



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:48 PM BST

PDB ID : 1IU2  
Title : The first PDZ domain of PSD-95  
Authors : Long, J.-F.; Tochio, H.; Wang, P.; Sala, C.; Niethammer, M.; Sheng, M.; Zhang, M.  
Deposited on : 2002-02-19

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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  
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

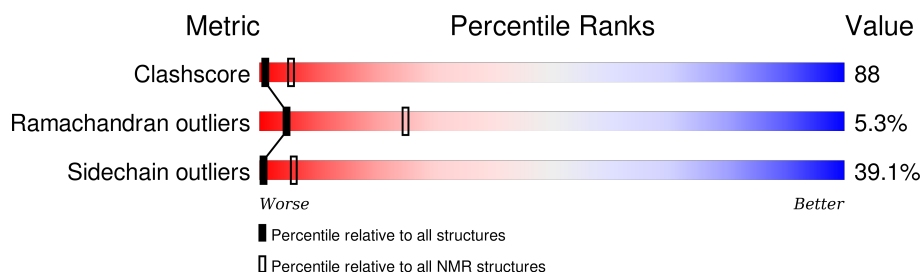
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*


The overall completeness of chemical shifts assignment was not calculated.

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  $\geq 3$ , 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	91	

## 2 Ensemble composition and analysis

This entry contains 50 models. Model 15 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:11, A:15-A:88 (83)	0.17	15

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. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49
2	19, 50

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1379 atoms, of which 688 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PSD-95.

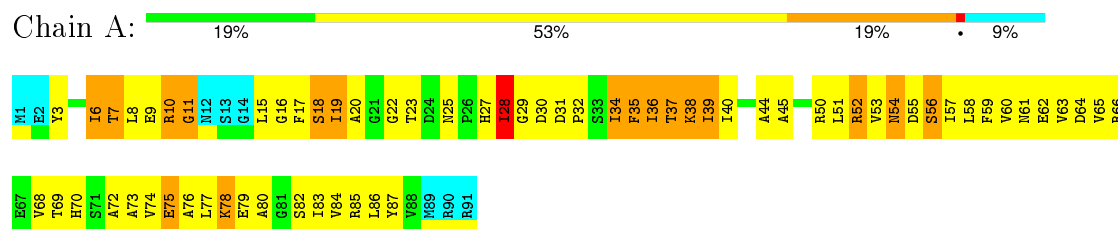
Mol	Chain	Residues	Atoms						Trace
1	A	91	Total	C	H	N	O	S	0
			1379	429	688	123	137	2	

## 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: PSD-95

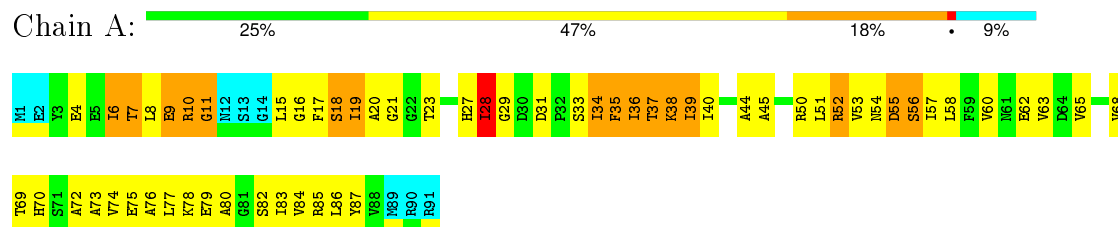


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

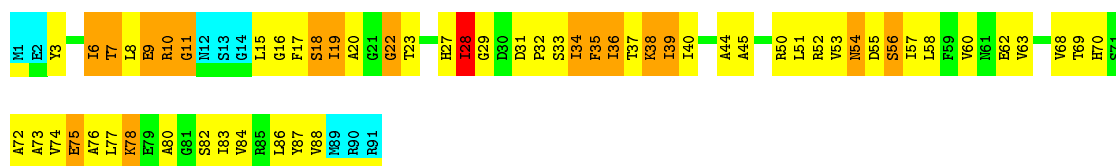
- Molecule 1: PSD-95



#### 4.2.2 Score per residue for model 2

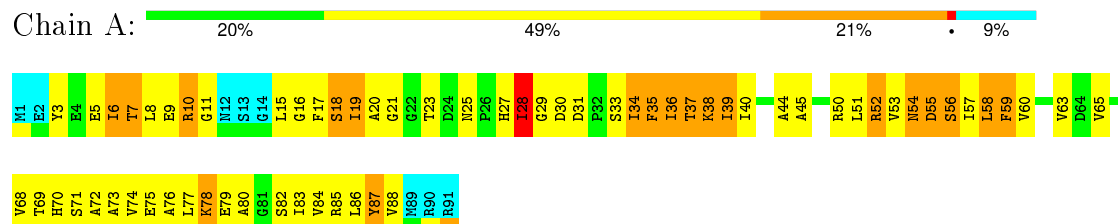
- Molecule 1: PSD-95





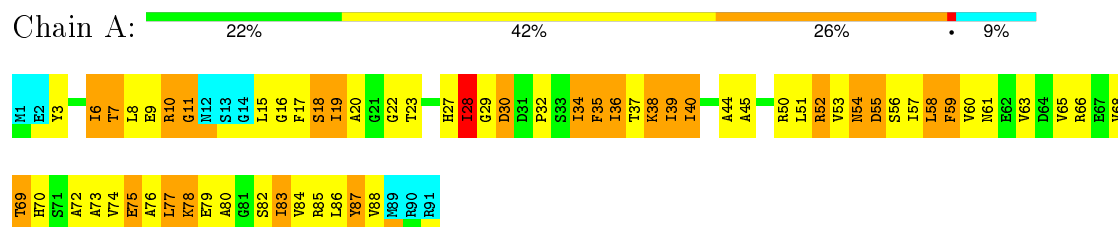
### 4.2.3 Score per residue for model 3

- Molecule 1: PSD-95



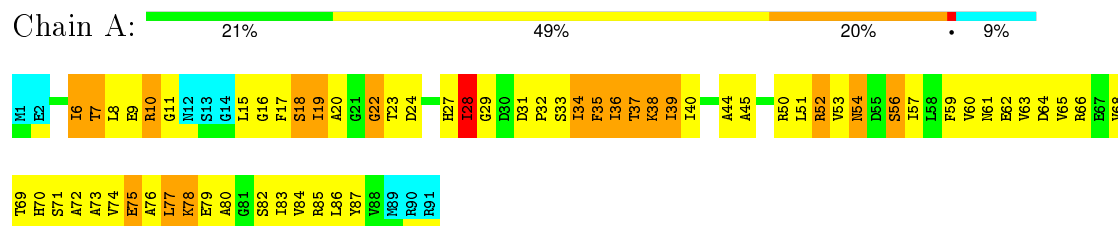
### 4.2.4 Score per residue for model 4

- Molecule 1: PSD-95



### 4.2.5 Score per residue for model 5

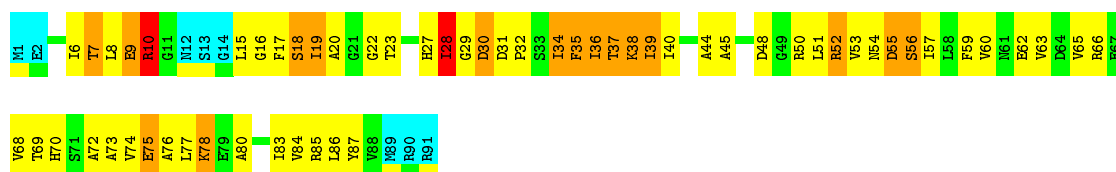
- Molecule 1: PSD-95



### 4.2.6 Score per residue for model 6

- Molecule 1: PSD-95

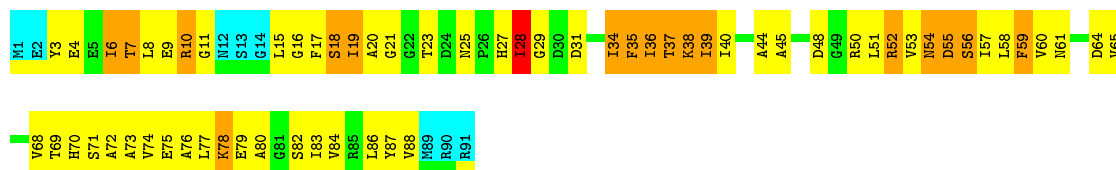




#### 4.2.7 Score per residue for model 7

- Molecule 1: PSD-95

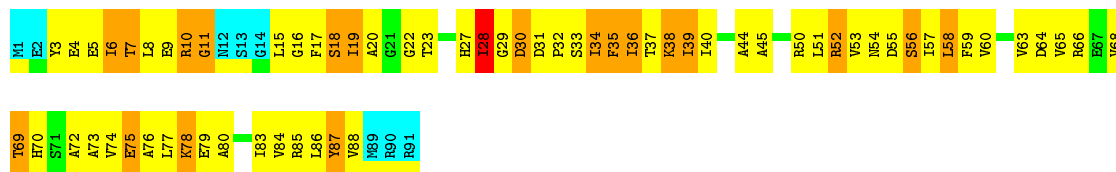
Chain A: 21% 51% 19% 9%



#### 4.2.8 Score per residue for model 8

- Molecule 1: PSD-95

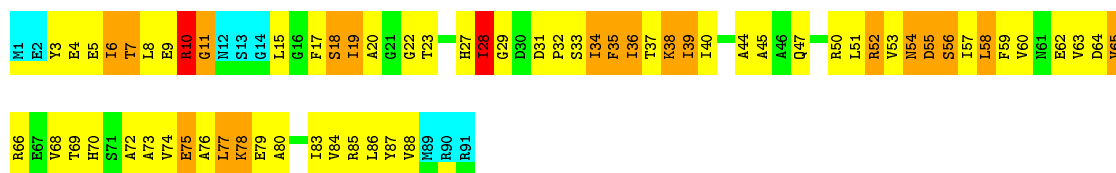
Chain A: 19% 51% 21% 9%



#### 4.2.9 Score per residue for model 9

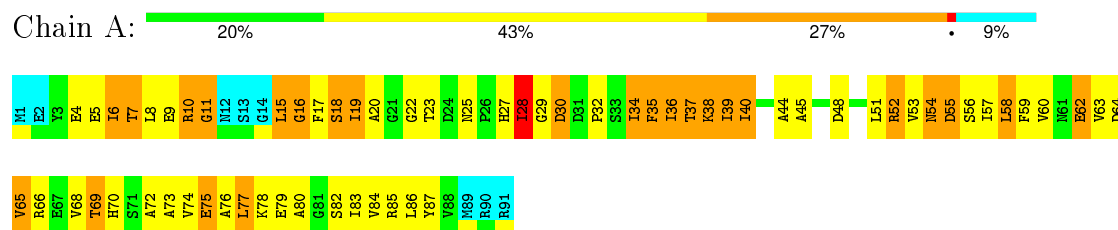
- Molecule 1: PSD-95

Chain A: 19% 49% 21% 9%



#### 4.2.10 Score per residue for model 10

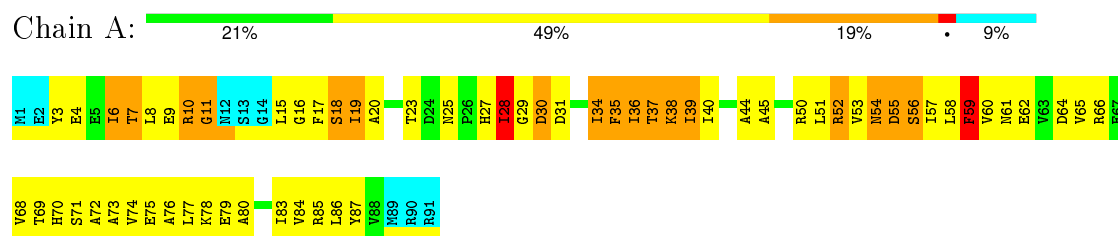
- Molecule 1: PSD-95





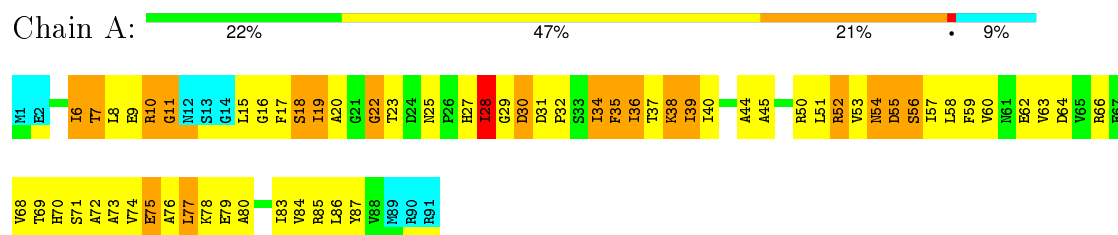
#### 4.2.14 Score per residue for model 14

- Molecule 1: PSD-95



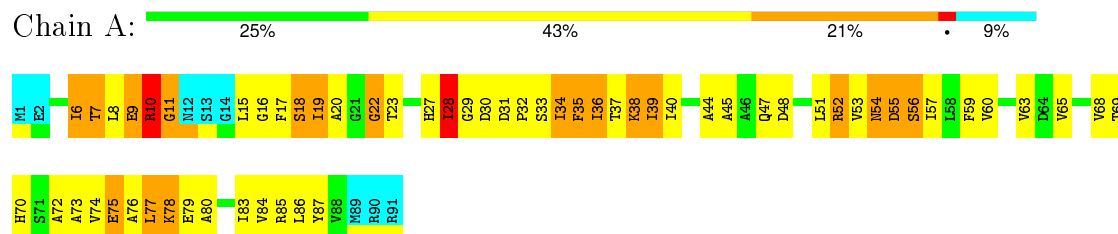
#### 4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: PSD-95



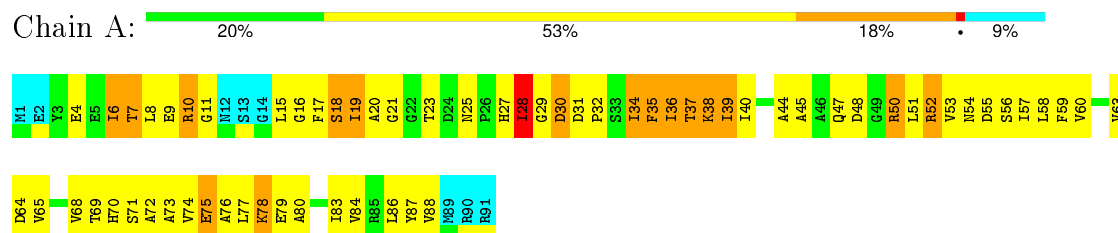
#### 4.2.16 Score per residue for model 16

- Molecule 1: PSD-95



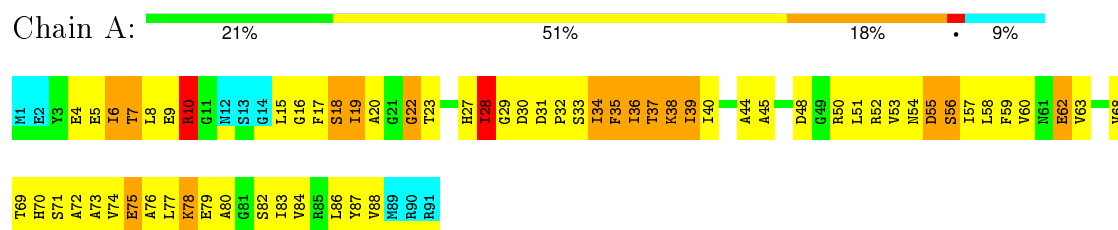
#### 4.2.17 Score per residue for model 17

- Molecule 1: PSD-95



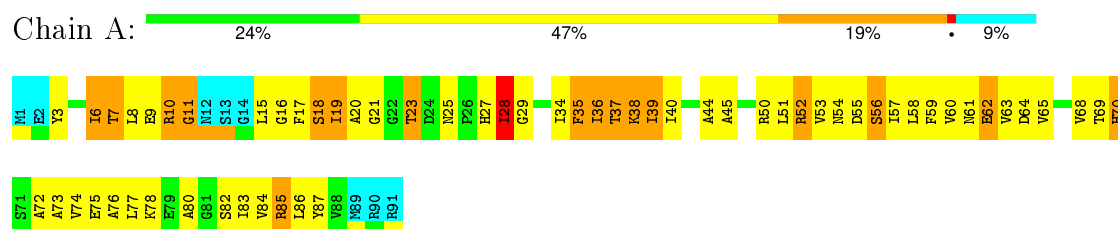
## 4.2.18 Score per residue for model 18

- Molecule 1: PSD-95



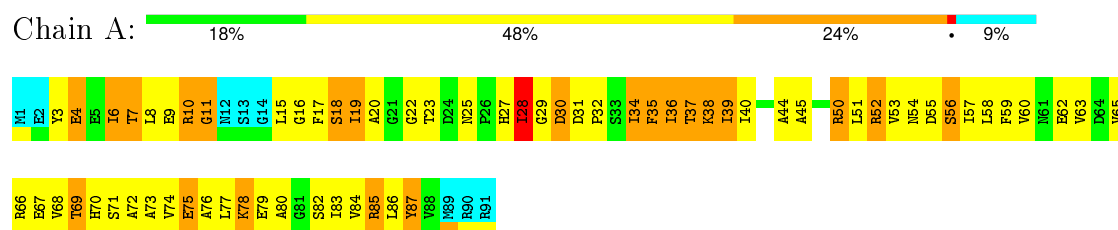
## 4.2.19 Score per residue for model 19

- Molecule 1: PSD-95



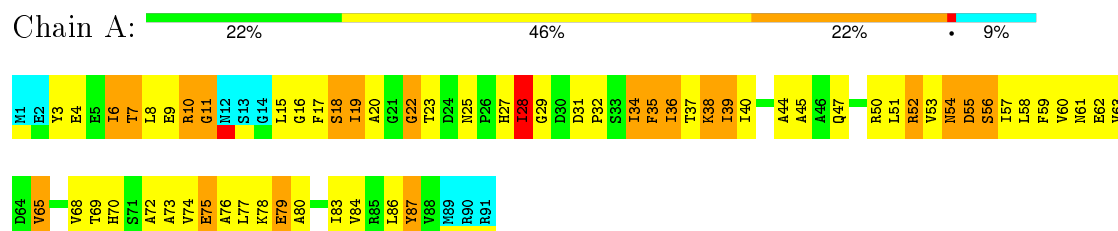
## 4.2.20 Score per residue for model 20

- Molecule 1: PSD-95



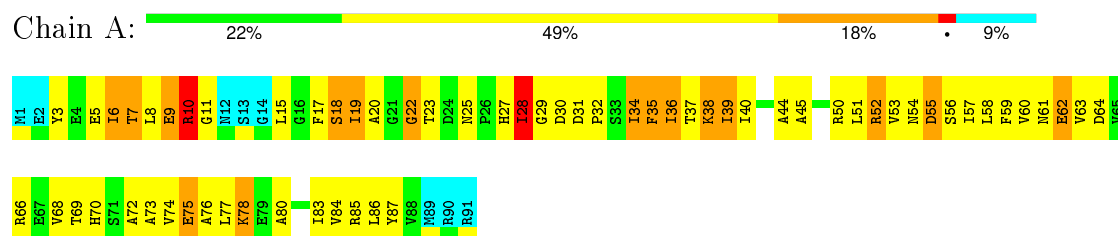
## 4.2.21 Score per residue for model 21

- Molecule 1: PSD-95



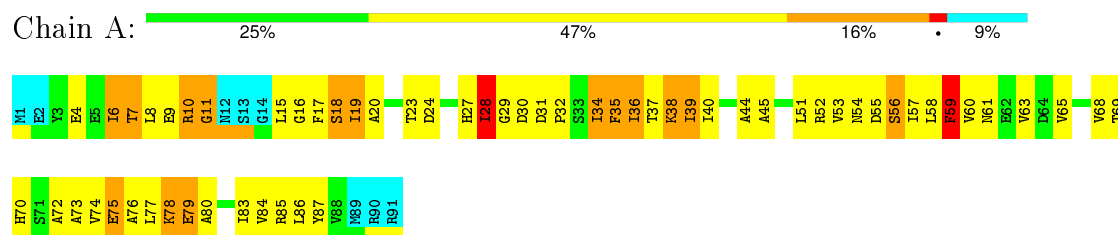
### 4.2.22 Score per residue for model 22

- Molecule 1: PSD-95



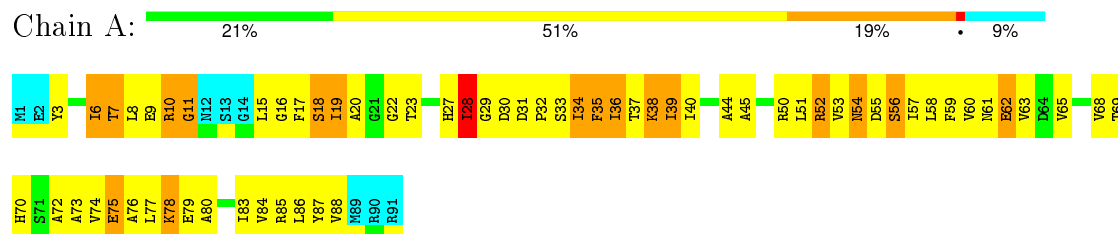
### 4.2.23 Score per residue for model 23

- Molecule 1: PSD-95



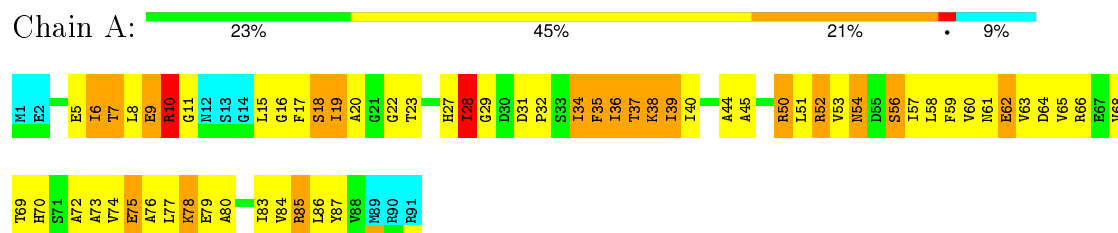
### 4.2.24 Score per residue for model 24

- Molecule 1: PSD-95



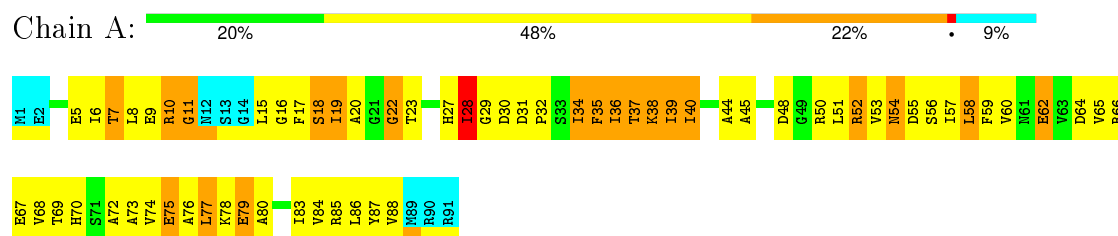
### 4.2.25 Score per residue for model 25

- Molecule 1: PSD-95



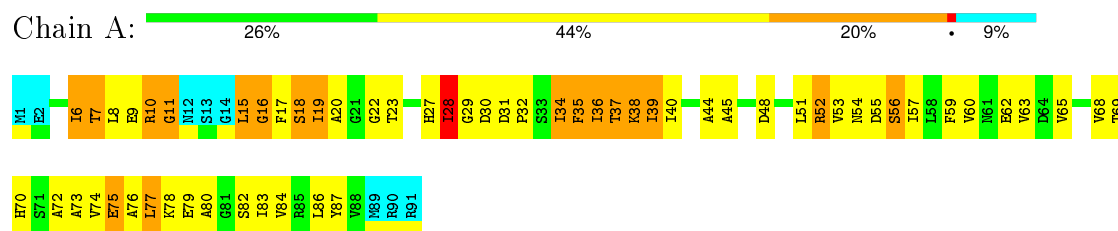
### 4.2.26 Score per residue for model 26

- Molecule 1: PSD-95



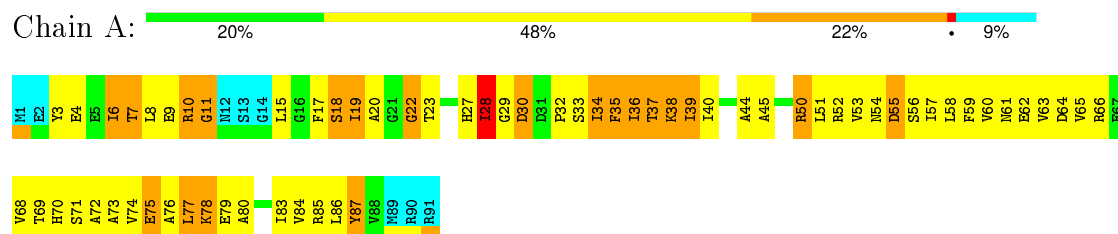
### 4.2.27 Score per residue for model 27

- Molecule 1: PSD-95



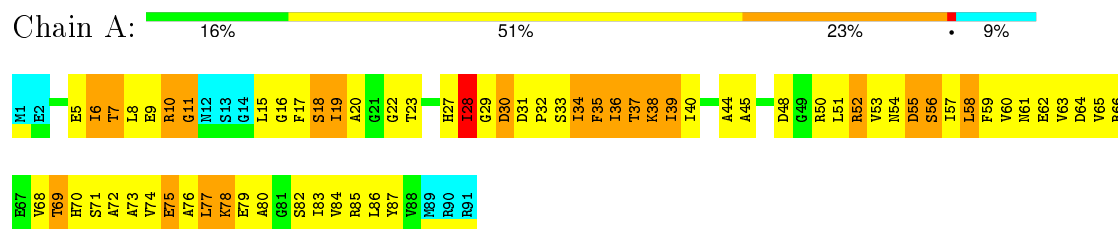
### 4.2.28 Score per residue for model 28

- Molecule 1: PSD-95



### 4.2.29 Score per residue for model 29

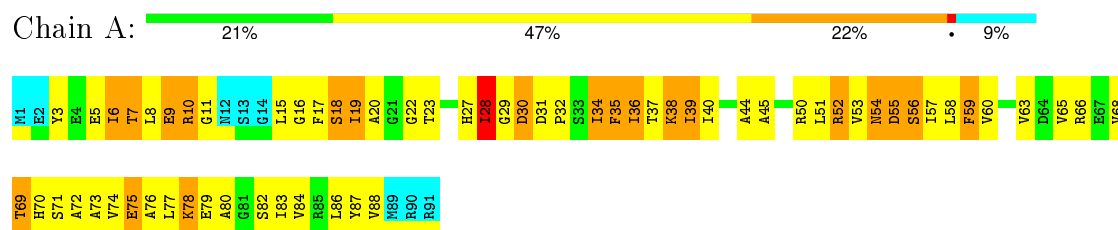
- Molecule 1: PSD-95





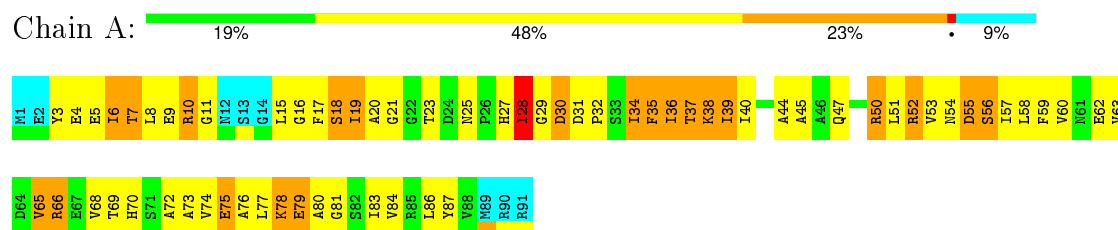
### 4.2.34 Score per residue for model 34

- Molecule 1: PSD-95



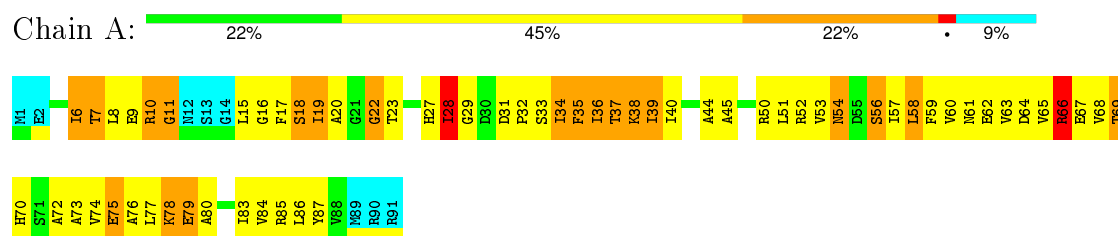
### 4.2.38 Score per residue for model 38

- Molecule 1: PSD-95



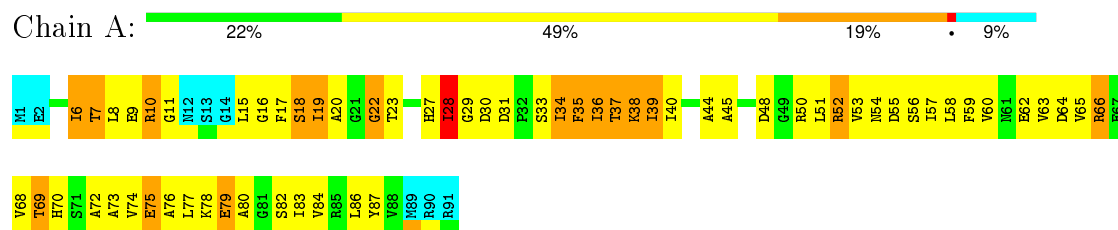
### 4.2.39 Score per residue for model 39

- Molecule 1: PSD-95



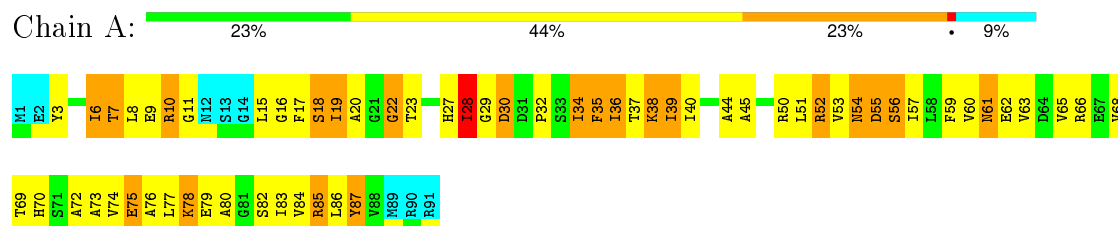
### 4.2.40 Score per residue for model 40

- Molecule 1: PSD-95



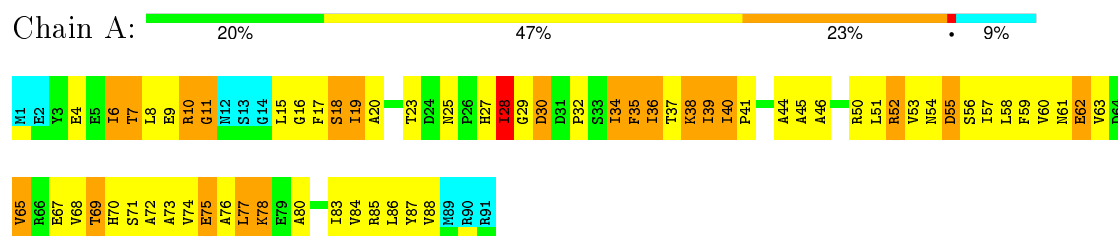
### 4.2.41 Score per residue for model 41

- Molecule 1: PSD-95



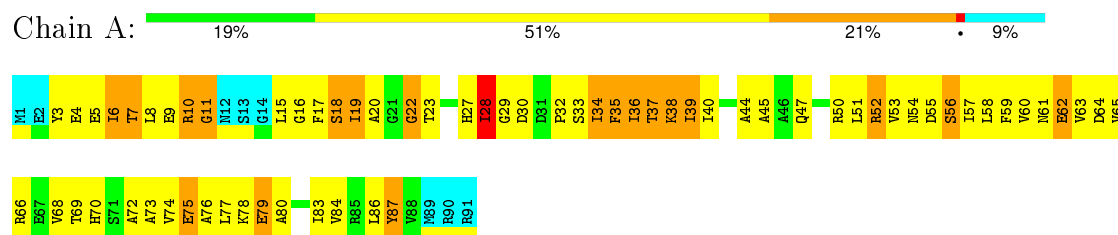
## 4.2.42 Score per residue for model 42

- Molecule 1: PSD-95



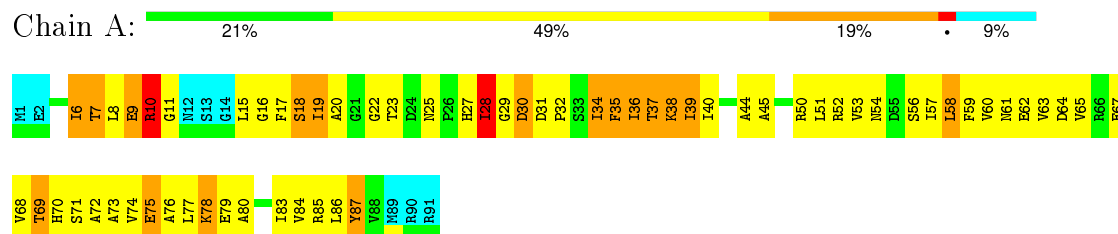
## 4.2.43 Score per residue for model 43

- Molecule 1: PSD-95



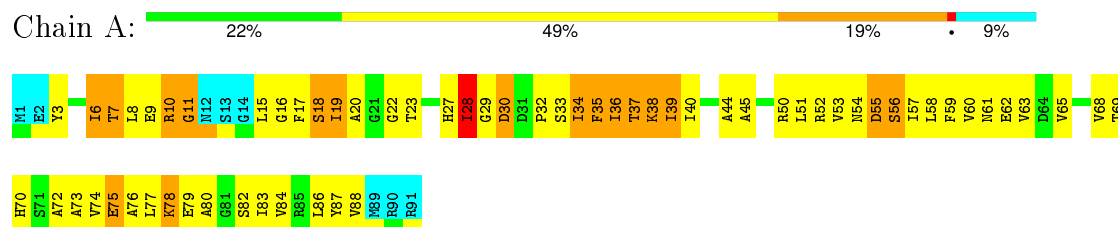
## 4.2.44 Score per residue for model 44

- Molecule 1: PSD-95



## 4.2.45 Score per residue for model 45

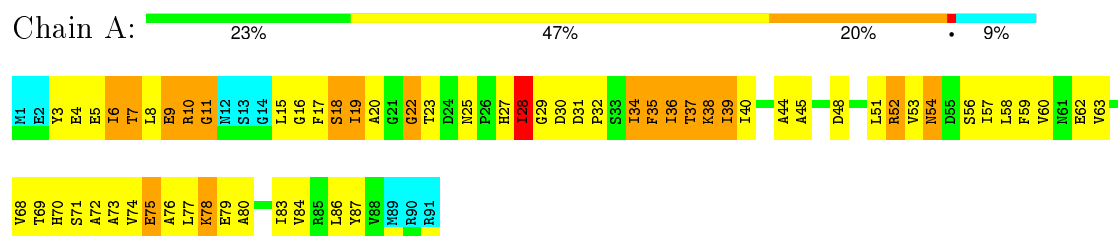
- Molecule 1: PSD-95





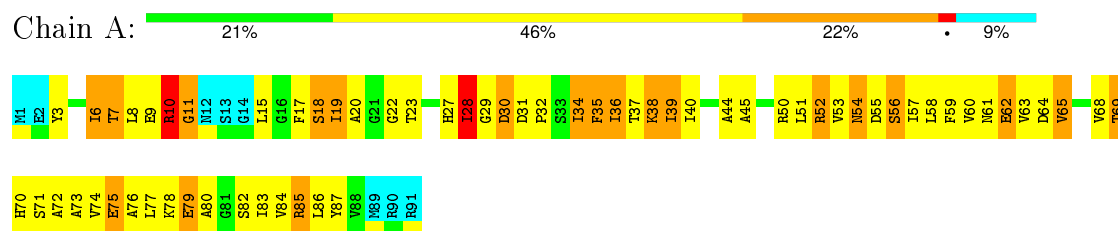
## 4.2.46 Score per residue for model 46

- Molecule 1: PSD-95



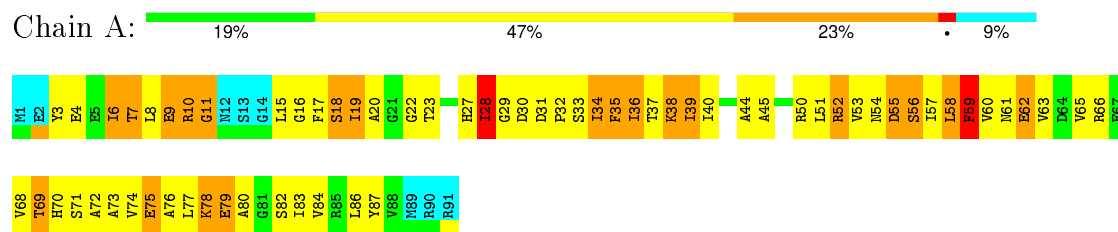
## 4.2.47 Score per residue for model 47

- Molecule 1: PSD-95



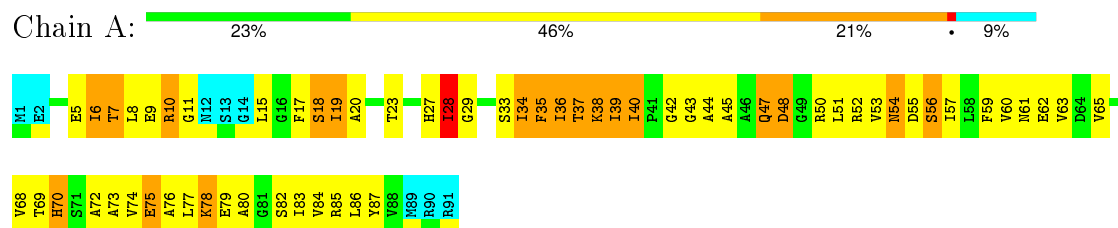
## 4.2.48 Score per residue for model 48

- Molecule 1: PSD-95



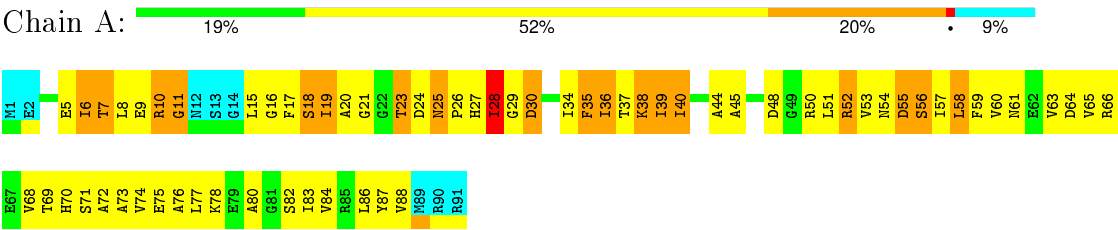
## 4.2.49 Score per residue for model 49

- Molecule 1: PSD-95



4.2.50 Score per residue for model 50

● Molecule 1: PSD-95



## 5 Refinement protocol and experimental data overview ⓘ

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

Of the 200 calculated structures, 50 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

No chemical shift data was provided. 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	622	620	110±5
All	All	31250	31100	31000	5476

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 88.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:ILE:HG21	1:A:57:ILE:HD11	1.10	1.24	29	50
1:A:36:ILE:HD12	1:A:51:LEU:HD21	1.09	1.25	39	50
1:A:57:ILE:HG22	1:A:65:VAL:HG21	1.06	1.22	19	12
1:A:6:ILE:HD11	1:A:8:LEU:HD13	1.03	1.26	17	47
1:A:60:VAL:HG11	1:A:76:ALA:HB1	1.01	1.24	1	42
1:A:19:ILE:HD12	1:A:77:LEU:HD11	0.96	1.37	41	40
1:A:39:ILE:HD11	1:A:51:LEU:HD23	0.93	1.40	32	49
1:A:28:ILE:HD12	1:A:35:PHE:CZ	0.89	2.03	14	50
1:A:8:LEU:HD23	1:A:15:LEU:HB3	0.88	1.45	43	19
1:A:80:ALA:HB1	1:A:84:VAL:CB	0.87	1.99	17	50
1:A:39:ILE:CD1	1:A:51:LEU:HD23	0.86	2.00	43	50
1:A:34:ILE:HD11	1:A:68:VAL:O	0.86	1.69	19	2
1:A:8:LEU:HD23	1:A:15:LEU:HG	0.84	1.49	37	31
1:A:36:ILE:CD1	1:A:51:LEU:HD21	0.84	2.02	44	50

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:ILE:HD12	1:A:77:LEU:HD12	0.83	1.50	25	8
1:A:70:HIS:O	1:A:74:VAL:HG23	0.83	1.72	29	50
1:A:60:VAL:HG13	1:A:86:LEU:CD2	0.83	2.02	29	46
1:A:60:VAL:HG11	1:A:76:ALA:CB	0.82	2.03	1	25
1:A:34:ILE:HG21	1:A:73:ALA:CB	0.82	2.04	50	50
1:A:3:TYR:CD2	1:A:58:LEU:HD13	0.81	2.09	8	10
1:A:60:VAL:HG23	1:A:86:LEU:CD2	0.81	2.05	34	3
1:A:57:ILE:CG2	1:A:65:VAL:HG21	0.80	2.06	19	2
1:A:7:THR:HG22	1:A:83:ILE:HG13	0.80	1.52	26	49
1:A:27:HIS:CD2	1:A:35:PHE:CZ	0.80	2.70	50	50
1:A:8:LEU:HD21	1:A:45:ALA:CA	0.79	2.08	22	49
1:A:8:LEU:HD23	1:A:15:LEU:CB	0.79	2.07	10	7
1:A:34:ILE:CD1	1:A:73:ALA:HB2	0.79	2.08	30	49
1:A:61:ASN:OD1	1:A:84:VAL:HG23	0.78	1.77	43	13
1:A:34:ILE:HD12	1:A:73:ALA:HB2	0.78	1.55	14	48
1:A:7:THR:HG22	1:A:83:ILE:CD1	0.78	2.08	13	11
1:A:19:ILE:HD12	1:A:77:LEU:CD1	0.78	2.09	12	48
1:A:15:LEU:O	1:A:44:ALA:HB3	0.78	1.79	50	50
1:A:80:ALA:HB1	1:A:84:VAL:HB	0.78	1.56	46	50
1:A:15:LEU:HD23	1:A:17:PHE:CE2	0.77	2.14	17	23
1:A:57:ILE:HG22	1:A:65:VAL:CG2	0.77	2.10	50	3
1:A:80:ALA:CB	1:A:84:VAL:HG11	0.76	2.10	41	50
1:A:80:ALA:HB1	1:A:84:VAL:CG1	0.76	2.11	41	50
1:A:60:VAL:HG13	1:A:86:LEU:HD21	0.76	1.57	50	37
1:A:6:ILE:HG23	1:A:50:ARG:HB3	0.76	1.56	37	3
1:A:6:ILE:HG23	1:A:50:ARG:CB	0.75	2.11	26	3
1:A:60:VAL:HG21	1:A:76:ALA:HB1	0.75	1.59	50	15
1:A:19:ILE:HD11	1:A:74:VAL:HG22	0.75	1.59	42	2
1:A:3:TYR:CD1	1:A:58:LEU:HD22	0.75	2.17	48	2
1:A:6:ILE:CD1	1:A:8:LEU:HD13	0.74	2.12	40	47
1:A:60:VAL:CG1	1:A:76:ALA:HB1	0.74	2.09	1	31
1:A:77:LEU:HD23	1:A:86:LEU:CD1	0.74	2.11	27	2
1:A:60:VAL:HG21	1:A:76:ALA:CB	0.74	2.12	18	22
1:A:23:THR:HG22	1:A:32:PRO:CB	0.74	2.13	45	24
1:A:8:LEU:HD21	1:A:45:ALA:HB2	0.73	1.60	20	38
1:A:28:ILE:HD12	1:A:35:PHE:CE2	0.73	2.19	50	50
1:A:8:LEU:HD21	1:A:45:ALA:CB	0.73	2.13	49	48
1:A:19:ILE:CG2	1:A:57:ILE:HD11	0.73	2.11	29	17
1:A:9:GLU:CG	1:A:83:ILE:HD13	0.72	2.14	37	1
1:A:19:ILE:CD1	1:A:77:LEU:HD11	0.72	2.14	33	4
1:A:60:VAL:HG13	1:A:86:LEU:HD22	0.72	1.62	11	35

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:ILE:CD1	1:A:51:LEU:HD13	0.72	2.15	37	3
1:A:19:ILE:HG21	1:A:57:ILE:CD1	0.72	2.14	34	43
1:A:61:ASN:CG	1:A:84:VAL:HG23	0.72	2.05	42	5
1:A:6:ILE:HD13	1:A:51:LEU:HD13	0.71	1.63	26	3
1:A:19:ILE:HD13	1:A:19:ILE:H	0.71	1.46	42	24
1:A:8:LEU:HD21	1:A:45:ALA:HA	0.71	1.62	35	47
1:A:7:THR:HG23	1:A:85:ARG:HG3	0.71	1.63	25	15
1:A:23:THR:HG22	1:A:32:PRO:HB2	0.70	1.63	24	12
1:A:77:LEU:HD22	1:A:86:LEU:HD13	0.70	1.64	29	11
1:A:77:LEU:HD22	1:A:86:LEU:CD1	0.70	2.17	44	15
1:A:80:ALA:HB1	1:A:84:VAL:CG2	0.70	2.16	27	42
1:A:8:LEU:HD11	1:A:45:ALA:HA	0.69	1.64	34	32
1:A:75:GLU:O	1:A:79:GLU:CG	0.69	2.39	45	23
1:A:17:PHE:CZ	1:A:77:LEU:HD13	0.69	2.22	44	18
1:A:80:ALA:HB1	1:A:84:VAL:HG21	0.69	1.62	27	35
1:A:43:GLY:O	1:A:47:GLN:HB2	0.69	1.87	49	1
1:A:23:THR:HG23	1:A:68:VAL:C	0.69	2.08	17	48
1:A:27:HIS:CD2	1:A:35:PHE:CE2	0.68	2.81	50	50
1:A:23:THR:OG1	1:A:69:THR:HA	0.68	1.89	19	16
1:A:23:THR:HG23	1:A:68:VAL:O	0.68	1.89	22	50
1:A:7:THR:HG23	1:A:85:ARG:HG2	0.68	1.64	44	7
1:A:19:ILE:H	1:A:19:ILE:HD13	0.68	1.49	27	25
1:A:80:ALA:HB1	1:A:84:VAL:HG11	0.68	1.66	41	41
1:A:61:ASN:ND2	1:A:84:VAL:HG23	0.67	2.05	25	5
1:A:23:THR:HG22	1:A:32:PRO:HB3	0.67	1.66	28	30
1:A:55:ASP:OD2	1:A:88:VAL:HG21	0.66	1.90	45	6
1:A:58:LEU:HD23	1:A:88:VAL:C	0.66	2.10	32	3
1:A:3:TYR:CE2	1:A:58:LEU:HD22	0.66	2.25	20	3
1:A:60:VAL:HG23	1:A:86:LEU:HD22	0.66	1.66	34	3
1:A:58:LEU:HD11	1:A:88:VAL:O	0.66	1.91	9	1
1:A:34:ILE:HG21	1:A:73:ALA:HB1	0.66	1.66	50	44
1:A:21:GLY:HA2	1:A:34:ILE:HG23	0.66	1.67	19	2
1:A:34:ILE:HD13	1:A:73:ALA:HB2	0.65	1.67	50	40
1:A:9:GLU:N	1:A:83:ILE:HD12	0.65	2.07	18	18
1:A:17:PHE:HB3	1:A:39:ILE:HG23	0.64	1.69	49	50
1:A:73:ALA:O	1:A:77:LEU:HD12	0.64	1.92	38	2
1:A:74:VAL:HA	1:A:77:LEU:HD12	0.64	1.68	27	2
1:A:3:TYR:CE2	1:A:58:LEU:HD13	0.63	2.28	24	5
1:A:83:ILE:HG23	1:A:83:ILE:O	0.63	1.93	18	16
1:A:77:LEU:N	1:A:77:LEU:HD23	0.63	2.07	50	21
1:A:60:VAL:CB	1:A:76:ALA:HB1	0.63	2.23	38	27

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:PHE:CZ	1:A:77:LEU:HD22	0.63	2.28	42	2
1:A:28:ILE:HG23	1:A:29:GLY:N	0.63	2.09	19	50
1:A:7:THR:HG22	1:A:83:ILE:HD11	0.62	1.72	13	10
1:A:28:ILE:HB	1:A:35:PHE:CE1	0.62	2.28	21	50
1:A:77:LEU:HD23	1:A:77:LEU:N	0.62	2.09	12	19
1:A:60:VAL:HG23	1:A:86:LEU:HD21	0.61	1.71	1	3
1:A:28:ILE:CD1	1:A:35:PHE:CZ	0.61	2.83	43	50
1:A:9:GLU:O	1:A:44:ALA:HB2	0.61	1.95	47	42
1:A:8:LEU:HD11	1:A:44:ALA:O	0.61	1.95	19	16
1:A:8:LEU:C	1:A:83:ILE:HD12	0.61	2.16	23	38
1:A:34:ILE:HG22	1:A:57:ILE:HD12	0.61	1.73	19	2
1:A:74:VAL:O	1:A:78:LYS:HG2	0.60	1.95	17	42
1:A:26:PRO:O	1:A:28:ILE:N	0.60	2.32	12	1
1:A:17:PHE:CE1	1:A:77:LEU:HD13	0.60	2.30	25	38
1:A:15:LEU:CD1	1:A:86:LEU:HD11	0.60	2.27	23	10
1:A:7:THR:HG23	1:A:83:ILE:HD11	0.60	1.73	18	1
1:A:57:ILE:HA	1:A:88:VAL:HG12	0.60	1.73	4	8
1:A:9:GLU:HG2	1:A:83:ILE:HD13	0.60	1.72	37	1
1:A:19:ILE:HA	1:A:36:ILE:HA	0.59	1.75	27	50
1:A:8:LEU:HD12	1:A:48:ASP:OD2	0.58	1.98	7	5
1:A:83:ILE:O	1:A:83:ILE:HG23	0.58	1.99	49	30
1:A:60:VAL:CG2	1:A:76:ALA:HB1	0.58	2.29	50	9
1:A:17:PHE:CE1	1:A:36:ILE:HD13	0.58	2.34	50	49
1:A:7:THR:HG22	1:A:83:ILE:CG1	0.58	2.29	45	33
1:A:65:VAL:O	1:A:65:VAL:HG23	0.57	1.98	10	9
1:A:58:LEU:C	1:A:65:VAL:HG22	0.57	2.19	19	2
1:A:3:TYR:HD2	1:A:58:LEU:HD13	0.57	1.58	9	2
1:A:63:VAL:HG12	1:A:65:VAL:H	0.57	1.59	39	2
1:A:72:ALA:O	1:A:75:GLU:HG2	0.57	2.00	14	21
1:A:6:ILE:HG21	1:A:51:LEU:HD13	0.57	1.77	4	28
1:A:15:LEU:CD2	1:A:86:LEU:HD11	0.57	2.30	49	9
1:A:51:LEU:HG	1:A:52:ARG:N	0.56	2.15	37	50
1:A:78:LYS:CD	1:A:79:GLU:HG2	0.56	2.29	45	3
1:A:20:ALA:HB1	1:A:27:HIS:HB2	0.56	1.77	50	38
1:A:58:LEU:HD12	1:A:87:TYR:HB3	0.56	1.76	9	1
1:A:35:PHE:N	1:A:35:PHE:CD1	0.56	2.74	19	28
1:A:8:LEU:O	1:A:83:ILE:HA	0.56	2.00	26	50
1:A:77:LEU:HD23	1:A:86:LEU:HD11	0.56	1.75	27	1
1:A:10:ARG:CG	1:A:15:LEU:HD23	0.56	2.31	26	18
1:A:61:ASN:HD22	1:A:84:VAL:HG23	0.56	1.60	5	3
1:A:65:VAL:HG12	1:A:68:VAL:HG21	0.55	1.78	37	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:ILE:O	1:A:6:ILE:HG23	0.55	2.02	11	30
1:A:18:SER:O	1:A:36:ILE:HG22	0.55	2.02	27	49
1:A:34:ILE:CG2	1:A:57:ILE:HD12	0.55	2.32	50	2
1:A:77:LEU:HD23	1:A:86:LEU:HD13	0.55	1.78	42	2
1:A:6:ILE:HG23	1:A:6:ILE:O	0.54	2.02	24	17
1:A:65:VAL:HG23	1:A:65:VAL:O	0.54	2.02	30	7
1:A:19:ILE:HD13	1:A:19:ILE:N	0.54	2.17	25	28
1:A:9:GLU:HG3	1:A:83:ILE:HD13	0.54	1.79	37	1
1:A:8:LEU:CD2	1:A:15:LEU:HB3	0.54	2.28	10	4
1:A:59:PHE:HA	1:A:63:VAL:O	0.54	2.03	8	34
1:A:55:ASP:HB3	1:A:88:VAL:HG11	0.54	1.80	45	2
1:A:75:GLU:O	1:A:79:GLU:CB	0.54	2.56	24	8
1:A:16:GLY:O	1:A:45:ALA:HB3	0.54	2.03	27	10
1:A:34:ILE:O	1:A:57:ILE:N	0.54	2.40	33	50
1:A:80:ALA:CB	1:A:84:VAL:CG1	0.54	2.86	18	48
1:A:75:GLU:HA	1:A:78:LYS:CG	0.53	2.33	23	8
1:A:19:ILE:N	1:A:19:ILE:HD13	0.53	2.18	39	17
1:A:39:ILE:CG2	1:A:45:ALA:HB3	0.53	2.33	44	5
1:A:74:VAL:O	1:A:78:LYS:CG	0.53	2.56	25	10
1:A:35:PHE:CD1	1:A:35:PHE:N	0.53	2.77	50	22
1:A:73:ALA:O	1:A:76:ALA:HB3	0.53	2.04	33	41
1:A:25:ASN:O	1:A:27:HIS:N	0.53	2.42	33	11
1:A:38:LYS:HA	1:A:53:VAL:CG2	0.53	2.34	30	50
1:A:16:GLY:O	1:A:39:ILE:HG23	0.53	2.04	33	40
1:A:9:GLU:O	1:A:44:ALA:CB	0.53	2.56	40	33
1:A:75:GLU:O	1:A:79:GLU:HB3	0.53	2.03	24	5
1:A:6:ILE:C	1:A:6:ILE:HD13	0.52	2.25	22	14
1:A:38:LYS:HA	1:A:53:VAL:HG21	0.52	1.79	32	50
1:A:8:LEU:HB3	1:A:15:LEU:HD11	0.52	1.81	44	5
1:A:60:VAL:HG13	1:A:63:VAL:HB	0.52	1.80	34	2
1:A:15:LEU:HD23	1:A:17:PHE:CZ	0.52	2.40	42	3
1:A:6:ILE:HD13	1:A:6:ILE:C	0.52	2.25	28	16
1:A:21:GLY:O	1:A:25:ASN:O	0.52	2.28	17	5
1:A:20:ALA:HB2	1:A:37:THR:HG21	0.51	1.83	35	11
1:A:15:LEU:HD11	1:A:86:LEU:HD11	0.51	1.82	23	4
1:A:58:LEU:HD23	1:A:87:TYR:C	0.51	2.26	3	2
1:A:20:ALA:CB	1:A:27:HIS:CG	0.51	2.94	1	12
1:A:72:ALA:HA	1:A:75:GLU:HG2	0.51	1.83	35	41
1:A:19:ILE:HG22	1:A:36:ILE:HG23	0.51	1.81	27	1
1:A:7:THR:HG23	1:A:85:ARG:CG	0.51	2.36	10	11
1:A:39:ILE:HD11	1:A:51:LEU:CD2	0.51	2.36	26	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ALA:O	1:A:35:PHE:O	0.51	2.29	12	37
1:A:74:VAL:O	1:A:78:LYS:HG3	0.51	2.05	45	8
1:A:72:ALA:O	1:A:75:GLU:CG	0.50	2.59	39	34
1:A:75:GLU:O	1:A:79:GLU:HG2	0.50	2.05	45	1
1:A:17:PHE:CD2	1:A:51:LEU:HD22	0.50	2.42	8	10
1:A:17:PHE:CE2	1:A:51:LEU:HD22	0.49	2.42	8	11
1:A:15:LEU:O	1:A:45:ALA:N	0.49	2.44	22	4
1:A:19:ILE:CG2	1:A:36:ILE:HD13	0.49	2.37	50	7
1:A:70:HIS:CD2	1:A:74:VAL:HG23	0.49	2.42	33	24
1:A:80:ALA:CB	1:A:84:VAL:HG21	0.49	2.37	6	9
1:A:7:THR:CG2	1:A:83:ILE:HD11	0.49	2.37	13	6
1:A:3:TYR:CD1	1:A:58:LEU:HD11	0.49	2.42	43	4
1:A:60:VAL:HG13	1:A:60:VAL:O	0.49	2.08	13	2
1:A:19:ILE:HD11	1:A:77:LEU:CD1	0.49	2.37	17	1
1:A:34:ILE:O	1:A:56:SER:HA	0.49	2.08	14	43
1:A:70:HIS:CD2	1:A:74:VAL:CG2	0.49	2.96	50	20
1:A:53:VAL:CG1	1:A:54:ASN:N	0.49	2.75	42	50
1:A:56:SER:O	1:A:58:LEU:HD22	0.49	2.06	32	1
1:A:17:PHE:CE1	1:A:77:LEU:CD1	0.49	2.95	50	28
1:A:17:PHE:O	1:A:17:PHE:CD1	0.49	2.65	42	21
1:A:17:PHE:HZ	1:A:86:LEU:HD12	0.49	1.68	7	37
1:A:35:PHE:HA	1:A:56:SER:HA	0.49	1.84	15	48
1:A:68:VAL:HB	1:A:72:ALA:CB	0.49	2.38	39	6
1:A:3:TYR:CZ	1:A:58:LEU:HD22	0.49	2.43	8	1
1:A:21:GLY:HA2	1:A:34:ILE:CG2	0.49	2.38	19	2
1:A:3:TYR:CD2	1:A:58:LEU:HD22	0.49	2.43	14	1
1:A:15:LEU:HA	1:A:44:ALA:HB3	0.48	1.85	44	4
1:A:61:ASN:HB2	1:A:84:VAL:HG23	0.48	1.84	44	1
1:A:15:LEU:HD12	1:A:17:PHE:CE2	0.48	2.43	27	3
1:A:27:HIS:CD2	1:A:35:PHE:CE1	0.48	3.01	49	22
1:A:10:ARG:HG3	1:A:15:LEU:HD23	0.48	1.85	23	5
1:A:9:GLU:O	1:A:11:GLY:N	0.48	2.47	28	43
1:A:15:LEU:HD21	1:A:86:LEU:HD11	0.48	1.84	42	5
1:A:10:ARG:O	1:A:10:ARG:CG	0.48	2.61	6	2
1:A:75:GLU:HG3	1:A:76:ALA:N	0.48	2.23	40	29
1:A:21:GLY:HA2	1:A:34:ILE:HA	0.48	1.84	50	2
1:A:20:ALA:HB3	1:A:27:HIS:CD2	0.48	2.42	19	4
1:A:55:ASP:CG	1:A:88:VAL:HG21	0.48	2.29	42	2
1:A:60:VAL:O	1:A:62:GLU:N	0.48	2.46	44	30
1:A:15:LEU:O	1:A:44:ALA:N	0.48	2.47	26	14
1:A:17:PHE:CD1	1:A:17:PHE:O	0.48	2.67	12	24

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:PHE:CE1	1:A:36:ILE:CD1	0.48	2.97	3	28
1:A:39:ILE:HG23	1:A:45:ALA:HB3	0.48	1.84	44	3
1:A:20:ALA:O	1:A:27:HIS:CD2	0.48	2.67	49	11
1:A:8:LEU:CD2	1:A:15:LEU:HG	0.48	2.39	34	1
1:A:28:ILE:HB	1:A:35:PHE:CZ	0.47	2.44	32	40
1:A:64:ASP:O	1:A:65:VAL:HG22	0.47	2.08	32	3
1:A:70:HIS:CD2	1:A:70:HIS:C	0.47	2.87	49	1
1:A:15:LEU:O	1:A:44:ALA:CB	0.47	2.62	26	10
1:A:10:ARG:HG2	1:A:15:LEU:HD23	0.47	1.87	26	2
1:A:19:ILE:HD11	1:A:74:VAL:HA	0.47	1.85	40	8
1:A:60:VAL:CG2	1:A:86:LEU:HD22	0.47	2.40	34	1
1:A:78:LYS:HD3	1:A:79:GLU:HG2	0.47	1.85	45	3
1:A:8:LEU:O	1:A:82:SER:O	0.47	2.33	34	13
1:A:3:TYR:CG	1:A:58:LEU:CD1	0.47	2.97	37	4
1:A:6:ILE:HD11	1:A:8:LEU:CD1	0.47	2.39	34	1
1:A:59:PHE:CE1	1:A:64:ASP:N	0.47	2.83	32	3
1:A:22:GLY:HA3	1:A:70:HIS:N	0.47	2.25	22	33
1:A:3:TYR:CD1	1:A:58:LEU:CD2	0.47	2.98	45	2
1:A:18:SER:O	1:A:36:ILE:CG2	0.47	2.62	42	50
1:A:65:VAL:HG23	1:A:66:ARG:N	0.47	2.25	38	1
1:A:83:ILE:CG2	1:A:83:ILE:O	0.47	2.63	18	1
1:A:53:VAL:HG12	1:A:54:ASN:N	0.46	2.25	19	50
1:A:60:VAL:O	1:A:63:VAL:HG23	0.46	2.10	35	13
1:A:10:ARG:CG	1:A:10:ARG:O	0.46	2.63	25	2
1:A:74:VAL:HA	1:A:77:LEU:CD1	0.46	2.40	17	2
1:A:3:TYR:CD1	1:A:58:LEU:CD1	0.46	2.98	46	4
1:A:63:VAL:HG21	1:A:79:GLU:OE2	0.46	2.11	38	1
1:A:77:LEU:CD2	1:A:86:LEU:CD1	0.46	2.94	42	1
1:A:3:TYR:CG	1:A:58:LEU:CD2	0.46	2.99	14	1
1:A:75:GLU:HA	1:A:78:LYS:HG2	0.46	1.87	28	40
1:A:59:PHE:CZ	1:A:64:ASP:HB3	0.46	2.46	44	18
1:A:34:ILE:HD11	1:A:68:VAL:HG23	0.46	1.88	4	6
1:A:6:ILE:HD13	1:A:51:LEU:CD1	0.46	2.39	26	2
1:A:74:VAL:O	1:A:78:LYS:HD3	0.46	2.11	33	17
1:A:28:ILE:CG2	1:A:29:GLY:N	0.46	2.79	31	10
1:A:3:TYR:CB	1:A:87:TYR:CE2	0.46	2.98	28	4
1:A:3:TYR:CD2	1:A:58:LEU:CD1	0.45	2.99	34	3
1:A:4:GLU:HG2	1:A:88:VAL:HG23	0.45	1.88	17	1
1:A:9:GLU:HA	1:A:83:ILE:HA	0.45	1.87	8	40
1:A:60:VAL:HG11	1:A:76:ALA:C	0.45	2.31	31	7
1:A:6:ILE:HG12	1:A:50:ARG:CB	0.45	2.42	42	38

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:TYR:CD2	1:A:58:LEU:CD2	0.45	2.99	14	1
1:A:20:ALA:HB3	1:A:27:HIS:CG	0.45	2.47	35	7
1:A:17:PHE:CE1	1:A:77:LEU:CD2	0.45	2.99	17	2
1:A:35:PHE:HA	1:A:55:ASP:O	0.45	2.12	49	37
1:A:77:LEU:N	1:A:77:LEU:CD2	0.45	2.80	11	8
1:A:60:VAL:HB	1:A:76:ALA:HB1	0.45	1.89	31	2
1:A:58:LEU:HD12	1:A:58:LEU:O	0.45	2.12	14	1
1:A:68:VAL:HB	1:A:72:ALA:HB3	0.44	1.88	37	8
1:A:40:ILE:O	1:A:42:GLY:N	0.44	2.50	49	1
1:A:75:GLU:O	1:A:79:GLU:N	0.44	2.50	20	15
1:A:58:LEU:O	1:A:59:PHE:CD2	0.44	2.71	7	8
1:A:77:LEU:CD2	1:A:77:LEU:N	0.44	2.79	12	7
1:A:6:ILE:HG23	1:A:50:ARG:HB2	0.44	1.90	6	2
1:A:57:ILE:CA	1:A:88:VAL:HG12	0.44	2.41	4	1
1:A:17:PHE:HA	1:A:39:ILE:HA	0.44	1.89	49	7
1:A:3:TYR:N	1:A:3:TYR:CD1	0.44	2.86	19	4
1:A:8:LEU:N	1:A:83:ILE:HD12	0.44	2.27	45	8
1:A:77:LEU:CD2	1:A:86:LEU:HD13	0.44	2.42	42	1
1:A:59:PHE:CD2	1:A:63:VAL:O	0.43	2.71	42	23
1:A:8:LEU:HB3	1:A:15:LEU:CD1	0.43	2.43	34	1
1:A:37:THR:C	1:A:53:VAL:HG13	0.43	2.33	19	22
1:A:58:LEU:O	1:A:59:PHE:CD1	0.43	2.71	24	2
1:A:3:TYR:CD1	1:A:3:TYR:N	0.43	2.85	22	1
1:A:36:ILE:HD12	1:A:51:LEU:CD2	0.43	2.22	13	2
1:A:21:GLY:HA2	1:A:27:HIS:HB3	0.43	1.90	12	1
1:A:3:TYR:CG	1:A:58:LEU:HD22	0.43	2.48	14	1
1:A:8:LEU:HD12	1:A:48:ASP:CG	0.43	2.34	49	1
1:A:17:PHE:CZ	1:A:77:LEU:CD2	0.43	3.00	27	1
1:A:10:ARG:HG3	1:A:15:LEU:CD2	0.43	2.44	45	3
1:A:58:LEU:HD23	1:A:88:VAL:CA	0.43	2.44	4	2
1:A:16:GLY:O	1:A:39:ILE:CG2	0.43	2.66	33	15
1:A:15:LEU:HD22	1:A:77:LEU:HB3	0.43	1.91	42	2
1:A:3:TYR:CG	1:A:58:LEU:HD13	0.43	2.49	28	1
1:A:19:ILE:HG22	1:A:36:ILE:HD13	0.43	1.91	27	2
1:A:21:GLY:HA3	1:A:70:HIS:HB2	0.42	1.89	50	1
1:A:39:ILE:HD13	1:A:51:LEU:HD23	0.42	1.88	6	5
1:A:7:THR:O	1:A:7:THR:CG2	0.42	2.67	18	1
1:A:8:LEU:HD23	1:A:15:LEU:CG	0.42	2.35	7	4
1:A:58:LEU:N	1:A:87:TYR:O	0.42	2.51	8	2
1:A:8:LEU:HD21	1:A:45:ALA:N	0.42	2.29	25	1
1:A:17:PHE:CE1	1:A:77:LEU:HD21	0.42	2.48	38	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:LEU:HG	1:A:87:TYR:HB3	0.42	1.92	4	3
1:A:23:THR:CG2	1:A:68:VAL:N	0.42	2.82	17	2
1:A:65:VAL:HG23	1:A:66:ARG:H	0.42	1.75	37	1
1:A:17:PHE:HD2	1:A:45:ALA:HB2	0.42	1.73	22	1
1:A:21:GLY:O	1:A:70:HIS:HA	0.42	2.15	1	2
1:A:58:LEU:HD23	1:A:87:TYR:O	0.42	2.14	3	1
1:A:19:ILE:CD1	1:A:77:LEU:HD12	0.42	2.36	25	2
1:A:8:LEU:N	1:A:83:ILE:CD1	0.42	2.83	14	6
1:A:17:PHE:CZ	1:A:86:LEU:HD12	0.42	2.49	8	8
1:A:17:PHE:N	1:A:40:ILE:HD11	0.42	2.30	33	7
1:A:65:VAL:CA	1:A:68:VAL:HG22	0.42	2.45	11	3
1:A:59:PHE:CZ	1:A:64:ASP:CB	0.42	3.03	32	1
1:A:71:SER:O	1:A:75:GLU:HB3	0.42	2.15	7	1
1:A:51:LEU:HD11	1:A:88:VAL:HG11	0.42	1.91	17	2
1:A:21:GLY:HA3	1:A:70:HIS:HA	0.42	1.92	19	1
1:A:35:PHE:HB3	1:A:56:SER:HA	0.42	1.92	19	1
1:A:28:ILE:CD1	1:A:35:PHE:CE2	0.41	3.00	27	5
1:A:69:THR:O	1:A:72:ALA:N	0.41	2.53	50	2
1:A:40:ILE:HD13	1:A:40:ILE:H	0.41	1.75	49	1
1:A:7:THR:HA	1:A:85:ARG:HA	0.41	1.91	4	1
1:A:10:ARG:CG	1:A:15:LEU:CD2	0.41	2.98	26	1
1:A:60:VAL:HG21	1:A:76:ALA:HB3	0.41	1.89	7	1
1:A:41:PRO:HA	1:A:46:ALA:CB	0.41	2.45	42	2
1:A:70:HIS:O	1:A:70:HIS:CD2	0.41	2.73	1	2
1:A:20:ALA:HB3	1:A:37:THR:CG2	0.41	2.44	27	1
1:A:70:HIS:CD2	1:A:70:HIS:O	0.41	2.74	3	6
1:A:10:ARG:O	1:A:11:GLY:O	0.41	2.39	10	1
1:A:21:GLY:O	1:A:70:HIS:HB3	0.41	2.15	31	1
1:A:65:VAL:O	1:A:65:VAL:CG2	0.41	2.68	10	1
1:A:56:SER:O	1:A:58:LEU:CD2	0.41	2.68	32	1
1:A:8:LEU:CD2	1:A:45:ALA:HB2	0.41	2.42	5	2
1:A:31:ASP:CB	1:A:32:PRO:CD	0.41	2.99	11	1
1:A:17:PHE:C	1:A:17:PHE:CD1	0.41	2.94	32	3
1:A:15:LEU:HD21	1:A:86:LEU:CD1	0.41	2.46	42	1
1:A:66:ARG:O	1:A:67:GLU:CG	0.41	2.68	39	1
1:A:53:VAL:O	1:A:54:ASN:HB2	0.41	2.15	29	3
1:A:8:LEU:HB3	1:A:15:LEU:HD22	0.41	1.93	23	1
1:A:21:GLY:O	1:A:70:HIS:HB2	0.41	2.14	17	3
1:A:19:ILE:HD11	1:A:77:LEU:HD11	0.41	1.93	17	1
1:A:59:PHE:CE1	1:A:64:ASP:OD1	0.41	2.74	17	4
1:A:36:ILE:O	1:A:54:ASN:HA	0.41	2.16	43	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:GLU:O	1:A:87:TYR:CD1	0.41	2.74	20	4
1:A:17:PHE:CD1	1:A:17:PHE:C	0.40	2.94	35	3
1:A:5:GLU:OE2	1:A:87:TYR:CE2	0.40	2.74	31	1
1:A:58:LEU:HD23	1:A:66:ARG:HD3	0.40	1.92	38	1
1:A:5:GLU:CG	1:A:87:TYR:CZ	0.40	3.05	31	1
1:A:51:LEU:CG	1:A:52:ARG:N	0.40	2.84	37	1
1:A:75:GLU:HA	1:A:78:LYS:HG3	0.40	1.93	29	1
1:A:59:PHE:CE2	1:A:64:ASP:OD1	0.40	2.74	7	1
1:A:15:LEU:C	1:A:44:ALA:HB3	0.40	2.37	25	1
1:A:19:ILE:CD1	1:A:77:LEU:CD1	0.40	2.95	50	1
1:A:61:ASN:CB	1:A:84:VAL:HG23	0.40	2.46	42	1
1:A:60:VAL:O	1:A:63:VAL:CG2	0.40	2.70	8	1
1:A:6:ILE:CG1	1:A:50:ARG:CB	0.40	3.00	44	1
1:A:39:ILE:CG2	1:A:45:ALA:CB	0.40	3.00	16	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	83/91 (91%)	66±2 (79±2%)	13±2 (15±2%)	4±1 (5±1%)	4	25
All	All	4150/4550 (91%)	3289 (79%)	641 (15%)	220 (5%)	4	25

All 12 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	10	ARG	50
1	A	28	ILE	50
1	A	30	ASP	37
1	A	11	GLY	32
1	A	65	VAL	21
1	A	22	GLY	18
1	A	59	PHE	3
1	A	66	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	16	GLY	2
1	A	81	GLY	2
1	A	27	HIS	1
1	A	26	PRO	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	66/73 (90%)	40±2 (61±3%)	26±2 (39±3%)	1	6
All	All	3300/3650 (90%)	2011 (61%)	1289 (39%)	1	6

All 47 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	40	ILE	50
1	A	28	ILE	50
1	A	37	THR	50
1	A	38	LYS	50
1	A	19	ILE	50
1	A	39	ILE	50
1	A	36	ILE	50
1	A	35	PHE	50
1	A	18	SER	50
1	A	7	THR	50
1	A	87	TYR	49
1	A	34	ILE	48
1	A	69	THR	48
1	A	6	ILE	47
1	A	75	GLU	43
1	A	52	ARG	40
1	A	10	ARG	37
1	A	56	SER	36
1	A	78	LYS	36
1	A	55	ASP	35
1	A	31	ASP	35

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Mol	Chain	Res	Type	Models (Total)
1	A	66	ARG	25
1	A	54	ASN	25
1	A	30	ASP	25
1	A	79	GLU	25
1	A	62	GLU	21
1	A	58	LEU	19
1	A	71	SER	19
1	A	33	SER	18
1	A	5	GLU	16
1	A	25	ASN	15
1	A	85	ARG	15
1	A	82	SER	13
1	A	9	GLU	13
1	A	4	GLU	13
1	A	77	LEU	12
1	A	48	ASP	11
1	A	47	GLN	10
1	A	59	PHE	9
1	A	50	ARG	8
1	A	61	ASN	6
1	A	67	GLU	5
1	A	24	ASP	3
1	A	83	ILE	3
1	A	70	HIS	2
1	A	15	LEU	2
1	A	23	THR	2

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.



## 7 Chemical shift validation

No chemical shift data were provided