



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:16 pm BST

PDB ID : 2LP3  
Title : Solution structure of S100A1 Ca<sup>2+</sup>  
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Deposited on : 2012-01-31

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

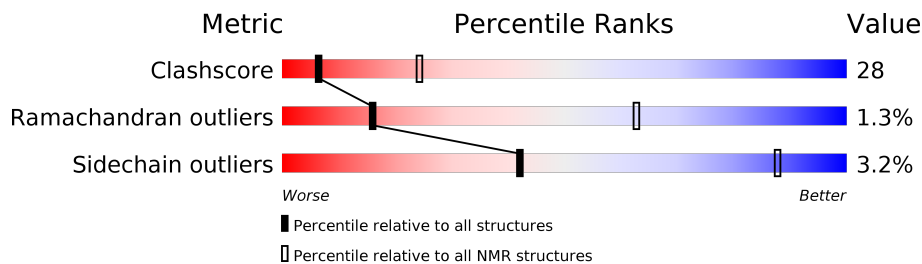
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 44%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	93	
1	B	93	

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 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:2-A:87, B:2-B:87 (172)	0.47	16

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 4 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2880 atoms, of which 1412 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein S100-A1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	93	1438	461	706	115	153	3	0
1	B	93	1438	461	706	115	153	3	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

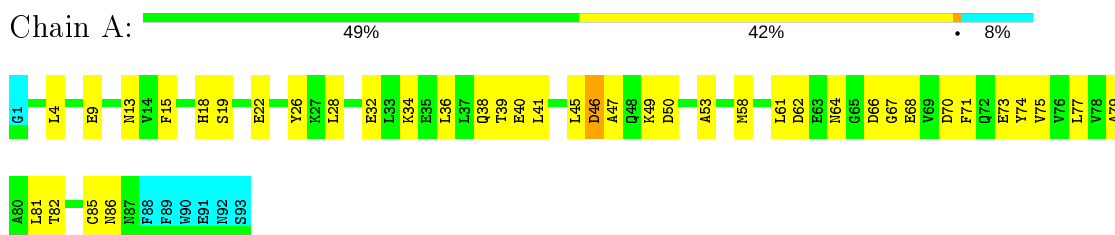
Mol	Chain	Residues	Atoms	
			Total	Ca
2	B	2	2	2
2	A	2	2	2

## 4 Residue-property plots [i](#)

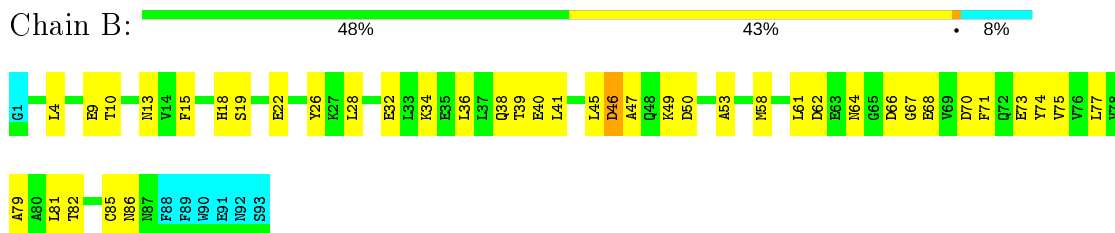
### 4.1 Average score per residue in the NMR ensemble

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: Protein S100-A1



- Molecule 1: Protein S100-A1

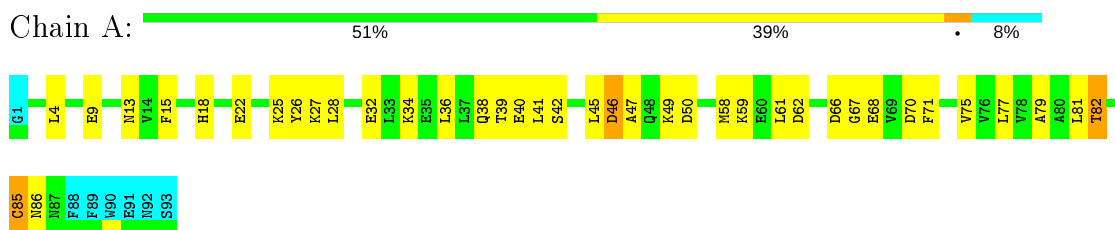


### 4.2 Scores per residue for each member of the ensemble

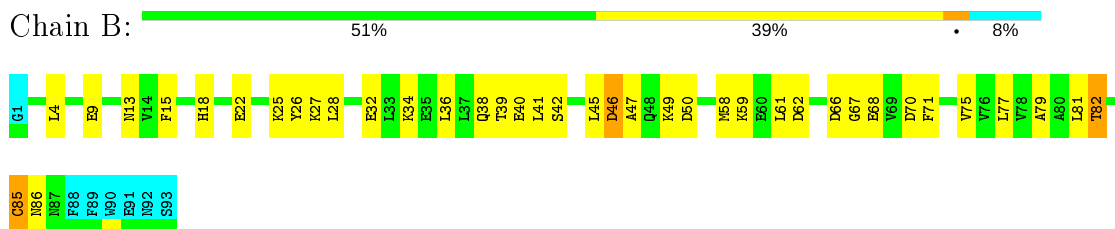
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Protein S100-A1

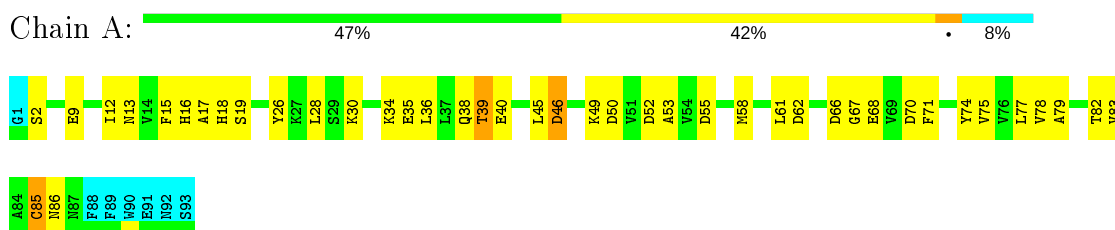


- Molecule 1: Protein S100-A1

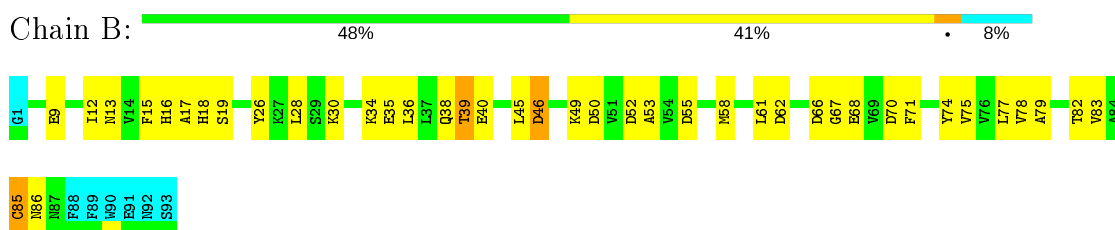


#### 4.2.2 Score per residue for model 2

- Molecule 1: Protein S100-A1

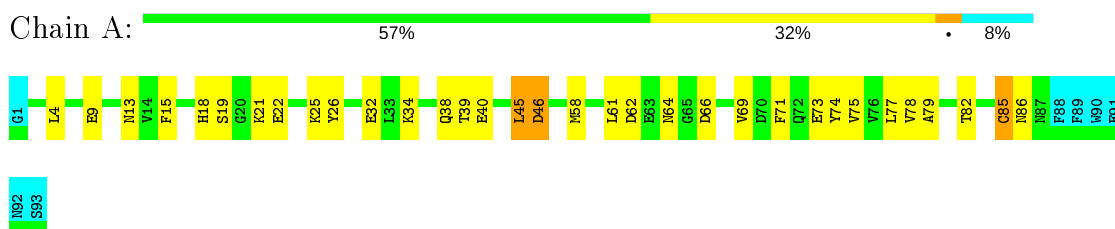


- Molecule 1: Protein S100-A1

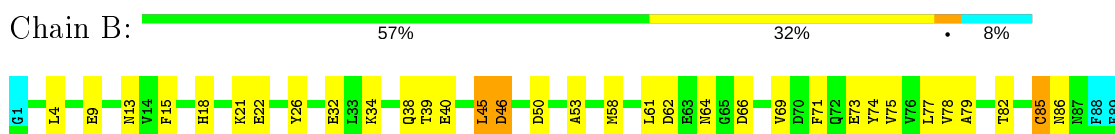


#### 4.2.3 Score per residue for model 3

- Molecule 1: Protein S100-A1



- Molecule 1: Protein S100-A1



W90  
E91  
N92  
S93

#### 4.2.4 Score per residue for model 4

- Molecule 1: Protein S100-A1

Chain A: 46% 42% 8%

G1 L4 E9 T10 L11 I12 N13 N14 F15 H18 S19 E22 Y26 K27 L28 S29 E32 L33 K34 E35 L36 L37 L37 Q38 T39 E40 E40 L41 L45 D46 A47 K49 D50 M58 L61 M64 G65 D66 G67 E68 V69 D70 F71 Q72 E73 Y74 Y75 V76 L77 V78 A79

L80 L81 N86 N87 F88 F89 W90 E91 N92 S93

- Molecule 1: Protein S100-A1

Chain B: 46% 42% 8%

G1 L4 E9 T10 L11 I12 N13 N14 F15 H18 S19 E22 Y26 K27 L28 S29 E32 L33 K34 E35 L36 L37 L37 Q38 T39 E40 E40 L41 L45 D46 A47 K49 D50 M58 L61 M64 G65 D66 G67 E68 V69 D70 F71 Q72 E73 Y74 Y75 V76 L77 V78 A79

L80 L81 N86 N87 F88 F89 W90 E91 N92 S93

#### 4.2.5 Score per residue for model 5

- Molecule 1: Protein S100-A1

Chain A: 49% 39% 8%

G1 E5 I12 N13 V14 F15 H16 A17 H18 E22 Y26 K27 L28 E32 L33 K34 E35 L36 L37 Q38 T39 E40 E40 L41 L45 D46 A47 K49 D50 M58 L61 D62 D66 G67 E68 V69 F71 Q72 E73 Y74 Y75 V76 L77 V78 A79 T82 C85 N86

N87 F88 W90 E91 N92 S93

- Molecule 1: Protein S100-A1

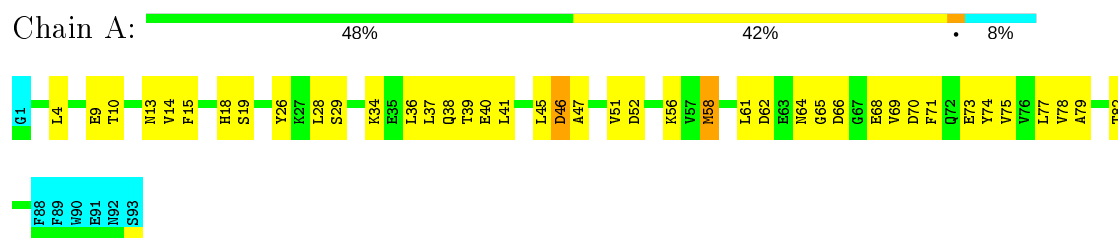
Chain B: 47% 41% 8%

G1 E5 T6 T10 L11 I12 N13 F14 F15 H16 A17 H18 E22 Y26 K27 L28 E32 L33 K34 E35 L36 L37 Q38 T39 E40 L41 L45 D46 A47 K49 D50 M58 L61 D62 D66 G67 E68 V69 D70 F71 Q72 E73 Y74 Y75 V76 L77 V78 A79 T82

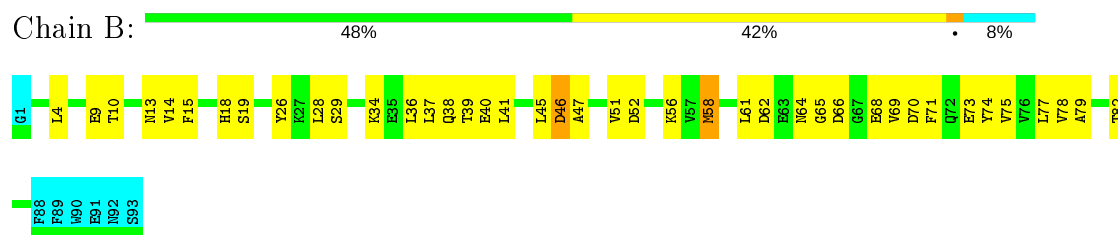
C85 N86 N87 F88 W90 E91 N92 S93

### 4.2.6 Score per residue for model 6

- Molecule 1: Protein S100-A1

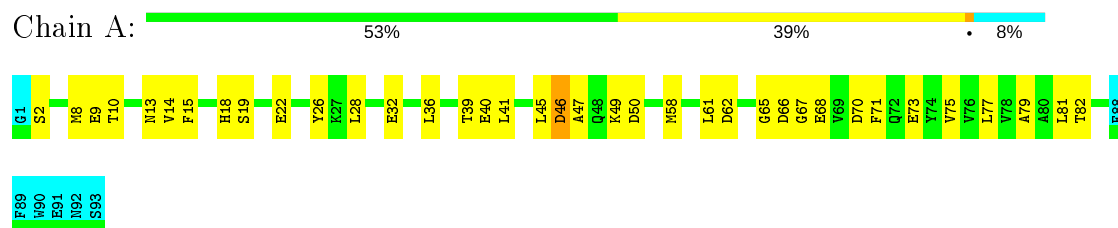


- Molecule 1: Protein S100-A1

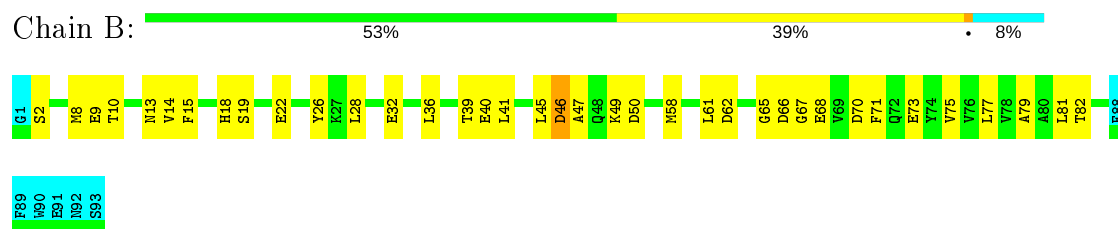


### 4.2.7 Score per residue for model 7

- Molecule 1: Protein S100-A1



- Molecule 1: Protein S100-A1

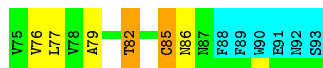
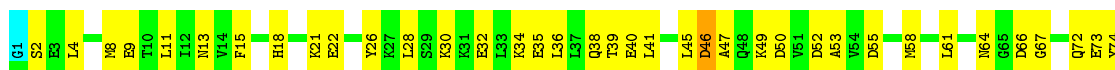


### 4.2.8 Score per residue for model 8

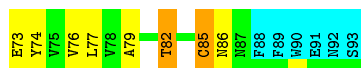
- Molecule 1: Protein S100-A1





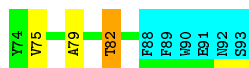
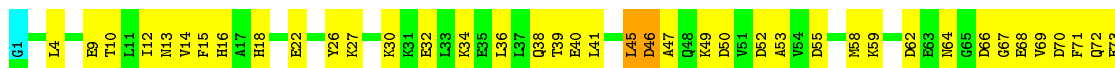


- Molecule 1: Protein S100-A1



#### 4.2.9 Score per residue for model 9

- Molecule 1: Protein S100-A1

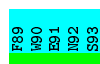
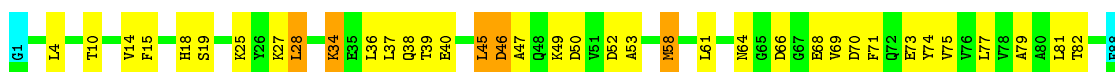


- Molecule 1: Protein S100-A1

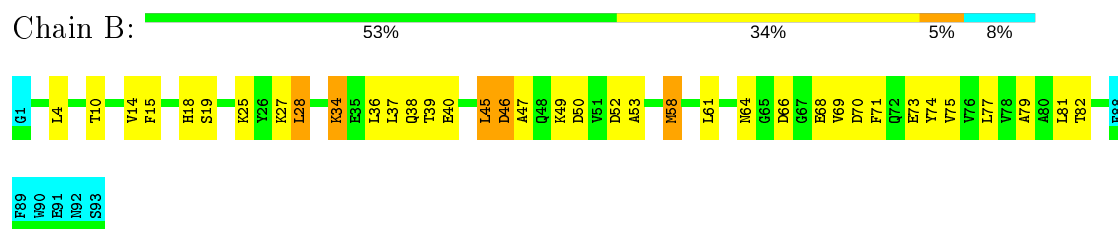


#### 4.2.10 Score per residue for model 10

- Molecule 1: Protein S100-A1

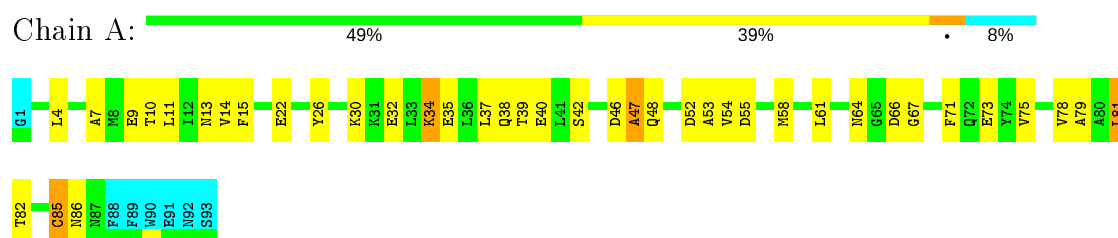


- Molecule 1: Protein S100-A1

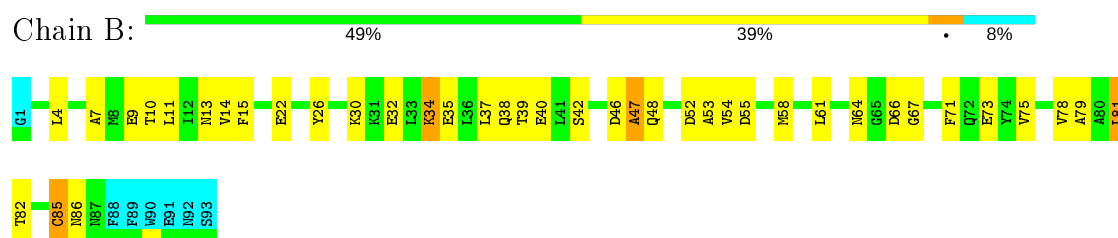


#### 4.2.11 Score per residue for model 11

- Molecule 1: Protein S100-A1

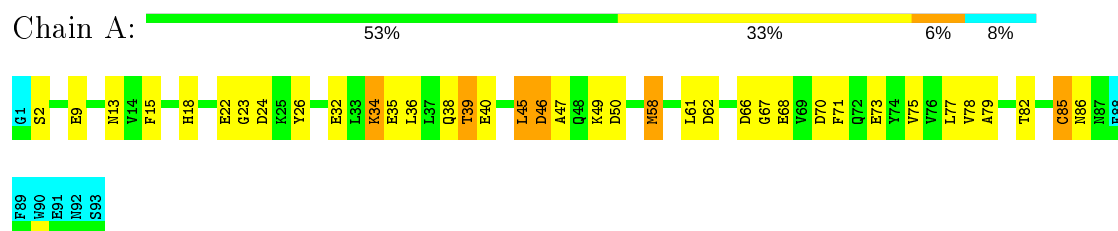


- Molecule 1: Protein S100-A1

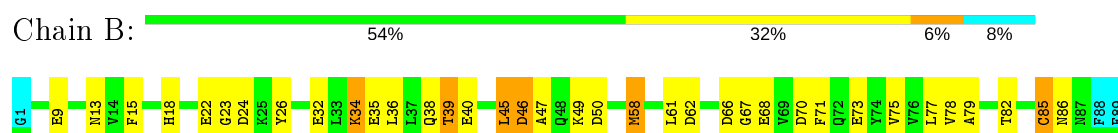


#### 4.2.12 Score per residue for model 12

- Molecule 1: Protein S100-A1



- Molecule 1: Protein S100-A1



W90  
E91  
N92  
S93

#### 4.2.13 Score per residue for model 13

- Molecule 1: Protein S100-A1

Chain A:  53% 35% 8%

G1 L4 E9 N13 V14 F15 S19 D24 K25 Y26 K27 L28 K34 L37 Q38 T39 E40 L45 D46 A47 D50 A53 V54 D55 M58 L61 N64 G65 D66 G67 E68 V69 D70 F71 E72 E73 Y74 V75 V78 A79 A80 L81 T82 C85 N86

H87  
F88  
F89  
W90  
E91  
N92  
S93

- Molecule 1: Protein S100-A1

Chain B:  53% 35% 8%

G1 L4 E9 N13 V14 F15 S19 D24 K25 Y26 K27 L28 K34 L37 Q38 T39 E40 L45 D46 A47 D50 A53 V54 D55 M58 L61 N64 G65 D66 G67 E68 V69 D70 F71 E72 E73 Y74 V75 V78 A79 A80 L81 T82 C85 N86

H87  
F88  
F89  
W90  
E91  
N92  
S93

#### 4.2.14 Score per residue for model 14

- Molecule 1: Protein S100-A1

Chain A:  58% 33% 8%

G1 L4 L11 V14 F15 H18 S19 Y26 K27 K34 E35 L36 L37 Q38 E40 L45 D46 A47 V51 D52 A53 V57 M58 L61 N64 G65 G67 D70 F71 E72 E73 Y74 V75 A79 F88 F89 W90 E91 N92 S93

- Molecule 1: Protein S100-A1

Chain B:  55% 37% 8%

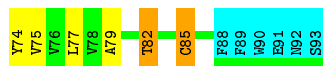
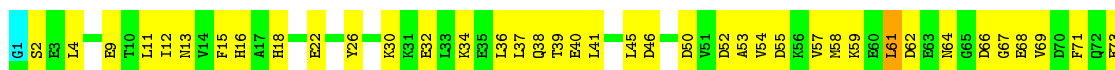
G1 L4 M8 E9 T10 L11 V14 F15 H18 S19 K25 Y26 K27 K34 E35 L36 L37 Q38 T39 E40 L41 L45 D46 A47 V51 D52 A53 V57 M58 L61 N64 G65 D66 G67 D70 F71 E72 E73 Y74 V75 A79 F88 F89 W90 E91 N92

S93

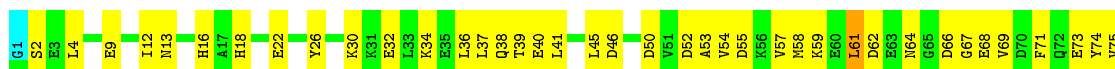
#### 4.2.15 Score per residue for model 15

- Molecule 1: Protein S100-A1

Chain A:  44% 45% 8%

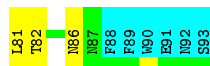
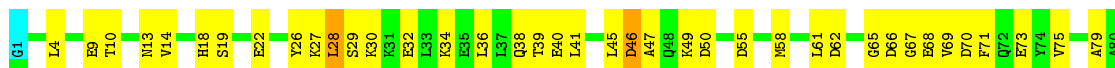


- Molecule 1: Protein S100-A1

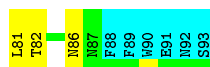
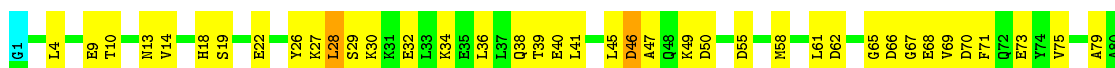


#### 4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: Protein S100-A1

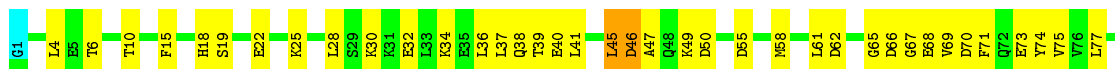


- Molecule 1: Protein S100-A1

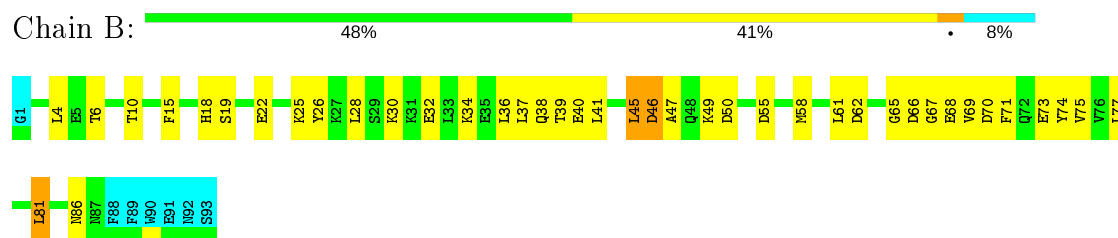


#### 4.2.17 Score per residue for model 17

- Molecule 1: Protein S100-A1

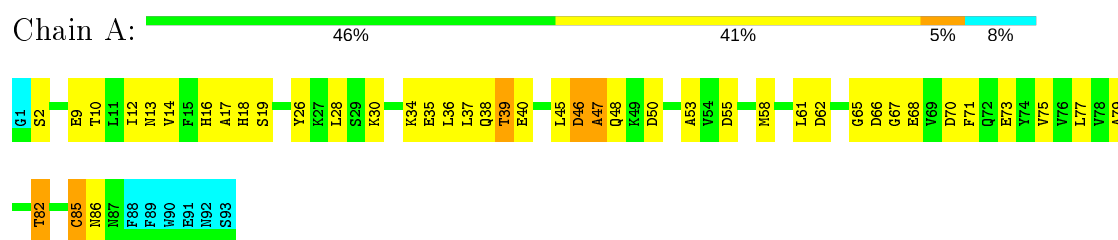


- Molecule 1: Protein S100-A1

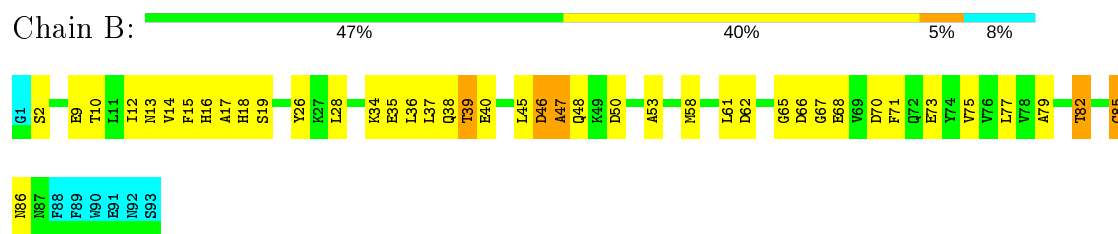


#### 4.2.18 Score per residue for model 18

- Molecule 1: Protein S100-A1

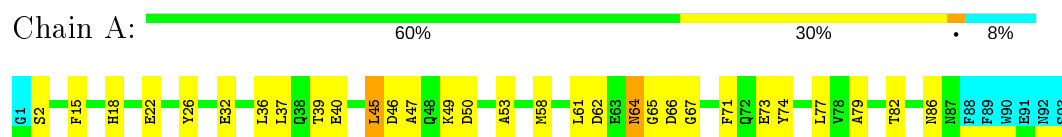


- Molecule 1: Protein S100-A1

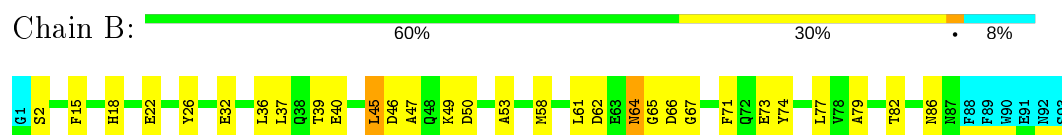


#### 4.2.19 Score per residue for model 19

- Molecule 1: Protein S100-A1

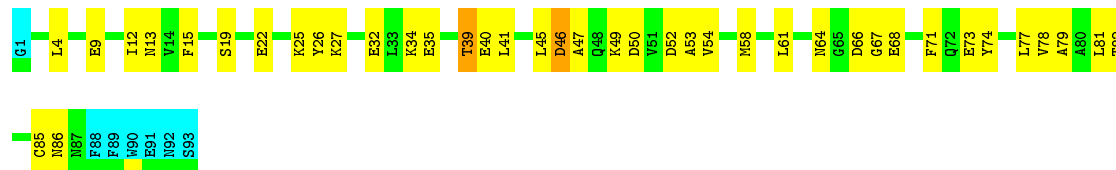


- Molecule 1: Protein S100-A1

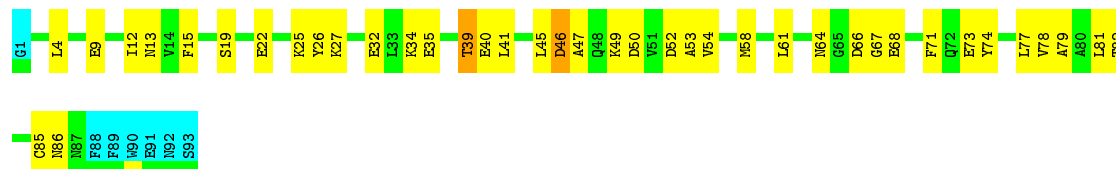


## 4.2.20 Score per residue for model 20

## • Molecule 1: Protein S100-A1

Chain A:  49% 41% 8%

## • Molecule 1: Protein S100-A1

Chain B:  49% 41% 8%

## 5 Refinement protocol and experimental data overview

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

Of the 210 calculated structures, 20 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
X-PLOR NIH	refinement	
CYANA	structure solution	

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

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1091
Number of shifts mapped to atoms	1091
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	44%

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

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
CA

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 [i](#)

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	668	658	655	40±6
1	B	668	658	655	41±6
All	All	26800	26320	26234	1499

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:LEU:HD11	1:A:69:VAL:HG13	0.86	1.47	15	1
1:B:61:LEU:HD12	1:B:61:LEU:C	0.86	1.91	15	1
1:B:61:LEU:HD11	1:B:69:VAL:HG13	0.85	1.47	15	1
1:A:61:LEU:C	1:A:61:LEU:HD12	0.84	1.91	15	1
1:A:79:ALA:HB1	1:B:75:VAL:HG12	0.84	1.50	14	7
1:A:75:VAL:HG12	1:B:79:ALA:HB1	0.84	1.48	3	7
1:A:61:LEU:O	1:A:61:LEU:HD12	0.83	1.74	15	1
1:B:61:LEU:HD12	1:B:61:LEU:O	0.83	1.74	15	1
1:A:10:THR:O	1:A:14:VAL:HG23	0.81	1.75	4	7
1:B:45:LEU:O	1:B:47:ALA:N	0.81	2.14	18	11
1:A:61:LEU:HD11	1:A:77:LEU:HD22	0.81	1.53	20	1

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:10:THR:O	1:B:14:VAL:HG23	0.81	1.75	4	7
1:A:45:LEU:O	1:A:47:ALA:N	0.80	2.14	18	11
1:B:61:LEU:HD11	1:B:77:LEU:HD22	0.77	1.53	20	1
1:A:79:ALA:HB2	1:B:79:ALA:HB2	0.77	1.57	20	5
1:B:66:ASP:OD1	1:B:67:GLY:N	0.74	2.20	9	16
1:A:35:GLU:O	1:A:39:THR:HG22	0.74	1.82	11	6
1:A:66:ASP:OD1	1:A:67:GLY:N	0.74	2.20	9	16
1:B:18:HIS:CG	1:B:36:LEU:HD21	0.74	2.18	5	5
1:B:74:TYR:O	1:B:78:VAL:HG23	0.74	1.83	13	2
1:A:18:HIS:CG	1:A:36:LEU:HD21	0.73	2.18	5	5
1:B:35:GLU:O	1:B:39:THR:HG22	0.73	1.82	11	6
1:A:47:ALA:HB1	1:A:50:ASP:O	0.73	1.83	18	1
1:B:47:ALA:HB1	1:B:50:ASP:O	0.72	1.83	18	1
1:A:74:TYR:O	1:A:78:VAL:HG23	0.72	1.84	13	2
1:A:34:LYS:HZ1	1:A:38:GLN:NE2	0.71	1.81	9	5
1:B:46:ASP:O	1:B:48:GLN:N	0.71	2.24	11	2
1:A:18:HIS:CB	1:A:36:LEU:HD21	0.71	2.16	1	12
1:A:64:ASN:HD22	1:A:65:GLY:H	0.70	1.29	19	1
1:B:18:HIS:CB	1:B:36:LEU:HD21	0.70	2.16	1	12
1:B:40:GLU:C	1:B:41:LEU:HD22	0.70	2.07	20	1
1:A:46:ASP:O	1:A:48:GLN:N	0.70	2.24	11	2
1:A:40:GLU:C	1:A:41:LEU:HD22	0.69	2.07	20	1
1:A:15:PHE:CD1	1:A:71:PHE:CD1	0.69	2.81	14	6
1:B:15:PHE:CD1	1:B:71:PHE:CD1	0.69	2.81	14	6
1:B:34:LYS:HZ1	1:B:38:GLN:NE2	0.69	1.86	5	5
1:B:64:ASN:HD22	1:B:65:GLY:H	0.69	1.29	19	1
1:B:58:MET:SD	1:B:64:ASN:ND2	0.69	2.66	9	1
1:A:58:MET:SD	1:A:64:ASN:ND2	0.68	2.66	9	1
1:A:40:GLU:C	1:A:41:LEU:HD12	0.67	2.10	8	11
1:A:34:LYS:NZ	1:A:38:GLN:NE2	0.67	2.43	9	6
1:B:40:GLU:C	1:B:41:LEU:HD12	0.66	2.10	8	11
1:A:42:SER:O	1:A:46:ASP:N	0.66	2.29	11	1
1:B:42:SER:O	1:B:46:ASP:N	0.66	2.29	11	1
1:B:34:LYS:NZ	1:B:38:GLN:NE2	0.66	2.43	9	6
1:A:52:ASP:OD1	1:A:53:ALA:N	0.65	2.29	9	3
1:B:52:ASP:OD1	1:B:53:ALA:N	0.65	2.30	8	3
1:A:64:ASN:HD22	1:A:65:GLY:N	0.65	1.90	19	1
1:A:61:LEU:HD21	1:A:77:LEU:HD22	0.64	1.70	12	10
1:B:46:ASP:OD2	1:B:53:ALA:HB1	0.63	1.93	11	1
1:B:64:ASN:HD22	1:B:65:GLY:N	0.63	1.90	19	1
1:A:46:ASP:OD2	1:A:53:ALA:HB1	0.63	1.93	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:61:LEU:HD21	1:B:77:LEU:HD22	0.63	1.70	8	10
1:A:19:SER:OG	1:A:28:LEU:HD21	0.63	1.94	7	3
1:A:75:VAL:HG12	1:B:79:ALA:CB	0.63	2.22	3	1
1:B:62:ASP:OD2	1:B:66:ASP:N	0.63	2.32	6	5
1:A:4:LEU:HD23	1:A:4:LEU:O	0.62	1.95	8	1
1:A:61:LEU:HD11	1:A:69:VAL:CG1	0.62	2.23	15	1
1:B:19:SER:OG	1:B:28:LEU:HD21	0.62	1.94	7	3
1:A:62:ASP:OD2	1:A:66:ASP:N	0.62	2.32	6	5
1:A:71:PHE:CE1	1:A:75:VAL:CG2	0.62	2.83	3	1
1:B:71:PHE:CE1	1:B:75:VAL:CG2	0.62	2.83	3	1
1:B:4:LEU:O	1:B:4:LEU:HD23	0.62	1.95	8	1
1:A:79:ALA:CB	1:B:75:VAL:HG12	0.61	2.22	3	1
1:A:34:LYS:NZ	1:A:38:GLN:OE1	0.61	2.33	2	9
1:B:71:PHE:CZ	1:B:75:VAL:CG1	0.61	2.84	10	5
1:A:12:ILE:HG23	1:A:16:HIS:CE1	0.61	2.30	18	1
1:A:27:LYS:NZ	1:A:70:ASP:OD1	0.61	2.33	14	4
1:A:71:PHE:CZ	1:A:75:VAL:CG1	0.61	2.84	10	5
1:B:27:LYS:NZ	1:B:70:ASP:OD1	0.61	2.33	1	4
1:B:30:LYS:NZ	1:B:55:ASP:OD1	0.61	2.34	17	5
1:A:15:PHE:CD2	1:A:71:PHE:CE1	0.61	2.89	12	3
1:B:12:ILE:HG23	1:B:16:HIS:CE1	0.61	2.30	18	1
1:A:9:GLU:O	1:A:13:ASN:ND2	0.61	2.34	13	14
1:A:26:TYR:CD1	1:A:26:TYR:N	0.60	2.68	18	14
1:B:34:LYS:NZ	1:B:38:GLN:OE1	0.60	2.34	18	9
1:B:15:PHE:CD2	1:B:71:PHE:CE1	0.60	2.89	12	3
1:B:9:GLU:O	1:B:13:ASN:ND2	0.60	2.35	7	14
1:A:30:LYS:NZ	1:A:55:ASP:OD1	0.60	2.34	17	6
1:B:26:TYR:N	1:B:26:TYR:CD1	0.60	2.69	1	11
1:B:26:TYR:CD1	1:B:26:TYR:N	0.60	2.68	12	8
1:B:62:ASP:OD2	1:B:67:GLY:N	0.59	2.35	16	7
1:A:71:PHE:CE2	1:A:75:VAL:CG1	0.59	2.85	18	5
1:B:71:PHE:CE2	1:B:75:VAL:CG1	0.59	2.85	18	5
1:A:34:LYS:HZ1	1:A:38:GLN:HE22	0.59	1.38	9	2
1:A:78:VAL:O	1:A:82:THR:HG22	0.59	1.96	13	3
1:A:62:ASP:OD2	1:A:67:GLY:N	0.59	2.36	16	6
1:B:28:LEU:O	1:B:69:VAL:O	0.59	2.20	13	7
1:A:4:LEU:HD13	1:B:40:GLU:OE1	0.59	1.97	3	1
1:A:37:LEU:CD1	1:A:37:LEU:N	0.59	2.66	6	1
1:B:37:LEU:CD1	1:B:37:LEU:N	0.59	2.66	6	1
1:B:66:ASP:O	1:B:66:ASP:OD1	0.59	2.21	3	2
1:B:14:VAL:O	1:B:18:HIS:ND1	0.59	2.36	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:GLU:N	1:A:32:GLU:OE2	0.59	2.35	3	5
1:A:28:LEU:O	1:A:69:VAL:O	0.59	2.20	13	7
1:A:40:GLU:OE1	1:B:4:LEU:HD13	0.59	1.97	3	1
1:A:18:HIS:HB2	1:A:36:LEU:HD21	0.59	1.74	6	8
1:A:66:ASP:O	1:A:66:ASP:OD1	0.59	2.21	3	2
1:B:78:VAL:O	1:B:82:THR:HG22	0.59	1.96	13	3
1:B:50:ASP:HB3	1:B:53:ALA:HB2	0.59	1.75	19	3
1:B:15:PHE:CE2	1:B:25:LYS:O	0.58	2.56	1	1
1:A:41:LEU:HB2	1:A:45:LEU:HD22	0.58	1.75	20	1
1:B:46:ASP:O	1:B:46:ASP:OD1	0.58	2.21	6	4
1:A:14:VAL:O	1:A:18:HIS:ND1	0.58	2.36	5	1
1:A:26:TYR:N	1:A:26:TYR:CD1	0.58	2.68	2	4
1:B:64:ASN:N	1:B:64:ASN:HD22	0.58	1.96	19	1
1:A:15:PHE:CE2	1:A:25:LYS:O	0.58	2.56	1	1
1:A:74:TYR:CZ	1:A:78:VAL:CG2	0.58	2.86	6	2
1:A:58:MET:SD	1:A:58:MET:C	0.58	2.82	6	14
1:B:74:TYR:CE2	1:B:78:VAL:CG2	0.58	2.86	6	2
1:B:58:MET:SD	1:B:58:MET:C	0.58	2.82	6	11
1:B:61:LEU:HD11	1:B:69:VAL:CG1	0.58	2.23	15	1
1:B:22:GLU:N	1:B:32:GLU:OE2	0.58	2.35	3	5
1:A:64:ASN:N	1:A:64:ASN:HD22	0.58	1.96	19	1
1:A:22:GLU:O	1:A:32:GLU:OE2	0.58	2.22	7	14
1:B:74:TYR:CZ	1:B:78:VAL:CG2	0.58	2.86	6	2
1:B:41:LEU:HB2	1:B:45:LEU:HD22	0.58	1.75	20	1
1:B:45:LEU:N	1:B:45:LEU:CD2	0.58	2.67	12	2
1:A:27:LYS:HZ1	1:A:68:GLU:CD	0.58	2.02	16	2
1:A:74:TYR:CE2	1:A:78:VAL:CG2	0.58	2.86	6	2
1:A:45:LEU:N	1:A:45:LEU:CD2	0.58	2.67	12	2
1:A:15:PHE:CE1	1:A:28:LEU:HD23	0.57	2.34	10	1
1:B:15:PHE:CE1	1:B:28:LEU:HD23	0.57	2.35	10	1
1:B:64:ASN:N	1:B:64:ASN:ND2	0.57	2.51	19	1
1:A:34:LYS:HZ2	1:A:38:GLN:NE2	0.57	1.96	4	1
1:B:71:PHE:CE2	1:B:75:VAL:CG2	0.57	2.87	4	5
1:A:62:ASP:CG	1:A:69:VAL:HG13	0.57	2.20	9	1
1:B:77:LEU:N	1:B:77:LEU:CD2	0.57	2.67	19	1
1:B:18:HIS:HB2	1:B:36:LEU:HD21	0.57	1.75	2	8
1:A:46:ASP:OD1	1:A:46:ASP:O	0.57	2.21	6	4
1:B:22:GLU:O	1:B:32:GLU:OE2	0.57	2.22	7	14
1:A:15:PHE:CE1	1:A:71:PHE:CD1	0.57	2.93	14	3
1:A:64:ASN:ND2	1:A:64:ASN:N	0.57	2.51	19	1
1:A:77:LEU:CD2	1:A:77:LEU:N	0.57	2.67	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:PHE:CE2	1:A:75:VAL:CG2	0.57	2.87	4	5
1:A:15:PHE:CE2	1:A:74:TYR:CE2	0.57	2.93	8	1
1:B:34:LYS:HZ3	1:B:38:GLN:CD	0.57	2.03	9	2
1:A:50:ASP:HB3	1:A:53:ALA:HB2	0.57	1.75	19	3
1:B:77:LEU:N	1:B:77:LEU:HD22	0.57	2.14	19	1
1:B:82:THR:O	1:B:85:CYS:SG	0.57	2.63	8	10
1:B:62:ASP:CG	1:B:69:VAL:HG13	0.57	2.20	9	1
1:B:37:LEU:O	1:B:42:SER:N	0.57	2.31	11	1
1:A:77:LEU:HD22	1:A:77:LEU:N	0.57	2.14	19	1
1:B:71:PHE:CZ	1:B:75:VAL:CG2	0.57	2.88	3	3
1:A:37:LEU:O	1:A:42:SER:N	0.57	2.31	11	1
1:B:47:ALA:O	1:B:50:ASP:O	0.56	2.23	19	1
1:A:4:LEU:HD23	1:A:4:LEU:C	0.56	2.21	8	2
1:A:82:THR:O	1:A:85:CYS:SG	0.56	2.63	1	10
1:A:75:VAL:HG11	1:B:79:ALA:O	0.56	2.01	2	3
1:B:15:PHE:CE1	1:B:71:PHE:CD1	0.56	2.93	14	3
1:B:27:LYS:NZ	1:B:68:GLU:CD	0.56	2.59	5	2
1:B:4:LEU:HD23	1:B:4:LEU:C	0.56	2.21	8	2
1:B:81:LEU:N	1:B:81:LEU:CD2	0.56	2.67	11	1
1:A:81:LEU:CD2	1:A:81:LEU:N	0.56	2.67	11	1
1:B:53:ALA:O	1:B:57:VAL:HG23	0.56	2.01	15	2
1:B:28:LEU:HD12	1:B:74:TYR:CD2	0.56	2.35	8	1
1:B:15:PHE:CE2	1:B:74:TYR:CE2	0.56	2.93	8	1
1:B:46:ASP:OD1	1:B:46:ASP:O	0.56	2.24	13	4
1:A:71:PHE:CZ	1:A:75:VAL:CG2	0.56	2.88	3	3
1:B:64:ASN:OD1	1:B:73:GLU:OE2	0.56	2.23	3	8
1:A:27:LYS:NZ	1:A:68:GLU:CD	0.56	2.59	5	2
1:B:30:LYS:CE	1:B:55:ASP:OD1	0.56	2.54	15	4
1:A:86:ASN:HD21	1:B:12:ILE:HD13	0.56	1.60	20	2
1:B:15:PHE:CE2	1:B:71:PHE:CG	0.56	2.94	19	1
1:A:64:ASN:OD1	1:A:73:GLU:OE2	0.56	2.23	3	8
1:B:28:LEU:HD23	1:B:29:SER:N	0.56	2.16	16	3
1:A:53:ALA:O	1:A:57:VAL:HG23	0.56	2.01	15	2
1:A:15:PHE:CE2	1:A:71:PHE:CD1	0.56	2.94	12	2
1:A:13:ASN:O	1:A:17:ALA:HB2	0.55	2.01	18	2
1:B:37:LEU:HD12	1:B:37:LEU:N	0.55	2.16	6	2
1:A:30:LYS:CE	1:A:55:ASP:OD1	0.55	2.54	15	4
1:B:34:LYS:HD3	1:B:54:VAL:HG11	0.55	1.78	13	1
1:A:46:ASP:C	1:A:48:GLN:N	0.55	2.59	18	1
1:A:79:ALA:O	1:B:75:VAL:HG11	0.55	2.01	2	3
1:A:37:LEU:N	1:A:37:LEU:HD12	0.55	2.16	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LEU:HD12	1:A:74:TYR:CD2	0.55	2.35	8	1
1:A:15:PHE:CE2	1:A:71:PHE:CG	0.55	2.94	19	1
1:B:13:ASN:O	1:B:17:ALA:HB2	0.55	2.01	18	2
1:A:46:ASP:O	1:A:46:ASP:OD1	0.55	2.24	13	4
1:A:34:LYS:HD3	1:A:54:VAL:HG11	0.55	1.78	13	1
1:A:27:LYS:CE	1:A:70:ASP:OD1	0.55	2.55	1	1
1:B:27:LYS:CE	1:B:70:ASP:OD1	0.55	2.55	1	1
1:B:15:PHE:CE2	1:B:71:PHE:CD1	0.55	2.94	12	2
1:A:47:ALA:O	1:A:50:ASP:O	0.55	2.23	19	1
1:A:85:CYS:SG	1:A:86:ASN:N	0.55	2.80	8	8
1:B:47:ALA:O	1:B:51:VAL:HG22	0.55	2.02	6	2
1:B:46:ASP:C	1:B:48:GLN:N	0.55	2.59	18	1
1:A:47:ALA:O	1:A:51:VAL:HG22	0.54	2.02	6	2
1:B:14:VAL:CG1	1:B:40:GLU:OE2	0.54	2.55	4	3
1:B:81:LEU:CD2	1:B:81:LEU:N	0.54	2.69	4	2
1:B:85:CYS:SG	1:B:86:ASN:N	0.54	2.80	8	8
1:A:81:LEU:N	1:A:81:LEU:CD2	0.54	2.69	4	2
1:A:11:LEU:O	1:A:15:PHE:CD1	0.54	2.61	8	1
1:B:64:ASN:ND2	1:B:65:GLY:N	0.54	2.56	19	1
1:B:58:MET:C	1:B:58:MET:SD	0.54	2.86	4	9
1:A:39:THR:HG23	1:A:40:GLU:HG3	0.54	1.80	11	1
1:A:45:LEU:O	1:A:46:ASP:C	0.54	2.46	16	19
1:B:39:THR:HG23	1:B:40:GLU:HG3	0.54	1.80	11	1
1:A:14:VAL:CG1	1:A:40:GLU:OE2	0.54	2.55	4	3
1:B:11:LEU:O	1:B:15:PHE:CD1	0.54	2.60	8	1
1:A:64:ASN:ND2	1:A:65:GLY:N	0.54	2.56	19	1
1:A:28:LEU:HD23	1:A:29:SER:N	0.54	2.17	16	3
1:A:12:ILE:HD13	1:B:86:ASN:HD21	0.54	1.60	20	2
1:B:45:LEU:O	1:B:46:ASP:C	0.53	2.46	16	19
1:B:66:ASP:OD1	1:B:68:GLU:O	0.53	2.26	6	2
1:A:78:VAL:O	1:A:82:THR:HG23	0.53	2.03	20	1
1:A:2:SER:CB	1:B:40:GLU:OE1	0.53	2.56	15	4
1:A:2:SER:OG	1:B:40:GLU:OE1	0.53	2.26	15	5
1:B:34:LYS:HZ1	1:B:38:GLN:HE22	0.53	1.44	5	3
1:B:74:TYR:CE2	1:B:78:VAL:HG21	0.53	2.38	4	3
1:B:78:VAL:O	1:B:82:THR:HG23	0.53	2.03	20	1
1:A:18:HIS:C	1:A:18:HIS:CD2	0.53	2.82	17	1
1:A:66:ASP:OD1	1:A:68:GLU:O	0.53	2.26	6	2
1:A:74:TYR:CE2	1:A:78:VAL:HG21	0.53	2.38	4	3
1:A:34:LYS:HZ3	1:A:38:GLN:CD	0.53	2.06	5	2
1:A:77:LEU:O	1:A:77:LEU:HD13	0.53	2.04	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:LYS:O	1:A:50:ASP:OD1	0.53	2.27	12	12
1:A:58:MET:C	1:A:58:MET:SD	0.53	2.87	18	6
1:B:61:LEU:HD21	1:B:77:LEU:CD2	0.52	2.34	12	10
1:A:40:GLU:OE1	1:B:2:SER:CB	0.52	2.56	15	4
1:A:61:LEU:HD21	1:A:77:LEU:CD2	0.52	2.34	12	10
1:B:49:LYS:O	1:B:50:ASP:OD1	0.52	2.28	2	12
1:B:66:ASP:OD1	1:B:68:GLU:N	0.52	2.43	15	10
1:A:34:LYS:NZ	1:A:38:GLN:CD	0.52	2.63	9	2
1:A:15:PHE:C	1:A:15:PHE:CD1	0.52	2.80	13	1
1:B:77:LEU:O	1:B:77:LEU:HD13	0.52	2.04	4	1
1:B:27:LYS:HZ1	1:B:68:GLU:CD	0.52	2.08	5	1
1:B:34:LYS:NZ	1:B:38:GLN:CD	0.52	2.62	9	2
1:A:27:LYS:NZ	1:A:68:GLU:OE1	0.52	2.43	5	2
1:B:61:LEU:HD23	1:B:77:LEU:HD12	0.52	1.82	5	1
1:B:18:HIS:CD2	1:B:18:HIS:C	0.52	2.82	17	1
1:B:70:ASP:OD1	1:B:71:PHE:N	0.52	2.43	5	8
1:B:61:LEU:O	1:B:73:GLU:OE1	0.52	2.28	10	12
1:A:61:LEU:HD23	1:A:77:LEU:HD12	0.52	1.81	5	1
1:A:15:PHE:CD1	1:A:28:LEU:HD13	0.52	2.40	13	1
1:A:71:PHE:CE2	1:A:75:VAL:HG21	0.52	2.40	12	5
1:A:40:GLU:O	1:B:5:GLU:OE2	0.51	2.28	5	1
1:B:15:PHE:CD1	1:B:15:PHE:C	0.51	2.80	13	1
1:B:46:ASP:C	1:B:48:GLN:H	0.51	2.09	18	1
1:B:41:LEU:HD12	1:B:41:LEU:N	0.51	2.20	8	4
1:A:66:ASP:OD1	1:A:68:GLU:N	0.51	2.43	15	9
1:A:10:THR:O	1:A:14:VAL:HG13	0.51	2.05	9	1
1:B:15:PHE:CD1	1:B:28:LEU:HD13	0.51	2.40	13	1
1:A:70:ASP:OD1	1:A:71:PHE:N	0.51	2.43	5	8
1:A:75:VAL:HB	1:B:79:ALA:HB1	0.51	1.82	13	1
1:A:71:PHE:CE2	1:A:75:VAL:HG11	0.51	2.41	9	5
1:B:71:PHE:CE2	1:B:75:VAL:HG21	0.51	2.41	6	5
1:A:61:LEU:O	1:A:73:GLU:OE1	0.51	2.28	19	12
1:B:27:LYS:NZ	1:B:68:GLU:OE1	0.51	2.43	5	2
1:A:27:LYS:CB	1:A:68:GLU:OE2	0.51	2.59	9	2
1:A:79:ALA:HB1	1:B:75:VAL:HB	0.51	1.82	13	1
1:A:19:SER:OG	1:A:25:LYS:O	0.51	2.26	17	3
1:B:27:LYS:CB	1:B:68:GLU:OE2	0.51	2.59	9	2
1:B:58:MET:HA	1:B:61:LEU:HD23	0.51	1.82	15	1
1:A:58:MET:HA	1:A:61:LEU:HD23	0.50	1.82	15	1
1:A:5:GLU:OE2	1:B:40:GLU:O	0.50	2.28	5	1
1:A:62:ASP:OD2	1:A:66:ASP:O	0.50	2.29	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ASP:OD2	1:A:66:ASP:OD1	0.50	2.30	5	2
1:B:41:LEU:HD23	1:B:45:LEU:HD13	0.50	1.84	7	3
1:B:71:PHE:CE2	1:B:75:VAL:HG11	0.50	2.41	9	7
1:A:15:PHE:O	1:A:19:SER:OG	0.50	2.30	13	3
1:B:19:SER:OG	1:B:28:LEU:CD2	0.50	2.59	10	2
1:B:64:ASN:ND2	1:B:66:ASP:OD2	0.50	2.43	6	1
1:A:41:LEU:HD12	1:A:41:LEU:N	0.50	2.21	8	3
1:A:15:PHE:CD2	1:A:71:PHE:CD1	0.50	3.00	12	1
1:B:15:PHE:CD2	1:B:71:PHE:CD1	0.50	3.00	12	2
1:A:19:SER:OG	1:A:28:LEU:CD2	0.50	2.59	10	2
1:A:46:ASP:C	1:A:48:GLN:H	0.50	2.09	18	1
1:A:19:SER:O	1:A:32:GLU:OE2	0.50	2.30	4	2
1:A:18:HIS:CB	1:A:36:LEU:HD11	0.49	2.37	15	1
1:B:27:LYS:HZ3	1:B:68:GLU:CD	0.49	2.10	16	1
1:B:19:SER:O	1:B:32:GLU:OE2	0.49	2.30	4	2
1:A:62:ASP:OD1	1:A:66:ASP:OD1	0.49	2.31	2	2
1:B:39:THR:CG2	1:B:40:GLU:N	0.49	2.76	17	19
1:B:10:THR:O	1:B:14:VAL:HG13	0.49	2.06	9	1
1:B:41:LEU:N	1:B:41:LEU:HD12	0.49	2.22	14	4
1:A:4:LEU:HD22	1:B:40:GLU:OE1	0.49	2.07	6	8
1:A:34:LYS:HZ2	1:A:38:GLN:CD	0.49	2.11	4	1
1:B:62:ASP:OD2	1:B:66:ASP:OD1	0.49	2.30	15	2
1:A:41:LEU:HD23	1:A:45:LEU:HD13	0.49	1.84	7	3
1:B:18:HIS:O	1:B:21:LYS:NZ	0.49	2.45	3	2
1:B:71:PHE:CZ	1:B:75:VAL:HG21	0.49	2.42	3	1
1:B:62:ASP:OD2	1:B:66:ASP:O	0.49	2.29	6	1
1:B:19:SER:OG	1:B:25:LYS:O	0.49	2.31	20	3
1:A:39:THR:CG2	1:A:40:GLU:N	0.49	2.76	3	19
1:A:41:LEU:N	1:A:41:LEU:HD12	0.49	2.22	14	3
1:A:71:PHE:CZ	1:A:75:VAL:HG21	0.49	2.42	3	1
1:B:54:VAL:CG2	1:B:55:ASP:N	0.49	2.76	13	1
1:B:71:PHE:O	1:B:75:VAL:HG23	0.49	2.08	11	3
1:A:72:GLN:O	1:A:76:VAL:HG23	0.49	2.08	8	1
1:A:18:HIS:O	1:A:21:LYS:NZ	0.48	2.44	8	2
1:A:54:VAL:CG2	1:A:55:ASP:N	0.48	2.76	13	1
1:B:72:GLN:O	1:B:76:VAL:HG23	0.48	2.08	8	1
1:B:38:GLN:O	1:B:42:SER:OG	0.48	2.29	1	1
1:A:40:GLU:OE1	1:B:4:LEU:HD22	0.48	2.08	16	8
1:B:37:LEU:HD21	1:B:74:TYR:OH	0.48	2.08	13	6
1:B:61:LEU:CD1	1:B:61:LEU:C	0.48	2.69	15	1
1:A:71:PHE:O	1:A:75:VAL:HG23	0.48	2.08	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:62:ASP:OD1	1:B:66:ASP:OD1	0.48	2.30	2	2
1:A:37:LEU:HD21	1:A:74:TYR:OH	0.48	2.08	13	6
1:A:37:LEU:HD11	1:A:74:TYR:CE1	0.48	2.44	14	1
1:A:18:HIS:HB2	1:A:36:LEU:HD11	0.48	1.86	15	1
1:B:18:HIS:CB	1:B:36:LEU:HD11	0.48	2.37	15	1
1:A:6:THR:O	1:A:10:THR:OG1	0.48	2.28	17	1
1:A:50:ASP:CB	1:A:53:ALA:HB2	0.48	2.39	20	3
1:A:45:LEU:CD2	1:A:45:LEU:N	0.48	2.77	10	2
1:B:45:LEU:CD2	1:B:45:LEU:N	0.48	2.77	10	2
1:A:33:LEU:HD21	1:A:61:LEU:CD1	0.47	2.39	5	1
1:B:37:LEU:HD11	1:B:74:TYR:CE1	0.47	2.44	14	1
1:B:33:LEU:HD21	1:B:61:LEU:CD1	0.47	2.38	5	1
1:B:15:PHE:O	1:B:19:SER:OG	0.47	2.31	6	4
1:A:62:ASP:OD2	1:A:65:GLY:C	0.47	2.53	6	5
1:A:62:ASP:CG	1:A:67:GLY:H	0.47	2.13	16	1
1:A:62:ASP:CG	1:A:66:ASP:O	0.47	2.53	6	1
1:B:50:ASP:CB	1:B:53:ALA:HB2	0.47	2.39	20	2
1:B:18:HIS:HB2	1:B:36:LEU:HD11	0.47	1.86	15	1
1:B:62:ASP:OD2	1:B:65:GLY:C	0.47	2.53	16	5
1:B:71:PHE:O	1:B:75:VAL:HG13	0.47	2.09	7	4
1:A:62:ASP:OD2	1:A:70:ASP:N	0.47	2.46	9	1
1:A:40:GLU:OE1	1:B:4:LEU:CB	0.47	2.63	11	3
1:A:40:GLU:OE1	1:B:2:SER:OG	0.47	2.26	15	3
1:A:18:HIS:CG	1:A:36:LEU:CD2	0.47	2.97	1	2
1:B:34:LYS:HZ2	1:B:38:GLN:NE2	0.47	2.07	4	1
1:A:71:PHE:O	1:A:75:VAL:HG13	0.47	2.09	7	4
1:B:62:ASP:CG	1:B:67:GLY:H	0.47	2.13	16	1
1:B:13:ASN:O	1:B:17:ALA:CB	0.47	2.63	18	2
1:B:62:ASP:CG	1:B:66:ASP:O	0.47	2.53	6	1
1:B:58:MET:O	1:B:61:LEU:HG	0.47	2.10	15	1
1:A:15:PHE:CG	1:A:71:PHE:CE1	0.47	3.03	19	1
1:B:66:ASP:C	1:B:68:GLU:H	0.46	2.13	12	1
1:B:15:PHE:CZ	1:B:25:LYS:O	0.46	2.68	1	1
1:A:75:VAL:O	1:A:78:VAL:HG12	0.46	2.09	2	2
1:A:4:LEU:CB	1:B:40:GLU:OE1	0.46	2.63	11	3
1:A:66:ASP:C	1:A:68:GLU:H	0.46	2.13	12	1
1:A:64:ASN:ND2	1:A:66:ASP:OD2	0.46	2.43	6	1
1:A:66:ASP:OD1	1:A:66:ASP:C	0.46	2.53	10	1
1:A:11:LEU:HD11	1:B:11:LEU:HD11	0.46	1.86	11	1
1:A:15:PHE:CZ	1:A:25:LYS:O	0.46	2.68	1	1
1:B:75:VAL:O	1:B:78:VAL:HG12	0.46	2.09	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:15:PHE:CZ	1:B:74:TYR:CE2	0.46	3.03	17	3
1:A:61:LEU:O	1:A:73:GLU:CD	0.46	2.54	12	7
1:B:15:PHE:CG	1:B:71:PHE:CE1	0.46	3.03	19	1
1:A:4:LEU:CD2	1:B:40:GLU:OE1	0.46	2.64	20	11
1:A:13:ASN:O	1:A:17:ALA:CB	0.46	2.63	18	2
1:B:61:LEU:O	1:B:73:GLU:CD	0.46	2.54	6	7
1:A:28:LEU:CD1	1:A:74:TYR:CE2	0.46	2.99	8	1
1:B:28:LEU:CD1	1:B:74:TYR:CE2	0.46	2.99	8	1
1:A:47:ALA:O	1:A:50:ASP:C	0.46	2.54	13	6
1:A:79:ALA:HB2	1:B:79:ALA:CB	0.46	2.38	20	1
1:A:15:PHE:CZ	1:A:74:TYR:CE2	0.46	3.03	17	3
1:B:79:ALA:O	1:B:82:THR:CG2	0.46	2.64	18	12
1:B:62:ASP:OD1	1:B:69:VAL:HG22	0.46	2.11	3	1
1:A:40:GLU:OE1	1:B:4:LEU:CD2	0.46	2.64	14	11
1:B:66:ASP:OD1	1:B:66:ASP:C	0.46	2.53	10	2
1:B:54:VAL:HG23	1:B:55:ASP:N	0.46	2.25	13	1
1:A:58:MET:O	1:A:61:LEU:HG	0.46	2.10	15	1
1:B:52:ASP:C	1:B:52:ASP:OD1	0.45	2.55	6	3
1:B:47:ALA:O	1:B:50:ASP:C	0.45	2.54	13	6
1:B:50:ASP:CG	1:B:53:ALA:H	0.45	2.15	13	2
1:B:72:GLN:O	1:B:75:VAL:HG22	0.45	2.11	5	2
1:A:54:VAL:HG23	1:A:55:ASP:N	0.45	2.26	13	1
1:B:85:CYS:SG	1:B:86:ASN:ND2	0.45	2.90	5	1
1:B:81:LEU:CD1	1:B:81:LEU:O	0.45	2.65	13	1
1:A:79:ALA:O	1:A:82:THR:CG2	0.45	2.64	18	12
1:B:9:GLU:O	1:B:13:ASN:CG	0.45	2.54	11	5
1:A:41:LEU:HD21	1:B:8:MET:SD	0.45	2.52	7	2
1:A:14:VAL:HG23	1:A:15:PHE:N	0.45	2.27	9	1
1:A:38:GLN:O	1:A:42:SER:OG	0.45	2.29	1	1
1:A:9:GLU:O	1:A:13:ASN:CG	0.45	2.55	11	5
1:A:85:CYS:SG	1:A:86:ASN:ND2	0.45	2.90	5	1
1:A:8:MET:SD	1:B:41:LEU:HD21	0.45	2.52	7	1
1:A:28:LEU:CD1	1:A:74:TYR:CD2	0.45	3.00	8	1
1:B:14:VAL:HG23	1:B:15:PHE:N	0.45	2.27	9	1
1:A:77:LEU:O	1:A:77:LEU:CD1	0.45	2.65	4	1
1:A:12:ILE:O	1:A:16:HIS:CB	0.45	2.65	5	4
1:B:62:ASP:OD2	1:B:70:ASP:N	0.45	2.46	9	1
1:A:40:GLU:O	1:A:41:LEU:HD22	0.45	2.11	20	1
1:A:75:VAL:O	1:B:79:ALA:HB1	0.45	2.12	18	2
1:B:28:LEU:CD1	1:B:74:TYR:CD2	0.45	3.00	8	1
1:B:12:ILE:O	1:B:16:HIS:CB	0.45	2.65	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:66:ASP:CG	1:B:68:GLU:O	0.45	2.55	9	1
1:A:74:TYR:CZ	1:A:78:VAL:CG1	0.45	3.00	20	1
1:A:52:ASP:C	1:A:52:ASP:OD1	0.45	2.56	2	3
1:A:50:ASP:CG	1:A:53:ALA:H	0.45	2.15	13	1
1:A:81:LEU:CD1	1:A:81:LEU:O	0.45	2.65	13	1
1:A:64:ASN:ND2	1:A:65:GLY:H	0.45	2.03	19	1
1:A:74:TYR:CE2	1:A:78:VAL:HG11	0.44	2.47	20	1
1:B:74:TYR:CZ	1:B:78:VAL:CG1	0.44	3.00	20	1
1:A:39:THR:HG23	1:A:40:GLU:N	0.44	2.28	15	10
1:A:66:ASP:CG	1:A:68:GLU:O	0.44	2.55	9	1
1:B:81:LEU:HD13	1:B:81:LEU:O	0.44	2.13	13	1
1:B:40:GLU:O	1:B:41:LEU:HD22	0.44	2.11	20	1
1:B:39:THR:HG23	1:B:40:GLU:N	0.44	2.27	19	9
1:A:62:ASP:OD1	1:A:66:ASP:N	0.44	2.50	6	1
1:A:22:GLU:C	1:A:32:GLU:OE2	0.44	2.56	15	1
1:A:45:LEU:HD11	1:A:81:LEU:HD21	0.44	1.89	20	1
1:B:74:TYR:CE2	1:B:78:VAL:HG11	0.44	2.47	20	1
1:A:25:LYS:C	1:A:27:LYS:H	0.44	2.16	10	1
1:A:52:ASP:OD1	1:A:52:ASP:C	0.44	2.55	6	2
1:B:52:ASP:OD1	1:B:52:ASP:C	0.44	2.56	15	2
1:A:52:ASP:OD1	1:A:56:LYS:NZ	0.44	2.50	6	1
1:A:66:ASP:C	1:A:66:ASP:OD1	0.44	2.54	6	2
1:B:66:ASP:C	1:B:66:ASP:OD1	0.44	2.54	6	1
1:A:81:LEU:HD13	1:A:81:LEU:O	0.44	2.13	13	1
1:A:72:GLN:O	1:A:75:VAL:HG22	0.44	2.12	5	2
1:B:18:HIS:CG	1:B:36:LEU:CD2	0.44	2.98	5	2
1:A:62:ASP:OD1	1:A:69:VAL:HG22	0.44	2.11	3	1
1:B:52:ASP:OD1	1:B:56:LYS:NZ	0.44	2.50	6	1
1:A:64:ASN:HD21	1:A:66:ASP:CG	0.43	2.16	11	1
1:B:6:THR:O	1:B:10:THR:OG1	0.43	2.31	5	3
1:A:61:LEU:C	1:A:61:LEU:CD1	0.43	2.69	15	1
1:A:15:PHE:CD1	1:A:36:LEU:HD13	0.43	2.48	17	1
1:B:77:LEU:CD1	1:B:77:LEU:O	0.43	2.65	4	1
1:A:79:ALA:HB1	1:B:75:VAL:O	0.43	2.12	18	2
1:A:34:LYS:CE	1:A:38:GLN:OE1	0.43	2.67	18	4
1:B:22:GLU:C	1:B:32:GLU:OE2	0.43	2.56	15	1
1:B:50:ASP:OD2	1:B:52:ASP:OD1	0.43	2.37	15	1
1:B:34:LYS:CE	1:B:38:GLN:OE1	0.43	2.67	18	4
1:B:34:LYS:HZ2	1:B:38:GLN:CD	0.43	2.17	4	1
1:B:64:ASN:HD21	1:B:66:ASP:CG	0.43	2.16	11	1
1:A:62:ASP:CG	1:A:66:ASP:N	0.43	2.72	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:25:LYS:C	1:B:27:LYS:H	0.43	2.16	10	1
1:A:18:HIS:HB3	1:A:36:LEU:HD21	0.43	1.90	1	2
1:A:41:LEU:CD2	1:A:45:LEU:HD13	0.43	2.43	7	1
1:A:62:ASP:CB	1:A:64:ASN:OD1	0.43	2.67	9	1
1:B:62:ASP:CB	1:B:64:ASN:OD1	0.43	2.67	9	1
1:A:25:LYS:C	1:A:27:LYS:N	0.43	2.72	10	1
1:B:41:LEU:CD2	1:B:45:LEU:HD13	0.43	2.43	7	1
1:B:15:PHE:CD1	1:B:36:LEU:HD13	0.43	2.48	17	1
1:B:26:TYR:O	1:B:70:ASP:OD1	0.43	2.37	5	1
1:B:59:LYS:O	1:B:62:ASP:O	0.43	2.37	9	1
1:A:79:ALA:CB	1:B:79:ALA:HB2	0.43	2.38	20	1
1:A:34:LYS:HD3	1:A:54:VAL:HG21	0.42	1.91	15	3
1:B:25:LYS:C	1:B:27:LYS:N	0.42	2.72	10	1
1:B:62:ASP:CG	1:B:66:ASP:N	0.42	2.72	6	1
1:B:62:ASP:OD1	1:B:66:ASP:N	0.42	2.50	6	1
1:A:62:ASP:OD1	1:A:73:GLU:CB	0.42	2.68	9	1
1:A:34:LYS:O	1:A:38:GLN:CB	0.42	2.68	11	4
1:A:81:LEU:CD1	1:A:81:LEU:C	0.42	2.87	13	1
1:B:45:LEU:HD11	1:B:81:LEU:HD21	0.42	1.89	20	1
1:A:34:LYS:NZ	1:A:47:ALA:HB3	0.42	2.29	4	1
1:A:18:HIS:ND1	1:A:36:LEU:CD2	0.42	2.83	7	1
1:B:27:LYS:CG	1:B:68:GLU:OE2	0.42	2.68	10	1
1:A:50:ASP:OD2	1:A:52:ASP:OD1	0.42	2.37	15	1
1:B:58:MET:CG	1:B:59:LYS:N	0.42	2.83	15	1
1:B:34:LYS:HD3	1:B:54:VAL:HG21	0.42	1.91	15	3
1:B:18:HIS:HB3	1:B:36:LEU:HD21	0.42	1.91	5	1
1:B:34:LYS:O	1:B:38:GLN:CB	0.42	2.67	9	4
1:A:27:LYS:CG	1:A:68:GLU:OE2	0.42	2.68	10	1
1:A:12:ILE:O	1:A:16:HIS:ND1	0.42	2.50	18	1
1:B:37:LEU:HD23	1:B:45:LEU:HD12	0.42	1.92	18	1
1:A:77:LEU:C	1:A:77:LEU:CD1	0.42	2.88	4	1
1:B:77:LEU:CD1	1:B:77:LEU:C	0.42	2.88	4	1
1:A:26:TYR:O	1:A:70:ASP:OD1	0.42	2.37	5	1
1:A:58:MET:CG	1:A:59:LYS:N	0.42	2.83	15	1
1:B:62:ASP:C	1:B:64:ASN:ND2	0.42	2.73	19	1
1:A:4:LEU:CD1	1:B:11:LEU:CD2	0.42	2.98	4	1
1:B:19:SER:OG	1:B:28:LEU:HD23	0.42	2.15	10	1
1:A:11:LEU:HD21	1:B:7:ALA:HB1	0.42	1.91	11	1
1:B:15:PHE:C	1:B:15:PHE:CD1	0.42	2.92	19	1
1:B:34:LYS:NZ	1:B:47:ALA:HB3	0.42	2.30	4	1
1:B:62:ASP:CG	1:B:66:ASP:OD1	0.42	2.58	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LYS:O	1:A:62:ASP:O	0.42	2.37	9	1
1:A:45:LEU:HD22	1:A:45:LEU:N	0.42	2.30	12	1
1:B:81:LEU:CD1	1:B:81:LEU:C	0.42	2.87	13	1
1:A:62:ASP:C	1:A:64:ASN:ND2	0.42	2.73	19	1
1:B:62:ASP:OD1	1:B:73:GLU:CB	0.41	2.68	9	1
1:A:19:SER:OG	1:A:28:LEU:HD23	0.41	2.15	10	1
1:B:15:PHE:CE1	1:B:19:SER:OG	0.41	2.61	4	1
1:B:42:SER:OG	1:B:47:ALA:HB2	0.41	2.16	11	1
1:B:58:MET:SD	1:B:59:LYS:N	0.41	2.93	15	1
1:A:62:ASP:CG	1:A:66:ASP:OD1	0.41	2.58	1	2
1:A:37:LEU:HD11	1:A:74:TYR:OH	0.41	2.15	6	1
1:B:18:HIS:ND1	1:B:36:LEU:CD2	0.41	2.82	7	1
1:A:42:SER:OG	1:A:47:ALA:HB2	0.41	2.16	11	1
1:A:11:LEU:CD2	1:B:4:LEU:CD1	0.41	2.98	4	1
1:A:58:MET:HG3	1:A:59:LYS:N	0.41	2.30	1	1
1:A:81:LEU:N	1:A:81:LEU:HD12	0.41	2.31	16	1
1:A:75:VAL:HG21	1:B:83:VAL:CG2	0.41	2.45	2	1
1:A:83:VAL:CG2	1:B:75:VAL:HG21	0.41	2.45	2	1
1:B:15:PHE:CD1	1:B:71:PHE:CE1	0.41	3.09	7	1
1:B:11:LEU:O	1:B:15:PHE:CD2	0.41	2.74	11	1
1:B:58:MET:HG3	1:B:59:LYS:N	0.41	2.30	1	1
1:B:45:LEU:HD21	1:B:81:LEU:HD13	0.41	1.91	1	2
1:A:11:LEU:O	1:A:15:PHE:CD2	0.41	2.74	11	2
1:B:71:PHE:CE1	1:B:75:VAL:HG22	0.41	2.51	3	1
1:B:37:LEU:HD11	1:B:74:TYR:OH	0.41	2.15	6	1
1:A:4:LEU:HD23	1:B:41:LEU:HD11	0.41	1.92	6	1
1:B:81:LEU:N	1:B:81:LEU:HD12	0.41	2.31	16	2
1:A:66:ASP:C	1:A:68:GLU:N	0.41	2.75	12	1
1:B:45:LEU:N	1:B:45:LEU:HD22	0.41	2.30	12	1
1:B:66:ASP:C	1:B:68:GLU:N	0.41	2.75	12	1
1:A:11:LEU:O	1:A:14:VAL:HG22	0.41	2.16	14	1
1:A:28:LEU:HD23	1:A:29:SER:H	0.41	1.75	16	1
1:B:12:ILE:O	1:B:16:HIS:ND1	0.41	2.50	18	1
1:A:37:LEU:HD23	1:A:45:LEU:HD12	0.41	1.92	18	1
1:B:64:ASN:ND2	1:B:65:GLY:H	0.41	2.03	19	1
1:A:45:LEU:HD21	1:A:81:LEU:HD13	0.41	1.91	1	2
1:A:41:LEU:HD11	1:B:4:LEU:HD23	0.40	1.92	6	1
1:A:58:MET:SD	1:A:59:LYS:N	0.40	2.93	15	1
1:A:57:VAL:O	1:A:77:LEU:CD2	0.40	2.69	15	1
1:A:81:LEU:HD12	1:A:81:LEU:N	0.40	2.31	10	1
1:B:57:VAL:O	1:B:77:LEU:CD2	0.40	2.69	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LEU:N	1:A:45:LEU:CD1	0.40	2.84	20	1
1:A:74:TYR:CE2	1:A:78:VAL:CG1	0.40	3.04	20	1
1:A:15:PHE:CD1	1:A:71:PHE:CE1	0.40	3.09	7	1
1:B:81:LEU:N	1:B:81:LEU:HD22	0.40	2.31	11	1
1:B:11:LEU:O	1:B:14:VAL:HG22	0.40	2.16	14	1
1:A:7:ALA:HB1	1:B:11:LEU:HD21	0.40	1.92	11	1
1:B:8:MET:SD	1:B:9:GLU:N	0.40	2.95	14	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	86/93 (92%)	83±1 (96±1%)	2±1 (3±1%)	1±1 (1±1%)	16	63
1	B	86/93 (92%)	83±1 (96±1%)	2±1 (3±1%)	1±1 (1±1%)	16	63
All	All	3440/3720 (92%)	3300 (96%)	96 (3%)	44 (1%)	16	63

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	46	ASP	17
1	A	46	ASP	17
1	B	24	ASP	2
1	A	24	ASP	2
1	B	47	ALA	2
1	A	47	ALA	2
1	A	23	GLY	1
1	B	23	GLY	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	74/80 (92%)	72±1 (97±2%)	2±1 (3±2%)	42	88
1	B	74/80 (92%)	72±1 (97±2%)	2±1 (3±2%)	42	88
All	All	2960/3200 (92%)	2864 (97%)	96 (3%)	42	88

All 30 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	85	CYS	11
1	B	85	CYS	11
1	A	45	LEU	7
1	B	45	LEU	7
1	B	82	THR	6
1	A	82	THR	6
1	B	39	THR	4
1	B	81	LEU	4
1	A	39	THR	4
1	A	81	LEU	4
1	A	34	LYS	3
1	B	58	MET	3
1	B	28	LEU	3
1	A	58	MET	3
1	B	34	LYS	3
1	A	28	LEU	3
1	B	8	MET	1
1	A	15	PHE	1
1	A	77	LEU	1
1	B	64	ASN	1
1	A	64	ASN	1
1	A	26	TYR	1
1	B	36	LEU	1
1	A	8	MET	1
1	B	77	LEU	1
1	B	15	PHE	1
1	B	61	LEU	1
1	A	36	LEU	1
1	B	26	TYR	1
1	A	61	LEU	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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

### 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 [i](#)

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

### 7.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping [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	1091
Number of shifts mapped to atoms	1091
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	91	$-0.35 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	83	$0.19 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	83	$-0.04 \pm 0.07$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	83	$0.34 \pm 0.20$	None needed ( $< 0.5$ ppm)

#### 7.1.3 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 44%, i.e. 894 atoms were assigned a chemical shift out of a possible 2034. 18 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	402/860 (47%)	162/344 (47%)	162/344 (47%)	78/172 (45%)
Sidechain	458/1056 (43%)	281/604 (47%)	171/420 (41%)	6/32 (19%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	34/118 (29%)	19/62 (31%)	15/48 (31%)	0/8 (0%)
Overall	894/2034 (44%)	462/1010 (46%)	348/812 (43%)	84/212 (40%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 969 atoms were assigned a chemical shift out of a possible 2216. 18 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	431/930 (46%)	174/372 (47%)	174/372 (47%)	83/186 (45%)
Sidechain	482/1108 (44%)	297/636 (47%)	178/438 (41%)	7/34 (21%)
Aromatic	56/178 (31%)	32/94 (34%)	23/74 (31%)	1/10 (10%)
Overall	969/2216 (44%)	503/1102 (46%)	375/884 (42%)	91/230 (40%)

#### 7.1.4 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	A	19	SER	HB2	2.12	5.18 – 2.58	-6.8

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

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.

Random coil index (RCI) for chain A:

