



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:42 PM BST

PDB ID : 1K2H
Title : Three-dimensional Solution Structure of apo-S100A1.
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Deposited on : 2001-09-27

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

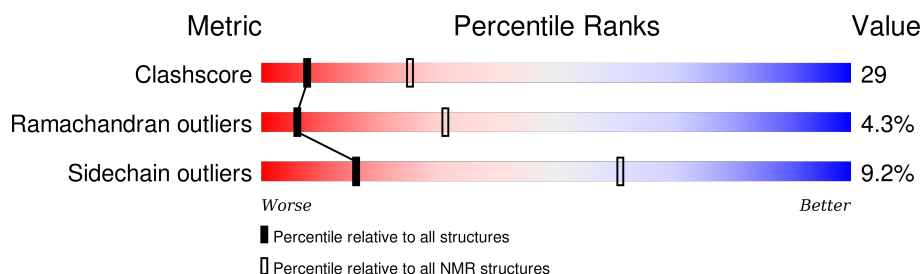
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 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	93	
1	B	93	

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 17 as representative, based on the following criterion: *lowest energy*.

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:3-A:20, A:25-A:86, B:3-B:20, B:25-B:86 (160)	0.34	19

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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2886 atoms, of which 1420 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called S-100 protein, alpha chain.

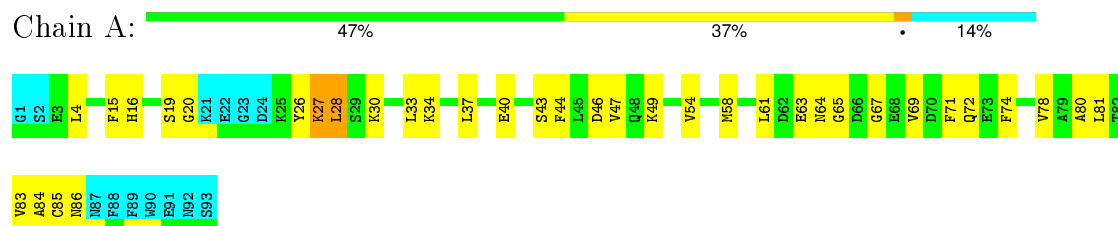
Mol	Chain	Residues	Atoms						Trace
1	A	93	Total	C	H	N	O	S	0
			1443	462	710	115	153	3	
1	B	93	Total	C	H	N	O	S	0
			1443	462	710	115	153	3	

4 Residue-property plots

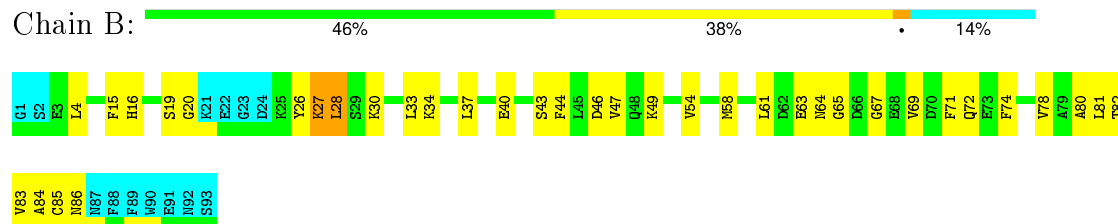
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: S-100 protein, alpha chain



- Molecule 1: S-100 protein, alpha chain

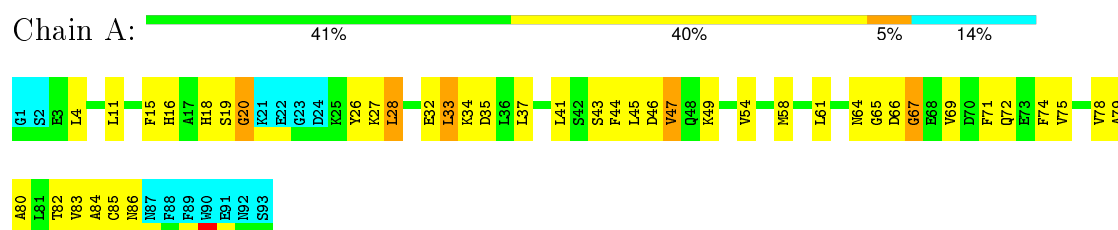


4.2 Scores per residue for each member of the ensemble

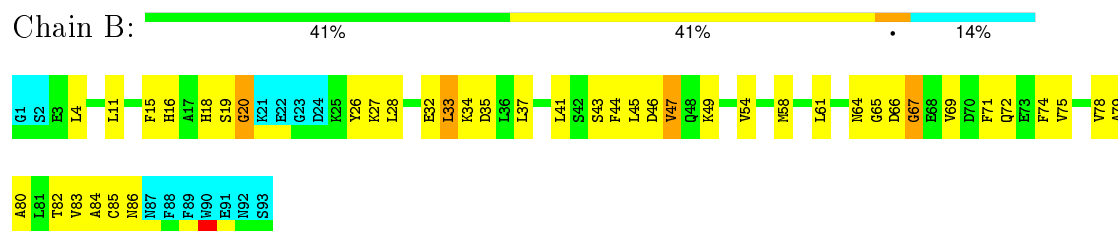
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: S-100 protein, alpha chain

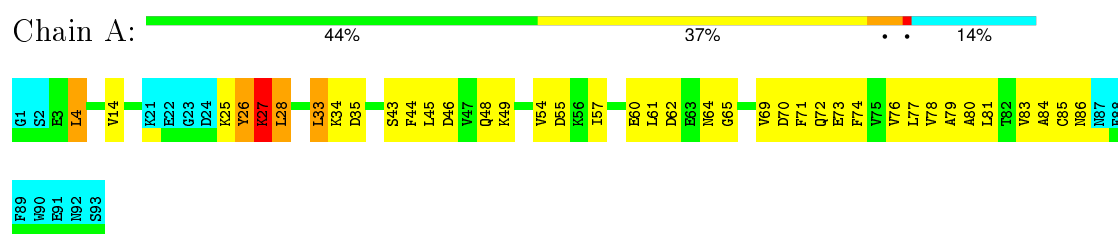


- Molecule 1: S-100 protein, alpha chain

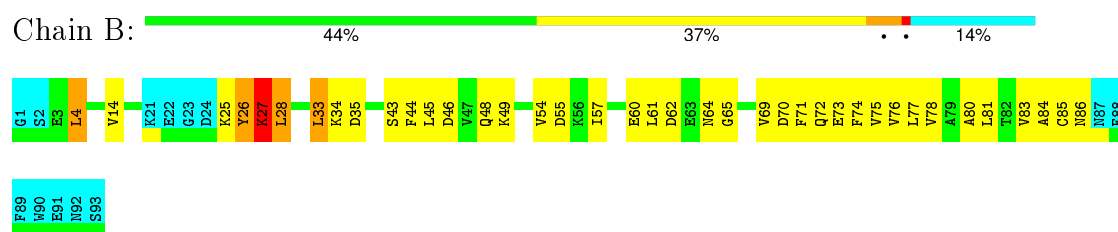


4.2.2 Score per residue for model 2

- Molecule 1: S-100 protein, alpha chain

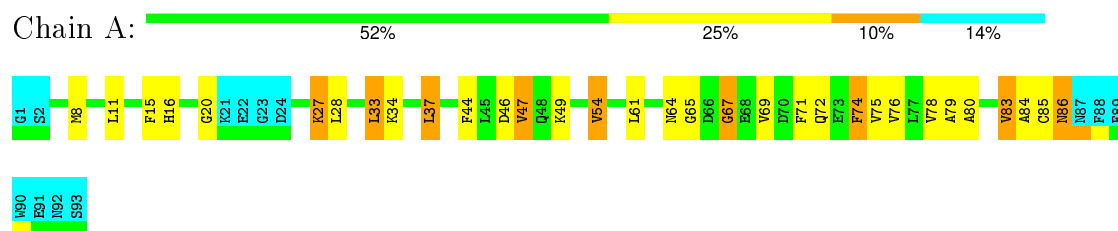


- Molecule 1: S-100 protein, alpha chain

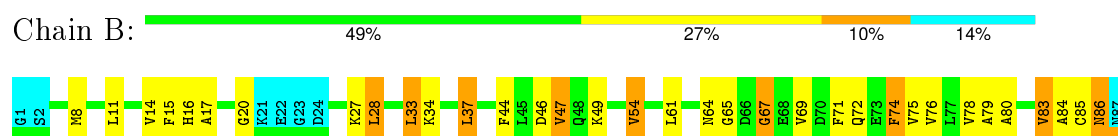


4.2.3 Score per residue for model 3

- Molecule 1: S-100 protein, alpha chain



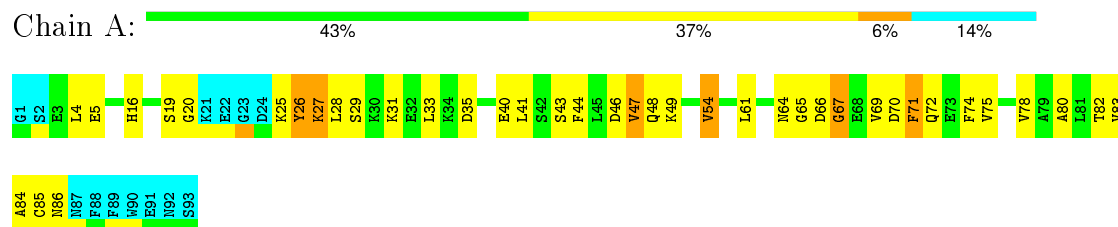
- Molecule 1: S-100 protein, alpha chain



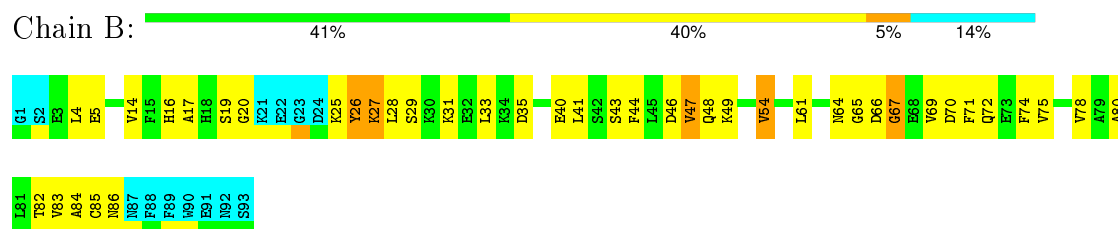


4.2.4 Score per residue for model 4

- Molecule 1: S-100 protein, alpha chain

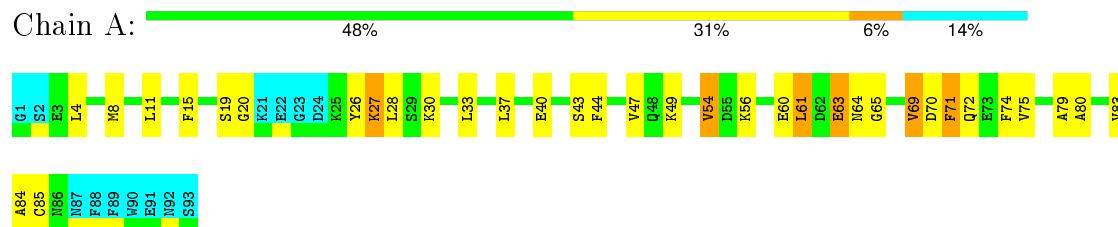


- Molecule 1: S-100 protein, alpha chain

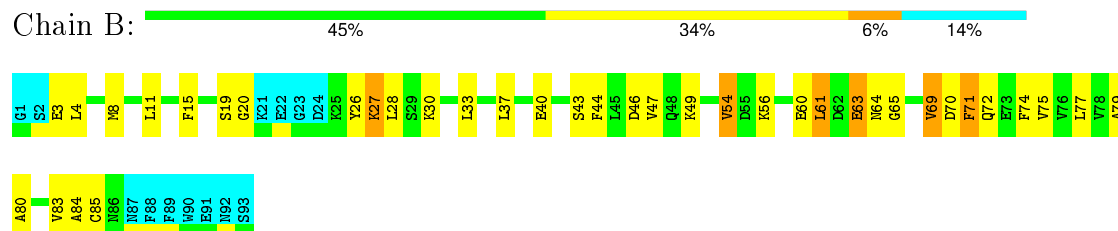


4.2.5 Score per residue for model 5

- Molecule 1: S-100 protein, alpha chain

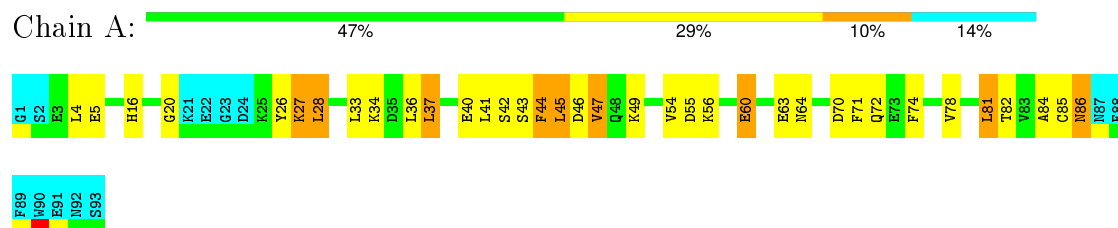


- Molecule 1: S-100 protein, alpha chain

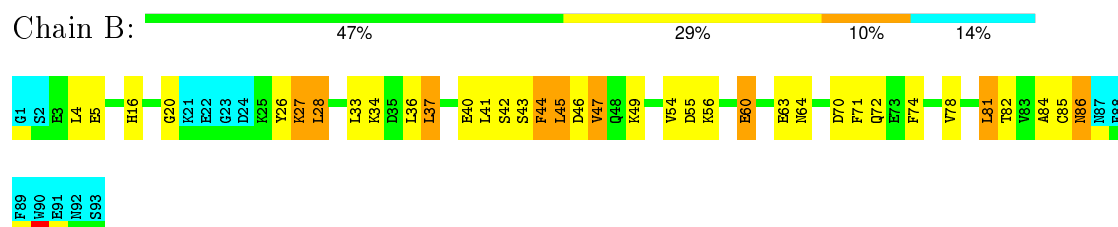


4.2.6 Score per residue for model 6

- Molecule 1: S-100 protein, alpha chain

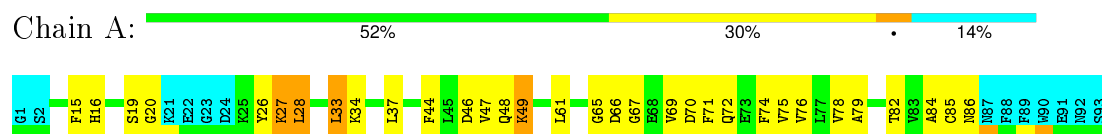


- Molecule 1: S-100 protein, alpha chain

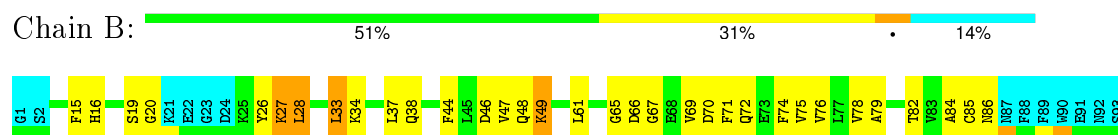


4.2.7 Score per residue for model 7

- Molecule 1: S-100 protein, alpha chain

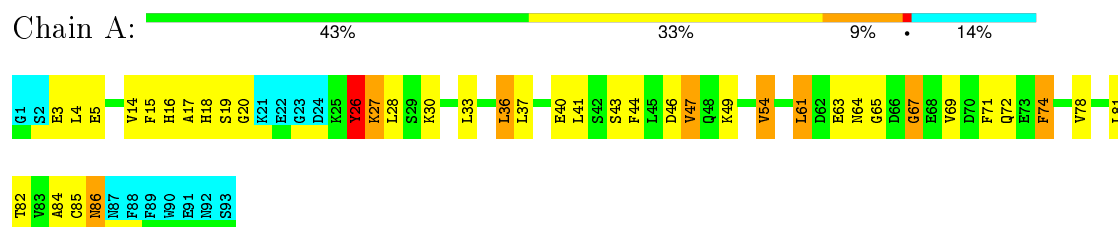


- Molecule 1: S-100 protein, alpha chain

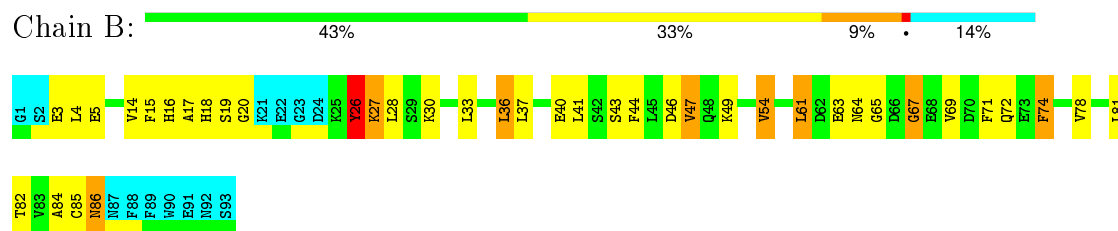


4.2.8 Score per residue for model 8

- Molecule 1: S-100 protein, alpha chain

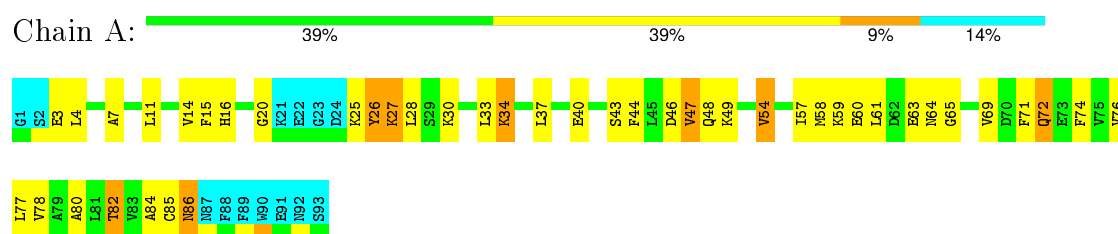


- Molecule 1: S-100 protein, alpha chain

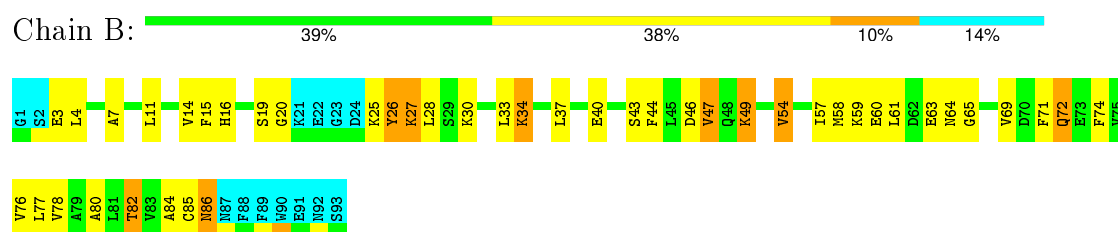


4.2.9 Score per residue for model 9

- Molecule 1: S-100 protein, alpha chain

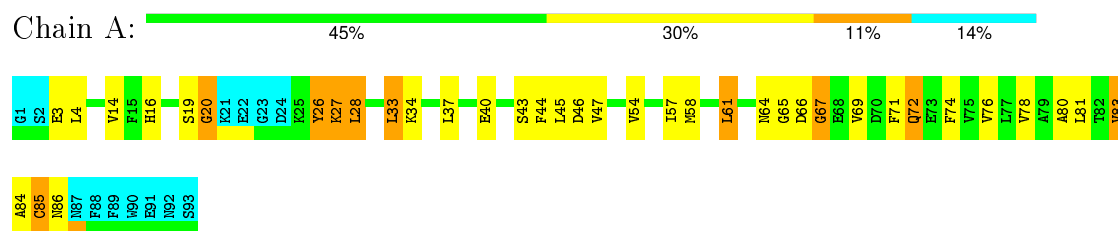


- Molecule 1: S-100 protein, alpha chain

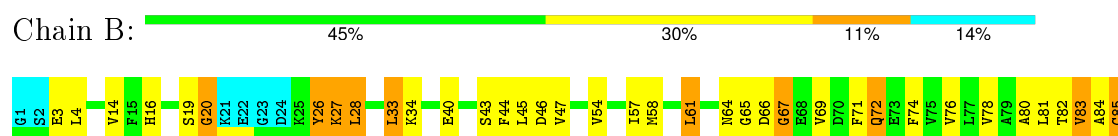


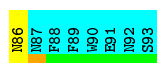
4.2.10 Score per residue for model 10

- Molecule 1: S-100 protein, alpha chain



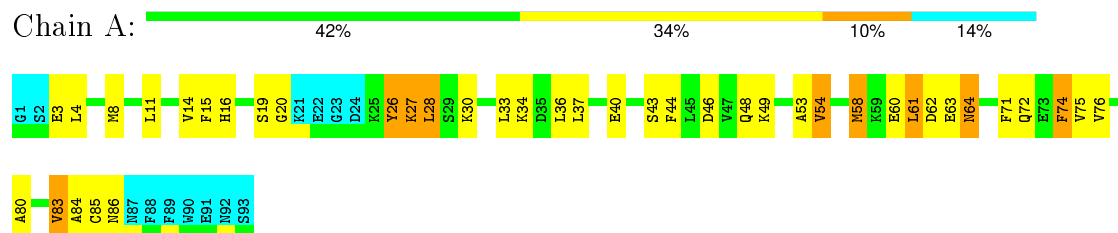
- Molecule 1: S-100 protein, alpha chain



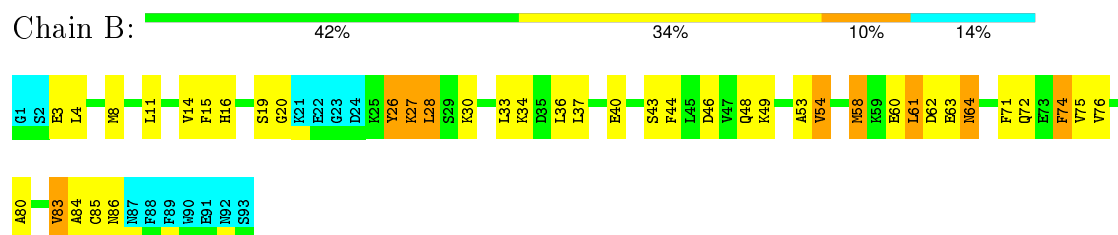


4.2.11 Score per residue for model 11

- Molecule 1: S-100 protein, alpha chain

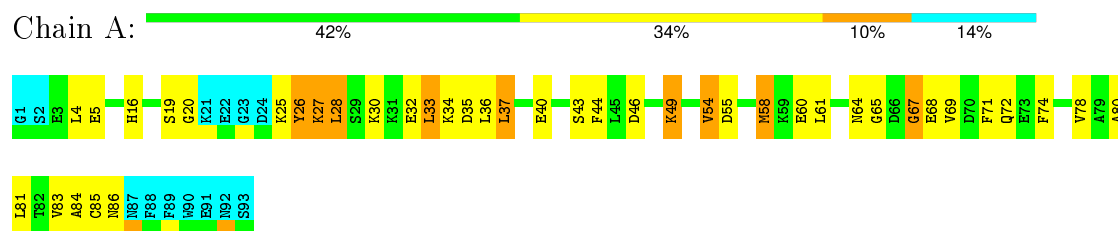


- Molecule 1: S-100 protein, alpha chain

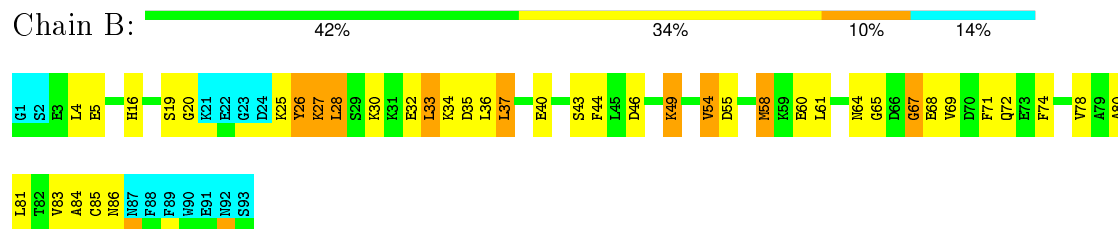


4.2.12 Score per residue for model 12

- Molecule 1: S-100 protein, alpha chain

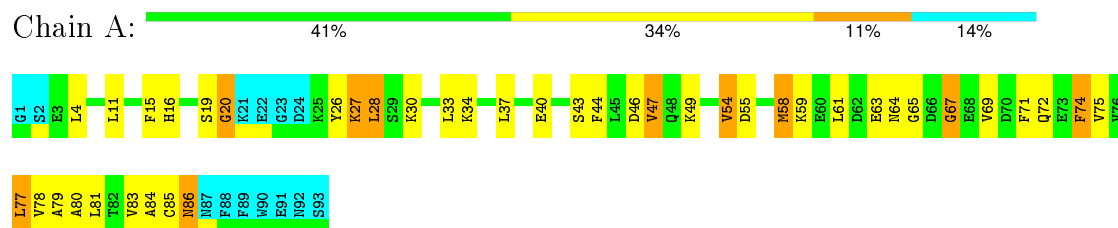


- Molecule 1: S-100 protein, alpha chain

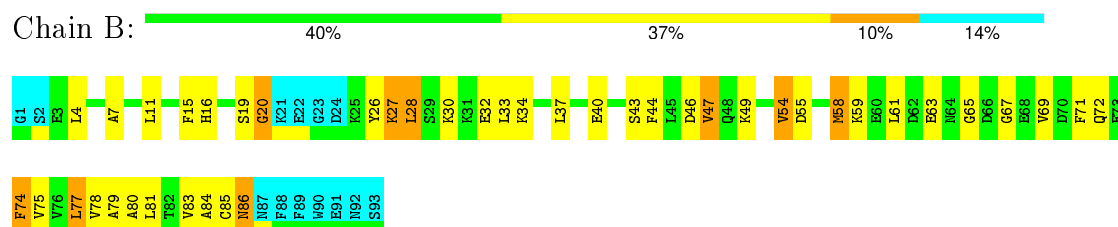


4.2.13 Score per residue for model 13

- Molecule 1: S-100 protein, alpha chain

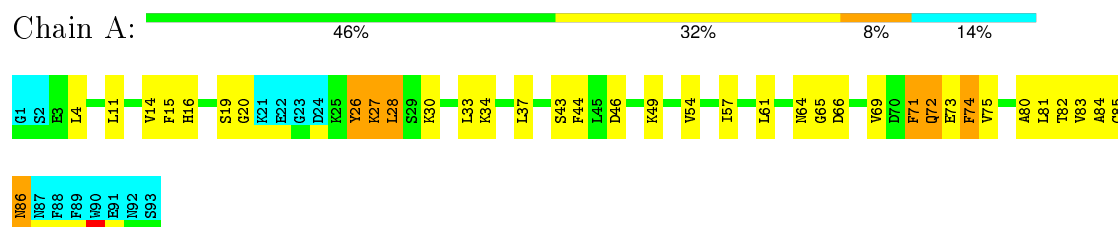


- Molecule 1: S-100 protein, alpha chain

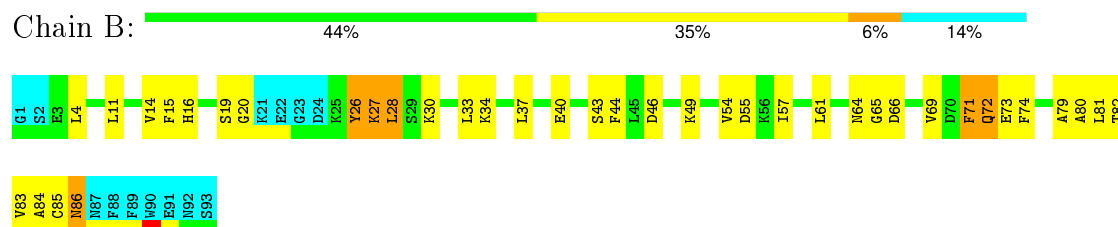


4.2.14 Score per residue for model 14

- Molecule 1: S-100 protein, alpha chain



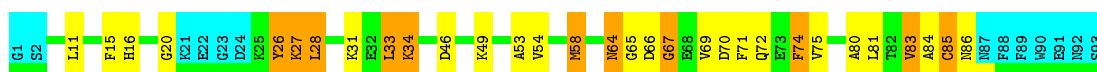
- Molecule 1: S-100 protein, alpha chain



4.2.15 Score per residue for model 15

- Molecule 1: S-100 protein, alpha chain





- Molecule 1: S-100 protein, alpha chain

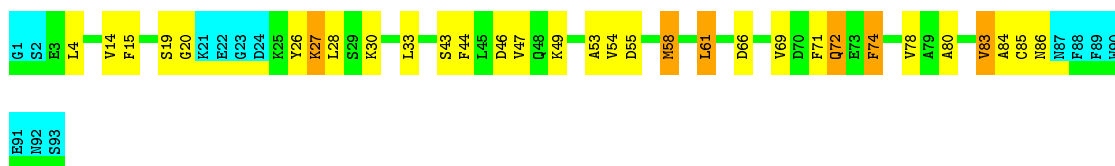


4.2.16 Score per residue for model 16

- Molecule 1: S-100 protein, alpha chain

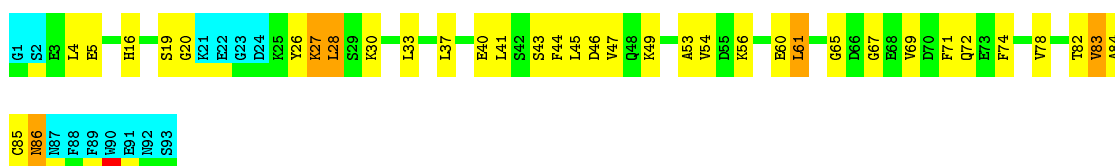


- Molecule 1: S-100 protein, alpha chain



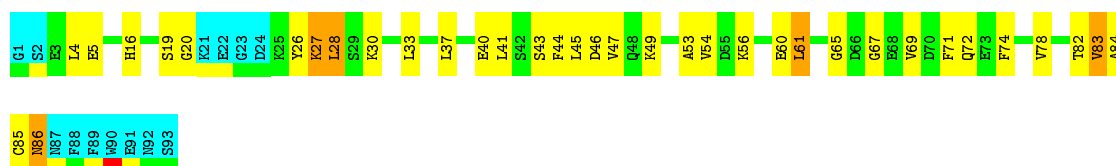
4.2.17 Score per residue for model 17

- Molecule 1: S-100 protein, alpha chain



- Molecule 1: S-100 protein, alpha chain

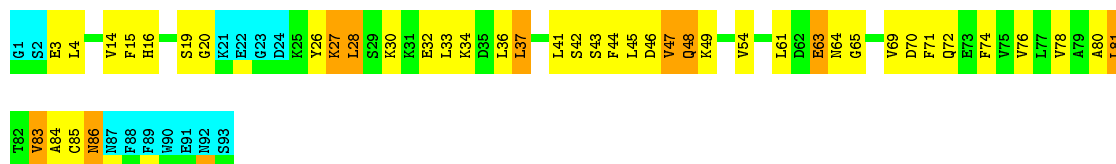




4.2.18 Score per residue for model 18

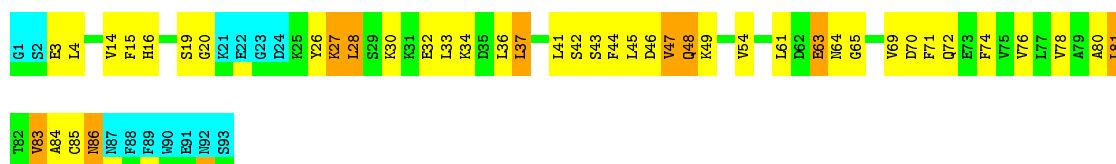
- Molecule 1: S-100 protein, alpha chain

Chain A: 40% 37% 10% 14%



- Molecule 1: S-100 protein, alpha chain

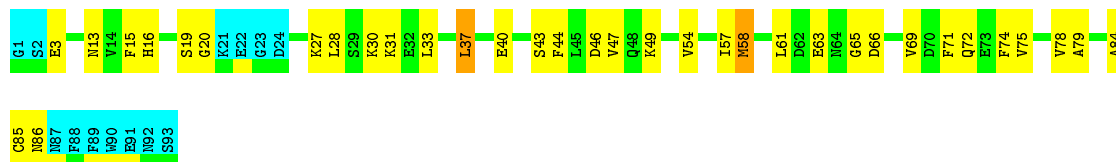
Chain B: 40% 37% 10% 14%



4.2.19 Score per residue for model 19 (medoid)

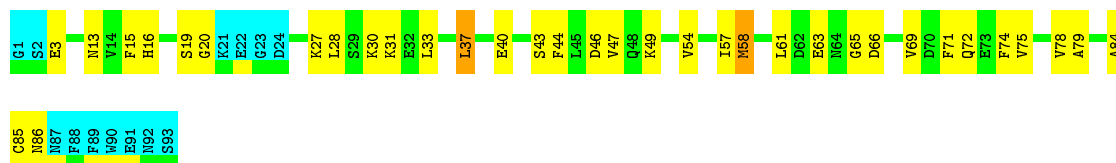
- Molecule 1: S-100 protein, alpha chain

Chain A: 48% 35% 14%



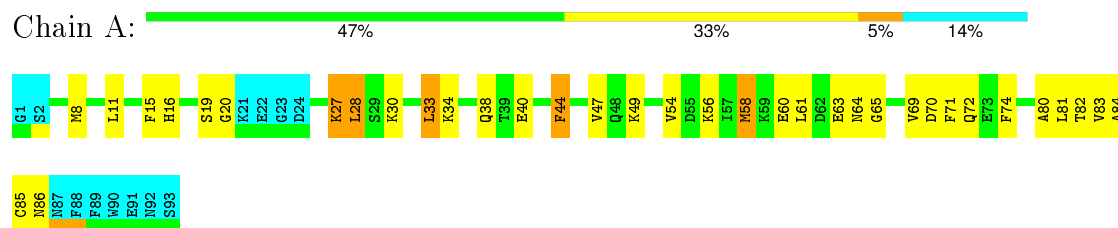
- Molecule 1: S-100 protein, alpha chain

Chain B: 48% 35% 14%

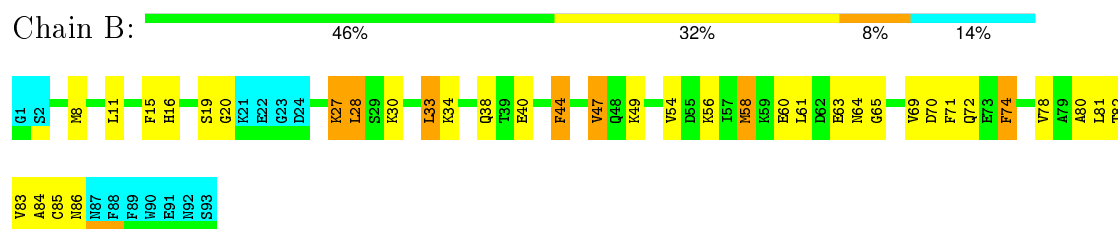


4.2.20 Score per residue for model 20

- Molecule 1: S-100 protein, alpha chain



- Molecule 1: S-100 protein, alpha chain



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry, simulated annealing, docking, molecular dynamics*.

Of the 75 calculated structures, 20 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
X-PLOR	structure solution	3.851
CHARMM	structure solution	
CHARMM	refinement	

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)	BMRB entry 4285
Number of chemical shift lists	3
Total number of shifts	2304
Number of shifts mapped to atoms	2286
Number of unparsed shifts	0
Number of shifts with mapping errors	18
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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

6 Model quality

6.1 Standard geometry

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

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	625	623	621	42±12
1	B	625	623	621	42±11
All	All	25000	24920	24840	1464

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 29.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD22	1:B:4:LEU:CD2	1.14	1.72	13	1
1:A:4:LEU:CD2	1:B:37:LEU:HD22	1.07	1.77	13	1
1:A:72:GLN:CD	1:B:83:VAL:CG2	1.04	2.25	1	1
1:A:83:VAL:CG2	1:B:72:GLN:CD	1.04	2.26	1	1
1:A:41:LEU:HD23	1:B:5:GLU:OE1	1.03	1.54	17	2
1:A:5:GLU:OE1	1:B:41:LEU:HD23	0.98	1.57	17	2
1:B:34:LYS:HZ1	1:B:61:LEU:HD13	0.96	1.17	9	1
1:A:72:GLN:NE2	1:B:83:VAL:HG21	0.96	1.74	1	2
1:A:83:VAL:HG21	1:B:72:GLN:NE2	0.94	1.76	1	2
1:A:72:GLN:CD	1:B:83:VAL:HG21	0.91	1.85	1	1
1:A:34:LYS:HZ1	1:A:61:LEU:HD13	0.90	1.21	9	1
1:A:72:GLN:NE2	1:B:83:VAL:CG2	0.90	2.34	1	2
1:A:33:LEU:HD13	1:A:34:LYS:N	0.89	1.83	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:33:LEU:HD13	1:B:34:LYS:N	0.89	1.82	7	5
1:A:83:VAL:HG21	1:B:72:GLN:CD	0.89	1.86	1	1
1:A:40:GLU:O	1:B:5:GLU:OE1	0.89	1.90	6	2
1:B:34:LYS:NZ	1:B:61:LEU:HD13	0.88	1.81	9	1
1:A:33:LEU:HD22	1:A:69:VAL:HG21	0.88	1.45	18	3
1:A:86:ASN:ND2	1:B:71:PHE:CZ	0.88	2.42	9	3
1:A:4:LEU:CD1	1:B:14:VAL:CG1	0.88	2.51	11	1
1:A:34:LYS:NZ	1:A:61:LEU:HD13	0.88	1.83	9	1
1:A:83:VAL:CG2	1:B:72:GLN:OE1	0.87	2.23	1	3
1:A:5:GLU:OE1	1:B:40:GLU:O	0.87	1.91	6	2
1:A:72:GLN:OE1	1:B:83:VAL:CG2	0.87	2.22	1	3
1:A:83:VAL:CG2	1:B:72:GLN:NE2	0.87	2.36	1	2
1:B:33:LEU:HD22	1:B:69:VAL:HG21	0.86	1.44	18	3
1:A:71:PHE:CZ	1:B:86:ASN:ND2	0.86	2.44	9	3
1:A:41:LEU:CD2	1:B:5:GLU:OE1	0.85	2.24	17	1
1:A:33:LEU:HD23	1:A:34:LYS:N	0.84	1.88	15	2
1:A:37:LEU:HD22	1:B:4:LEU:HD21	0.84	1.48	13	1
1:B:33:LEU:O	1:B:33:LEU:HD22	0.83	1.73	1	3
1:A:14:VAL:CG1	1:B:4:LEU:CD1	0.83	2.55	11	1
1:B:33:LEU:HD23	1:B:34:LYS:N	0.83	1.88	15	2
1:A:5:GLU:OE1	1:B:41:LEU:CD2	0.82	2.26	17	1
1:A:33:LEU:HD22	1:A:33:LEU:O	0.82	1.73	1	3
1:A:40:GLU:OE2	1:B:4:LEU:N	0.81	2.14	8	4
1:A:4:LEU:N	1:B:40:GLU:OE2	0.79	2.14	8	4
1:A:4:LEU:HD21	1:B:37:LEU:HD22	0.79	1.51	13	1
1:A:37:LEU:HD22	1:B:4:LEU:HD22	0.79	1.53	13	1
1:A:72:GLN:OE1	1:B:83:VAL:HG21	0.79	1.77	1	2
1:A:4:LEU:HD21	1:B:14:VAL:HG13	0.79	1.53	16	1
1:A:83:VAL:HG21	1:B:72:GLN:OE1	0.78	1.77	1	2
1:A:80:ALA:O	1:A:83:VAL:HG12	0.78	1.78	14	12
1:B:80:ALA:O	1:B:83:VAL:HG12	0.76	1.79	14	12
1:B:33:LEU:HD12	1:B:33:LEU:O	0.75	1.81	20	1
1:A:33:LEU:O	1:A:33:LEU:HD12	0.75	1.81	20	1
1:A:83:VAL:HB	1:B:72:GLN:OE1	0.75	1.81	5	1
1:A:14:VAL:HG13	1:B:4:LEU:HD21	0.75	1.58	16	1
1:A:76:VAL:HG13	1:B:76:VAL:HG13	0.75	1.59	2	3
1:A:75:VAL:HG11	1:B:79:ALA:HB2	0.74	1.58	1	7
1:A:37:LEU:CD2	1:B:4:LEU:CD2	0.74	2.61	13	1
1:A:4:LEU:HD22	1:B:37:LEU:HD22	0.74	1.58	13	1
1:A:79:ALA:HB2	1:B:75:VAL:HG11	0.73	1.58	1	7
1:A:37:LEU:N	1:A:37:LEU:HD23	0.73	1.99	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:HD21	1:B:14:VAL:CG1	0.73	2.14	16	3
1:A:80:ALA:HA	1:B:72:GLN:HE21	0.73	1.44	1	1
1:A:72:GLN:OE1	1:B:83:VAL:HB	0.72	1.83	5	1
1:A:72:GLN:HE21	1:B:80:ALA:HA	0.72	1.42	1	1
1:A:83:VAL:CB	1:B:72:GLN:OE1	0.72	2.38	5	1
1:A:71:PHE:CD2	1:A:72:GLN:N	0.72	2.58	9	3
1:A:40:GLU:CD	1:B:4:LEU:HB2	0.72	2.05	6	1
1:A:61:LEU:H	1:A:61:LEU:HD12	0.71	1.45	9	1
1:B:71:PHE:CD2	1:B:72:GLN:N	0.71	2.58	9	3
1:A:37:LEU:CD2	1:B:4:LEU:HD22	0.71	2.14	13	1
1:A:14:VAL:HG13	1:B:3:GLU:HB3	0.71	1.63	8	1
1:A:71:PHE:CD1	1:A:72:GLN:N	0.71	2.59	10	15
1:A:86:ASN:ND2	1:B:71:PHE:CE1	0.71	2.59	9	2
1:B:37:LEU:HD23	1:B:37:LEU:N	0.70	2.01	3	3
1:B:49:LYS:N	1:B:84:ALA:O	0.70	2.25	3	19
1:B:71:PHE:CD1	1:B:72:GLN:N	0.70	2.59	10	15
1:B:61:LEU:H	1:B:61:LEU:HD12	0.70	1.45	9	1
1:A:72:GLN:OE1	1:B:83:VAL:CB	0.70	2.39	5	1
1:A:4:LEU:CD2	1:B:37:LEU:CD2	0.70	2.65	13	1
1:A:14:VAL:CG1	1:B:4:LEU:HD21	0.70	2.17	16	3
1:A:14:VAL:HG12	1:B:4:LEU:CD1	0.69	2.18	11	1
1:A:71:PHE:CE1	1:B:86:ASN:ND2	0.69	2.60	9	2
1:A:4:LEU:CD1	1:B:14:VAL:HG12	0.69	2.15	11	1
1:A:4:LEU:HB2	1:B:40:GLU:CD	0.69	2.08	6	1
1:A:4:LEU:HD11	1:B:14:VAL:HG12	0.68	1.64	11	1
1:A:4:LEU:HB3	1:B:40:GLU:CD	0.68	2.09	13	1
1:B:74:PHE:O	1:B:78:VAL:HG23	0.68	1.89	9	16
1:A:40:GLU:CD	1:B:4:LEU:HB3	0.68	2.09	13	1
1:A:49:LYS:N	1:A:84:ALA:O	0.68	2.27	3	19
1:A:33:LEU:C	1:A:33:LEU:HD13	0.67	2.10	10	7
1:B:33:LEU:C	1:B:33:LEU:HD13	0.67	2.10	11	9
1:A:4:LEU:HD12	1:B:14:VAL:CG1	0.67	2.18	11	1
1:A:33:LEU:HD13	1:A:33:LEU:C	0.67	2.10	16	7
1:A:4:LEU:HD22	1:B:37:LEU:CD2	0.67	2.19	13	1
1:A:14:VAL:HG12	1:B:4:LEU:HD11	0.67	1.66	11	1
1:A:74:PHE:O	1:A:78:VAL:HG23	0.66	1.90	18	15
1:A:30:LYS:O	1:A:61:LEU:HD23	0.66	1.90	9	2
1:B:33:LEU:HD13	1:B:33:LEU:C	0.66	2.12	9	5
1:A:3:GLU:HB3	1:B:14:VAL:HG13	0.65	1.68	8	1
1:B:30:LYS:O	1:B:61:LEU:HD23	0.65	1.91	9	2
1:A:75:VAL:CG1	1:B:79:ALA:HB2	0.65	2.21	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:HG	1:B:14:VAL:HG11	0.64	1.68	18	3
1:A:79:ALA:HB2	1:B:75:VAL:CG1	0.64	2.21	1	5
1:B:71:PHE:CG	1:B:72:GLN:N	0.64	2.66	7	14
1:A:71:PHE:CG	1:A:72:GLN:N	0.64	2.66	7	15
1:A:83:VAL:HB	1:B:72:GLN:NE2	0.63	2.08	18	1
1:A:72:GLN:NE2	1:B:83:VAL:HB	0.63	2.07	18	1
1:A:14:VAL:CG1	1:B:4:LEU:HD12	0.62	2.22	11	1
1:A:58:MET:N	1:A:58:MET:SD	0.62	2.73	12	4
1:A:44:PHE:CD2	1:A:85:CYS:SG	0.62	2.93	9	1
1:A:33:LEU:HD22	1:A:69:VAL:CG2	0.62	2.24	18	3
1:B:44:PHE:CD2	1:B:85:CYS:SG	0.62	2.93	9	1
1:A:4:LEU:HB3	1:B:40:GLU:OE1	0.62	1.95	13	1
1:B:58:MET:SD	1:B:58:MET:N	0.61	2.73	12	3
1:A:14:VAL:HG11	1:B:4:LEU:HG	0.61	1.72	18	3
1:A:83:VAL:HG21	1:B:72:GLN:HE22	0.61	1.53	1	1
1:A:83:VAL:HG22	1:B:71:PHE:CZ	0.61	2.30	2	1
1:A:28:LEU:O	1:A:69:VAL:HG22	0.61	1.96	12	14
1:B:34:LYS:HZ1	1:B:61:LEU:CD1	0.61	2.04	9	1
1:A:71:PHE:CZ	1:B:83:VAL:HG22	0.61	2.31	2	1
1:B:54:VAL:HG23	1:B:84:ALA:CB	0.60	2.25	13	12
1:B:46:ASP:OD1	1:B:47:VAL:N	0.60	2.35	18	3
1:A:34:LYS:HZ2	1:A:61:LEU:HD22	0.60	1.55	9	1
1:A:46:ASP:OD1	1:A:47:VAL:N	0.60	2.34	18	3
1:B:28:LEU:O	1:B:69:VAL:HG22	0.60	1.96	20	15
1:A:37:LEU:HD13	1:A:78:VAL:HG22	0.60	1.74	8	3
1:B:37:LEU:N	1:B:37:LEU:HD23	0.60	2.12	18	2
1:A:76:VAL:CG1	1:B:76:VAL:HG13	0.60	2.27	2	1
1:A:54:VAL:HG23	1:A:84:ALA:CB	0.60	2.26	13	12
1:A:61:LEU:N	1:A:61:LEU:HD12	0.60	2.12	9	1
1:A:16:HIS:O	1:A:20:GLY:N	0.60	2.35	1	17
1:B:37:LEU:HD13	1:B:78:VAL:HG22	0.59	1.73	8	3
1:A:76:VAL:HG13	1:B:76:VAL:CG1	0.59	2.27	2	1
1:A:82:THR:O	1:A:86:ASN:N	0.59	2.35	9	7
1:A:57:ILE:O	1:A:61:LEU:HD12	0.59	1.97	14	3
1:B:58:MET:N	1:B:58:MET:SD	0.59	2.76	20	2
1:A:46:ASP:OD1	1:A:47:VAL:HG22	0.59	1.97	18	1
1:A:37:LEU:HD23	1:A:37:LEU:N	0.59	2.13	18	1
1:B:33:LEU:HD22	1:B:69:VAL:CG2	0.59	2.23	18	3
1:A:4:LEU:CD2	1:B:14:VAL:HG13	0.59	2.28	16	1
1:B:4:LEU:HD22	1:B:4:LEU:N	0.59	2.13	5	2
1:A:4:LEU:HG	1:B:14:VAL:CG1	0.59	2.28	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:46:ASP:OD1	1:B:47:VAL:HG22	0.59	1.97	18	1
1:A:72:GLN:HE22	1:B:83:VAL:HG21	0.59	1.51	1	1
1:B:57:ILE:O	1:B:61:LEU:HD12	0.59	1.97	14	3
1:A:4:LEU:HD22	1:A:4:LEU:N	0.59	2.12	5	1
1:A:40:GLU:OE1	1:B:4:LEU:HB3	0.59	1.97	13	1
1:B:82:THR:O	1:B:86:ASN:N	0.59	2.36	9	7
1:A:15:PHE:CE1	1:A:74:PHE:CE1	0.59	2.91	13	8
1:A:37:LEU:HD22	1:B:4:LEU:HG	0.59	1.75	5	1
1:A:4:LEU:HG	1:B:37:LEU:CD2	0.59	2.28	5	1
1:B:16:HIS:O	1:B:20:GLY:N	0.58	2.35	1	17
1:B:37:LEU:HD23	1:B:78:VAL:HG22	0.58	1.75	9	1
1:A:37:LEU:HD23	1:A:78:VAL:HG22	0.58	1.75	9	1
1:A:33:LEU:C	1:A:33:LEU:HD22	0.58	2.18	1	1
1:A:37:LEU:CD2	1:B:4:LEU:HG	0.58	2.28	5	1
1:B:15:PHE:CE1	1:B:74:PHE:CE1	0.58	2.91	13	8
1:A:33:LEU:C	1:A:33:LEU:HD23	0.58	2.19	15	1
1:B:61:LEU:HD12	1:B:61:LEU:N	0.58	2.13	9	1
1:A:58:MET:SD	1:A:58:MET:N	0.58	2.76	19	1
1:B:33:LEU:C	1:B:33:LEU:HD22	0.58	2.18	1	2
1:A:40:GLU:OE1	1:B:4:LEU:HB2	0.58	1.99	6	1
1:B:61:LEU:CD2	1:B:61:LEU:N	0.57	2.67	17	2
1:A:33:LEU:HD22	1:A:33:LEU:C	0.57	2.19	7	1
1:A:86:ASN:N	1:A:86:ASN:HD22	0.57	1.97	6	1
1:B:61:LEU:N	1:B:61:LEU:CD2	0.57	2.68	16	2
1:A:40:GLU:OE1	1:B:4:LEU:CD1	0.57	2.52	6	1
1:B:33:LEU:C	1:B:33:LEU:HD23	0.57	2.19	15	2
1:B:44:PHE:O	1:B:85:CYS:SG	0.57	2.63	5	10
1:A:61:LEU:N	1:A:61:LEU:CD2	0.57	2.68	16	4
1:B:44:PHE:CG	1:B:85:CYS:SG	0.57	2.98	9	1
1:A:44:PHE:CG	1:A:85:CYS:SG	0.56	2.98	9	1
1:A:4:LEU:HG	1:B:37:LEU:HD22	0.56	1.77	5	1
1:A:33:LEU:HD12	1:A:69:VAL:HG21	0.56	1.77	12	2
1:B:86:ASN:N	1:B:86:ASN:HD22	0.56	1.97	6	1
1:A:71:PHE:CE2	1:B:86:ASN:ND2	0.56	2.74	18	2
1:B:33:LEU:HD12	1:B:69:VAL:HG21	0.56	1.76	12	2
1:B:61:LEU:O	1:B:65:GLY:N	0.56	2.39	4	4
1:A:14:VAL:CG1	1:B:4:LEU:HG	0.56	2.30	18	2
1:A:44:PHE:O	1:A:85:CYS:SG	0.56	2.63	5	10
1:A:64:ASN:HD22	1:A:67:GLY:CA	0.56	2.14	12	1
1:B:81:LEU:O	1:B:84:ALA:HB3	0.56	2.01	6	3
1:B:64:ASN:HD22	1:B:67:GLY:CA	0.56	2.14	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:60:GLU:N	1:B:60:GLU:OE1	0.56	2.39	6	2
1:A:81:LEU:O	1:A:84:ALA:HB3	0.56	2.01	6	3
1:A:4:LEU:HD11	1:B:14:VAL:HG11	0.56	1.78	16	1
1:A:86:ASN:ND2	1:B:71:PHE:CE2	0.56	2.74	18	2
1:A:61:LEU:O	1:A:65:GLY:N	0.56	2.39	4	4
1:A:4:LEU:N	1:A:4:LEU:CD2	0.56	2.69	2	3
1:A:72:GLN:NE2	1:B:80:ALA:HA	0.56	2.15	1	1
1:B:34:LYS:HZ2	1:B:61:LEU:HD22	0.55	1.62	9	1
1:B:73:GLU:N	1:B:73:GLU:OE1	0.55	2.40	14	2
1:A:54:VAL:O	1:A:58:MET:SD	0.55	2.65	19	7
1:B:27:LYS:N	1:B:69:VAL:O	0.55	2.40	1	1
1:A:4:LEU:CB	1:B:40:GLU:OE1	0.55	2.55	13	2
1:A:26:TYR:CD1	1:A:26:TYR:N	0.55	2.73	8	1
1:A:33:LEU:HD23	1:A:33:LEU:C	0.55	2.21	12	1
1:B:54:VAL:O	1:B:58:MET:SD	0.55	2.65	9	7
1:A:4:LEU:CD1	1:B:40:GLU:OE1	0.55	2.55	6	1
1:B:15:PHE:O	1:B:19:SER:N	0.55	2.38	14	3
1:A:60:GLU:N	1:A:60:GLU:OE1	0.55	2.39	6	2
1:A:80:ALA:HA	1:B:72:GLN:NE2	0.55	2.15	1	1
1:B:37:LEU:HD21	1:B:74:PHE:CE2	0.55	2.36	7	1
1:A:15:PHE:O	1:A:19:SER:N	0.54	2.38	14	4
1:B:15:PHE:O	1:B:20:GLY:N	0.54	2.41	16	1
1:A:72:GLN:CD	1:B:83:VAL:HG23	0.54	2.18	1	1
1:A:72:GLN:OE1	1:B:83:VAL:HG22	0.54	2.01	1	1
1:A:83:VAL:HG22	1:B:72:GLN:OE1	0.54	2.02	1	1
1:A:15:PHE:O	1:A:20:GLY:N	0.54	2.40	16	1
1:A:57:ILE:HD11	1:A:80:ALA:HB1	0.54	1.79	9	1
1:B:4:LEU:CD2	1:B:4:LEU:N	0.54	2.71	5	2
1:B:47:VAL:HG13	1:B:47:VAL:O	0.54	2.03	8	2
1:A:5:GLU:HB2	1:B:40:GLU:HG2	0.54	1.79	4	1
1:A:27:LYS:O	1:A:28:LEU:HD22	0.54	2.03	12	4
1:A:81:LEU:HD23	1:A:81:LEU:O	0.54	2.02	14	4
1:B:70:ASP:OD1	1:B:71:PHE:N	0.54	2.41	5	6
1:A:40:GLU:CD	1:B:4:LEU:CB	0.54	2.76	6	2
1:B:26:TYR:CD1	1:B:26:TYR:N	0.54	2.72	8	1
1:A:83:VAL:HG22	1:B:71:PHE:HZ	0.54	1.61	2	1
1:A:45:LEU:O	1:A:48:GLN:NE2	0.54	2.41	2	1
1:A:4:LEU:HB2	1:B:40:GLU:OE1	0.54	2.02	6	2
1:A:85:CYS:O	1:A:85:CYS:SG	0.54	2.66	3	3
1:A:48:GLN:N	1:A:48:GLN:OE1	0.54	2.41	18	1
1:B:48:GLN:OE1	1:B:48:GLN:N	0.54	2.41	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:LEU:O	1:A:65:GLY:CA	0.54	2.56	14	14
1:A:11:LEU:O	1:A:15:PHE:CD1	0.54	2.61	3	6
1:A:37:LEU:HD21	1:A:74:PHE:CE2	0.54	2.37	7	1
1:B:82:THR:O	1:B:85:CYS:N	0.53	2.41	20	3
1:A:70:ASP:OD1	1:A:71:PHE:N	0.53	2.41	5	6
1:A:40:GLU:OE2	1:B:4:LEU:CB	0.53	2.56	6	1
1:A:73:GLU:OE1	1:A:73:GLU:N	0.53	2.40	14	1
1:B:61:LEU:O	1:B:65:GLY:CA	0.53	2.56	14	14
1:B:57:ILE:HD11	1:B:80:ALA:HB1	0.53	1.80	9	1
1:A:40:GLU:HG2	1:B:5:GLU:HB2	0.53	1.78	4	1
1:B:27:LYS:NZ	1:B:74:PHE:CE2	0.53	2.70	6	2
1:A:31:LYS:N	1:A:65:GLY:O	0.53	2.38	19	3
1:A:85:CYS:SG	1:A:85:CYS:O	0.53	2.67	16	2
1:A:27:LYS:NZ	1:A:74:PHE:CE2	0.53	2.70	6	2
1:B:33:LEU:CD2	1:B:69:VAL:HG11	0.53	2.34	17	3
1:A:33:LEU:HG	1:A:69:VAL:HG21	0.53	1.81	10	6
1:A:27:LYS:N	1:A:69:VAL:O	0.53	2.39	1	1
1:B:81:LEU:O	1:B:81:LEU:HD23	0.52	2.04	14	4
1:B:33:LEU:HG	1:B:69:VAL:HG21	0.52	1.81	10	7
1:A:44:PHE:O	1:A:85:CYS:CB	0.52	2.57	10	1
1:A:14:VAL:CG1	1:B:4:LEU:CD2	0.52	2.87	9	3
1:A:43:SER:O	1:A:46:ASP:OD1	0.52	2.27	18	2
1:A:33:LEU:CD2	1:A:69:VAL:HG11	0.52	2.34	17	3
1:A:40:GLU:OE1	1:B:4:LEU:CB	0.52	2.57	13	2
1:B:11:LEU:O	1:B:15:PHE:CD1	0.52	2.62	3	6
1:B:45:LEU:O	1:B:48:GLN:NE2	0.52	2.42	2	1
1:A:37:LEU:N	1:A:37:LEU:CD2	0.52	2.67	3	3
1:A:33:LEU:HD21	1:A:37:LEU:HD11	0.52	1.81	3	1
1:B:30:LYS:O	1:B:61:LEU:CD1	0.52	2.57	17	4
1:A:60:GLU:OE1	1:A:60:GLU:N	0.52	2.41	17	1
1:B:16:HIS:O	1:B:20:GLY:CA	0.52	2.57	7	4
1:A:30:LYS:O	1:A:61:LEU:CD1	0.52	2.58	17	4
1:A:72:GLN:O	1:A:72:GLN:NE2	0.52	2.42	17	1
1:B:27:LYS:O	1:B:28:LEU:HD22	0.52	2.04	12	4
1:B:44:PHE:O	1:B:85:CYS:CB	0.52	2.57	10	1
1:B:85:CYS:SG	1:B:85:CYS:O	0.52	2.67	16	3
1:B:43:SER:O	1:B:46:ASP:OD1	0.52	2.27	18	2
1:B:63:GLU:O	1:B:64:ASN:ND2	0.52	2.43	20	1
1:A:3:GLU:CB	1:B:14:VAL:HG13	0.52	2.34	8	1
1:B:72:GLN:NE2	1:B:72:GLN:O	0.52	2.42	17	1
1:B:53:ALA:CB	1:B:83:VAL:CG1	0.52	2.88	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:THR:O	1:A:85:CYS:N	0.52	2.41	20	3
1:A:64:ASN:O	1:A:66:ASP:N	0.52	2.43	10	3
1:A:4:LEU:HD11	1:B:14:VAL:CG1	0.52	2.29	11	1
1:A:16:HIS:O	1:A:20:GLY:CA	0.52	2.57	7	4
1:A:14:VAL:HG13	1:B:3:GLU:CB	0.52	2.32	8	1
1:A:14:VAL:HG13	1:B:4:LEU:CD2	0.51	2.31	16	1
1:B:27:LYS:HB3	1:B:69:VAL:HG23	0.51	1.82	9	7
1:B:33:LEU:HD21	1:B:37:LEU:HD11	0.51	1.83	3	1
1:A:11:LEU:HD11	1:B:11:LEU:HD11	0.51	1.82	13	1
1:A:53:ALA:CB	1:A:83:VAL:CG1	0.51	2.88	11	4
1:A:83:VAL:HG23	1:B:72:GLN:CD	0.51	2.20	1	1
1:A:4:LEU:CB	1:B:40:GLU:CD	0.51	2.78	6	2
1:B:64:ASN:O	1:B:66:ASP:N	0.51	2.43	10	3
1:B:37:LEU:CD2	1:B:37:LEU:N	0.51	2.73	1	4
1:A:14:VAL:HG11	1:B:4:LEU:HD11	0.51	1.80	16	1
1:A:30:LYS:NZ	1:A:64:ASN:O	0.51	2.41	8	1
1:A:30:LYS:CE	1:A:60:GLU:O	0.51	2.59	17	2
1:A:63:GLU:O	1:A:64:ASN:ND2	0.51	2.44	20	1
1:A:14:VAL:CG1	1:B:3:GLU:HB3	0.51	2.33	8	1
1:A:33:LEU:CD2	1:A:69:VAL:HG21	0.51	2.32	17	2
1:B:74:PHE:C	1:B:74:PHE:CD1	0.51	2.84	11	7
1:A:11:LEU:HD21	1:B:7:ALA:CB	0.51	2.35	9	1
1:A:73:GLU:N	1:A:73:GLU:OE1	0.51	2.43	2	1
1:A:47:VAL:O	1:A:47:VAL:HG13	0.51	2.04	8	4
1:A:49:LYS:CB	1:A:49:LYS:NZ	0.51	2.74	18	1
1:A:86:ASN:CG	1:B:71:PHE:CZ	0.51	2.84	9	1
1:A:4:LEU:CD2	1:B:14:VAL:CG1	0.51	2.88	9	3
1:B:19:SER:OG	1:B:27:LYS:O	0.51	2.29	4	4
1:B:37:LEU:HD22	1:B:37:LEU:N	0.51	2.21	1	1
1:B:77:LEU:CD2	1:B:77:LEU:N	0.51	2.74	13	1
1:A:27:LYS:HB3	1:A:69:VAL:HG23	0.51	1.82	9	9
1:B:85:CYS:O	1:B:85:CYS:SG	0.51	2.69	3	2
1:A:26:TYR:O	1:A:27:LYS:O	0.51	2.29	9	9
1:B:30:LYS:CE	1:B:60:GLU:O	0.50	2.59	17	2
1:A:4:LEU:HD11	1:B:18:HIS:CE1	0.50	2.41	1	1
1:A:74:PHE:CD1	1:A:74:PHE:C	0.50	2.84	11	6
1:A:4:LEU:CB	1:B:40:GLU:OE2	0.50	2.58	6	1
1:B:26:TYR:O	1:B:27:LYS:O	0.50	2.30	9	9
1:B:37:LEU:HD13	1:B:78:VAL:CG2	0.50	2.37	3	2
1:A:33:LEU:HD22	1:A:69:VAL:HG11	0.50	1.81	18	2
1:A:77:LEU:CD2	1:A:77:LEU:N	0.50	2.74	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:PHE:HZ	1:B:83:VAL:HG22	0.50	1.63	2	1
1:B:33:LEU:HD22	1:B:69:VAL:HG11	0.50	1.83	18	2
1:B:33:LEU:HD12	1:B:33:LEU:C	0.50	2.26	20	1
1:A:5:GLU:HB2	1:B:40:GLU:O	0.50	2.06	6	1
1:A:37:LEU:HD22	1:A:37:LEU:N	0.50	2.21	1	1
1:A:37:LEU:HD13	1:A:78:VAL:CG2	0.50	2.37	3	2
1:A:72:GLN:NE2	1:B:83:VAL:HG23	0.50	2.18	1	1
1:A:40:GLU:O	1:B:5:GLU:HB2	0.50	2.06	6	1
1:A:28:LEU:HD11	1:A:36:LEU:CD1	0.50	2.37	6	1
1:B:34:LYS:HB2	1:B:61:LEU:HD13	0.50	1.84	18	1
1:A:33:LEU:HD12	1:A:33:LEU:C	0.50	2.25	20	1
1:A:19:SER:OG	1:A:27:LYS:O	0.50	2.29	4	4
1:A:46:ASP:O	1:A:47:VAL:HG13	0.49	2.07	9	3
1:B:28:LEU:HD11	1:B:36:LEU:CD1	0.49	2.37	6	1
1:B:33:LEU:CD2	1:B:69:VAL:HG21	0.49	2.30	18	3
1:A:4:LEU:CD2	1:B:14:VAL:HG11	0.49	2.37	14	1
1:A:14:VAL:HG11	1:B:4:LEU:CD2	0.49	2.36	14	1
1:B:57:ILE:O	1:B:61:LEU:CD1	0.49	2.61	9	2
1:A:46:ASP:CG	1:A:47:VAL:HG22	0.49	2.27	4	3
1:A:18:HIS:CE1	1:B:4:LEU:HD11	0.49	2.42	1	1
1:A:74:PHE:C	1:A:74:PHE:CD1	0.49	2.85	15	5
1:B:49:LYS:NZ	1:B:49:LYS:CB	0.49	2.75	18	1
1:B:46:ASP:CG	1:B:47:VAL:HG22	0.49	2.27	4	3
1:B:47:VAL:O	1:B:47:VAL:HG13	0.49	2.08	6	2
1:B:46:ASP:O	1:B:47:VAL:HG13	0.49	2.08	4	3
1:A:42:SER:O	1:A:45:LEU:CD2	0.49	2.61	6	2
1:A:57:ILE:O	1:A:61:LEU:CD1	0.49	2.60	9	1
1:A:71:PHE:CZ	1:B:86:ASN:CG	0.49	2.85	9	1
1:A:33:LEU:HD11	1:A:37:LEU:HD11	0.49	1.83	6	1
1:B:56:LYS:O	1:B:60:GLU:OE1	0.49	2.30	20	2
1:A:33:LEU:CD1	1:A:33:LEU:C	0.49	2.81	16	6
1:A:33:LEU:CD1	1:A:69:VAL:HG21	0.49	2.38	15	2
1:B:33:LEU:HD13	1:B:69:VAL:HG11	0.49	1.85	12	1
1:B:42:SER:O	1:B:45:LEU:CD2	0.49	2.61	6	2
1:A:7:ALA:CB	1:B:11:LEU:HD21	0.49	2.37	9	1
1:A:83:VAL:HG23	1:B:72:GLN:NE2	0.49	2.20	1	1
1:A:71:PHE:O	1:A:75:VAL:HG23	0.49	2.08	15	2
1:B:11:LEU:O	1:B:15:PHE:CE1	0.49	2.66	20	3
1:A:47:VAL:HG22	1:A:47:VAL:O	0.49	2.08	1	2
1:A:47:VAL:O	1:A:49:LYS:NZ	0.49	2.46	7	1
1:A:74:PHE:O	1:A:78:VAL:CG2	0.48	2.61	18	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LEU:O	1:A:15:PHE:CE1	0.48	2.66	20	3
1:A:45:LEU:HD12	1:A:45:LEU:N	0.48	2.23	1	2
1:B:33:LEU:HD11	1:B:37:LEU:HD11	0.48	1.84	6	1
1:A:81:LEU:C	1:A:81:LEU:HD23	0.48	2.28	2	1
1:A:3:GLU:HB3	1:B:14:VAL:CG1	0.48	2.38	8	1
1:A:40:GLU:OE2	1:B:4:LEU:HB3	0.48	2.08	6	1
1:B:33:LEU:CD1	1:B:33:LEU:C	0.48	2.81	16	7
1:B:30:LYS:NZ	1:B:64:ASN:O	0.48	2.41	8	1
1:A:4:LEU:HB3	1:B:40:GLU:OE2	0.48	2.08	6	1
1:B:33:LEU:C	1:B:33:LEU:CD1	0.48	2.82	10	4
1:B:43:SER:O	1:B:46:ASP:N	0.48	2.43	18	2
1:A:34:LYS:HB2	1:A:61:LEU:HD13	0.48	1.84	18	1
1:B:33:LEU:CD1	1:B:69:VAL:HG21	0.48	2.39	15	2
1:A:56:LYS:O	1:A:60:GLU:OE1	0.48	2.30	20	2
1:A:60:GLU:O	1:A:64:ASN:ND2	0.48	2.46	11	1
1:B:74:PHE:O	1:B:78:VAL:CG2	0.48	2.61	12	8
1:B:37:LEU:CD2	1:B:74:PHE:CE2	0.48	2.97	12	2
1:A:64:ASN:ND2	1:A:67:GLY:CA	0.48	2.77	12	2
1:A:64:ASN:C	1:A:66:ASP:N	0.48	2.67	10	3
1:B:45:LEU:N	1:B:45:LEU:HD12	0.48	2.24	1	2
1:B:71:PHE:O	1:B:75:VAL:HG23	0.48	2.09	15	2
1:A:37:LEU:CD2	1:A:37:LEU:N	0.47	2.74	12	1
1:B:3:GLU:N	1:B:3:GLU:OE1	0.47	2.42	9	2
1:B:28:LEU:HD23	1:B:28:LEU:N	0.47	2.24	1	1
1:A:28:LEU:HD23	1:A:28:LEU:N	0.47	2.24	1	1
1:A:15:PHE:CZ	1:A:74:PHE:CE1	0.47	3.02	13	1
1:A:37:LEU:CD2	1:A:74:PHE:CE2	0.47	2.98	12	2
1:B:64:ASN:ND2	1:B:67:GLY:CA	0.47	2.77	12	2
1:A:33:LEU:C	1:A:33:LEU:CD1	0.47	2.83	14	6
1:B:30:LYS:NZ	1:B:64:ASN:HD22	0.47	2.07	18	1
1:A:30:LYS:O	1:A:61:LEU:CD2	0.47	2.62	19	1
1:B:64:ASN:C	1:B:66:ASP:N	0.47	2.67	10	3
1:A:30:LYS:NZ	1:A:64:ASN:HD22	0.47	2.08	18	1
1:A:4:LEU:CG	1:B:14:VAL:CG1	0.47	2.93	11	1
1:B:30:LYS:O	1:B:61:LEU:CD2	0.47	2.62	19	1
1:B:4:LEU:N	1:B:4:LEU:CD2	0.47	2.78	16	1
1:B:46:ASP:O	1:B:46:ASP:OD1	0.47	2.33	15	1
1:B:15:PHE:CZ	1:B:74:PHE:CE1	0.47	3.02	13	1
1:A:26:TYR:CG	1:A:68:GLU:OE2	0.47	2.67	12	1
1:A:37:LEU:N	1:A:37:LEU:HD12	0.47	2.25	11	1
1:B:29:SER:O	1:B:33:LEU:N	0.47	2.41	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:47:VAL:O	1:B:49:LYS:NZ	0.47	2.46	7	1
1:A:79:ALA:CB	1:B:75:VAL:CG1	0.46	2.93	1	1
1:B:60:GLU:O	1:B:64:ASN:ND2	0.46	2.47	11	1
1:A:46:ASP:OD1	1:A:46:ASP:O	0.46	2.33	15	1
1:A:54:VAL:CG2	1:A:84:ALA:HB2	0.46	2.40	10	2
1:A:33:LEU:HD13	1:A:69:VAL:HG11	0.46	1.85	12	1
1:B:54:VAL:CG2	1:B:84:ALA:HB2	0.46	2.40	10	2
1:A:75:VAL:CG1	1:B:79:ALA:CB	0.46	2.93	1	1
1:A:43:SER:O	1:A:46:ASP:CB	0.46	2.64	1	7
1:A:41:LEU:O	1:A:44:PHE:CB	0.46	2.64	1	3
1:A:25:LYS:O	1:A:26:TYR:O	0.46	2.34	12	4
1:B:26:TYR:CG	1:B:68:GLU:OE2	0.46	2.68	12	1
1:A:72:GLN:O	1:A:76:VAL:HG23	0.46	2.11	18	4
1:B:41:LEU:O	1:B:44:PHE:CB	0.46	2.64	1	3
1:A:44:PHE:CE2	1:A:85:CYS:SG	0.46	3.09	9	1
1:A:3:GLU:OE1	1:A:3:GLU:N	0.46	2.42	10	1
1:A:4:LEU:N	1:A:4:LEU:HD22	0.46	2.24	16	2
1:B:44:PHE:CE2	1:B:85:CYS:SG	0.46	3.08	9	1
1:A:3:GLU:HB3	1:B:14:VAL:HG22	0.46	1.86	11	1
1:B:43:SER:O	1:B:46:ASP:CB	0.46	2.64	1	7
1:A:44:PHE:C	1:A:46:ASP:N	0.46	2.69	11	3
1:B:72:GLN:O	1:B:76:VAL:HG23	0.46	2.10	3	4
1:B:25:LYS:O	1:B:26:TYR:O	0.46	2.34	12	4
1:B:64:ASN:O	1:B:67:GLY:N	0.46	2.40	3	2
1:B:44:PHE:C	1:B:46:ASP:N	0.46	2.69	11	3
1:A:81:LEU:O	1:A:84:ALA:CB	0.46	2.64	10	1
1:A:4:LEU:HD21	1:B:74:PHE:CZ	0.46	2.46	17	1
1:B:81:LEU:O	1:B:84:ALA:CB	0.46	2.64	10	1
1:A:30:LYS:NZ	1:A:60:GLU:O	0.45	2.50	12	1
1:B:41:LEU:O	1:B:44:PHE:N	0.45	2.41	4	3
1:B:32:GLU:O	1:B:35:ASP:N	0.45	2.50	12	1
1:A:55:ASP:OD1	1:A:59:LYS:NZ	0.45	2.49	13	1
1:A:66:ASP:O	1:A:66:ASP:OD1	0.45	2.34	16	2
1:A:29:SER:O	1:A:33:LEU:N	0.45	2.42	4	1
1:A:75:VAL:CG1	1:B:75:VAL:CG1	0.45	2.94	4	1
1:A:83:VAL:N	1:B:71:PHE:HZ	0.45	2.10	14	1
1:A:41:LEU:O	1:A:44:PHE:N	0.45	2.42	1	3
1:B:66:ASP:O	1:B:67:GLY:O	0.45	2.35	15	3
1:A:14:VAL:HG22	1:B:3:GLU:HB3	0.45	1.87	11	1
1:A:33:LEU:O	1:A:33:LEU:HD13	0.45	2.12	5	2
1:B:63:GLU:OE2	1:B:64:ASN:OD1	0.45	2.35	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:PHE:HE2	1:B:5:GLU:OE2	0.45	1.95	17	1
1:A:44:PHE:C	1:A:46:ASP:H	0.45	2.14	7	4
1:B:44:PHE:C	1:B:46:ASP:H	0.45	2.14	7	3
1:B:37:LEU:N	1:B:37:LEU:CD2	0.45	2.78	18	2
1:A:84:ALA:C	1:A:85:CYS:SG	0.45	2.94	11	3
1:A:34:LYS:NZ	1:A:61:LEU:CD1	0.45	2.71	9	1
1:B:48:GLN:CG	1:B:48:GLN:O	0.45	2.65	11	1
1:A:14:VAL:HG11	1:B:4:LEU:HD13	0.45	1.89	2	1
1:B:31:LYS:N	1:B:65:GLY:O	0.45	2.38	19	3
1:A:47:VAL:O	1:A:47:VAL:HG23	0.45	2.12	18	2
1:A:15:PHE:CZ	1:A:74:PHE:CD1	0.45	3.05	1	1
1:B:33:LEU:O	1:B:33:LEU:HD13	0.45	2.12	5	2
1:B:30:LYS:HB3	1:B:61:LEU:HD23	0.45	1.89	13	1
1:B:64:ASN:OD1	1:B:66:ASP:OD1	0.45	2.35	4	1
1:B:84:ALA:C	1:B:85:CYS:SG	0.45	2.95	11	2
1:A:32:GLU:O	1:A:35:ASP:N	0.45	2.50	12	1
1:B:77:LEU:O	1:B:80:ALA:HB3	0.45	2.12	9	1
1:B:37:LEU:N	1:B:37:LEU:HD12	0.45	2.25	11	1
1:B:64:ASN:OD1	1:B:67:GLY:N	0.45	2.50	8	1
1:B:15:PHE:CZ	1:B:74:PHE:CD1	0.45	3.05	1	1
1:A:62:ASP:O	1:A:62:ASP:OD1	0.45	2.35	11	1
1:A:63:GLU:OE2	1:A:64:ASN:OD1	0.45	2.35	5	1
1:B:44:PHE:CD1	1:B:44:PHE:C	0.45	2.90	4	1
1:A:64:ASN:OD1	1:A:64:ASN:N	0.45	2.50	2	1
1:B:66:ASP:O	1:B:66:ASP:OD1	0.44	2.35	16	3
1:A:30:LYS:O	1:A:61:LEU:HD22	0.44	2.12	13	1
1:A:64:ASN:OD1	1:A:67:GLY:N	0.44	2.50	8	1
1:A:76:VAL:HA	1:B:76:VAL:HG22	0.44	1.89	2	1
1:A:64:ASN:O	1:A:67:GLY:N	0.44	2.40	10	3
1:A:17:ALA:CB	1:B:3:GLU:OE1	0.44	2.65	8	1
1:A:3:GLU:N	1:A:3:GLU:OE1	0.44	2.42	9	2
1:A:61:LEU:H	1:A:61:LEU:CD1	0.44	2.22	9	1
1:A:11:LEU:HD21	1:B:7:ALA:HB3	0.44	1.89	9	1
1:B:46:ASP:OD1	1:B:46:ASP:O	0.44	2.36	13	1
1:B:15:PHE:N	1:B:15:PHE:CD1	0.44	2.84	14	2
1:B:47:VAL:HG22	1:B:47:VAL:O	0.44	2.12	1	2
1:B:19:SER:OG	1:B:26:TYR:O	0.44	2.34	11	1
1:A:48:GLN:O	1:A:48:GLN:CG	0.44	2.65	11	1
1:A:44:PHE:C	1:A:44:PHE:CD1	0.44	2.91	4	1
1:B:48:GLN:O	1:B:48:GLN:CG	0.44	2.65	4	1
1:A:48:GLN:CG	1:A:48:GLN:O	0.44	2.66	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:81:LEU:HD23	1:B:81:LEU:C	0.44	2.31	2	1
1:A:27:LYS:O	1:A:28:LEU:CD2	0.44	2.66	12	2
1:B:61:LEU:H	1:B:61:LEU:CD1	0.44	2.23	9	1
1:A:30:LYS:HG2	1:A:69:VAL:HG13	0.44	1.90	5	2
1:A:46:ASP:O	1:A:46:ASP:OD1	0.44	2.35	13	1
1:A:43:SER:O	1:A:46:ASP:N	0.44	2.39	4	2
1:A:14:VAL:CG1	1:B:4:LEU:CG	0.44	2.95	11	1
1:A:83:VAL:CG1	1:A:84:ALA:N	0.44	2.81	13	1
1:A:4:LEU:HD13	1:B:14:VAL:HG11	0.44	1.88	2	1
1:B:60:GLU:O	1:B:64:ASN:OD1	0.44	2.36	9	1
1:A:60:GLU:OE2	1:A:63:GLU:OE2	0.44	2.36	11	1
1:A:64:ASN:OD1	1:A:66:ASP:OD1	0.44	2.36	4	1
1:A:43:SER:O	1:A:46:ASP:CG	0.44	2.56	2	9
1:B:36:LEU:CD1	1:B:36:LEU:N	0.44	2.81	12	1
1:A:15:PHE:N	1:A:15:PHE:CD1	0.44	2.84	14	2
1:A:66:ASP:O	1:A:67:GLY:O	0.44	2.35	15	4
1:A:14:VAL:HG13	1:B:3:GLU:HB2	0.44	1.90	18	1
1:B:27:LYS:NZ	1:B:36:LEU:CD2	0.44	2.81	18	1
1:B:30:LYS:HG2	1:B:69:VAL:HG13	0.44	1.90	5	2
1:B:55:ASP:OD1	1:B:59:LYS:NZ	0.44	2.49	13	1
1:B:74:PHE:CD1	1:B:74:PHE:C	0.43	2.91	17	3
1:B:43:SER:O	1:B:46:ASP:CG	0.43	2.56	18	9
1:B:30:LYS:NZ	1:B:60:GLU:O	0.43	2.51	12	1
1:A:5:GLU:OE2	1:B:44:PHE:HE2	0.43	1.97	17	1
1:A:60:GLU:O	1:A:64:ASN:OD1	0.43	2.36	9	1
1:A:19:SER:OG	1:A:26:TYR:O	0.43	2.33	11	2
1:A:3:GLU:OE1	1:B:17:ALA:CB	0.43	2.66	8	1
1:A:72:GLN:OE1	1:A:72:GLN:O	0.43	2.36	14	1
1:B:46:ASP:O	1:B:47:VAL:CG1	0.43	2.67	18	2
1:B:47:VAL:O	1:B:47:VAL:HG23	0.43	2.13	18	1
1:B:71:PHE:O	1:B:75:VAL:CG2	0.43	2.66	11	2
1:A:77:LEU:O	1:A:80:ALA:HB3	0.43	2.14	9	1
1:B:60:GLU:OE2	1:B:63:GLU:OE2	0.43	2.36	11	1
1:B:62:ASP:O	1:B:62:ASP:OD1	0.43	2.35	11	1
1:B:33:LEU:HD13	1:B:34:LYS:CA	0.43	2.44	7	1
1:B:4:LEU:N	1:B:4:LEU:HD22	0.43	2.28	2	1
1:B:64:ASN:OD1	1:B:64:ASN:N	0.43	2.50	2	1
1:A:74:PHE:CZ	1:B:4:LEU:HD21	0.43	2.48	17	1
1:B:32:GLU:O	1:B:33:LEU:C	0.43	2.57	18	3
1:B:60:GLU:OE1	1:B:60:GLU:N	0.43	2.48	20	1
1:B:27:LYS:O	1:B:28:LEU:CD2	0.43	2.66	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:36:LEU:N	1:B:36:LEU:HD12	0.43	2.29	12	1
1:B:46:ASP:OD1	1:B:46:ASP:N	0.43	2.52	3	1
1:A:71:PHE:O	1:A:75:VAL:CG2	0.43	2.67	15	2
1:A:33:LEU:HD23	1:A:34:LYS:CA	0.43	2.43	15	1
1:A:3:GLU:CD	1:A:3:GLU:N	0.43	2.72	19	1
1:A:34:LYS:NZ	1:A:81:LEU:HD21	0.43	2.28	18	1
1:B:69:VAL:C	1:B:70:ASP:OD1	0.43	2.57	2	1
1:A:7:ALA:HB3	1:B:11:LEU:HD21	0.43	1.91	9	1
1:B:30:LYS:O	1:B:61:LEU:HD22	0.43	2.13	13	1
1:A:69:VAL:C	1:A:70:ASP:OD1	0.43	2.57	2	1
1:A:34:LYS:NZ	1:A:81:LEU:CD1	0.43	2.82	16	1
1:A:44:PHE:CZ	1:A:81:LEU:HD11	0.43	2.49	20	1
1:A:30:LYS:HB3	1:A:61:LEU:HD23	0.43	1.89	13	1
1:A:35:ASP:O	1:A:35:ASP:OD1	0.43	2.37	4	2
1:B:28:LEU:N	1:B:28:LEU:HD22	0.43	2.29	6	1
1:B:63:GLU:O	1:B:63:GLU:OE1	0.43	2.37	18	1
1:A:49:LYS:HB3	1:A:49:LYS:HZ2	0.43	1.74	8	1
1:A:32:GLU:O	1:A:33:LEU:C	0.42	2.57	18	2
1:B:81:LEU:O	1:B:85:CYS:SG	0.42	2.77	15	1
1:A:28:LEU:N	1:A:28:LEU:HD22	0.42	2.29	6	1
1:A:76:VAL:HG22	1:B:76:VAL:HA	0.42	1.90	2	1
1:B:57:ILE:HD11	1:B:80:ALA:CB	0.42	2.44	2	1
1:B:86:ASN:OD1	1:B:86:ASN:N	0.42	2.50	17	1
1:A:46:ASP:O	1:A:47:VAL:CG1	0.42	2.67	18	2
1:B:35:ASP:OD1	1:B:35:ASP:O	0.42	2.37	2	3
1:A:62:ASP:OD1	1:A:62:ASP:O	0.42	2.37	2	1
1:A:71:PHE:HZ	1:B:83:VAL:N	0.42	2.12	14	1
1:A:4:LEU:CG	1:B:14:VAL:HG11	0.42	2.45	11	2
1:B:34:LYS:NZ	1:B:81:LEU:HD21	0.42	2.29	18	1
1:A:63:GLU:O	1:A:63:GLU:OE1	0.42	2.37	18	2
1:B:37:LEU:N	1:B:37:LEU:CD1	0.42	2.82	11	1
1:A:47:VAL:O	1:A:85:CYS:SG	0.42	2.78	4	1
1:B:47:VAL:O	1:B:85:CYS:SG	0.42	2.77	4	1
1:B:18:HIS:ND1	1:B:36:LEU:HD21	0.42	2.29	8	1
1:A:40:GLU:OE1	1:B:4:LEU:HD12	0.42	2.14	6	1
1:A:36:LEU:N	1:A:36:LEU:CD1	0.42	2.82	12	1
1:A:86:ASN:OD1	1:A:86:ASN:N	0.42	2.50	17	1
1:A:3:GLU:HB2	1:B:14:VAL:HG13	0.42	1.92	18	1
1:B:33:LEU:HD23	1:B:34:LYS:CA	0.42	2.43	15	1
1:A:36:LEU:N	1:A:36:LEU:HD12	0.42	2.29	12	1
1:B:72:GLN:O	1:B:72:GLN:OE1	0.42	2.37	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:3:GLU:N	1:B:3:GLU:CD	0.42	2.72	19	1
1:A:27:LYS:NZ	1:A:36:LEU:CD2	0.42	2.82	18	1
1:B:63:GLU:CG	1:B:64:ASN:HD22	0.42	2.27	11	1
1:B:62:ASP:OD1	1:B:62:ASP:O	0.42	2.37	2	1
1:A:33:LEU:C	1:A:33:LEU:CD2	0.42	2.87	1	2
1:A:81:LEU:O	1:A:85:CYS:SG	0.42	2.77	15	1
1:B:7:ALA:O	1:B:11:LEU:HD13	0.42	2.15	13	1
1:B:82:THR:O	1:B:85:CYS:C	0.42	2.58	4	1
1:A:18:HIS:ND1	1:A:36:LEU:HD21	0.42	2.29	8	1
1:B:35:ASP:O	1:B:35:ASP:OD1	0.42	2.38	12	1
1:B:3:GLU:OE1	1:B:3:GLU:N	0.42	2.43	10	2
1:A:57:ILE:CD1	1:A:57:ILE:N	0.42	2.83	19	1
1:A:11:LEU:O	1:A:15:PHE:CE2	0.42	2.72	5	1
1:B:86:ASN:N	1:B:86:ASN:ND2	0.42	2.67	6	1
1:A:81:LEU:O	1:A:81:LEU:HD13	0.42	2.14	6	1
1:B:41:LEU:O	1:B:42:SER:C	0.42	2.58	6	1
1:B:57:ILE:N	1:B:57:ILE:CD1	0.42	2.83	19	1
1:A:54:VAL:HG23	1:A:84:ALA:HB2	0.42	1.91	18	1
1:B:83:VAL:CG1	1:B:84:ALA:N	0.42	2.82	13	1
1:A:35:ASP:OD1	1:A:35:ASP:O	0.42	2.38	12	2
1:B:55:ASP:C	1:B:55:ASP:OD1	0.41	2.59	12	1
1:A:55:ASP:C	1:A:55:ASP:OD1	0.41	2.59	2	2
1:A:37:LEU:N	1:A:37:LEU:CD1	0.41	2.83	11	1
1:A:41:LEU:O	1:A:42:SER:C	0.41	2.58	6	1
1:A:86:ASN:N	1:A:86:ASN:OD1	0.41	2.52	3	1
1:B:14:VAL:O	1:B:17:ALA:N	0.41	2.53	4	2
1:A:27:LYS:HZ1	1:A:36:LEU:HD23	0.41	1.75	18	1
1:A:59:LYS:O	1:A:63:GLU:CG	0.41	2.68	9	1
1:B:70:ASP:OD2	1:B:71:PHE:CE2	0.41	2.73	18	1
1:A:70:ASP:OD2	1:A:71:PHE:CE2	0.41	2.73	18	1
1:A:33:LEU:HD13	1:A:34:LYS:CA	0.41	2.44	7	1
1:A:74:PHE:CZ	1:B:4:LEU:HD22	0.41	2.51	6	1
1:A:86:ASN:H	1:A:86:ASN:HD22	0.41	1.56	6	1
1:A:82:THR:CG2	1:B:71:PHE:CE2	0.41	3.03	14	1
1:B:27:LYS:NZ	1:B:36:LEU:HD23	0.41	2.31	18	1
1:B:59:LYS:O	1:B:63:GLU:CG	0.41	2.69	9	1
1:B:27:LYS:O	1:B:28:LEU:CB	0.41	2.69	1	1
1:B:11:LEU:O	1:B:15:PHE:CE2	0.41	2.74	5	1
1:A:82:THR:O	1:A:85:CYS:C	0.41	2.58	4	1
1:B:34:LYS:O	1:B:38:GLN:CB	0.41	2.68	7	1
1:B:47:VAL:O	1:B:48:GLN:C	0.41	2.58	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:55:ASP:OD1	1:B:55:ASP:C	0.41	2.59	14	4
1:A:34:LYS:HZ1	1:A:81:LEU:HD21	0.41	1.76	18	1
1:B:81:LEU:O	1:B:81:LEU:HD13	0.41	2.14	6	1
1:A:55:ASP:OD1	1:A:55:ASP:C	0.41	2.59	6	1
1:A:57:ILE:HD11	1:A:80:ALA:CB	0.41	2.46	2	1
1:B:33:LEU:C	1:B:33:LEU:CD2	0.41	2.88	12	1
1:A:74:PHE:CD2	1:A:75:VAL:HG23	0.41	2.51	14	1
1:A:72:GLN:O	1:A:76:VAL:CG2	0.41	2.68	18	1
1:B:48:GLN:CD	1:B:48:GLN:N	0.41	2.73	18	1
1:B:77:LEU:C	1:B:77:LEU:HD23	0.41	2.36	5	1
1:A:70:ASP:CG	1:A:71:PHE:H	0.41	2.19	15	3
1:A:46:ASP:OD1	1:A:85:CYS:SG	0.41	2.79	4	1
1:A:46:ASP:N	1:A:46:ASP:OD1	0.41	2.53	3	1
1:B:47:VAL:HG23	1:B:47:VAL:O	0.41	2.16	4	1
1:B:45:LEU:CD2	1:B:45:LEU:N	0.41	2.84	17	1
1:A:61:LEU:HD12	1:A:61:LEU:H	0.41	1.75	14	1
1:B:54:VAL:CG2	1:B:84:ALA:CB	0.41	2.99	19	1
1:B:47:VAL:HG13	1:B:85:CYS:SG	0.41	2.56	20	1
1:B:63:GLU:OE1	1:B:63:GLU:O	0.41	2.39	5	1
1:B:63:GLU:OE1	1:B:64:ASN:ND2	0.41	2.54	5	1
1:A:63:GLU:OE1	1:A:64:ASN:ND2	0.41	2.54	5	1
1:B:44:PHE:CE2	1:B:82:THR:HG23	0.41	2.51	10	1
1:B:81:LEU:O	1:B:84:ALA:N	0.41	2.54	10	1
1:B:13:ASN:O	1:B:13:ASN:OD1	0.41	2.39	19	1
1:A:83:VAL:CB	1:B:72:GLN:NE2	0.41	2.82	18	1
1:B:35:ASP:OD1	1:B:35:ASP:C	0.41	2.59	1	1
1:B:47:VAL:O	1:B:47:VAL:HG22	0.41	2.15	20	1
1:B:44:PHE:CZ	1:B:81:LEU:HD11	0.41	2.50	20	1
1:A:63:GLU:CG	1:A:64:ASN:HD22	0.41	2.29	11	1
1:A:47:VAL:O	1:A:48:GLN:C	0.41	2.58	7	1
1:A:13:ASN:OD1	1:A:13:ASN:C	0.41	2.60	19	1
1:A:48:GLN:N	1:A:48:GLN:CD	0.41	2.73	18	2
1:A:27:LYS:NZ	1:A:36:LEU:HD23	0.41	2.31	18	1
1:B:37:LEU:HD23	1:B:78:VAL:CG2	0.41	2.45	9	1
1:A:35:ASP:OD1	1:A:35:ASP:C	0.41	2.59	1	1
1:B:28:LEU:O	1:B:69:VAL:CG2	0.41	2.69	15	1
1:A:45:LEU:CD2	1:A:45:LEU:N	0.40	2.85	17	1
1:B:46:ASP:OD1	1:B:85:CYS:SG	0.40	2.79	4	1
1:B:70:ASP:CG	1:B:71:PHE:H	0.40	2.20	4	1
1:A:66:ASP:OD1	1:A:66:ASP:O	0.40	2.38	7	1
1:B:34:LYS:NZ	1:B:61:LEU:CD1	0.40	2.70	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:PHE:O	1:A:44:PHE:CD1	0.40	2.74	20	1
1:A:15:PHE:CD1	1:A:15:PHE:N	0.40	2.86	13	1
1:B:49:LYS:HB3	1:B:49:LYS:HZ2	0.40	1.76	8	1
1:A:34:LYS:CB	1:A:61:LEU:HD13	0.40	2.46	7	1
1:B:86:ASN:N	1:B:86:ASN:OD1	0.40	2.54	3	1
1:A:54:VAL:CG2	1:A:84:ALA:CB	0.40	2.99	19	1
1:B:46:ASP:C	1:B:46:ASP:OD1	0.40	2.60	5	1
1:B:60:GLU:OE1	1:B:77:LEU:CD1	0.40	2.70	2	1
1:B:43:SER:O	1:B:44:PHE:C	0.40	2.59	18	1
1:B:44:PHE:CD1	1:B:44:PHE:O	0.40	2.74	20	1
1:A:46:ASP:OD1	1:A:46:ASP:C	0.40	2.60	17	1
1:B:61:LEU:HD12	1:B:61:LEU:H	0.40	1.75	14	1
1:A:33:LEU:CD2	1:A:37:LEU:HD21	0.40	2.47	10	1
1:B:54:VAL:HG23	1:B:84:ALA:HB2	0.40	1.93	3	1
1:A:13:ASN:O	1:A:13:ASN:OD1	0.40	2.39	19	1
1:A:27:LYS:O	1:A:28:LEU:CB	0.40	2.69	1	1
1:A:75:VAL:HG13	1:B:75:VAL:HG13	0.40	1.93	4	1
1:A:60:GLU:OE1	1:A:77:LEU:CD1	0.40	2.69	2	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	80/93 (86%)	69±1 (87±2%)	7±2 (9±2%)	4±1 (4±2%)	6	30
1	B	80/93 (86%)	70±1 (87±2%)	7±2 (9±2%)	3±1 (4±2%)	6	31
All	All	3200/3720 (86%)	2779 (87%)	282 (9%)	139 (4%)	6	31

All 15 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	27	LYS	19
1	B	27	LYS	19
1	B	86	ASN	14

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Mol	Chain	Res	Type	Models (Total)
1	A	86	ASN	14
1	A	47	VAL	11
1	B	47	VAL	11
1	B	26	TYR	11
1	A	26	TYR	11
1	A	67	GLY	10
1	B	67	GLY	10
1	B	20	GLY	3
1	A	20	GLY	3
1	B	64	ASN	1
1	A	64	ASN	1
1	A	28	LEU	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	70/81 (86%)	64±2 (91±4%)	6±2 (9±4%)	16	61
1	B	70/81 (86%)	64±3 (91±4%)	6±3 (9±4%)	16	61
All	All	2800/3240 (86%)	2542 (91%)	258 (9%)	16	61

All 66 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	B	28	LEU	16
1	A	28	LEU	16
1	B	54	VAL	10
1	A	54	VAL	10
1	B	74	PHE	9
1	A	58	MET	9
1	A	74	PHE	9
1	B	58	MET	9
1	A	33	LEU	8
1	B	33	LEU	8
1	A	34	LYS	7
1	A	83	VAL	7

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Mol	Chain	Res	Type	Models (Total)
1	B	37	LEU	7
1	A	37	LEU	7
1	B	83	VAL	7
1	B	34	LYS	7
1	B	61	LEU	6
1	A	61	LEU	6
1	B	63	GLU	6
1	A	63	GLU	6
1	B	72	GLN	4
1	B	8	MET	4
1	A	8	MET	4
1	A	72	GLN	4
1	B	40	GLU	3
1	B	81	LEU	3
1	A	40	GLU	3
1	B	64	ASN	3
1	B	49	LYS	3
1	A	64	ASN	3
1	A	81	LEU	3
1	A	71	PHE	3
1	B	71	PHE	2
1	B	85	CYS	2
1	B	36	LEU	2
1	B	4	LEU	2
1	A	56	LYS	2
1	B	26	TYR	2
1	A	4	LEU	2
1	A	44	PHE	2
1	A	49	LYS	2
1	A	85	CYS	2
1	B	44	PHE	2
1	A	36	LEU	2
1	A	26	TYR	2
1	B	56	LYS	2
1	A	47	VAL	1
1	B	47	VAL	1
1	A	27	LYS	1
1	B	86	ASN	1
1	B	48	GLN	1
1	B	77	LEU	1
1	B	45	LEU	1
1	A	82	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	38	GLN	1
1	B	60	GLU	1
1	A	48	GLN	1
1	B	82	THR	1
1	A	60	GLU	1
1	B	38	GLN	1
1	A	86	ASN	1
1	B	69	VAL	1
1	A	69	VAL	1
1	A	45	LEU	1
1	A	77	LEU	1
1	B	27	LYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4285

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	1998
Number of shifts mapped to atoms	1998
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
$^{13}\text{C}_\alpha$	186	-0.54 ± 0.07	Should be applied
$^{13}\text{C}_\beta$	176	0.01 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	182	-0.03 ± 0.49	None needed (< 0.5 ppm)

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 82%, i.e. 1572 atoms were assigned a chemical shift out of a possible 1914. 38 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	636/800 (80%)	318/320 (99%)	160/320 (50%)	158/160 (99%)
Sidechain	884/994 (89%)	534/568 (94%)	340/398 (85%)	10/28 (36%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	52/120 (43%)	40/64 (62%)	12/48 (25%)	0/8 (0%)
Overall	1572/1914 (82%)	892/952 (94%)	512/766 (67%)	168/196 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1790 atoms were assigned a chemical shift out of a possible 2224. 38 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	736/930 (79%)	368/372 (99%)	186/372 (50%)	182/186 (98%)
Sidechain	992/1114 (89%)	606/640 (95%)	372/440 (85%)	14/34 (41%)
Aromatic	62/180 (34%)	48/96 (50%)	12/74 (16%)	2/10 (20%)
Overall	1790/2224 (80%)	1022/1108 (92%)	570/886 (64%)	198/230 (86%)

7.1.4 Statistically unusual chemical shifts ⓘ

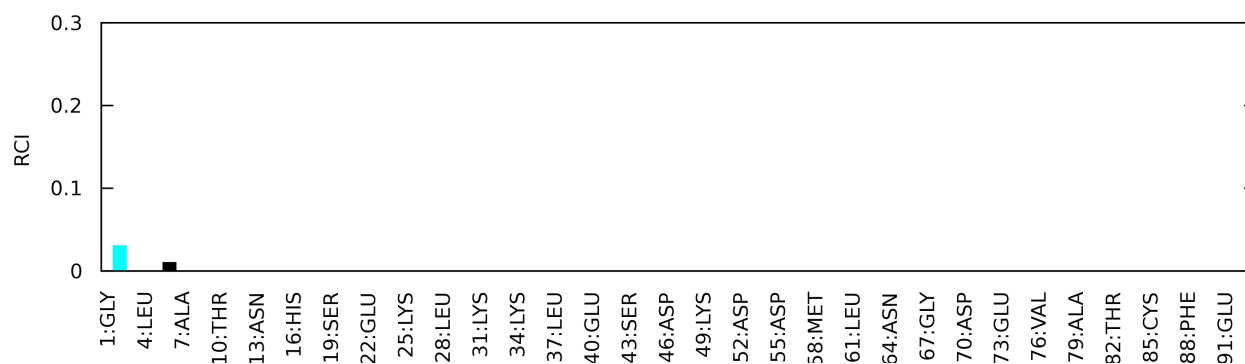
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	44	PHE	CZ	138.60	137.04 – 121.44	6.0
1	A	44	PHE	CZ	138.60	137.04 – 121.44	6.0

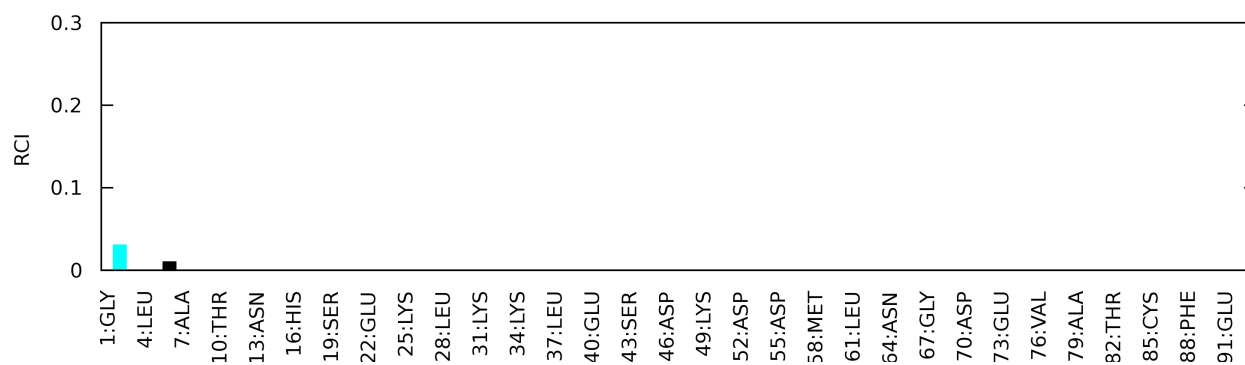
7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



7.2 Chemical shift list 2

File name: BMRB entry 4285

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	272
Number of shifts mapped to atoms	254
Number of unparsed shifts	0
Number of shifts with mapping errors	18
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 18 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1	MET	CG	32.06	-1.0	1
A	1	MET	CB	33.5	-1.0	1
A	1	MET	CA	54.13	-1.0	1
B	1	MET	HG2	2.2	-1.0	1
A	1	MET	HG2	2.2	-1.0	1
B	1	MET	CA	54.13	-1.0	1
A	1	MET	HA	4.66	-1.0	1
A	1	MET	HB2	2.63	-1.0	2
A	1	MET	HG3	2.03	-1.0	1
B	1	MET	CB	33.5	-1.0	1
B	1	MET	CG	32.06	-1.0	1
B	1	MET	N	128.88	-1.0	1
A	1	MET	H	8.4	-1.0	1
A	1	MET	N	128.88	-1.0	1
B	1	MET	HB2	2.63	-1.0	2
B	1	MET	HG3	2.03	-1.0	1
B	1	MET	HA	4.66	-1.0	1
B	1	MET	H	8.4	-1.0	1

7.2.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	26	-1.27 ± 0.90	None needed (imprecise)
$^{13}\text{C}_\beta$	26	0.70 ± 0.46	None needed (imprecise)
$^{13}\text{C}'$	0	—	—
^{15}N	28	-0.80 ± 0.59	None needed (imprecise)

7.2.3 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 10%, i.e. 194 atoms were assigned a chemical shift out of a possible 1914. 4 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	86/800 (11%)	44/320 (14%)	20/320 (6%)	22/160 (14%)
Sidechain	102/994 (10%)	64/568 (11%)	38/398 (10%)	0/28 (0%)
Aromatic	6/120 (5%)	4/64 (6%)	2/48 (4%)	0/8 (0%)
Overall	194/1914 (10%)	112/952 (12%)	60/766 (8%)	22/196 (11%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 10%, i.e. 222 atoms were assigned a chemical shift out of a possible 2224. 4 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	102/930 (11%)	52/372 (14%)	24/372 (6%)	26/186 (14%)
Sidechain	114/1114 (10%)	72/640 (11%)	42/440 (10%)	0/34 (0%)
Aromatic	6/180 (3%)	4/96 (4%)	2/74 (3%)	0/10 (0%)
Overall	222/2224 (10%)	128/1108 (12%)	68/886 (8%)	26/230 (11%)

7.2.4 Statistically unusual chemical shifts [i](#)

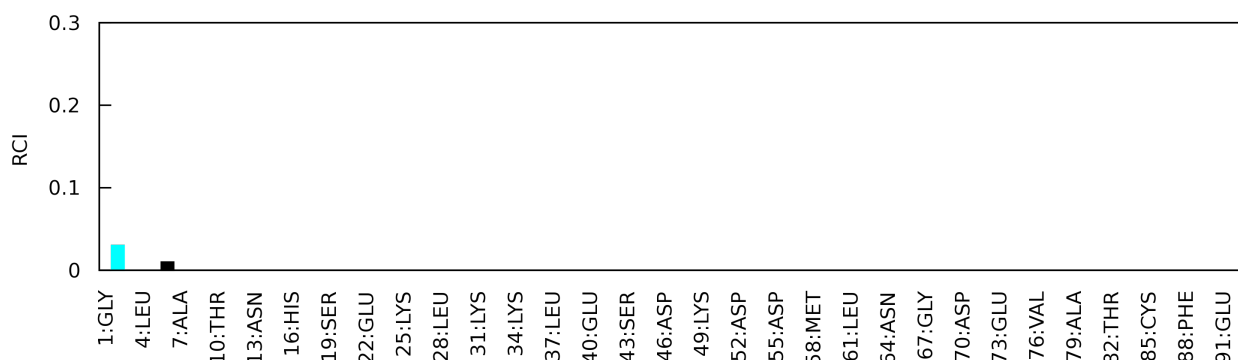
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	44	PHE	CZ	138.60	137.04 – 121.44	6.0
1	A	44	PHE	CZ	138.60	137.04 – 121.44	6.0

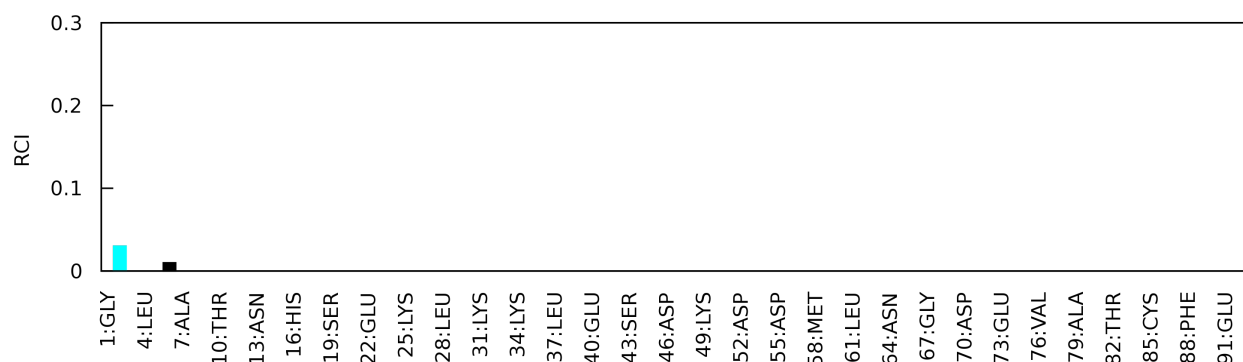
7.2.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



7.3 Chemical shift list 3

File name: BMRB entry 4285

Chemical shift list name: *assigned_chem_shift_list_3*

7.3.1 Bookkeeping [i](#)

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	34
Number of shifts mapped to atoms	34
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.3.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	4	-0.40 ± 0.64	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	4	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	4	-2.66 ± 1.56	None needed (imprecise)

7.3.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 1%, i.e. 12 atoms were assigned a chemical shift out of a possible 1914. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	8/800 (1%)	4/320 (1%)	2/320 (1%)	2/160 (1%)
Sidechain	4/994 (0%)	2/568 (0%)	2/398 (1%)	0/28 (0%)
Aromatic	0/120 (0%)	0/64 (0%)	0/48 (0%)	0/8 (0%)
Overall	12/1914 (1%)	6/952 (1%)	4/766 (1%)	2/196 (1%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 1%, i.e. 26 atoms were assigned a chemical shift out of a possible 2224. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	16/930 (2%)	8/372 (2%)	4/372 (1%)	4/186 (2%)
Sidechain	10/1114 (1%)	6/640 (1%)	4/440 (1%)	0/34 (0%)
Aromatic	0/180 (0%)	0/96 (0%)	0/74 (0%)	0/10 (0%)
Overall	26/2224 (1%)	14/1108 (1%)	8/886 (1%)	4/230 (2%)

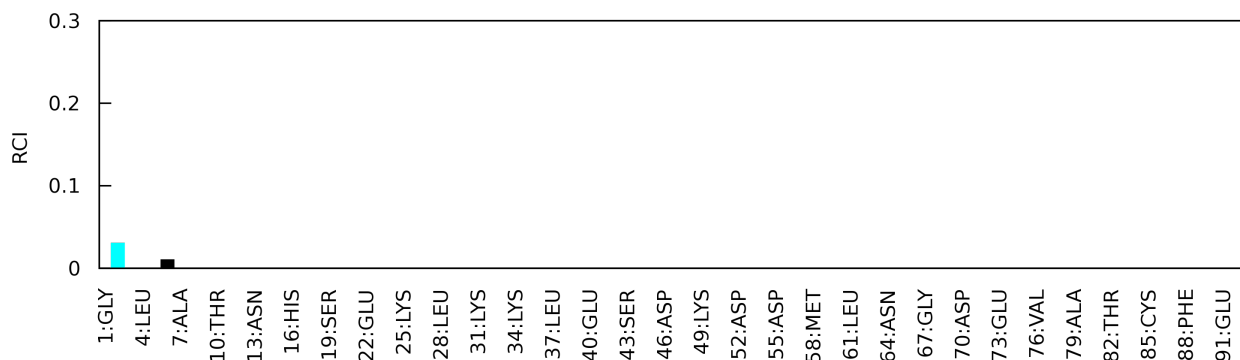
7.3.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.3.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

