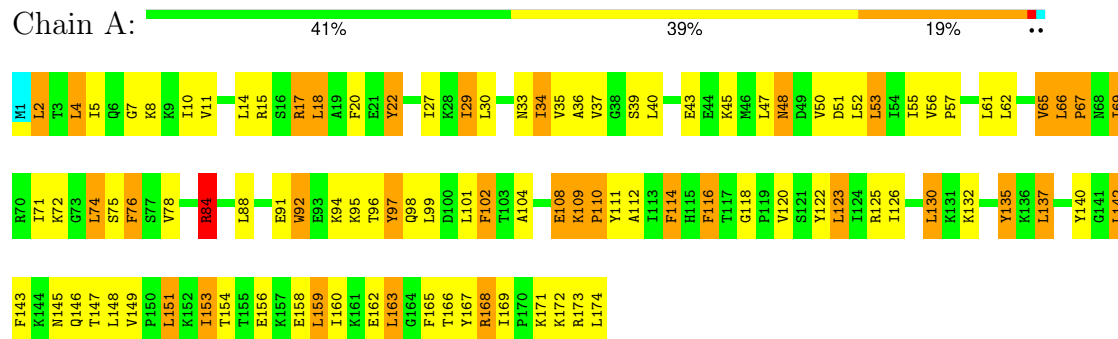
4.2.3 Score per residue for model 3

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



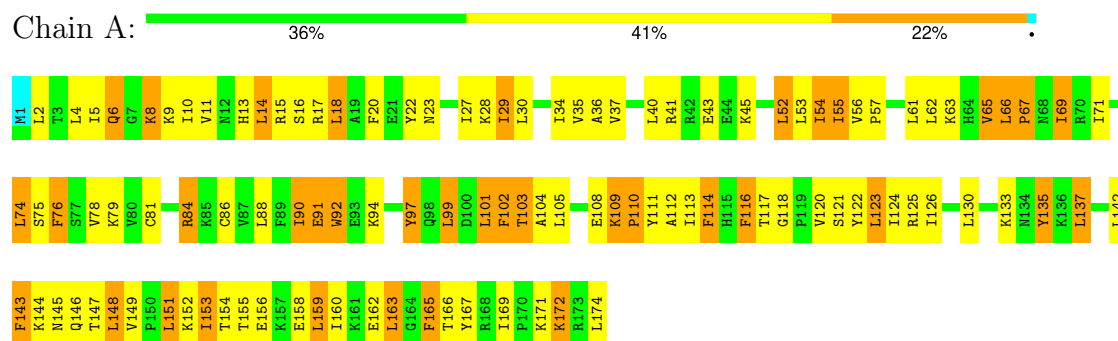
4.2.4 Score per residue for model 4

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



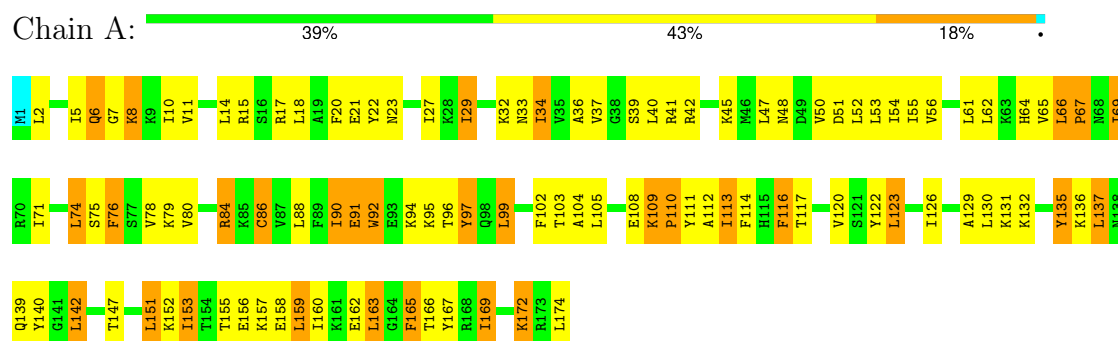
4.2.5 Score per residue for model 5

• Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



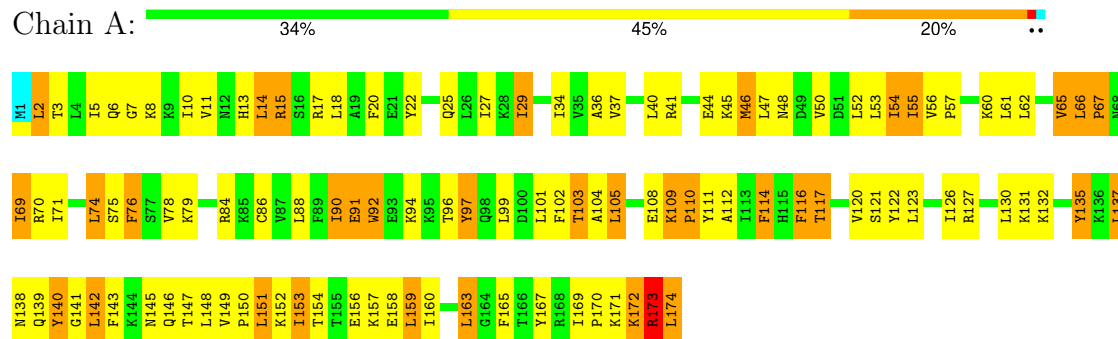
4.2.6 Score per residue for model 6

• Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



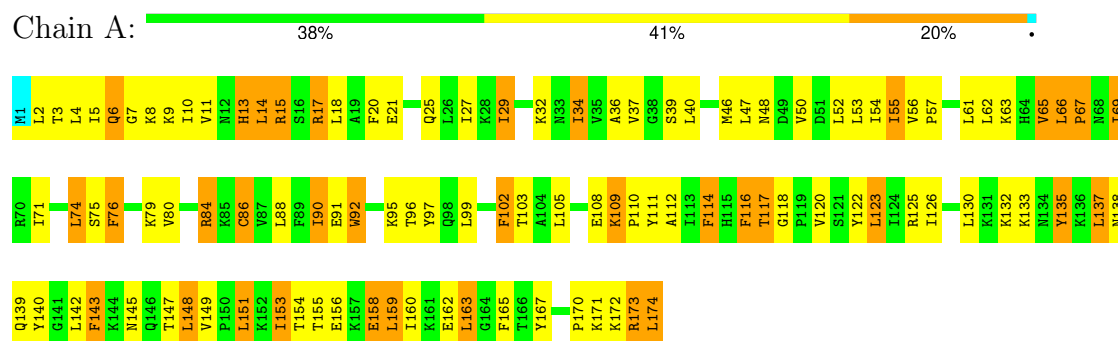
4.2.7 Score per residue for model 7

• Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



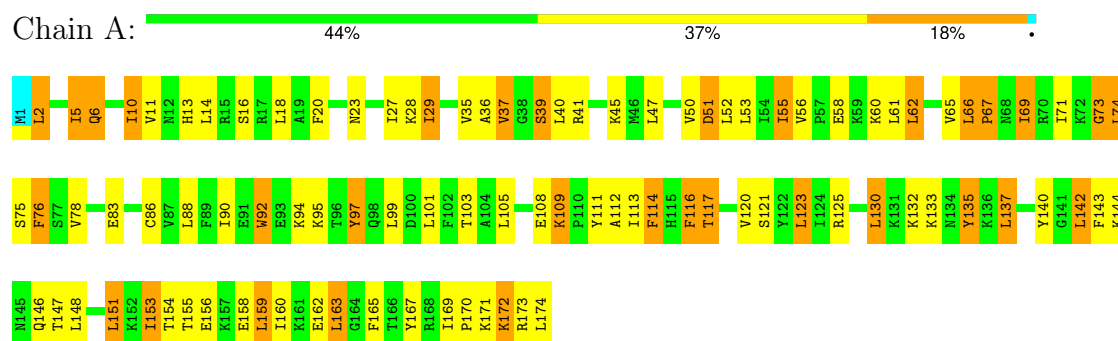
4.2.8 Score per residue for model 8

• Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



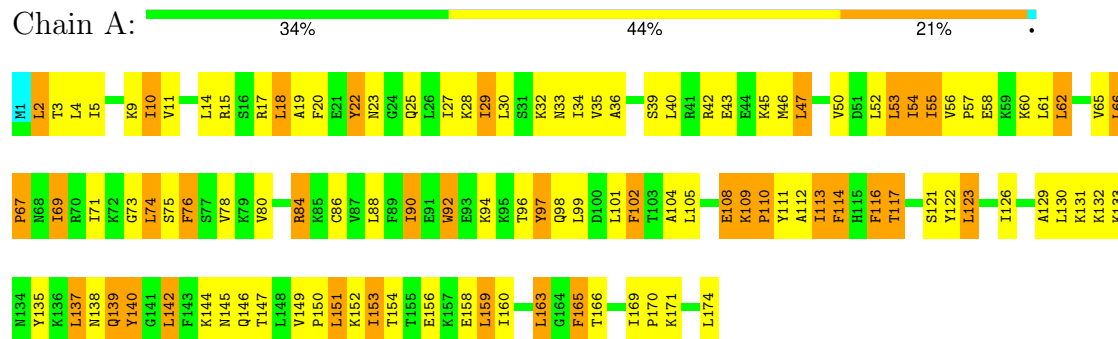
4.2.9 Score per residue for model 9

• Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



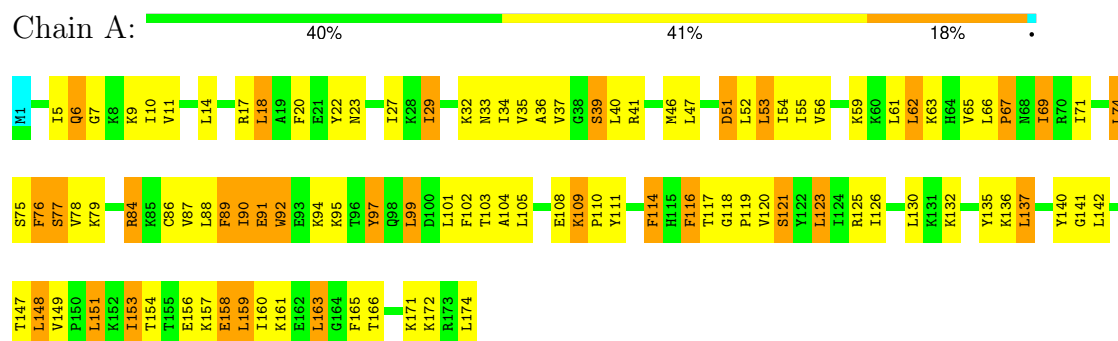
4.2.10 Score per residue for model 10

• Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



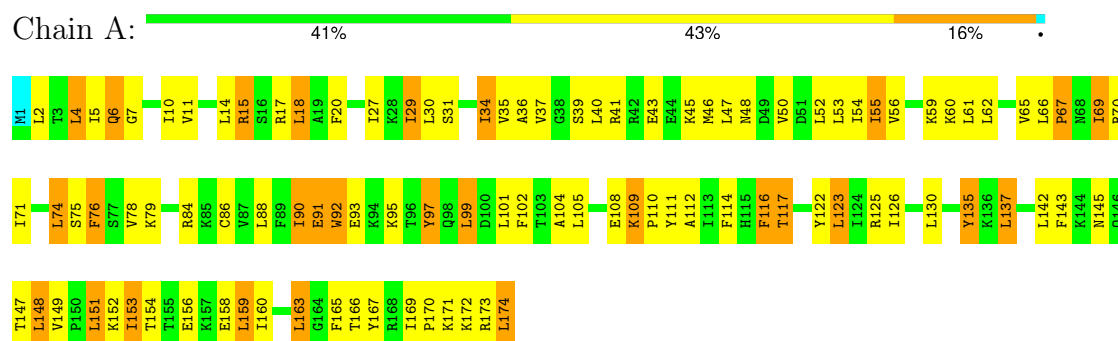
4.2.11 Score per residue for model 11

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



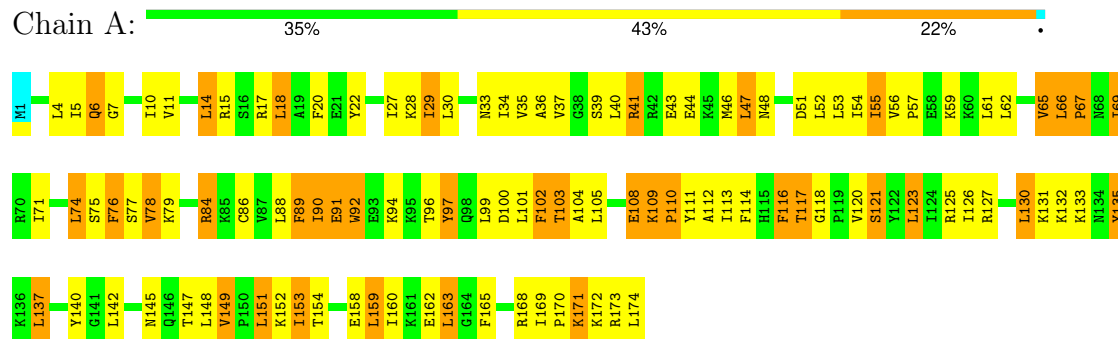
4.2.12 Score per residue for model 12

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



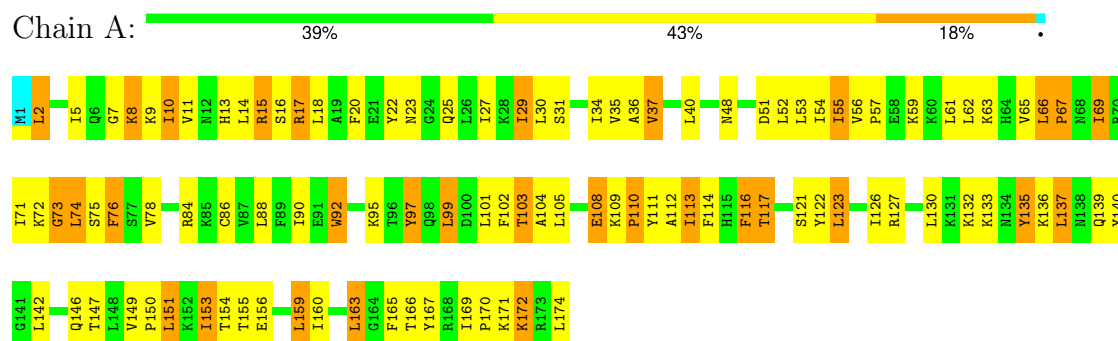
4.2.13 Score per residue for model 13

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



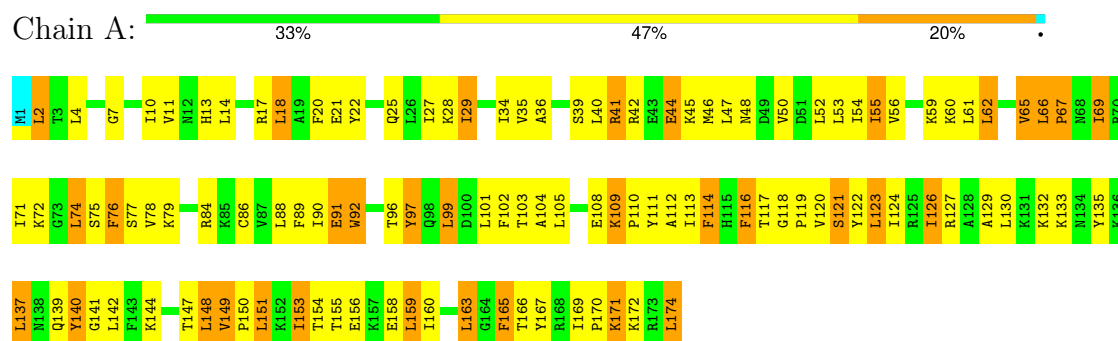
4.2.14 Score per residue for model 14

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



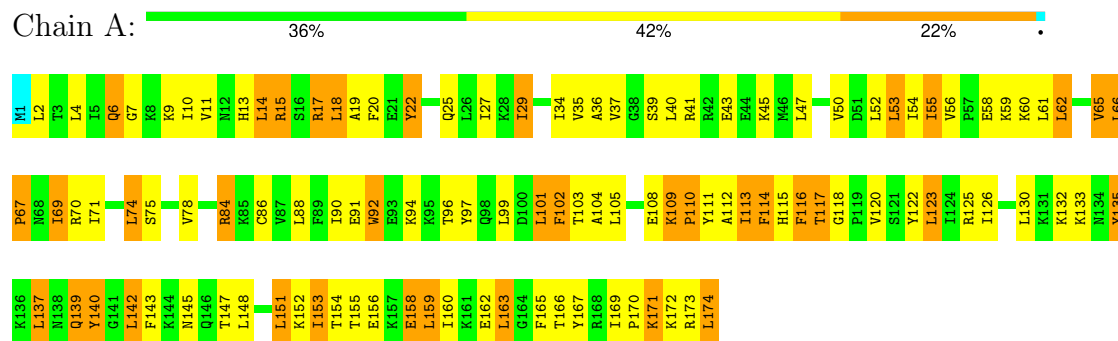
4.2.15 Score per residue for model 15

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



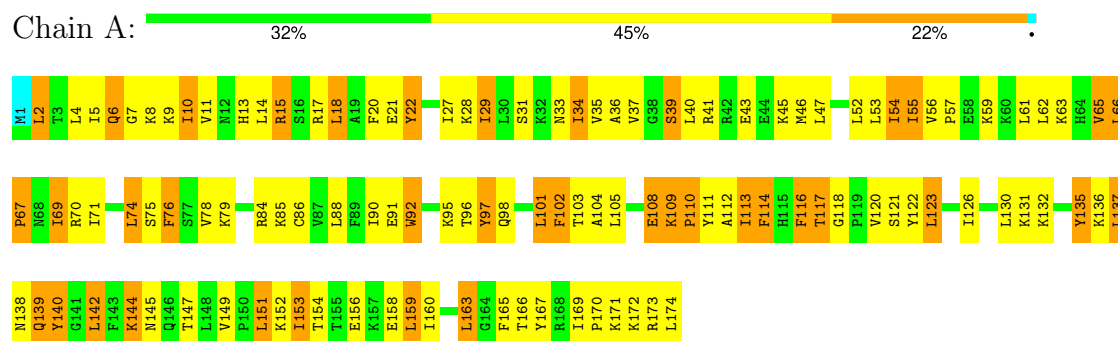
4.2.16 Score per residue for model 16

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



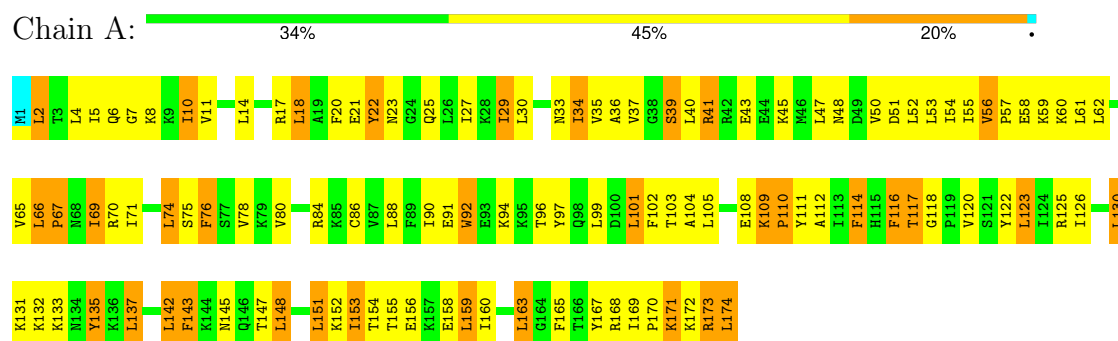
4.2.17 Score per residue for model 17

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



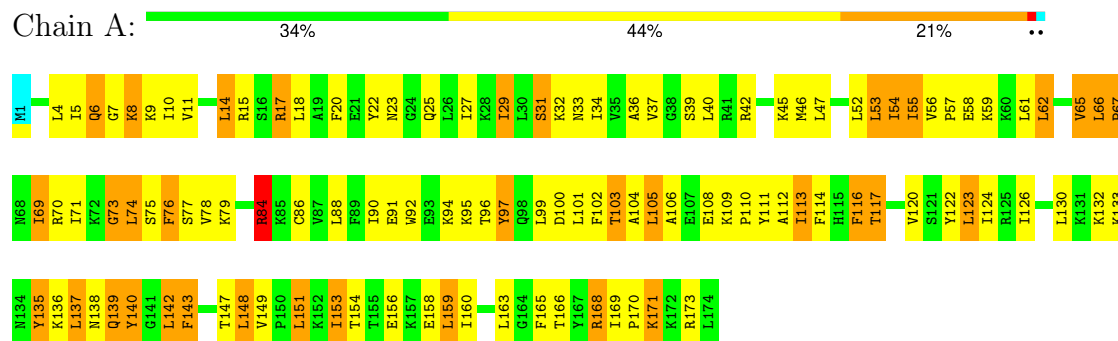
4.2.18 Score per residue for model 18

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



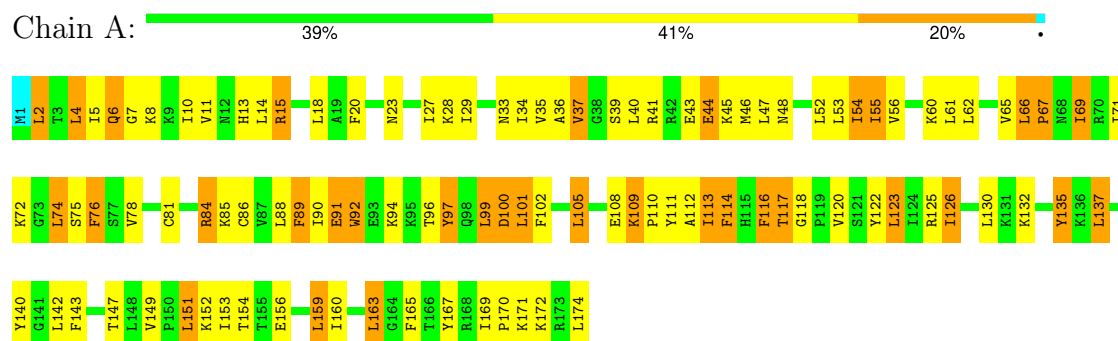
4.2.19 Score per residue for model 19

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



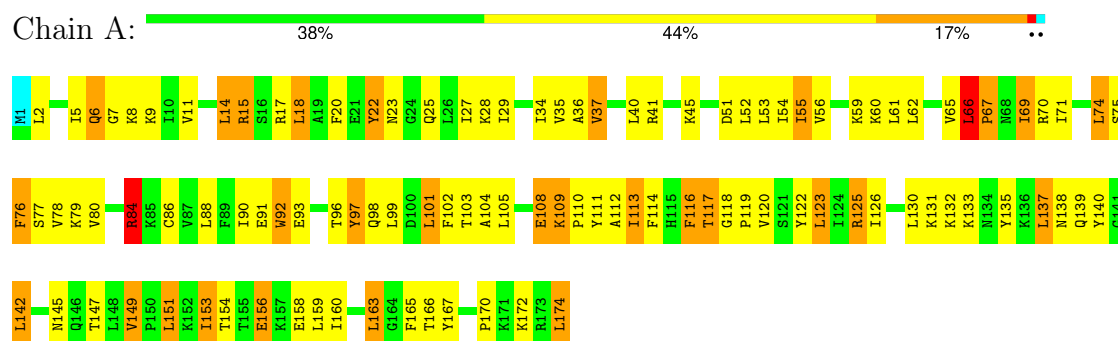
4.2.20 Score per residue for model 20

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



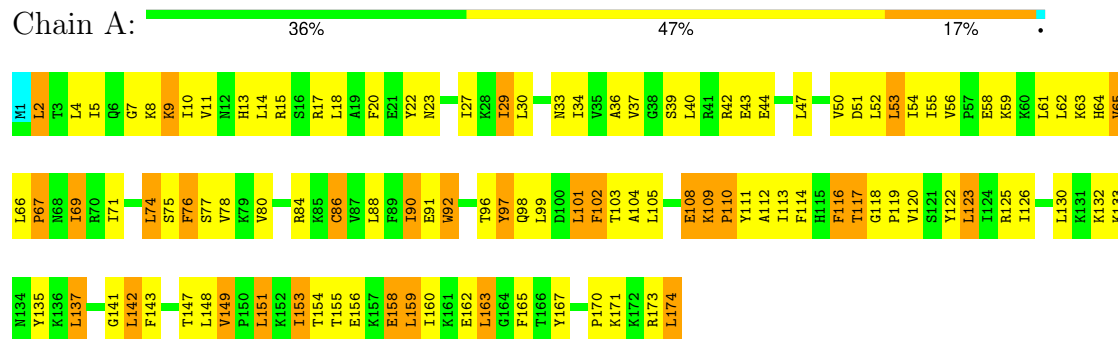
4.2.21 Score per residue for model 21

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



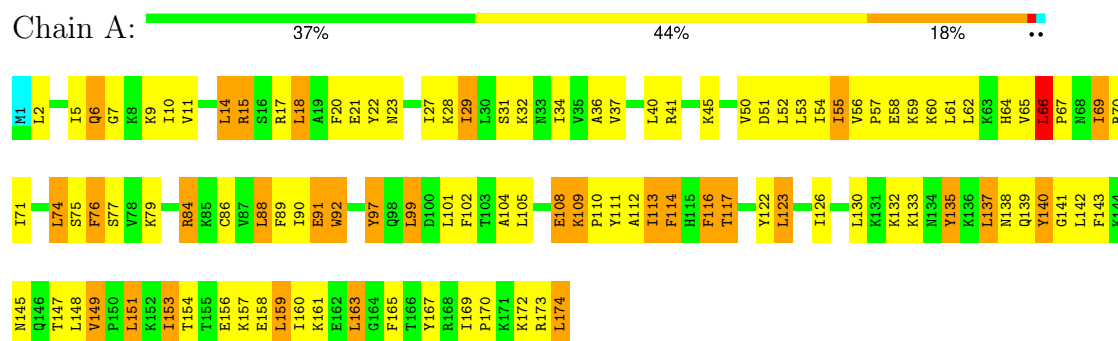
4.2.22 Score per residue for model 22

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



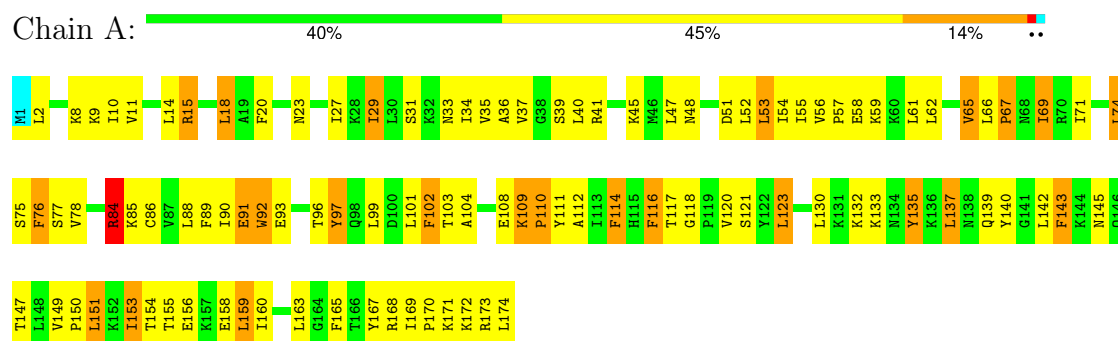
4.2.23 Score per residue for model 23

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



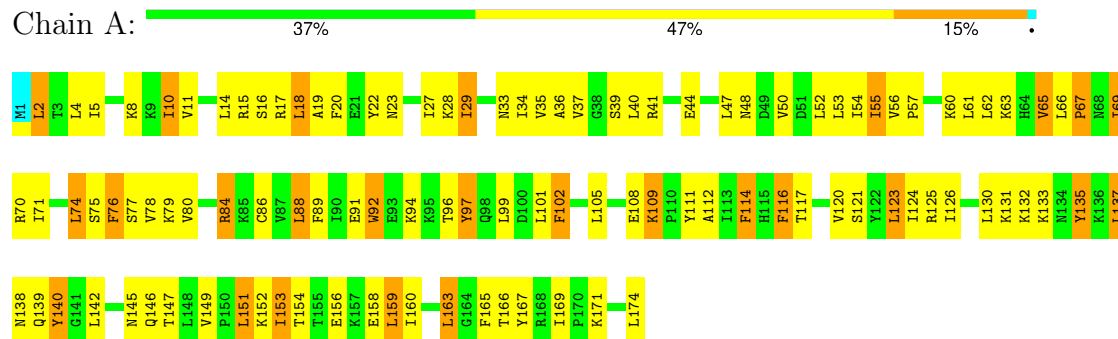
4.2.24 Score per residue for model 24

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



4.2.25 Score per residue for model 25

- Molecule 1: DNA POLYMERASE BETA-LIKE PROTEIN



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics energy minimization*.

Of the 200 calculated structures, 25 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
X-PLOR	refinement	3.851

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	2116
Number of shifts mapped to atoms	2116
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1425	1561	1558	109±10
All	All	35625	39025	38950	2721

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:VAL:HG13	1:A:52:LEU:HD11	1.02	1.28	19	11
1:A:99:LEU:HD23	1:A:101:LEU:HD11	1.00	1.33	11	3
1:A:53:LEU:HD21	1:A:112:ALA:HB3	0.98	1.34	6	4
1:A:18:LEU:HD23	1:A:29:ILE:HD12	0.97	1.32	2	3
1:A:53:LEU:HD23	1:A:112:ALA:HB1	0.97	1.33	25	3
1:A:50:VAL:HG23	1:A:99:LEU:HD12	0.96	1.35	18	5
1:A:53:LEU:HD22	1:A:113:ILE:HD12	0.96	1.35	16	5
1:A:88:LEU:HD11	1:A:99:LEU:HD11	0.96	1.38	20	5
1:A:53:LEU:HD13	1:A:113:ILE:HD12	0.94	1.35	1	3
1:A:52:LEU:HD12	1:A:99:LEU:HD11	0.94	1.36	2	1
1:A:130:LEU:HD13	1:A:137:LEU:HD21	0.94	1.39	6	13
1:A:53:LEU:HD21	1:A:113:ILE:HD12	0.93	1.39	21	1
1:A:11:VAL:HG13	1:A:52:LEU:HD21	0.93	1.38	23	5
1:A:88:LEU:HD11	1:A:101:LEU:HD11	0.92	1.37	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ALA:HB1	1:A:40:LEU:HD13	0.91	1.42	14	5
1:A:142:LEU:HD12	1:A:149:VAL:HG13	0.90	1.40	5	5
1:A:37:VAL:HG21	1:A:53:LEU:HD13	0.90	1.42	16	3
1:A:74:LEU:HD13	1:A:92:TRP:CD2	0.90	2.02	4	23
1:A:2:LEU:HD13	1:A:10:ILE:HD12	0.89	1.43	9	3
1:A:130:LEU:HD13	1:A:137:LEU:HD11	0.89	1.43	10	12
1:A:11:VAL:HG21	1:A:40:LEU:HD11	0.87	1.43	14	4
1:A:20:PHE:CZ	1:A:65:VAL:HG22	0.87	2.04	14	7
1:A:88:LEU:HD22	1:A:101:LEU:HD22	0.87	1.44	9	1
1:A:88:LEU:HD21	1:A:101:LEU:HD13	0.86	1.43	25	6
1:A:111:TYR:CZ	1:A:142:LEU:HD11	0.86	2.05	7	3
1:A:137:LEU:HD12	1:A:163:LEU:HD22	0.86	1.47	24	6
1:A:2:LEU:HD21	1:A:97:TYR:CE1	0.86	2.06	25	8
1:A:114:PHE:CG	1:A:159:LEU:HD11	0.84	2.08	7	4
1:A:69:ILE:HG21	1:A:78:VAL:CG2	0.84	2.03	1	6
1:A:156:GLU:O	1:A:160:ILE:HD12	0.84	1.73	22	21
1:A:52:LEU:CB	1:A:101:LEU:HD22	0.83	2.03	3	1
1:A:66:LEU:HD12	1:A:78:VAL:HG21	0.83	1.47	3	1
1:A:135:TYR:CE2	1:A:142:LEU:HD21	0.83	2.08	20	1
1:A:111:TYR:CE1	1:A:159:LEU:HD23	0.83	2.08	20	4
1:A:18:LEU:HD12	1:A:29:ILE:HD11	0.83	1.48	16	5
1:A:53:LEU:HD13	1:A:113:ILE:CD1	0.82	2.02	1	2
1:A:120:VAL:HG22	1:A:124:ILE:HD11	0.82	1.48	5	2
1:A:137:LEU:HD12	1:A:142:LEU:HD23	0.82	1.51	25	1
1:A:74:LEU:HD22	1:A:92:TRP:CZ3	0.82	2.08	9	3
1:A:142:LEU:CD1	1:A:149:VAL:HG13	0.81	2.05	1	7
1:A:130:LEU:CD1	1:A:137:LEU:HD21	0.81	2.04	1	12
1:A:18:LEU:HD12	1:A:29:ILE:HD12	0.81	1.51	15	1
1:A:20:PHE:CE1	1:A:27:ILE:HD13	0.81	2.11	4	3
1:A:61:LEU:O	1:A:65:VAL:HG23	0.81	1.75	14	25
1:A:88:LEU:HD11	1:A:101:LEU:CD1	0.81	2.05	3	1
1:A:53:LEU:HD21	1:A:112:ALA:CB	0.81	2.06	16	4
1:A:76:PHE:CD2	1:A:88:LEU:HD11	0.81	2.11	18	3
1:A:111:TYR:CE1	1:A:159:LEU:HD21	0.80	2.10	21	1
1:A:53:LEU:HD22	1:A:113:ILE:CD1	0.80	2.06	16	2
1:A:53:LEU:HD21	1:A:113:ILE:CD1	0.80	2.06	21	1
1:A:66:LEU:HD21	1:A:78:VAL:HG22	0.80	1.52	22	2
1:A:2:LEU:HD11	1:A:97:TYR:CE2	0.80	2.11	14	5
1:A:35:VAL:HG11	1:A:113:ILE:HD11	0.80	1.54	21	1
1:A:111:TYR:OH	1:A:142:LEU:HD23	0.79	1.77	8	5
1:A:53:LEU:HD11	1:A:116:PHE:CD2	0.79	2.12	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:TYR:CE2	1:A:151:LEU:HD12	0.79	2.13	24	17
1:A:142:LEU:HD13	1:A:151:LEU:HD12	0.79	1.51	7	1
1:A:135:TYR:CE1	1:A:142:LEU:HD12	0.78	2.14	16	6
1:A:159:LEU:HD13	1:A:160:ILE:N	0.78	1.93	22	4
1:A:111:TYR:OH	1:A:142:LEU:HD22	0.78	1.78	16	9
1:A:142:LEU:CD2	1:A:149:VAL:HG13	0.77	2.09	3	1
1:A:111:TYR:CZ	1:A:159:LEU:HD21	0.77	2.14	21	1
1:A:71:ILE:HD12	1:A:76:PHE:CD1	0.77	2.14	14	3
1:A:36:ALA:CB	1:A:40:LEU:HD22	0.77	2.09	2	5
1:A:142:LEU:O	1:A:149:VAL:HG23	0.77	1.79	15	2
1:A:3:THR:HG22	1:A:46:MET:CE	0.77	2.09	7	2
1:A:34:ILE:CG2	1:A:52:LEU:HD11	0.76	2.11	21	1
1:A:50:VAL:HG22	1:A:97:TYR:CE1	0.76	2.16	22	1
1:A:142:LEU:HB2	1:A:149:VAL:HG13	0.76	1.57	12	4
1:A:111:TYR:CD1	1:A:159:LEU:HD23	0.76	2.16	7	4
1:A:104:ALA:HB1	1:A:108:GLU:HB2	0.76	1.57	19	4
1:A:18:LEU:HD11	1:A:76:PHE:CE2	0.76	2.16	9	1
1:A:88:LEU:HD11	1:A:99:LEU:HD23	0.75	1.56	7	3
1:A:142:LEU:HD12	1:A:149:VAL:O	0.75	1.81	4	4
1:A:2:LEU:HD21	1:A:97:TYR:CZ	0.75	2.17	25	4
1:A:74:LEU:HD13	1:A:92:TRP:CE3	0.75	2.17	16	18
1:A:71:ILE:HG21	1:A:74:LEU:HD23	0.75	1.58	14	1
1:A:142:LEU:CD1	1:A:151:LEU:HD12	0.74	2.11	7	2
1:A:53:LEU:HD23	1:A:113:ILE:HD12	0.74	1.57	19	2
1:A:169:ILE:HD12	1:A:171:LYS:CG	0.74	2.12	14	15
1:A:2:LEU:HD11	1:A:97:TYR:OH	0.74	1.83	5	7
1:A:34:ILE:HD11	1:A:54:ILE:HD13	0.74	1.57	1	1
1:A:2:LEU:HD11	1:A:97:TYR:CZ	0.74	2.17	4	8
1:A:142:LEU:HD23	1:A:163:LEU:HD22	0.74	1.58	10	1
1:A:36:ALA:HB1	1:A:40:LEU:HD23	0.74	1.58	5	1
1:A:114:PHE:CD2	1:A:123:LEU:HD11	0.73	2.18	24	23
1:A:117:THR:HG21	1:A:170:PRO:CB	0.73	2.13	21	14
1:A:169:ILE:HD11	1:A:172:LYS:HD3	0.73	1.60	2	3
1:A:29:ILE:HG22	1:A:34:ILE:HD11	0.73	1.60	3	1
1:A:11:VAL:CG1	1:A:52:LEU:HD21	0.73	2.14	24	14
1:A:56:VAL:HG11	1:A:62:LEU:N	0.73	1.99	22	22
1:A:56:VAL:HG21	1:A:62:LEU:HG	0.73	1.60	21	8
1:A:34:ILE:HG23	1:A:52:LEU:HD22	0.73	1.59	6	10
1:A:11:VAL:CG1	1:A:52:LEU:HD11	0.73	2.13	13	4
1:A:56:VAL:O	1:A:105:LEU:HD13	0.73	1.84	16	21
1:A:55:ILE:HG22	1:A:105:LEU:O	0.73	1.83	21	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:VAL:HG23	1:A:99:LEU:CD1	0.73	2.14	4	2
1:A:35:VAL:CG1	1:A:113:ILE:HD11	0.73	2.13	21	1
1:A:35:VAL:HG21	1:A:109:LYS:HE2	0.72	1.60	25	1
1:A:53:LEU:HD23	1:A:112:ALA:CB	0.72	2.13	25	1
1:A:104:ALA:HB1	1:A:108:GLU:HB3	0.72	1.60	12	15
1:A:111:TYR:CE1	1:A:159:LEU:HD13	0.72	2.18	12	18
1:A:35:VAL:HG21	1:A:109:LYS:NZ	0.72	1.99	20	4
1:A:88:LEU:CD2	1:A:101:LEU:HD12	0.72	2.15	21	2
1:A:10:ILE:HD13	1:A:97:TYR:CE2	0.72	2.19	17	4
1:A:53:LEU:HD11	1:A:112:ALA:CB	0.71	2.15	1	3
1:A:104:ALA:HB1	1:A:108:GLU:CB	0.71	2.15	19	6
1:A:71:ILE:HD11	1:A:76:PHE:CD2	0.71	2.20	6	19
1:A:66:LEU:HD11	1:A:78:VAL:HG22	0.71	1.60	21	2
1:A:55:ILE:HD12	1:A:109:LYS:HD2	0.71	1.62	25	1
1:A:35:VAL:HG21	1:A:109:LYS:HE3	0.71	1.61	21	7
1:A:88:LEU:HD11	1:A:99:LEU:CD2	0.71	2.14	7	2
1:A:39:SER:OG	1:A:50:VAL:HG12	0.71	1.84	15	5
1:A:53:LEU:HD11	1:A:112:ALA:HB3	0.71	1.62	10	1
1:A:34:ILE:HG23	1:A:52:LEU:HD11	0.71	1.60	21	1
1:A:7:GLY:O	1:A:11:VAL:HG23	0.71	1.85	13	19
1:A:88:LEU:HD21	1:A:101:LEU:HD11	0.71	1.63	20	1
1:A:66:LEU:HD22	1:A:80:VAL:HB	0.71	1.61	22	3
1:A:37:VAL:CG2	1:A:53:LEU:HD13	0.71	2.16	25	1
1:A:69:ILE:HG21	1:A:78:VAL:HG21	0.71	1.62	1	3
1:A:18:LEU:HD23	1:A:29:ILE:CD1	0.71	2.15	8	3
1:A:18:LEU:HD12	1:A:29:ILE:CD1	0.71	2.16	15	7
1:A:149:VAL:HG12	1:A:150:PRO:HD2	0.71	1.63	15	2
1:A:53:LEU:HD13	1:A:53:LEU:O	0.70	1.86	3	7
1:A:15:ARG:CB	1:A:34:ILE:HG21	0.70	2.16	7	21
1:A:36:ALA:HB1	1:A:40:LEU:HG	0.70	1.63	13	18
1:A:137:LEU:CD1	1:A:163:LEU:HD22	0.70	2.16	18	5
1:A:142:LEU:HD22	1:A:149:VAL:HG13	0.70	1.64	3	1
1:A:36:ALA:HB1	1:A:40:LEU:HD22	0.70	1.64	2	4
1:A:117:THR:HG21	1:A:170:PRO:HB3	0.70	1.62	21	12
1:A:39:SER:HB3	1:A:47:LEU:HD13	0.70	1.63	10	7
1:A:88:LEU:HD23	1:A:101:LEU:HD11	0.70	1.63	22	2
1:A:142:LEU:HD13	1:A:163:LEU:HD23	0.70	1.61	24	1
1:A:69:ILE:HG23	1:A:76:PHE:CZ	0.70	2.22	13	17
1:A:53:LEU:HD13	1:A:112:ALA:HB1	0.70	1.63	19	4
1:A:29:ILE:CG2	1:A:34:ILE:HD11	0.69	2.17	3	2
1:A:8:LYS:CE	1:A:40:LEU:HD23	0.69	2.16	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:TYR:OH	1:A:142:LEU:HD12	0.69	1.86	20	2
1:A:53:LEU:CD2	1:A:113:ILE:HD12	0.69	2.16	19	6
1:A:34:ILE:HG23	1:A:52:LEU:HD21	0.69	1.62	21	1
1:A:66:LEU:O	1:A:66:LEU:HD22	0.69	1.88	23	1
1:A:142:LEU:HD21	1:A:163:LEU:HD22	0.69	1.62	25	1
1:A:135:TYR:CD1	1:A:142:LEU:HD11	0.68	2.21	17	1
1:A:111:TYR:CE1	1:A:159:LEU:HD11	0.68	2.22	21	1
1:A:10:ILE:O	1:A:14:LEU:HD23	0.68	1.87	9	13
1:A:52:LEU:HB2	1:A:101:LEU:HD22	0.68	1.64	3	2
1:A:137:LEU:HG	1:A:163:LEU:HD13	0.68	1.64	4	17
1:A:20:PHE:HB3	1:A:69:ILE:HD12	0.68	1.66	1	24
1:A:155:THR:HG22	1:A:158:GLU:OE2	0.68	1.88	8	2
1:A:90:ILE:HG23	1:A:99:LEU:HD21	0.68	1.64	20	5
1:A:111:TYR:CD1	1:A:159:LEU:HD13	0.68	2.23	15	16
1:A:88:LEU:HD11	1:A:99:LEU:CD1	0.68	2.19	15	4
1:A:69:ILE:HG21	1:A:78:VAL:HG23	0.67	1.66	6	3
1:A:169:ILE:HD12	1:A:171:LYS:HG2	0.67	1.65	14	10
1:A:88:LEU:CD2	1:A:101:LEU:HD22	0.67	2.19	14	5
1:A:88:LEU:CD2	1:A:101:LEU:HD13	0.67	2.19	1	7
1:A:111:TYR:OH	1:A:142:LEU:HD21	0.67	1.88	7	3
1:A:126:ILE:O	1:A:130:LEU:HD12	0.67	1.88	25	3
1:A:142:LEU:HD21	1:A:162:GLU:HG3	0.67	1.65	13	6
1:A:135:TYR:CE1	1:A:142:LEU:HD23	0.67	2.23	7	2
1:A:52:LEU:HB3	1:A:101:LEU:HD22	0.67	1.67	3	1
1:A:39:SER:CB	1:A:47:LEU:HD13	0.67	2.20	10	2
1:A:29:ILE:C	1:A:30:LEU:HD22	0.66	2.10	5	2
1:A:142:LEU:HB3	1:A:149:VAL:HG13	0.66	1.66	20	1
1:A:55:ILE:HG21	1:A:109:LYS:HB2	0.66	1.66	21	19
1:A:71:ILE:HG21	1:A:74:LEU:CD2	0.66	2.20	10	2
1:A:142:LEU:HD13	1:A:149:VAL:HG13	0.66	1.68	10	2
1:A:56:VAL:HG21	1:A:62:LEU:HD13	0.66	1.68	14	3
1:A:141:GLY:C	1:A:142:LEU:HD12	0.66	2.10	11	1
1:A:34:ILE:CG2	1:A:52:LEU:HD22	0.66	2.19	18	6
1:A:99:LEU:HD23	1:A:101:LEU:CD1	0.66	2.18	11	1
1:A:53:LEU:HD22	1:A:112:ALA:HB3	0.66	1.66	19	2
1:A:15:ARG:HB3	1:A:34:ILE:HG21	0.66	1.67	7	12
1:A:71:ILE:HD13	1:A:74:LEU:HD23	0.65	1.67	2	6
1:A:88:LEU:HD22	1:A:101:LEU:CD2	0.65	2.21	9	1
1:A:88:LEU:CD2	1:A:101:LEU:HD11	0.65	2.21	16	2
1:A:88:LEU:HD21	1:A:101:LEU:HD12	0.65	1.69	17	2
1:A:135:TYR:CZ	1:A:142:LEU:HD21	0.65	2.27	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:HD11	1:A:78:VAL:CG2	0.65	2.21	21	1
1:A:108:GLU:O	1:A:112:ALA:HB2	0.65	1.90	23	16
1:A:62:LEU:HD21	1:A:103:THR:HB	0.65	1.69	1	4
1:A:74:LEU:HD13	1:A:92:TRP:CG	0.65	2.26	24	13
1:A:159:LEU:HG	1:A:160:ILE:HD13	0.65	1.68	13	4
1:A:8:LYS:HA	1:A:40:LEU:HD11	0.65	1.67	19	1
1:A:11:VAL:CG1	1:A:52:LEU:HD13	0.65	2.22	17	4
1:A:74:LEU:HD12	1:A:91:GLU:O	0.65	1.91	24	21
1:A:36:ALA:CB	1:A:40:LEU:HD23	0.65	2.21	5	1
1:A:69:ILE:HG21	1:A:78:VAL:CG1	0.64	2.22	10	14
1:A:111:TYR:CD1	1:A:159:LEU:HD11	0.64	2.27	21	1
1:A:160:ILE:HG21	1:A:166:THR:O	0.64	1.92	19	12
1:A:159:LEU:HD22	1:A:159:LEU:O	0.64	1.92	20	4
1:A:136:LYS:C	1:A:137:LEU:HD13	0.64	2.12	19	3
1:A:135:TYR:CE1	1:A:142:LEU:HD11	0.64	2.26	17	1
1:A:62:LEU:HD13	1:A:103:THR:HB	0.64	1.69	17	1
1:A:109:LYS:O	1:A:112:ALA:HB3	0.64	1.92	9	3
1:A:29:ILE:C	1:A:30:LEU:HD12	0.64	2.12	10	8
1:A:137:LEU:N	1:A:137:LEU:HD13	0.64	2.08	21	11
1:A:39:SER:CB	1:A:47:LEU:HD21	0.64	2.23	13	1
1:A:122:TYR:CZ	1:A:126:ILE:HD11	0.64	2.28	18	4
1:A:33:ASN:HA	1:A:55:ILE:HD11	0.64	1.70	6	8
1:A:66:LEU:HD13	1:A:66:LEU:O	0.64	1.93	9	1
1:A:142:LEU:N	1:A:142:LEU:HD23	0.64	2.08	19	6
1:A:151:LEU:N	1:A:151:LEU:HD13	0.64	2.08	23	8
1:A:88:LEU:HD12	1:A:99:LEU:HD11	0.64	1.70	3	1
1:A:2:LEU:HD13	1:A:10:ILE:CD1	0.64	2.23	18	4
1:A:35:VAL:HG21	1:A:109:LYS:CE	0.63	2.23	21	13
1:A:78:VAL:CG1	1:A:88:LEU:HD23	0.63	2.23	11	1
1:A:53:LEU:HD12	1:A:53:LEU:O	0.63	1.93	21	1
1:A:76:PHE:CD2	1:A:88:LEU:HD21	0.63	2.28	11	1
1:A:135:TYR:CE2	1:A:142:LEU:HD23	0.63	2.29	11	1
1:A:88:LEU:HD21	1:A:101:LEU:CD1	0.63	2.23	14	6
1:A:17:ARG:HG3	1:A:71:ILE:HG23	0.63	1.71	17	5
1:A:88:LEU:HD23	1:A:101:LEU:CD1	0.63	2.23	22	3
1:A:20:PHE:CZ	1:A:27:ILE:HG21	0.63	2.29	17	25
1:A:137:LEU:HD22	1:A:137:LEU:H	0.63	1.54	23	25
1:A:88:LEU:HD23	1:A:101:LEU:HD13	0.63	1.68	23	3
1:A:55:ILE:HG21	1:A:109:LYS:HB3	0.63	1.69	4	3
1:A:66:LEU:HD23	1:A:66:LEU:O	0.63	1.93	18	3
1:A:169:ILE:HD11	1:A:172:LYS:CG	0.62	2.25	23	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:LEU:HD22	1:A:137:LEU:N	0.62	2.09	1	15
1:A:39:SER:CB	1:A:47:LEU:HD22	0.62	2.25	22	6
1:A:57:PRO:HD2	1:A:61:LEU:HD23	0.62	1.70	4	8
1:A:69:ILE:HG21	1:A:78:VAL:HG12	0.62	1.70	24	3
1:A:53:LEU:HD23	1:A:113:ILE:CD1	0.62	2.25	19	2
1:A:69:ILE:HG21	1:A:78:VAL:HG22	0.62	1.71	13	1
1:A:143:PHE:CE2	1:A:148:LEU:HD13	0.62	2.29	1	4
1:A:153:ILE:HG21	1:A:158:GLU:O	0.62	1.93	5	21
1:A:142:LEU:O	1:A:149:VAL:HG12	0.61	1.94	17	1
1:A:11:VAL:HG13	1:A:52:LEU:CD1	0.61	2.24	12	5
1:A:29:ILE:HD13	1:A:54:ILE:CD1	0.61	2.26	24	2
1:A:142:LEU:HD23	1:A:143:PHE:N	0.61	2.10	20	1
1:A:11:VAL:HG21	1:A:40:LEU:HD21	0.61	1.71	8	6
1:A:142:LEU:HD11	1:A:162:GLU:OE2	0.61	1.94	16	1
1:A:88:LEU:HD22	1:A:101:LEU:HD12	0.61	1.71	21	1
1:A:35:VAL:HG11	1:A:113:ILE:CD1	0.61	2.24	21	1
1:A:135:TYR:CE2	1:A:142:LEU:HD22	0.61	2.30	25	1
1:A:17:ARG:O	1:A:71:ILE:HG23	0.61	1.94	10	1
1:A:114:PHE:CE2	1:A:123:LEU:HD11	0.61	2.30	21	6
1:A:18:LEU:HD21	1:A:76:PHE:CE2	0.61	2.30	3	5
1:A:159:LEU:HD22	1:A:159:LEU:C	0.61	2.16	20	3
1:A:36:ALA:HB1	1:A:40:LEU:CD1	0.61	2.22	14	3
1:A:56:VAL:HG21	1:A:62:LEU:CG	0.61	2.25	3	3
1:A:114:PHE:CD1	1:A:159:LEU:HD11	0.61	2.30	7	4
1:A:4:LEU:HD12	1:A:47:LEU:HD11	0.61	1.71	25	3
1:A:156:GLU:OE2	1:A:160:ILE:HD11	0.61	1.96	21	1
1:A:4:LEU:HD11	1:A:43:GLU:CB	0.61	2.26	5	6
1:A:88:LEU:CD1	1:A:99:LEU:HD23	0.60	2.25	25	2
1:A:29:ILE:HG22	1:A:34:ILE:HG12	0.60	1.72	15	4
1:A:111:TYR:OH	1:A:142:LEU:HD11	0.60	1.96	11	4
1:A:78:VAL:HG12	1:A:88:LEU:HD23	0.60	1.72	11	1
1:A:8:LYS:HE2	1:A:40:LEU:HD23	0.60	1.73	2	1
1:A:2:LEU:HD21	1:A:97:TYR:OH	0.60	1.97	20	4
1:A:11:VAL:HG21	1:A:40:LEU:CD1	0.60	2.24	14	1
1:A:142:LEU:HD21	1:A:151:LEU:HD12	0.60	1.74	14	1
1:A:121:SER:CB	1:A:174:LEU:HD13	0.60	2.27	17	1
1:A:66:LEU:HD13	1:A:69:ILE:HD13	0.60	1.74	25	1
1:A:160:ILE:HD13	1:A:167:TYR:CD1	0.60	2.31	9	12
1:A:66:LEU:HD13	1:A:66:LEU:N	0.60	2.12	8	4
1:A:18:LEU:HD13	1:A:19:ALA:N	0.60	2.11	3	5
1:A:62:LEU:HD21	1:A:103:THR:OG1	0.60	1.97	9	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:ILE:HD11	1:A:76:PHE:CG	0.60	2.32	19	5
1:A:62:LEU:CD1	1:A:105:LEU:HD22	0.59	2.27	15	3
1:A:56:VAL:HG11	1:A:62:LEU:CA	0.59	2.26	25	4
1:A:14:LEU:HD21	1:A:74:LEU:CD2	0.59	2.27	23	9
1:A:71:ILE:HG21	1:A:74:LEU:HG	0.59	1.73	10	3
1:A:88:LEU:HB3	1:A:101:LEU:HD13	0.59	1.73	11	1
1:A:53:LEU:HG	1:A:113:ILE:HD12	0.59	1.73	22	1
1:A:66:LEU:N	1:A:67:PRO:CD	0.59	2.65	23	24
1:A:11:VAL:HG11	1:A:52:LEU:HD21	0.59	1.73	6	1
1:A:137:LEU:HD12	1:A:142:LEU:CD2	0.59	2.27	25	1
1:A:55:ILE:HD12	1:A:55:ILE:O	0.59	1.98	18	8
1:A:88:LEU:HD21	1:A:101:LEU:HD22	0.59	1.73	1	3
1:A:135:TYR:CE2	1:A:142:LEU:HD11	0.59	2.33	23	2
1:A:111:TYR:HH	1:A:142:LEU:HD22	0.58	1.57	16	2
1:A:99:LEU:HD22	1:A:101:LEU:HD11	0.58	1.74	14	1
1:A:142:LEU:HD21	1:A:163:LEU:CD2	0.58	2.28	25	1
1:A:160:ILE:HG21	1:A:166:THR:C	0.58	2.18	2	3
1:A:2:LEU:HD12	1:A:6:GLN:HG2	0.58	1.75	23	4
1:A:99:LEU:HD22	1:A:101:LEU:CD1	0.58	2.28	14	1
1:A:130:LEU:HD22	1:A:135:TYR:HB3	0.58	1.74	24	22
1:A:18:LEU:HD22	1:A:71:ILE:HG12	0.58	1.75	16	6
1:A:153:ILE:HD13	1:A:153:ILE:N	0.58	2.12	19	15
1:A:2:LEU:HD23	1:A:97:TYR:CE1	0.58	2.33	6	3
1:A:29:ILE:CG2	1:A:34:ILE:HD12	0.58	2.28	8	5
1:A:66:LEU:HD11	1:A:80:VAL:HB	0.58	1.75	6	1
1:A:2:LEU:HD12	1:A:6:GLN:CG	0.58	2.29	6	6
1:A:36:ALA:HA	1:A:52:LEU:HD12	0.58	1.74	3	2
1:A:135:TYR:CZ	1:A:142:LEU:HD12	0.58	2.33	2	2
1:A:143:PHE:CE1	1:A:148:LEU:HD13	0.58	2.34	4	3
1:A:101:LEU:N	1:A:101:LEU:HD13	0.58	2.13	5	1
1:A:37:VAL:HG21	1:A:53:LEU:HD22	0.58	1.76	25	1
1:A:66:LEU:HD22	1:A:66:LEU:N	0.58	2.14	3	2
1:A:39:SER:HB2	1:A:47:LEU:HD22	0.58	1.76	22	4
1:A:169:ILE:HD12	1:A:171:LYS:HD2	0.58	1.74	17	1
1:A:99:LEU:N	1:A:99:LEU:HD23	0.57	2.14	15	3
1:A:141:GLY:HA2	1:A:148:LEU:HD11	0.57	1.76	7	2
1:A:37:VAL:HG21	1:A:53:LEU:HD23	0.57	1.75	21	1
1:A:52:LEU:HD23	1:A:53:LEU:N	0.57	2.14	21	1
1:A:142:LEU:HD13	1:A:142:LEU:H	0.57	1.58	3	1
1:A:22:TYR:CD1	1:A:27:ILE:HD11	0.57	2.34	4	2
1:A:99:LEU:HD12	1:A:101:LEU:CD1	0.57	2.29	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:PHE:CE2	1:A:65:VAL:HG22	0.57	2.34	14	2
1:A:77:SER:O	1:A:88:LEU:HD22	0.57	1.99	11	1
1:A:53:LEU:HD22	1:A:112:ALA:HB1	0.57	1.76	21	2
1:A:15:ARG:HB2	1:A:34:ILE:HG21	0.57	1.76	25	13
1:A:29:ILE:HG22	1:A:34:ILE:CD1	0.57	2.28	3	1
1:A:137:LEU:HD11	1:A:163:LEU:HB3	0.57	1.77	8	4
1:A:53:LEU:HD22	1:A:112:ALA:CB	0.57	2.29	21	3
1:A:169:ILE:HD12	1:A:171:LYS:HD3	0.57	1.77	9	1
1:A:66:LEU:HD22	1:A:78:VAL:CG2	0.57	2.30	14	1
1:A:151:LEU:HB2	1:A:153:ILE:HD11	0.57	1.77	19	8
1:A:156:GLU:HA	1:A:159:LEU:HD23	0.57	1.75	19	6
1:A:117:THR:HG22	1:A:170:PRO:O	0.57	1.99	8	4
1:A:169:ILE:HD11	1:A:172:LYS:CD	0.57	2.29	9	3
1:A:10:ILE:HG21	1:A:97:TYR:CE2	0.57	2.34	12	1
1:A:4:LEU:O	1:A:4:LEU:HD23	0.56	1.99	15	4
1:A:35:VAL:HG21	1:A:109:LYS:HZ2	0.56	1.60	4	2
1:A:111:TYR:CZ	1:A:142:LEU:HD22	0.56	2.34	6	3
1:A:53:LEU:CD1	1:A:113:ILE:HD12	0.56	2.30	20	3
1:A:163:LEU:HD23	1:A:163:LEU:N	0.56	2.15	5	18
1:A:33:ASN:O	1:A:54:ILE:HD12	0.56	2.00	25	1
1:A:22:TYR:HB3	1:A:27:ILE:HD13	0.56	1.76	16	14
1:A:34:ILE:HG13	1:A:54:ILE:HG22	0.56	1.77	21	1
1:A:137:LEU:HD13	1:A:137:LEU:N	0.56	2.15	19	2
1:A:142:LEU:HD13	1:A:142:LEU:N	0.56	2.16	3	1
1:A:88:LEU:HD11	1:A:99:LEU:HD22	0.56	1.76	19	1
1:A:11:VAL:HG12	1:A:15:ARG:HD2	0.56	1.78	3	2
1:A:14:LEU:HD11	1:A:90:ILE:HG21	0.56	1.76	17	12
1:A:53:LEU:HD11	1:A:112:ALA:HB1	0.56	1.78	1	2
1:A:88:LEU:HD12	1:A:99:LEU:CD1	0.56	2.31	3	1
1:A:2:LEU:HD11	1:A:6:GLN:HG2	0.56	1.76	12	1
1:A:141:GLY:HA2	1:A:148:LEU:HD21	0.56	1.77	15	1
1:A:2:LEU:HD12	1:A:6:GLN:HB3	0.56	1.77	20	6
1:A:34:ILE:CG2	1:A:52:LEU:HD23	0.56	2.31	24	1
1:A:27:ILE:N	1:A:27:ILE:HD12	0.55	2.16	10	15
1:A:65:VAL:HG12	1:A:66:LEU:HG	0.55	1.78	14	1
1:A:50:VAL:HG23	1:A:99:LEU:HB3	0.55	1.78	15	2
1:A:29:ILE:HG22	1:A:34:ILE:CG1	0.55	2.31	23	1
1:A:53:LEU:HD22	1:A:54:ILE:N	0.55	2.16	3	2
1:A:142:LEU:CB	1:A:149:VAL:HG13	0.55	2.31	12	2
1:A:99:LEU:HD12	1:A:99:LEU:N	0.55	2.17	19	3
1:A:71:ILE:HG21	1:A:74:LEU:CG	0.55	2.32	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:ASP:C	1:A:101:LEU:HD23	0.55	2.21	20	1
1:A:88:LEU:CG	1:A:101:LEU:HD13	0.55	2.32	1	1
1:A:35:VAL:O	1:A:52:LEU:HD23	0.55	2.02	10	3
1:A:65:VAL:HG12	1:A:66:LEU:HD22	0.55	1.76	25	1
1:A:101:LEU:HD23	1:A:101:LEU:N	0.55	2.16	20	2
1:A:51:ASP:C	1:A:52:LEU:HD12	0.55	2.21	11	5
1:A:159:LEU:C	1:A:159:LEU:HD22	0.55	2.21	22	1
1:A:88:LEU:HD12	1:A:99:LEU:HB2	0.55	1.78	1	1
1:A:37:VAL:HG21	1:A:53:LEU:CD1	0.55	2.25	16	2
1:A:2:LEU:HD13	1:A:2:LEU:N	0.55	2.15	15	2
1:A:169:ILE:HD12	1:A:171:LYS:CD	0.55	2.32	9	5
1:A:119:PRO:HD2	1:A:174:LEU:HD13	0.55	1.76	11	1
1:A:29:ILE:HD13	1:A:54:ILE:HD12	0.55	1.77	2	2
1:A:130:LEU:HD21	1:A:163:LEU:O	0.55	2.02	11	3
1:A:4:LEU:HD11	1:A:43:GLU:CA	0.54	2.32	17	9
1:A:8:LYS:CE	1:A:40:LEU:HD11	0.54	2.32	5	1
1:A:149:VAL:HG23	1:A:150:PRO:HD2	0.54	1.79	7	3
1:A:61:LEU:C	1:A:65:VAL:HG23	0.54	2.23	9	9
1:A:56:VAL:HG21	1:A:62:LEU:HB2	0.54	1.79	17	4
1:A:121:SER:HB3	1:A:174:LEU:HD13	0.54	1.78	17	1
1:A:66:LEU:HD13	1:A:80:VAL:HB	0.54	1.80	21	2
1:A:126:ILE:HG22	1:A:130:LEU:HD12	0.54	1.78	5	1
1:A:39:SER:OG	1:A:47:LEU:HD13	0.54	2.03	9	2
1:A:114:PHE:HB2	1:A:159:LEU:HD21	0.54	1.80	9	16
1:A:66:LEU:CD2	1:A:78:VAL:HG22	0.54	2.32	22	1
1:A:109:LYS:N	1:A:110:PRO:CD	0.54	2.71	4	19
1:A:160:ILE:HD13	1:A:167:TYR:HB2	0.54	1.79	2	5
1:A:99:LEU:HD12	1:A:101:LEU:HD11	0.54	1.78	9	2
1:A:56:VAL:HG12	1:A:57:PRO:HD2	0.53	1.80	13	8
1:A:2:LEU:HD22	1:A:2:LEU:H	0.53	1.63	15	2
1:A:111:TYR:CE2	1:A:142:LEU:HD11	0.53	2.37	7	2
1:A:46:MET:O	1:A:47:LEU:HD23	0.53	2.03	11	1
1:A:33:ASN:CB	1:A:55:ILE:HD11	0.53	2.32	2	1
1:A:148:LEU:HD13	1:A:149:VAL:N	0.53	2.18	12	3
1:A:6:GLN:O	1:A:10:ILE:HD12	0.53	2.03	2	4
1:A:3:THR:HG23	1:A:46:MET:CE	0.53	2.32	10	1
1:A:111:TYR:HH	1:A:142:LEU:HD23	0.53	1.64	5	4
1:A:53:LEU:HD11	1:A:112:ALA:C	0.53	2.24	1	1
1:A:90:ILE:HG23	1:A:99:LEU:CD2	0.53	2.33	20	3
1:A:8:LYS:HE3	1:A:40:LEU:HD11	0.53	1.81	5	1
1:A:62:LEU:HD11	1:A:103:THR:HB	0.53	1.81	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:HD11	1:A:43:GLU:HA	0.53	1.80	13	2
1:A:34:ILE:HD11	1:A:54:ILE:CG1	0.53	2.34	20	1
1:A:143:PHE:CD1	1:A:148:LEU:HD22	0.53	2.39	18	2
1:A:2:LEU:HD23	1:A:2:LEU:N	0.53	2.19	25	1
1:A:53:LEU:CD2	1:A:112:ALA:HB3	0.52	2.33	19	5
1:A:20:PHE:CB	1:A:69:ILE:HD12	0.52	2.35	2	18
1:A:101:LEU:HD12	1:A:101:LEU:N	0.52	2.18	12	3
1:A:88:LEU:HD23	1:A:101:LEU:CD2	0.52	2.34	5	1
1:A:2:LEU:N	1:A:2:LEU:HD22	0.52	2.19	7	2
1:A:29:ILE:CG2	1:A:54:ILE:HD13	0.52	2.33	25	3
1:A:29:ILE:HG22	1:A:33:ASN:OD1	0.52	2.05	18	1
1:A:111:TYR:OH	1:A:163:LEU:HD22	0.52	2.04	4	3
1:A:11:VAL:HG11	1:A:52:LEU:HD13	0.52	1.82	17	1
1:A:56:VAL:HG11	1:A:62:LEU:H	0.52	1.65	9	3
1:A:88:LEU:HD23	1:A:101:LEU:HD21	0.52	1.81	5	1
1:A:71:ILE:HG22	1:A:73:GLY:H	0.52	1.65	14	3
1:A:34:ILE:HG23	1:A:52:LEU:HD12	0.52	1.82	13	2
1:A:142:LEU:HD22	1:A:142:LEU:O	0.52	2.04	3	1
1:A:37:VAL:HG21	1:A:116:PHE:CD2	0.52	2.39	14	3
1:A:88:LEU:HD21	1:A:101:LEU:CD2	0.52	2.35	14	3
1:A:56:VAL:HG11	1:A:62:LEU:CB	0.52	2.35	25	3
1:A:35:VAL:HG21	1:A:109:LYS:HD3	0.52	1.82	2	3
1:A:33:ASN:O	1:A:34:ILE:HD12	0.52	2.04	10	1
1:A:66:LEU:CD2	1:A:78:VAL:HG21	0.52	2.34	14	1
1:A:52:LEU:O	1:A:101:LEU:HD23	0.52	2.05	17	2
1:A:88:LEU:CG	1:A:99:LEU:HD23	0.52	2.35	25	1
1:A:86:CYS:HB2	1:A:103:THR:HG23	0.52	1.82	6	3
1:A:173:ARG:C	1:A:174:LEU:HD23	0.51	2.26	18	2
1:A:39:SER:HB3	1:A:47:LEU:HD22	0.51	1.81	24	5
1:A:62:LEU:HD21	1:A:103:THR:CB	0.51	2.35	16	5
1:A:52:LEU:HB2	1:A:101:LEU:HD12	0.51	1.81	5	1
1:A:102:PHE:CD1	1:A:116:PHE:CE2	0.51	2.99	25	17
1:A:109:LYS:HE2	1:A:113:ILE:HD13	0.51	1.80	17	7
1:A:102:PHE:CD1	1:A:116:PHE:CZ	0.51	2.99	1	12
1:A:160:ILE:HD13	1:A:167:TYR:HD1	0.51	1.65	20	8
1:A:56:VAL:HG23	1:A:104:ALA:O	0.51	2.06	18	2
1:A:4:LEU:HA	1:A:47:LEU:HD11	0.51	1.82	18	2
1:A:29:ILE:HG21	1:A:54:ILE:CD1	0.51	2.36	12	2
1:A:52:LEU:CB	1:A:101:LEU:HD23	0.51	2.35	16	2
1:A:169:ILE:HD12	1:A:171:LYS:HG3	0.51	1.80	24	3
1:A:122:TYR:O	1:A:126:ILE:HD12	0.51	2.06	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:VAL:CB	1:A:88:LEU:HD12	0.51	2.35	18	1
1:A:14:LEU:HD21	1:A:74:LEU:HD22	0.51	1.82	23	5
1:A:11:VAL:CG2	1:A:40:LEU:HD11	0.51	2.27	14	1
1:A:66:LEU:N	1:A:67:PRO:HD3	0.51	2.20	6	16
1:A:69:ILE:HG23	1:A:76:PHE:CE1	0.50	2.41	22	7
1:A:36:ALA:HB1	1:A:40:LEU:CG	0.50	2.35	1	5
1:A:53:LEU:HD13	1:A:53:LEU:C	0.50	2.27	7	6
1:A:117:THR:HG21	1:A:170:PRO:HB2	0.50	1.83	14	4
1:A:8:LYS:HE3	1:A:40:LEU:HD23	0.50	1.81	2	1
1:A:4:LEU:CD1	1:A:47:LEU:HD11	0.50	2.36	25	2
1:A:53:LEU:C	1:A:53:LEU:HD13	0.50	2.27	13	4
1:A:169:ILE:HD11	1:A:172:LYS:HG2	0.50	1.81	23	2
1:A:160:ILE:HG21	1:A:167:TYR:HA	0.50	1.83	5	3
1:A:102:PHE:CD1	1:A:116:PHE:CE1	0.50	3.00	14	1
1:A:18:LEU:CD1	1:A:29:ILE:HD11	0.50	2.29	16	2
1:A:142:LEU:CD2	1:A:163:LEU:HD22	0.50	2.36	10	2
1:A:87:VAL:HG12	1:A:89:PHE:CE1	0.50	2.42	11	1
1:A:39:SER:HB2	1:A:47:LEU:HD13	0.50	1.84	19	3
1:A:62:LEU:HD12	1:A:105:LEU:CD2	0.50	2.37	19	2
1:A:122:TYR:CE2	1:A:126:ILE:HD11	0.50	2.42	21	16
1:A:35:VAL:O	1:A:37:VAL:HG23	0.50	2.07	24	3
1:A:169:ILE:HD11	1:A:172:LYS:HG3	0.50	1.84	14	3
1:A:66:LEU:CD1	1:A:78:VAL:HG22	0.50	2.37	18	2
1:A:78:VAL:HB	1:A:88:LEU:HD12	0.50	1.82	18	1
1:A:121:SER:CB	1:A:174:LEU:HD12	0.49	2.37	13	1
1:A:114:PHE:CE2	1:A:163:LEU:HD11	0.49	2.43	7	1
1:A:10:ILE:HD13	1:A:97:TYR:CD2	0.49	2.42	23	1
1:A:74:LEU:HD21	1:A:90:ILE:HB	0.49	1.84	7	3
1:A:2:LEU:HD23	1:A:97:TYR:OH	0.49	2.07	12	1
1:A:29:ILE:HB	1:A:34:ILE:HD13	0.49	1.84	14	2
1:A:71:ILE:HD12	1:A:76:PHE:CG	0.49	2.42	14	1
1:A:126:ILE:HG23	1:A:130:LEU:HD12	0.49	1.84	15	3
1:A:4:LEU:HD11	1:A:43:GLU:CG	0.49	2.37	13	1
1:A:14:LEU:HD22	1:A:17:ARG:NH1	0.49	2.23	19	1
1:A:159:LEU:C	1:A:159:LEU:HD13	0.49	2.27	21	1
1:A:36:ALA:HA	1:A:52:LEU:HD23	0.49	1.84	18	2
1:A:11:VAL:HG11	1:A:52:LEU:HD11	0.49	1.81	15	1
1:A:8:LYS:CD	1:A:40:LEU:HD11	0.49	2.37	5	1
1:A:62:LEU:HD11	1:A:103:THR:CG2	0.49	2.38	14	1
1:A:33:ASN:CA	1:A:55:ILE:HD11	0.49	2.38	2	8
1:A:54:ILE:HD13	1:A:54:ILE:C	0.49	2.29	3	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:HD11	1:A:43:GLU:HB3	0.49	1.83	5	1
1:A:2:LEU:HD23	1:A:47:LEU:CB	0.49	2.38	15	1
1:A:11:VAL:HG12	1:A:15:ARG:CD	0.48	2.38	3	1
1:A:111:TYR:CZ	1:A:151:LEU:HD12	0.48	2.42	24	4
1:A:2:LEU:CD2	1:A:97:TYR:CE1	0.48	2.96	12	2
1:A:34:ILE:HG23	1:A:52:LEU:CD2	0.48	2.37	21	2
1:A:109:LYS:N	1:A:110:PRO:HD2	0.48	2.23	7	20
1:A:18:LEU:HD21	1:A:76:PHE:HE2	0.48	1.67	25	4
1:A:130:LEU:HD11	1:A:163:LEU:HB3	0.48	1.84	7	1
1:A:88:LEU:HD21	1:A:101:LEU:HG	0.48	1.83	3	1
1:A:129:ALA:HB1	1:A:165:PHE:CZ	0.48	2.43	15	2
1:A:10:ILE:HD13	1:A:97:TYR:HD2	0.48	1.68	23	1
1:A:8:LYS:HE2	1:A:40:LEU:HD12	0.48	1.84	1	1
1:A:142:LEU:HD11	1:A:162:GLU:HG3	0.48	1.85	9	2
1:A:114:PHE:CD2	1:A:159:LEU:HD11	0.48	2.43	20	2
1:A:18:LEU:CD2	1:A:29:ILE:HD12	0.48	2.23	2	2
1:A:36:ALA:HB1	1:A:40:LEU:CD2	0.48	2.36	2	4
1:A:138:ASN:O	1:A:140:TYR:N	0.48	2.47	25	7
1:A:88:LEU:HD13	1:A:88:LEU:C	0.48	2.29	11	1
1:A:2:LEU:HD12	1:A:6:GLN:CB	0.48	2.39	21	3
1:A:109:LYS:CE	1:A:113:ILE:HD13	0.48	2.39	17	3
1:A:135:TYR:HE2	1:A:142:LEU:HD23	0.48	1.65	11	1
1:A:53:LEU:HD12	1:A:113:ILE:HD12	0.48	1.84	20	1
1:A:88:LEU:CG	1:A:101:LEU:HD21	0.48	2.39	5	1
1:A:4:LEU:HD12	1:A:44:GLU:O	0.48	2.09	15	1
1:A:66:LEU:HA	1:A:69:ILE:HD13	0.47	1.86	14	3
1:A:142:LEU:H	1:A:142:LEU:HD23	0.47	1.68	24	1
1:A:22:TYR:HD1	1:A:27:ILE:HD11	0.47	1.69	4	2
1:A:111:TYR:CD2	1:A:151:LEU:HD12	0.47	2.44	6	2
1:A:18:LEU:HD22	1:A:71:ILE:CG1	0.47	2.39	16	1
1:A:50:VAL:HG22	1:A:97:TYR:HE1	0.47	1.66	22	1
1:A:88:LEU:C	1:A:88:LEU:HD12	0.47	2.30	5	7
1:A:92:TRP:N	1:A:92:TRP:CD1	0.47	2.81	23	19
1:A:56:VAL:HG11	1:A:62:LEU:HB2	0.47	1.84	3	5
1:A:62:LEU:HD11	1:A:103:THR:OG1	0.47	2.09	6	2
1:A:88:LEU:CD1	1:A:99:LEU:HD11	0.47	2.25	20	2
1:A:18:LEU:HD12	1:A:71:ILE:HG12	0.47	1.85	19	3
1:A:29:ILE:HG22	1:A:54:ILE:HD13	0.47	1.84	25	1
1:A:159:LEU:HD12	1:A:159:LEU:C	0.47	2.30	4	20
1:A:53:LEU:HD22	1:A:53:LEU:C	0.47	2.30	11	2
1:A:143:PHE:CD1	1:A:143:PHE:N	0.47	2.83	5	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:174:LEU:C	1:A:174:LEU:HD23	0.47	2.30	13	2
1:A:39:SER:OG	1:A:47:LEU:HD22	0.47	2.09	17	1
1:A:53:LEU:HD13	1:A:112:ALA:CB	0.47	2.37	19	1
1:A:34:ILE:HG23	1:A:52:LEU:CD1	0.47	2.35	21	1
1:A:20:PHE:CE2	1:A:27:ILE:CG2	0.47	2.98	4	20
1:A:143:PHE:CE2	1:A:148:LEU:CD2	0.47	2.98	5	2
1:A:20:PHE:CZ	1:A:27:ILE:CG2	0.47	2.98	17	23
1:A:92:TRP:CD1	1:A:92:TRP:N	0.47	2.82	5	5
1:A:29:ILE:HG21	1:A:54:ILE:HD13	0.47	1.87	15	3
1:A:44:GLU:HB2	1:A:47:LEU:HD21	0.46	1.86	20	2
1:A:29:ILE:HG21	1:A:54:ILE:HD12	0.46	1.87	23	1
1:A:55:ILE:HG21	1:A:109:LYS:CB	0.46	2.40	4	2
1:A:66:LEU:HD21	1:A:78:VAL:HG13	0.46	1.87	21	2
1:A:88:LEU:CB	1:A:101:LEU:HD12	0.46	2.40	13	1
1:A:53:LEU:CD2	1:A:112:ALA:HB1	0.46	2.40	23	1
1:A:173:ARG:O	1:A:174:LEU:HD23	0.46	2.11	22	5
1:A:104:ALA:HB1	1:A:108:GLU:CG	0.46	2.40	11	1
1:A:74:LEU:HD11	1:A:90:ILE:HB	0.46	1.87	14	2
1:A:140:TYR:CD1	1:A:140:TYR:N	0.46	2.82	23	1
1:A:56:VAL:HG12	1:A:58:GLU:H	0.46	1.70	16	2
1:A:4:LEU:HD11	1:A:43:GLU:HB2	0.46	1.86	18	2
1:A:17:ARG:CG	1:A:71:ILE:HG23	0.46	2.39	17	1
1:A:111:TYR:CE1	1:A:151:LEU:CB	0.46	2.99	17	2
1:A:2:LEU:CD2	1:A:97:TYR:CZ	0.46	2.99	12	2
1:A:160:ILE:HG21	1:A:167:TYR:N	0.46	2.26	2	2
1:A:66:LEU:HD13	1:A:66:LEU:H	0.46	1.71	15	3
1:A:99:LEU:HD12	1:A:101:LEU:HD21	0.46	1.87	3	2
1:A:111:TYR:CE1	1:A:159:LEU:CD2	0.46	2.97	22	2
1:A:78:VAL:CA	1:A:88:LEU:HD12	0.46	2.40	18	1
1:A:6:GLN:HE22	1:A:10:ILE:HD11	0.46	1.71	19	1
1:A:66:LEU:CD1	1:A:69:ILE:HD13	0.46	2.41	25	1
1:A:151:LEU:N	1:A:151:LEU:CD1	0.46	2.79	15	3
1:A:2:LEU:CD1	1:A:97:TYR:CZ	0.46	2.98	14	3
1:A:148:LEU:HD23	1:A:148:LEU:C	0.46	2.31	13	1
1:A:66:LEU:HD21	1:A:80:VAL:HB	0.45	1.87	1	1
1:A:10:ILE:CD1	1:A:97:TYR:CE2	0.45	3.00	7	4
1:A:8:LYS:HA	1:A:40:LEU:HD21	0.45	1.88	14	1
1:A:33:ASN:O	1:A:55:ILE:HD12	0.45	2.10	19	2
1:A:101:LEU:H	1:A:101:LEU:HD22	0.45	1.70	5	1
1:A:52:LEU:HB2	1:A:101:LEU:HD23	0.45	1.88	22	2
1:A:135:TYR:HE2	1:A:142:LEU:HD11	0.45	1.70	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:GLY:HA3	1:A:47:LEU:HD13	0.45	1.87	13	1
1:A:89:PHE:CD1	1:A:89:PHE:N	0.45	2.84	13	2
1:A:35:VAL:HG21	1:A:109:LYS:CD	0.45	2.42	2	1
1:A:151:LEU:O	1:A:151:LEU:HD23	0.45	2.12	22	4
1:A:143:PHE:CE1	1:A:148:LEU:CD2	0.45	3.00	12	1
1:A:66:LEU:HD22	1:A:78:VAL:HG21	0.45	1.89	14	1
1:A:53:LEU:HD23	1:A:109:LYS:HD2	0.45	1.87	16	1
1:A:114:PHE:CE2	1:A:123:LEU:CD1	0.45	3.00	21	2
1:A:142:LEU:HD22	1:A:149:VAL:CG1	0.45	2.42	20	1
1:A:22:TYR:CE1	1:A:64:HIS:CB	0.45	3.00	6	2
1:A:135:TYR:CE2	1:A:142:LEU:CD1	0.45	2.99	23	1
1:A:127:ARG:HG2	1:A:137:LEU:HD22	0.45	1.89	7	1
1:A:2:LEU:HD11	1:A:6:GLN:HB3	0.45	1.89	12	1
1:A:36:ALA:HB1	1:A:40:LEU:CB	0.45	2.42	6	2
1:A:137:LEU:N	1:A:137:LEU:CD1	0.45	2.80	24	5
1:A:151:LEU:HD13	1:A:151:LEU:H	0.45	1.71	21	4
1:A:55:ILE:HD13	1:A:55:ILE:N	0.45	2.26	10	1
1:A:142:LEU:HD12	1:A:142:LEU:N	0.45	2.26	11	1
1:A:111:TYR:HE2	1:A:151:LEU:HD12	0.45	1.71	21	1
1:A:122:TYR:CE1	1:A:125:ARG:NH2	0.45	2.84	21	1
1:A:56:VAL:HB	1:A:62:LEU:HD12	0.45	1.87	2	1
1:A:99:LEU:HG	1:A:101:LEU:HD11	0.45	1.89	4	1
1:A:111:TYR:CE2	1:A:142:LEU:CD2	0.45	2.99	14	1
1:A:66:LEU:HD12	1:A:78:VAL:HG22	0.45	1.89	24	1
1:A:10:ILE:CD1	1:A:97:TYR:CE1	0.45	3.00	15	2
1:A:122:TYR:CE2	1:A:126:ILE:CD1	0.45	2.99	6	4
1:A:104:ALA:HB1	1:A:108:GLU:HG2	0.45	1.89	11	1
1:A:114:PHE:CD2	1:A:123:LEU:CD1	0.45	3.00	15	2
1:A:88:LEU:HD23	1:A:101:LEU:HD22	0.45	1.89	15	1
1:A:155:THR:HG22	1:A:158:GLU:OE1	0.44	2.12	3	1
1:A:50:VAL:CG2	1:A:99:LEU:HD12	0.44	2.38	10	1
1:A:88:LEU:CB	1:A:101:LEU:HD13	0.44	2.42	11	1
1:A:87:VAL:CG1	1:A:89:PHE:CE1	0.44	3.01	11	1
1:A:149:VAL:HG12	1:A:150:PRO:CD	0.44	2.37	15	1
1:A:20:PHE:CE2	1:A:27:ILE:HG21	0.44	2.47	2	6
1:A:173:ARG:O	1:A:174:LEU:HD12	0.44	2.11	23	2
1:A:160:ILE:HG22	1:A:165:PHE:O	0.44	2.12	5	1
1:A:54:ILE:HG23	1:A:54:ILE:O	0.44	2.13	2	6
1:A:53:LEU:HG	1:A:112:ALA:HB1	0.44	1.89	9	1
1:A:16:SER:HA	1:A:30:LEU:HD23	0.44	1.88	14	1
1:A:34:ILE:HD11	1:A:54:ILE:CD1	0.44	2.38	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:TYR:CE1	1:A:142:LEU:HD13	0.44	2.47	5	1
1:A:141:GLY:CA	1:A:148:LEU:HD11	0.44	2.41	23	2
1:A:71:ILE:CD1	1:A:76:PHE:CG	0.44	3.00	9	4
1:A:114:PHE:CG	1:A:159:LEU:HD21	0.44	2.48	25	2
1:A:166:THR:HG21	1:A:168:ARG:CZ	0.44	2.43	19	1
1:A:34:ILE:CD1	1:A:54:ILE:HG22	0.44	2.42	21	1
1:A:130:LEU:HD22	1:A:135:TYR:CB	0.44	2.42	24	1
1:A:129:ALA:CB	1:A:165:PHE:CZ	0.44	3.00	15	3
1:A:143:PHE:CD1	1:A:148:LEU:HD13	0.44	2.48	7	1
1:A:13:HIS:CE1	1:A:17:ARG:NH2	0.44	2.85	8	1
1:A:4:LEU:HA	1:A:47:LEU:HD21	0.44	1.88	1	1
1:A:61:LEU:O	1:A:65:VAL:N	0.44	2.51	9	10
1:A:33:ASN:C	1:A:34:ILE:HD12	0.44	2.33	13	4
1:A:126:ILE:CG2	1:A:130:LEU:HD12	0.44	2.43	3	3
1:A:74:LEU:HD13	1:A:92:TRP:CE2	0.44	2.48	14	1
1:A:122:TYR:CZ	1:A:173:ARG:NH1	0.44	2.86	22	1
1:A:122:TYR:CE1	1:A:173:ARG:NH1	0.44	2.85	22	1
1:A:62:LEU:HD12	1:A:105:LEU:HD22	0.44	1.88	9	4
1:A:15:ARG:O	1:A:30:LEU:HD13	0.44	2.13	5	1
1:A:87:VAL:HG12	1:A:89:PHE:CZ	0.44	2.47	11	1
1:A:88:LEU:HD23	1:A:99:LEU:HD13	0.44	1.89	13	1
1:A:20:PHE:HZ	1:A:65:VAL:HG22	0.44	1.71	17	1
1:A:6:GLN:NE2	1:A:10:ILE:HD11	0.44	2.28	19	1
1:A:86:CYS:SG	1:A:103:THR:HG23	0.44	2.53	21	1
1:A:160:ILE:HG21	1:A:167:TYR:CA	0.43	2.42	5	2
1:A:88:LEU:CD2	1:A:101:LEU:HD21	0.43	2.43	5	1
1:A:111:TYR:HH	1:A:142:LEU:HD21	0.43	1.72	11	1
1:A:62:LEU:HD11	1:A:103:THR:CB	0.43	2.43	14	1
1:A:90:ILE:CG2	1:A:99:LEU:HD12	0.43	2.43	14	1
1:A:62:LEU:HD13	1:A:103:THR:CB	0.43	2.40	17	1
1:A:56:VAL:HG21	1:A:62:LEU:CB	0.43	2.43	18	1
1:A:52:LEU:HD23	1:A:52:LEU:C	0.43	2.34	21	1
1:A:111:TYR:OH	1:A:163:LEU:HD21	0.43	2.13	12	2
1:A:56:VAL:N	1:A:104:ALA:O	0.43	2.51	2	3
1:A:160:ILE:HD13	1:A:167:TYR:CB	0.43	2.43	5	2
1:A:88:LEU:HB3	1:A:101:LEU:HD11	0.43	1.90	18	1
1:A:137:LEU:HD12	1:A:142:LEU:HD11	0.43	1.89	23	1
1:A:102:PHE:CG	1:A:116:PHE:CE2	0.43	3.06	20	3
1:A:10:ILE:HD13	1:A:97:TYR:CE1	0.43	2.48	2	1
1:A:52:LEU:CD1	1:A:99:LEU:HD11	0.43	2.25	2	1
1:A:111:TYR:CE1	1:A:151:LEU:HB3	0.43	2.48	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:SER:HB2	1:A:47:LEU:HD21	0.43	1.88	13	1
1:A:124:ILE:HD13	1:A:124:ILE:N	0.43	2.28	15	1
1:A:2:LEU:HD13	1:A:97:TYR:CE2	0.43	2.48	17	1
1:A:18:LEU:HD23	1:A:29:ILE:HD11	0.43	1.90	19	1
1:A:34:ILE:CG1	1:A:54:ILE:HG22	0.43	2.42	21	1
1:A:90:ILE:HG23	1:A:99:LEU:HD12	0.43	1.91	14	1
1:A:135:TYR:HE1	1:A:142:LEU:HD12	0.43	1.68	19	1
1:A:141:GLY:HA2	1:A:151:LEU:HD13	0.43	1.90	22	1
1:A:120:VAL:HG13	1:A:124:ILE:HD11	0.43	1.91	2	2
1:A:173:ARG:O	1:A:174:LEU:HD22	0.43	2.13	12	1
1:A:37:VAL:CB	1:A:53:LEU:HD13	0.43	2.44	25	1
1:A:53:LEU:CD1	1:A:112:ALA:HB1	0.43	2.42	15	2
1:A:108:GLU:CG	1:A:140:TYR:CE1	0.43	3.02	15	1
1:A:20:PHE:CD2	1:A:65:VAL:O	0.43	2.71	6	9
1:A:29:ILE:O	1:A:30:LEU:HD12	0.43	2.14	1	6
1:A:37:VAL:HG13	1:A:113:ILE:HG13	0.43	1.89	1	1
1:A:22:TYR:CE2	1:A:61:LEU:CD1	0.43	3.02	16	3
1:A:142:LEU:CD1	1:A:142:LEU:N	0.43	2.82	12	1
1:A:14:LEU:HD21	1:A:92:TRP:CH2	0.43	2.49	24	2
1:A:2:LEU:HD11	1:A:6:GLN:CG	0.43	2.42	12	1
1:A:136:LYS:O	1:A:142:LEU:HD12	0.43	2.14	17	1
1:A:8:LYS:HD2	1:A:40:LEU:HD11	0.42	1.90	5	1
1:A:2:LEU:CG	1:A:97:TYR:CE1	0.42	3.02	6	1
1:A:155:THR:HG22	1:A:158:GLU:HG3	0.42	1.90	6	1
1:A:153:ILE:HG21	1:A:158:GLU:C	0.42	2.35	19	2
1:A:34:ILE:HG23	1:A:52:LEU:HG	0.42	1.90	25	2
1:A:50:VAL:O	1:A:99:LEU:HD12	0.42	2.14	16	1
1:A:135:TYR:CE1	1:A:144:LYS:CG	0.42	3.03	17	1
1:A:151:LEU:H	1:A:151:LEU:HD13	0.42	1.74	17	5
1:A:53:LEU:HD21	1:A:112:ALA:HB1	0.42	1.91	22	1
1:A:142:LEU:N	1:A:142:LEU:CD2	0.42	2.82	2	4
1:A:22:TYR:CD1	1:A:22:TYR:O	0.42	2.72	4	2
1:A:53:LEU:HD11	1:A:55:ILE:HG23	0.42	1.91	13	2
1:A:66:LEU:HG	1:A:80:VAL:HG13	0.42	1.91	8	1
1:A:84:ARG:O	1:A:102:PHE:CG	0.42	2.72	22	12
1:A:142:LEU:HD11	1:A:151:LEU:HD12	0.42	1.91	15	1
1:A:111:TYR:CD2	1:A:151:LEU:HG	0.42	2.50	21	1
1:A:120:VAL:CG1	1:A:121:SER:N	0.42	2.82	5	2
1:A:37:VAL:HG11	1:A:116:PHE:HB3	0.42	1.91	20	1
1:A:130:LEU:HD13	1:A:137:LEU:CD2	0.42	2.32	1	1
1:A:29:ILE:CG2	1:A:34:ILE:CD1	0.42	2.98	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:ASP:O	1:A:52:LEU:HD22	0.42	2.14	13	1
1:A:10:ILE:HD13	1:A:97:TYR:CZ	0.42	2.49	15	1
1:A:142:LEU:O	1:A:149:VAL:HG13	0.42	2.15	23	1
1:A:151:LEU:HD22	1:A:151:LEU:N	0.42	2.29	22	3
1:A:120:VAL:HG22	1:A:124:ILE:CD1	0.42	2.34	5	1
1:A:142:LEU:N	1:A:142:LEU:CD1	0.42	2.83	15	2
1:A:108:GLU:OE1	1:A:140:TYR:CD1	0.42	2.73	7	1
1:A:29:ILE:HB	1:A:34:ILE:HD11	0.42	1.91	16	1
1:A:53:LEU:HD21	1:A:113:ILE:CG1	0.42	2.45	21	1
1:A:69:ILE:CG2	1:A:76:PHE:CZ	0.42	3.01	22	1
1:A:54:ILE:O	1:A:54:ILE:HG23	0.41	2.15	5	2
1:A:69:ILE:HG21	1:A:78:VAL:HG11	0.41	1.92	21	2
1:A:20:PHE:CG	1:A:65:VAL:O	0.41	2.73	17	2
1:A:142:LEU:HD12	1:A:142:LEU:C	0.41	2.35	17	1
1:A:66:LEU:HD11	1:A:78:VAL:O	0.41	2.15	24	1
1:A:142:LEU:HD23	1:A:149:VAL:O	0.41	2.14	24	1
1:A:98:GLN:C	1:A:99:LEU:HD12	0.41	2.35	1	1
1:A:90:ILE:HD12	1:A:92:TRP:CZ2	0.41	2.51	9	1
1:A:41:ARG:N	1:A:41:ARG:CD	0.41	2.83	13	2
1:A:10:ILE:CD1	1:A:97:TYR:CZ	0.41	3.03	15	1
1:A:137:LEU:HD12	1:A:142:LEU:CD1	0.41	2.45	23	1
1:A:84:ARG:O	1:A:102:PHE:CD1	0.41	2.73	8	8
1:A:142:LEU:O	1:A:149:VAL:CG1	0.41	2.68	7	2
1:A:129:ALA:HB1	1:A:165:PHE:CE1	0.41	2.50	10	1
1:A:88:LEU:HD11	1:A:99:LEU:HD13	0.41	1.93	14	1
1:A:84:ARG:CD	1:A:84:ARG:N	0.41	2.82	21	1
1:A:119:PRO:CD	1:A:174:LEU:CB	0.41	2.98	22	1
1:A:124:ILE:HG22	1:A:125:ARG:HH21	0.41	1.75	25	1
1:A:50:VAL:O	1:A:99:LEU:HA	0.41	2.14	9	2
1:A:34:ILE:HD11	1:A:54:ILE:HG13	0.41	1.93	14	1
1:A:137:LEU:HD12	1:A:142:LEU:HB3	0.41	1.92	16	1
1:A:37:VAL:HG21	1:A:53:LEU:HB2	0.41	1.92	17	1
1:A:71:ILE:HD13	1:A:74:LEU:CD2	0.41	2.43	2	1
1:A:99:LEU:CG	1:A:101:LEU:HD11	0.41	2.45	4	1
1:A:137:LEU:N	1:A:137:LEU:HD22	0.41	2.30	17	1
1:A:2:LEU:N	1:A:2:LEU:CD1	0.41	2.83	15	2
1:A:111:TYR:CD1	1:A:151:LEU:HG	0.41	2.51	7	1
1:A:142:LEU:HD12	1:A:142:LEU:H	0.41	1.75	4	1
1:A:62:LEU:HD23	1:A:62:LEU:O	0.41	2.15	13	1
1:A:56:VAL:CG1	1:A:61:LEU:CB	0.41	2.99	17	1
1:A:137:LEU:HB3	1:A:142:LEU:HD13	0.41	1.93	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:TYR:O	1:A:22:TYR:CD1	0.41	2.74	1	1
1:A:17:ARG:CD	1:A:71:ILE:CG2	0.41	2.99	11	2
1:A:41:ARG:N	1:A:41:ARG:HD2	0.41	2.31	13	1
1:A:135:TYR:CD2	1:A:163:LEU:O	0.41	2.74	18	1
1:A:88:LEU:HD11	1:A:101:LEU:HD13	0.41	1.92	1	1
1:A:108:GLU:OE1	1:A:151:LEU:HD21	0.41	2.15	1	1
1:A:81:CYS:CB	1:A:85:LYS:CB	0.41	2.99	20	2
1:A:167:TYR:CE1	1:A:168:ARG:O	0.41	2.74	3	3
1:A:22:TYR:CE1	1:A:64:HIS:HB2	0.41	2.51	6	1
1:A:5:ILE:CG2	1:A:6:GLN:N	0.41	2.84	9	1
1:A:88:LEU:CD2	1:A:101:LEU:CD1	0.41	2.99	23	2
1:A:111:TYR:CE2	1:A:142:LEU:HD21	0.41	2.51	14	1
1:A:41:ARG:CG	1:A:170:PRO:CB	0.41	2.99	15	1
1:A:53:LEU:CD2	1:A:113:ILE:CD1	0.41	2.99	15	1
1:A:84:ARG:N	1:A:84:ARG:CD	0.41	2.84	19	1
1:A:53:LEU:CD2	1:A:112:ALA:CB	0.41	2.99	24	1
1:A:29:ILE:HG22	1:A:34:ILE:HD12	0.41	1.90	8	1
1:A:53:LEU:HD21	1:A:109:LYS:HD2	0.41	1.92	14	1
1:A:56:VAL:HG21	1:A:62:LEU:CD1	0.41	2.42	14	1
1:A:53:LEU:HD22	1:A:112:ALA:C	0.41	2.36	21	1
1:A:48:ASN:O	1:A:97:TYR:CE1	0.40	2.74	1	2
1:A:4:LEU:HA	1:A:47:LEU:HD23	0.40	1.93	2	1
1:A:30:LEU:HD22	1:A:30:LEU:N	0.40	2.31	5	2
1:A:121:SER:CB	1:A:174:LEU:CD1	0.40	2.99	11	1
1:A:2:LEU:HD11	1:A:6:GLN:CB	0.40	2.46	12	1
1:A:15:ARG:CB	1:A:34:ILE:CG2	0.40	3.00	13	1
1:A:15:ARG:NE	1:A:31:SER:CB	0.40	2.85	14	3
1:A:66:LEU:N	1:A:66:LEU:CD1	0.40	2.84	15	1
1:A:139:GLN:OE1	1:A:140:TYR:CD1	0.40	2.74	16	1
1:A:2:LEU:HD23	1:A:47:LEU:O	0.40	2.16	17	1
1:A:15:ARG:CD	1:A:31:SER:CB	0.40	2.99	19	1
1:A:66:LEU:HG	1:A:80:VAL:HG12	0.40	1.92	25	1
1:A:137:LEU:HD12	1:A:142:LEU:HG	0.40	1.92	11	1
1:A:119:PRO:CD	1:A:174:LEU:N	0.40	2.84	21	1
1:A:9:LYS:O	1:A:13:HIS:CD2	0.40	2.75	22	1
1:A:169:ILE:CD1	1:A:171:LYS:CG	0.40	2.99	5	1
1:A:173:ARG:HG3	1:A:174:LEU:HD23	0.40	1.93	7	1
1:A:65:VAL:O	1:A:65:VAL:CG1	0.40	2.70	9	1
1:A:62:LEU:CD1	1:A:103:THR:CG2	0.40	3.00	14	1
1:A:56:VAL:HG12	1:A:57:PRO:CD	0.40	2.46	17	1
1:A:62:LEU:HD11	1:A:103:THR:O	0.40	2.17	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:LEU:CD2	1:A:17:ARG:NH1	0.40	2.85	19	1
1:A:114:PHE:CZ	1:A:123:LEU:CD1	0.40	3.04	21	1
1:A:54:ILE:HG22	1:A:102:PHE:O	0.40	2.15	7	1
1:A:71:ILE:CD1	1:A:76:PHE:CD2	0.40	3.02	8	1
1:A:119:PRO:HD2	1:A:174:LEU:N	0.40	2.32	15	1
1:A:153:ILE:N	1:A:153:ILE:CD1	0.40	2.82	19	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	172/174 (99%)	152±2 (89±1%)	16±2 (9±1%)	3±1 (2±1%)	11	52
All	All	4300/4350 (99%)	3807 (89%)	406 (9%)	87 (2%)	11	52

All 9 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	67	PRO	23
1	A	110	PRO	17
1	A	118	GLY	14
1	A	84	ARG	9
1	A	139	GLN	9
1	A	173	ARG	7
1	A	73	GLY	4
1	A	66	LEU	3
1	A	106	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	158/159 (99%)	98±5 (62±3%)	60±5 (38±3%)	1	6
All	All	3950/3975 (99%)	2458 (62%)	1492 (38%)	1	6

All 129 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	29	ILE	25
1	A	69	ILE	25
1	A	74	LEU	25
1	A	75	SER	25
1	A	116	PHE	25
1	A	123	LEU	25
1	A	137	LEU	25
1	A	147	THR	25
1	A	151	LEU	25
1	A	153	ILE	25
1	A	165	PHE	25
1	A	76	PHE	24
1	A	92	TRP	24
1	A	97	TYR	24
1	A	154	THR	24
1	A	159	LEU	24
1	A	163	LEU	24
1	A	86	CYS	23
1	A	117	THR	23
1	A	132	LYS	23
1	A	109	LYS	23
1	A	135	TYR	22
1	A	18	LEU	21
1	A	140	TYR	20
1	A	172	LYS	20
1	A	174	LEU	20
1	A	5	ILE	20
1	A	55	ILE	19
1	A	96	THR	19
1	A	37	VAL	17
1	A	145	ASN	17
1	A	66	LEU	17
1	A	45	LYS	17
1	A	17	ARG	16
1	A	84	ARG	16
1	A	133	LYS	16

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Mol	Chain	Res	Type	Models (Total)
1	A	8	LYS	16
1	A	90	ILE	16
1	A	6	GLN	16
1	A	114	PHE	16
1	A	120	VAL	16
1	A	41	ARG	16
1	A	9	LYS	15
1	A	79	LYS	15
1	A	94	LYS	15
1	A	125	ARG	15
1	A	59	LYS	15
1	A	48	ASN	14
1	A	65	VAL	14
1	A	23	ASN	14
1	A	60	LYS	13
1	A	152	LYS	13
1	A	91	GLU	13
1	A	108	GLU	13
1	A	142	LEU	13
1	A	2	LEU	12
1	A	14	LEU	12
1	A	28	LYS	12
1	A	15	ARG	11
1	A	102	PHE	11
1	A	99	LEU	11
1	A	13	HIS	10
1	A	53	LEU	10
1	A	95	LYS	10
1	A	113	ILE	10
1	A	131	LYS	10
1	A	139	GLN	10
1	A	25	GLN	10
1	A	171	LYS	10
1	A	77	SER	10
1	A	22	TYR	9
1	A	146	GLN	9
1	A	70	ARG	9
1	A	121	SER	9
1	A	62	LEU	8
1	A	51	ASP	8
1	A	101	LEU	8
1	A	149	VAL	7

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Mol	Chain	Res	Type	Models (Total)
1	A	21	GLU	7
1	A	54	ILE	7
1	A	63	LYS	7
1	A	148	LEU	7
1	A	155	THR	7
1	A	46	MET	7
1	A	10	ILE	7
1	A	89	PHE	7
1	A	47	LEU	6
1	A	72	LYS	6
1	A	103	THR	6
1	A	144	LYS	6
1	A	173	ARG	6
1	A	143	PHE	6
1	A	34	ILE	6
1	A	32	LYS	6
1	A	58	GLU	6
1	A	158	GLU	5
1	A	98	GLN	5
1	A	42	ARG	5
1	A	44	GLU	5
1	A	4	LEU	4
1	A	100	ASP	4
1	A	130	LEU	4
1	A	168	ARG	4
1	A	157	LYS	4
1	A	39	SER	4
1	A	85	LYS	3
1	A	88	LEU	3
1	A	16	SER	3
1	A	105	LEU	3
1	A	126	ILE	3
1	A	31	SER	3
1	A	93	GLU	3
1	A	127	ARG	3
1	A	3	THR	2
1	A	64	HIS	2
1	A	138	ASN	2
1	A	169	ILE	2
1	A	136	LYS	2
1	A	161	LYS	2
1	A	40	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	52	LEU	1
1	A	81	CYS	1
1	A	67	PRO	1
1	A	83	GLU	1
1	A	78	VAL	1
1	A	43	GLU	1
1	A	115	HIS	1
1	A	56	VAL	1
1	A	156	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no monosaccharides 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 81% for the well-defined parts and 80% 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	2116
Number of shifts mapped to atoms	2116
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	165	-0.33 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	154	0.12 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	161	-0.04 ± 0.16	None needed (< 0.5 ppm)
^{15}N	162	0.56 ± 0.39	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 81%, i.e. 2115 atoms were assigned a chemical shift out of a possible 2624. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	828/861 (96%)	341/348 (98%)	325/346 (94%)	162/167 (97%)
Sidechain	1215/1584 (77%)	801/1032 (78%)	399/485 (82%)	15/67 (22%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	72/179 (40%)	71/86 (83%)	0/86 (0%)	1/7 (14%)
Overall	2115/2624 (81%)	1213/1466 (83%)	724/917 (79%)	178/241 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 2116 atoms were assigned a chemical shift out of a possible 2639. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	829/866 (96%)	341/350 (97%)	326/348 (94%)	162/168 (96%)
Sidechain	1215/1594 (76%)	801/1039 (77%)	399/488 (82%)	15/67 (22%)
Aromatic	72/179 (40%)	71/86 (83%)	0/86 (0%)	1/7 (14%)
Overall	2116/2639 (80%)	1213/1475 (82%)	725/922 (79%)	178/242 (74%)

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	17	ARG	NE	116.10	76.53 – 92.65	19.6
1	A	15	ARG	NE	114.20	76.53 – 92.65	18.4
1	A	41	ARG	NE	113.30	76.53 – 92.65	17.8
1	A	42	ARG	NE	113.30	76.53 – 92.65	17.8
1	A	93	GLU	HG3	1.18	1.20 – 3.30	-5.1

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:

