



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:00 PM BST

PDB ID : 1BY1  
Title : DBL homology domain from beta-PIX  
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Deposited on : 1998-10-22

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

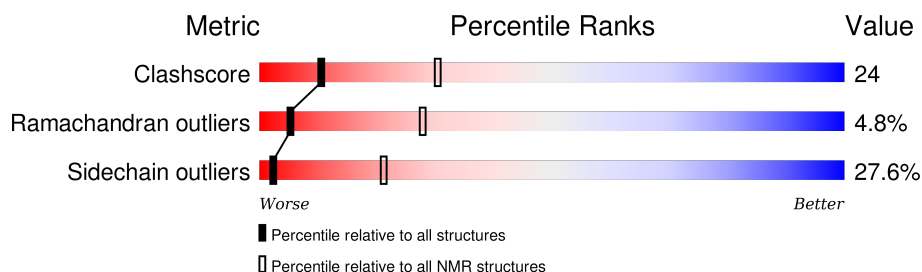
# 1 Overall quality at a glance

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	209	

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 4 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:13-A:43, A:49-A:164, A:175-A:192 (165)	0.65	4

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 5 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3361 atoms, of which 1688 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (PIX).

Mol	Chain	Residues	Atoms						Trace
1	A	209	Total	C	H	N	O	S	0
			3361	1051	1688	279	329	14	

There is a discrepancy between the modelled and reference sequences:

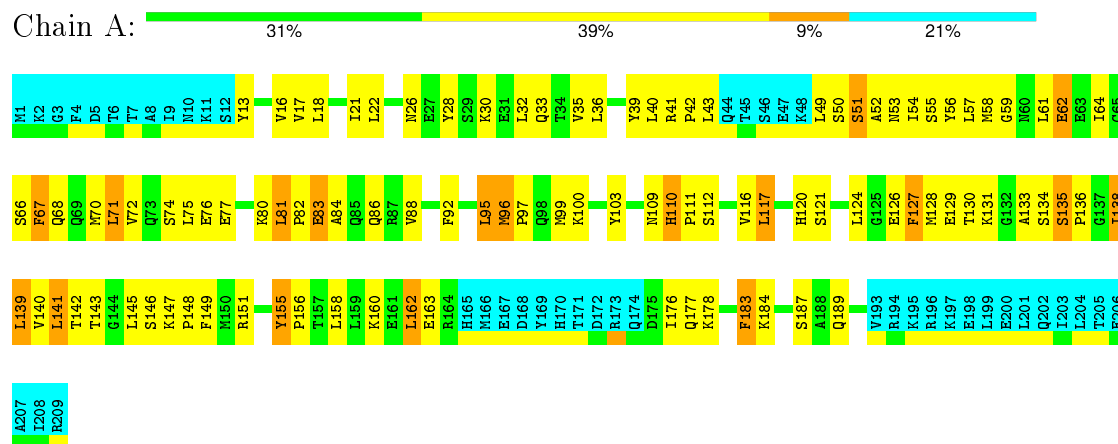
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	PRO	CLONING ARTIFACT	UNP Q14155

## 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 (PIX)

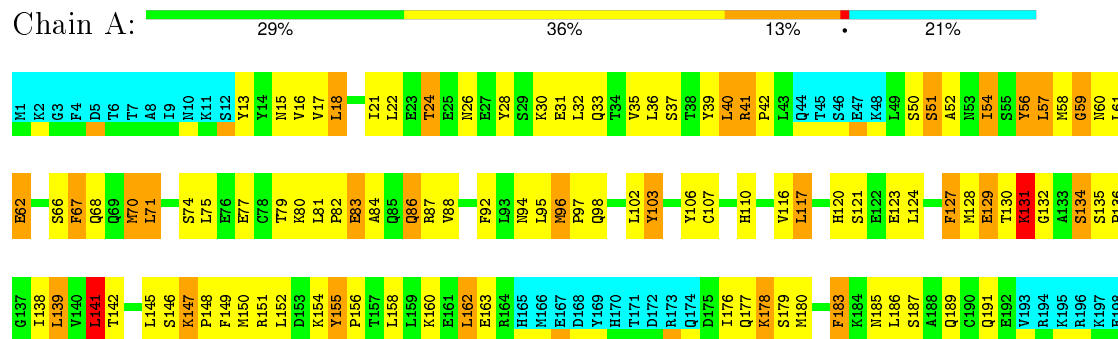


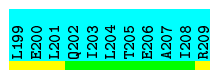
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

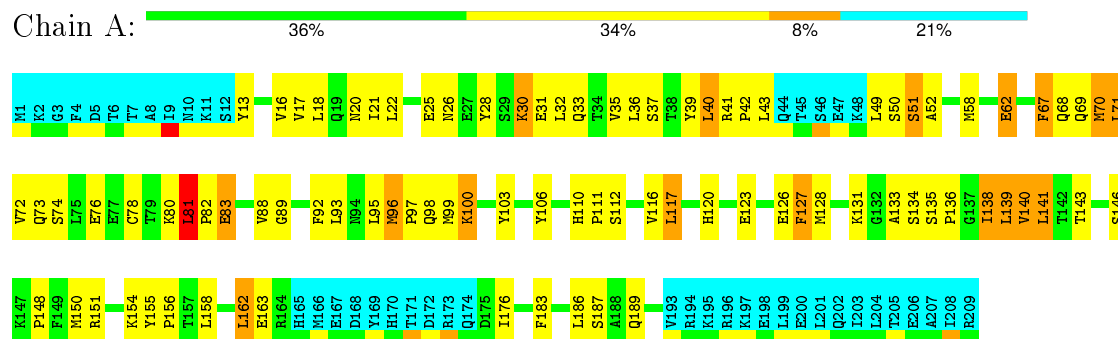
- Molecule 1: PROTEIN (PIX)





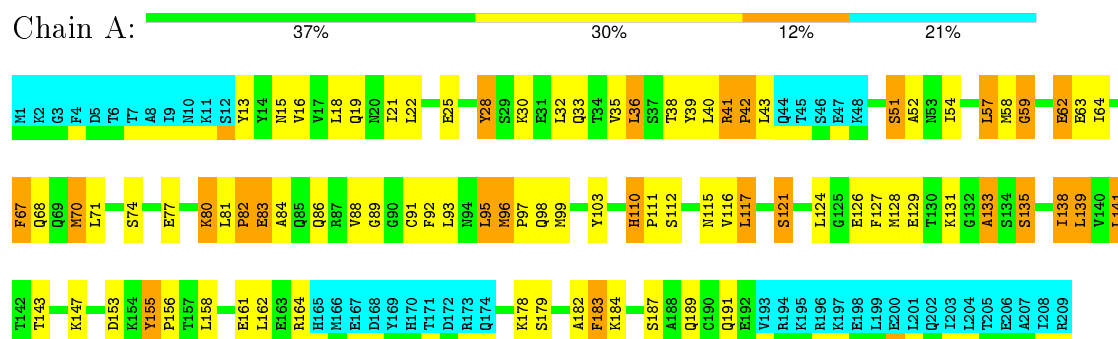
#### 4.2.2 Score per residue for model 2

- Molecule 1: PROTEIN (PIX)



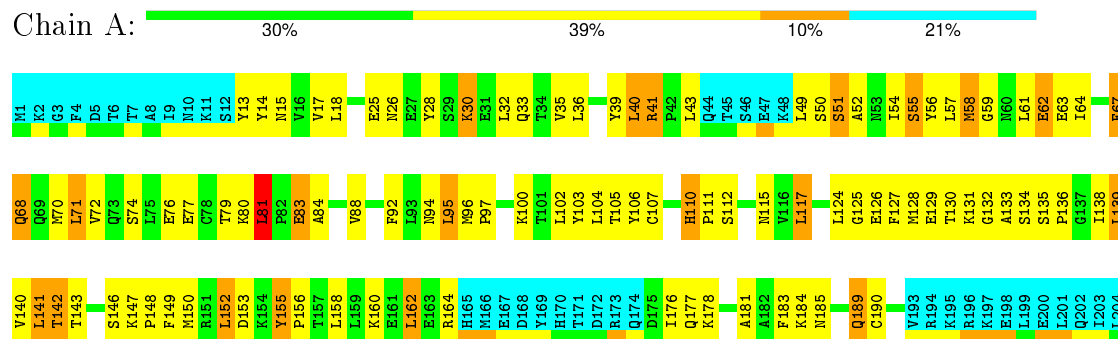
#### 4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (PIX)



#### 4.2.4 Score per residue for model 4 (medoid)

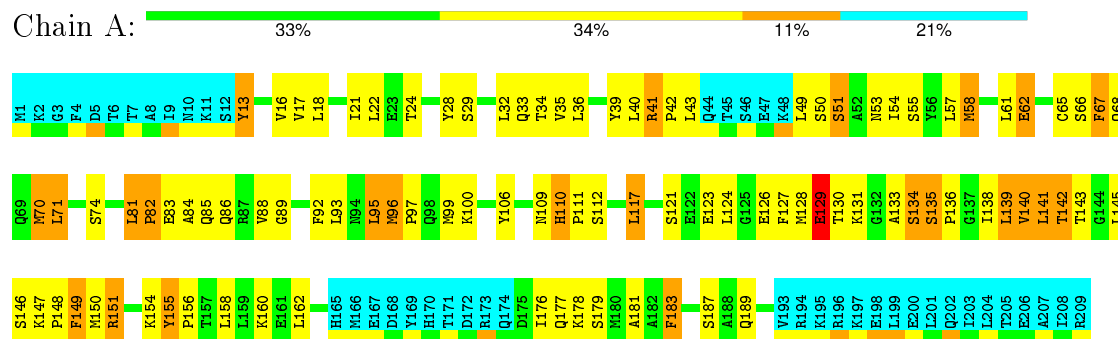
- Molecule 1: PROTEIN (PIX)



T205  
E206  
A207  
I208  
R209

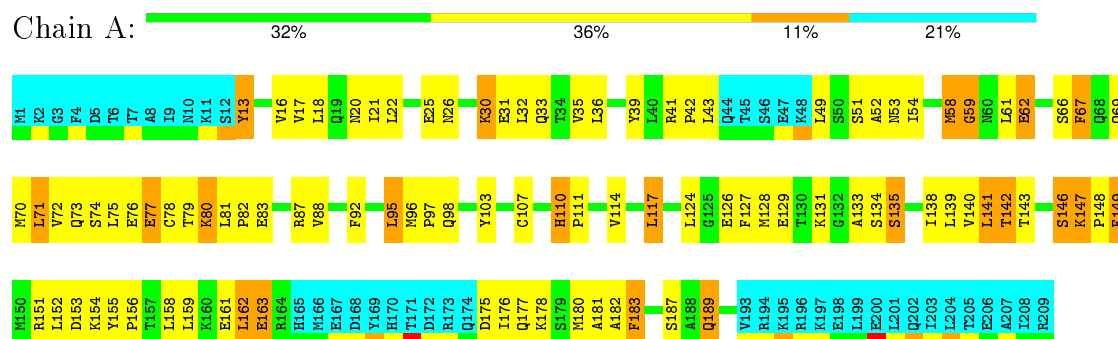
#### 4.2.5 Score per residue for model 5

- Molecule 1: PROTEIN (PIX)



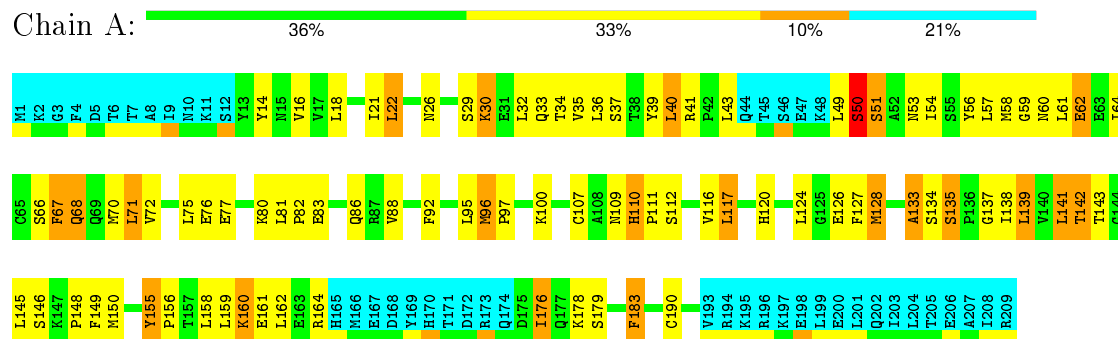
#### 4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (PIX)



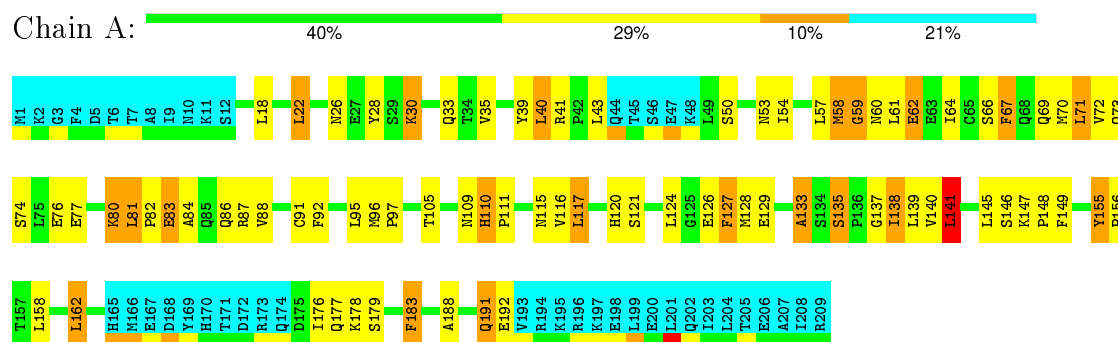
#### 4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN (PIX)



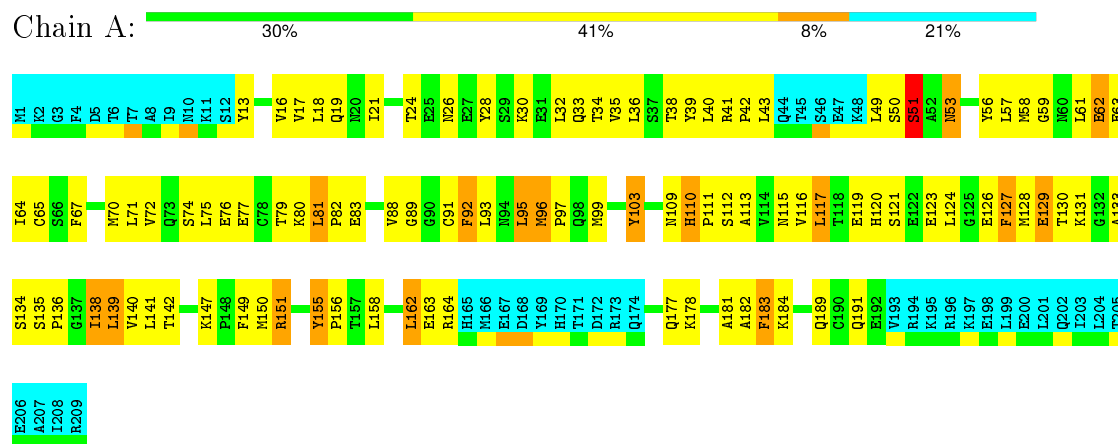
### 4.2.8 Score per residue for model 8

#### • Molecule 1: PROTEIN (PIX)



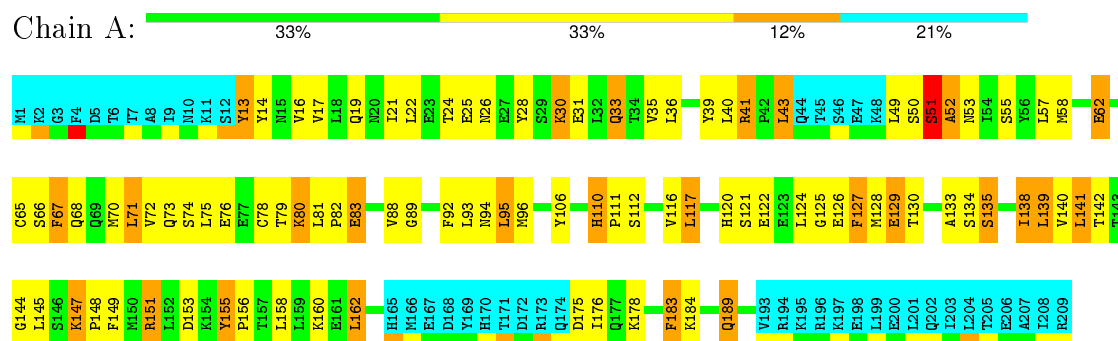
### 4.2.9 Score per residue for model 9

#### • Molecule 1: PROTEIN (PIX)



### 4.2.10 Score per residue for model 10

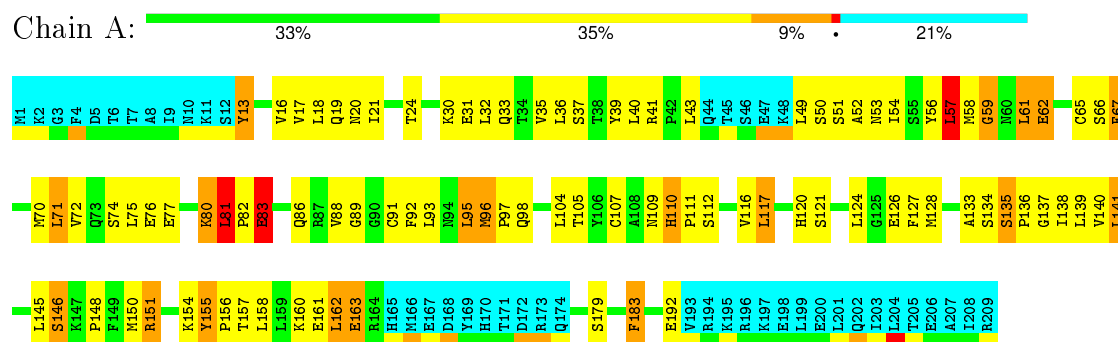
#### • Molecule 1: PROTEIN (PIX)





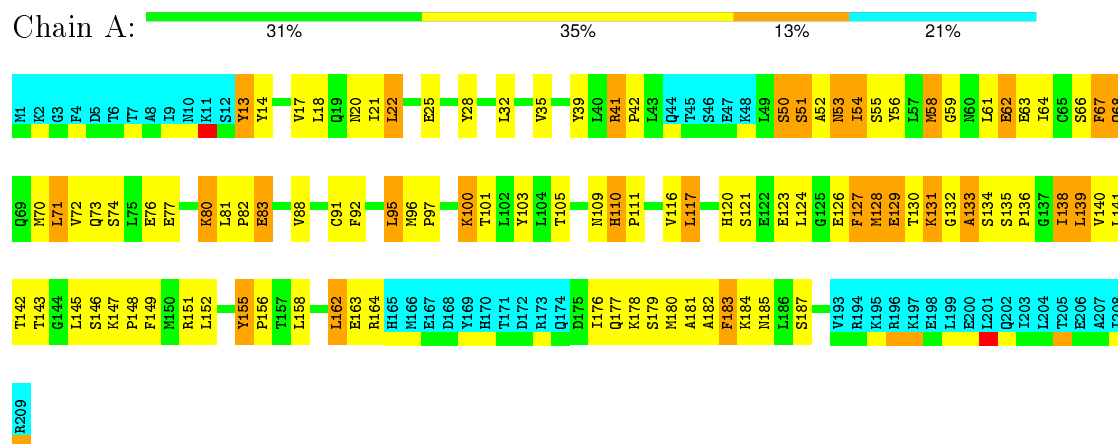
### 4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (PIX)



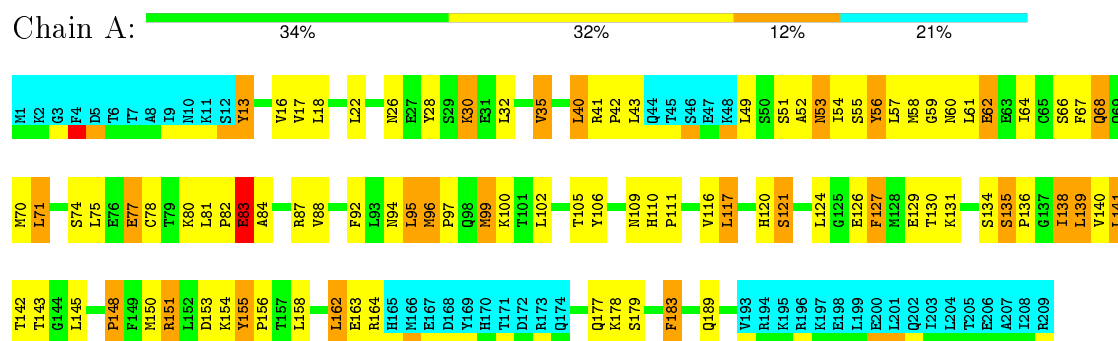
### 4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (PIX)



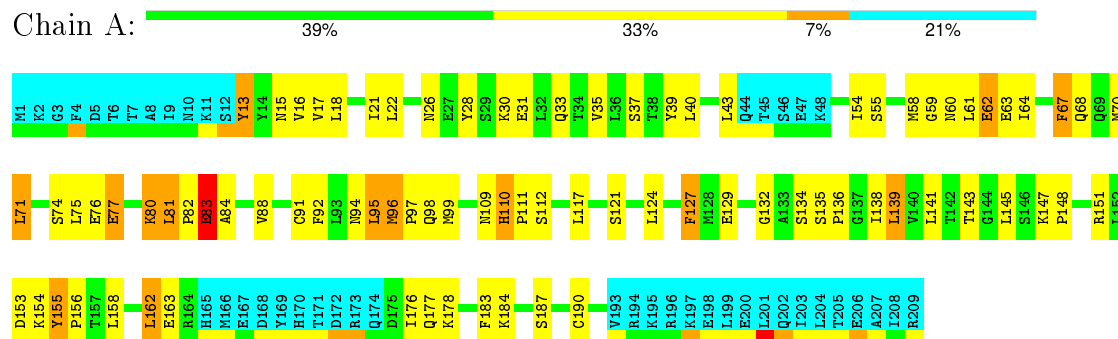
### 4.2.13 Score per residue for model 13

- Molecule 1: PROTEIN (PIX)



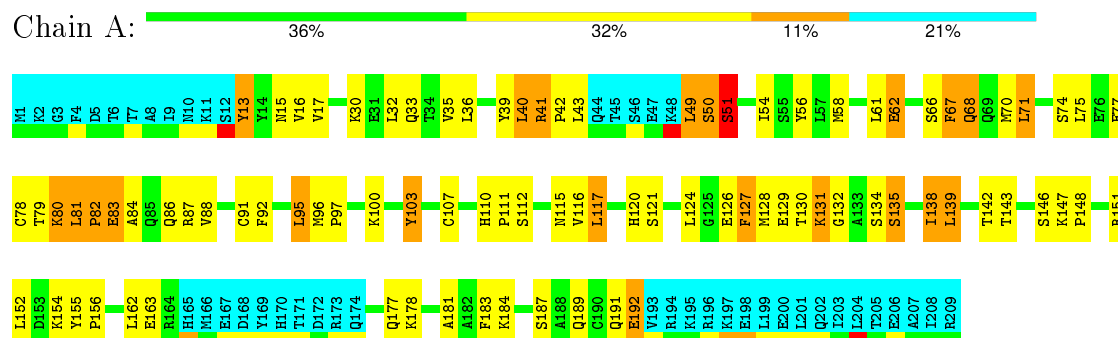
## 4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN (PIX)



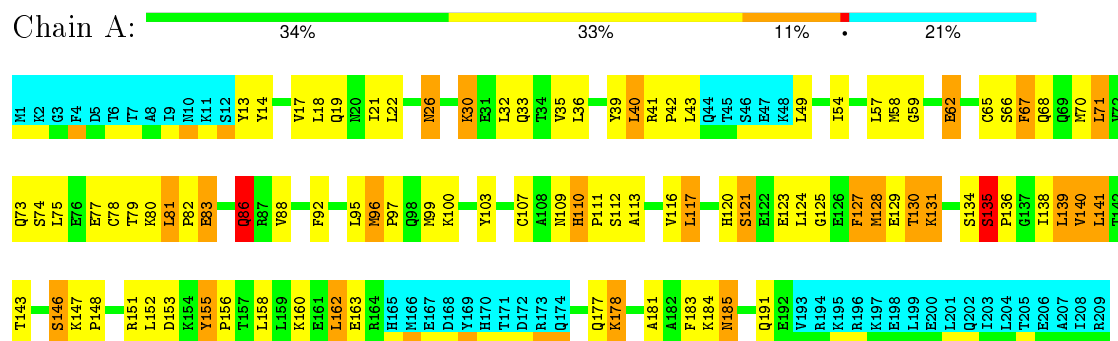
## 4.2.15 Score per residue for model 15

- Molecule 1: PROTEIN (PIX)



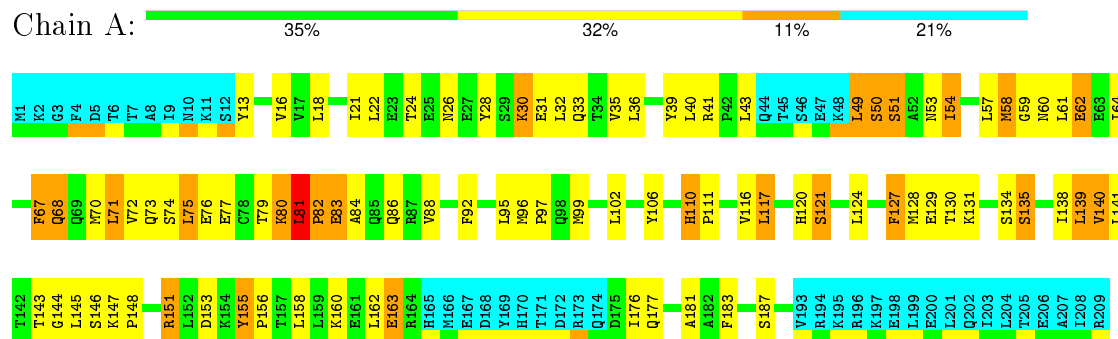
## 4.2.16 Score per residue for model 16

- Molecule 1: PROTEIN (PIX)



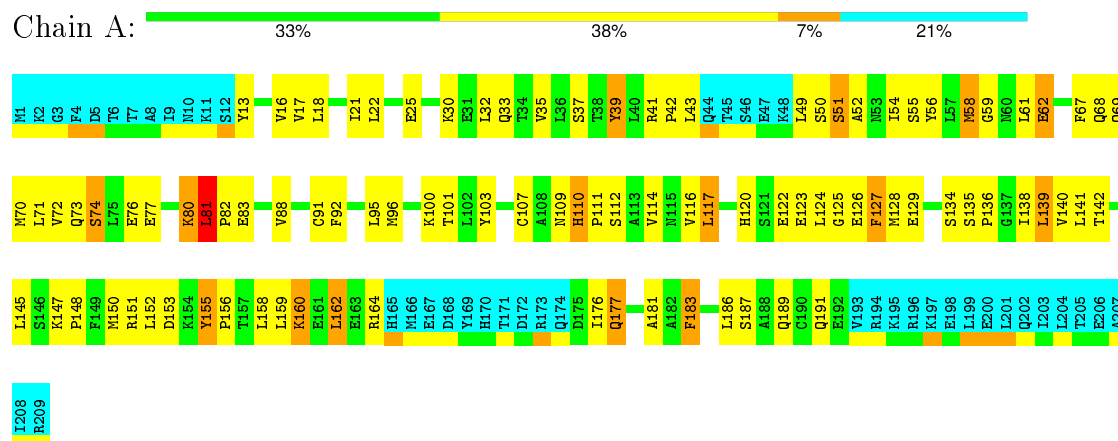
## 4.2.17 Score per residue for model 17

- Molecule 1: PROTEIN (PIX)



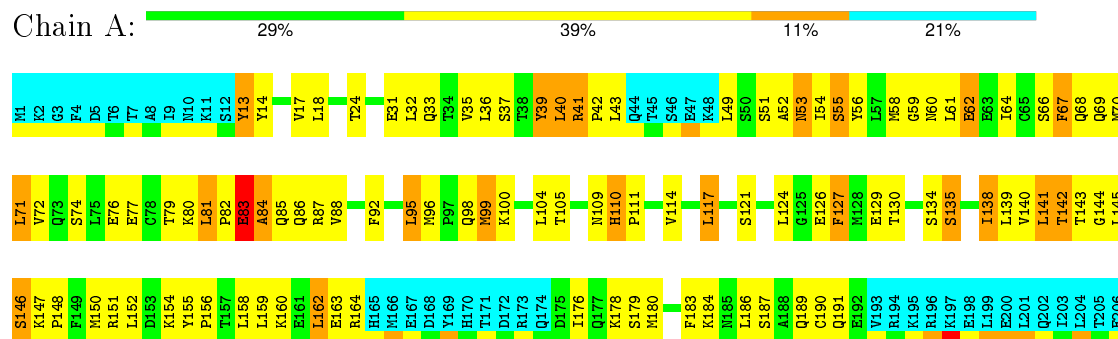
## 4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN (PIX)



## 4.2.19 Score per residue for model 19

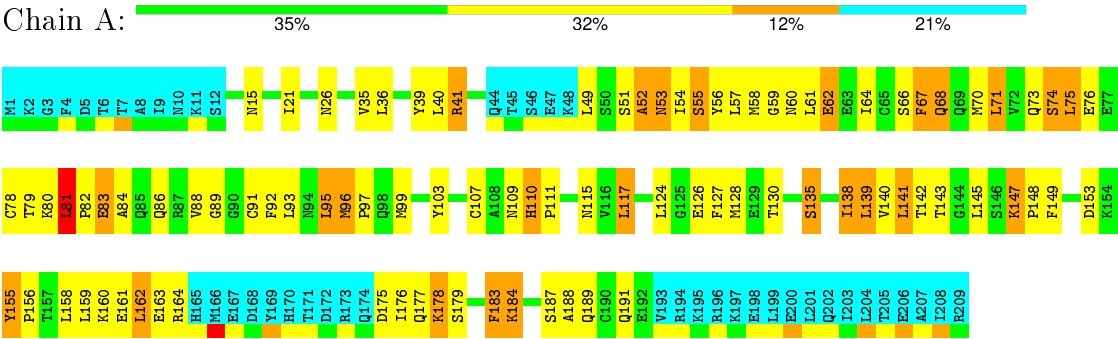
- Molecule 1: PROTEIN (PIX)



1207  
1208  
1209

4.2.20 Score per residue for model 20

- Molecule 1: PROTEIN (PIX)



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING*, *TORSION ANGLE DYNAMICS*.

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
CNS 0.3, X-PLOR	refinement	3.851
NMRPIPE	structure solution	
NMRVIEW	structure solution	
ARIA	structure solution	
X-PLOR	structure solution	
CNS	structure solution	

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	1304	1312	1310	64±9
All	All	26080	26240	26200	1279

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:LEU:HD13	1:A:145:LEU:HD12	1.03	1.23	5	2
1:A:67:PHE:CE1	1:A:95:LEU:HD21	0.96	1.95	16	3
1:A:67:PHE:CE1	1:A:71:LEU:HD22	0.94	1.98	5	17
1:A:61:LEU:HD22	1:A:145:LEU:HD11	0.93	1.40	12	4
1:A:35:VAL:HG13	1:A:39:TYR:CE2	0.92	1.99	15	15
1:A:57:LEU:HD13	1:A:141:LEU:HD23	0.89	1.45	17	1
1:A:67:PHE:CE1	1:A:71:LEU:HD13	0.88	2.03	18	2
1:A:57:LEU:HD21	1:A:141:LEU:HD21	0.88	1.43	9	1
1:A:88:VAL:HG12	1:A:92:PHE:CD2	0.86	2.05	15	18
1:A:49:LEU:HD21	1:A:124:LEU:HD21	0.86	1.46	10	5
1:A:18:LEU:HD22	1:A:76:GLU:OE2	0.83	1.73	12	2
1:A:49:LEU:HD12	1:A:58:MET:SD	0.83	2.13	5	2
1:A:138:ILE:HD13	1:A:138:ILE:O	0.82	1.74	20	4
1:A:124:LEU:CB	1:A:138:ILE:HG21	0.82	2.05	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:SER:O	1:A:116:VAL:HG23	0.82	1.74	11	7
1:A:13:TYR:O	1:A:17:VAL:HG23	0.81	1.74	18	14
1:A:77:GLU:O	1:A:81:LEU:HD12	0.80	1.76	14	8
1:A:57:LEU:HD21	1:A:141:LEU:CD2	0.80	2.07	9	1
1:A:43:LEU:HD23	1:A:58:MET:CE	0.80	2.06	3	1
1:A:67:PHE:CE1	1:A:95:LEU:HD13	0.80	2.12	12	3
1:A:141:LEU:HD23	1:A:145:LEU:CD1	0.79	2.07	8	1
1:A:138:ILE:O	1:A:138:ILE:HD13	0.78	1.79	8	3
1:A:124:LEU:HB2	1:A:138:ILE:HG21	0.77	1.56	9	3
1:A:43:LEU:HD22	1:A:43:LEU:O	0.77	1.79	10	1
1:A:61:LEU:CD2	1:A:145:LEU:HD13	0.77	2.10	14	1
1:A:21:ILE:HG21	1:A:158:LEU:HD11	0.76	1.55	10	8
1:A:124:LEU:O	1:A:138:ILE:HD13	0.75	1.81	17	4
1:A:43:LEU:HD13	1:A:127:PHE:CE2	0.74	2.17	17	4
1:A:136:PRO:HG2	1:A:140:VAL:HG22	0.73	1.59	9	4
1:A:67:PHE:CZ	1:A:95:LEU:HD11	0.73	2.18	6	2
1:A:88:VAL:HG23	1:A:162:LEU:HD22	0.73	1.59	8	1
1:A:35:VAL:CG1	1:A:40:LEU:HD22	0.73	2.13	13	1
1:A:163:GLU:OE1	1:A:176:ILE:HG23	0.72	1.84	14	1
1:A:75:LEU:O	1:A:79:THR:HG23	0.72	1.84	15	7
1:A:127:PHE:CZ	1:A:138:ILE:HD11	0.72	2.19	6	4
1:A:32:LEU:HD13	1:A:64:ILE:HG22	0.71	1.60	9	1
1:A:49:LEU:HD21	1:A:124:LEU:CD2	0.70	2.16	10	2
1:A:127:PHE:CE2	1:A:138:ILE:HD11	0.70	2.21	14	4
1:A:95:LEU:HD12	1:A:99:MET:SD	0.70	2.26	13	1
1:A:54:ILE:HD13	1:A:58:MET:CB	0.70	2.17	11	9
1:A:18:LEU:O	1:A:22:LEU:HD13	0.69	1.87	13	7
1:A:139:LEU:HD13	1:A:139:LEU:N	0.69	2.02	5	5
1:A:141:LEU:HD13	1:A:145:LEU:CD1	0.69	2.13	5	1
1:A:139:LEU:N	1:A:139:LEU:HD13	0.68	2.02	12	5
1:A:128:MET:O	1:A:133:ALA:HB2	0.68	1.88	5	3
1:A:79:THR:HG22	1:A:86:GLN:HA	0.68	1.63	20	1
1:A:18:LEU:HD22	1:A:76:GLU:OE1	0.68	1.88	9	2
1:A:25:GLU:CD	1:A:72:VAL:HG22	0.68	2.10	6	1
1:A:95:LEU:HD23	1:A:98:GLN:OE1	0.68	1.88	11	1
1:A:35:VAL:HG13	1:A:40:LEU:HD13	0.68	1.63	13	1
1:A:67:PHE:CE2	1:A:95:LEU:HD22	0.66	2.25	9	1
1:A:152:LEU:HD23	1:A:155:TYR:CG	0.66	2.25	15	1
1:A:36:LEU:HD23	1:A:40:LEU:CD2	0.66	2.21	15	3
1:A:18:LEU:HD13	1:A:80:LYS:HE2	0.65	1.68	13	2
1:A:141:LEU:HD23	1:A:145:LEU:HD11	0.65	1.68	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:LEU:HD21	1:A:141:LEU:HD13	0.65	1.67	1	1
1:A:43:LEU:HD13	1:A:127:PHE:CD2	0.65	2.27	17	2
1:A:36:LEU:HD23	1:A:40:LEU:HD23	0.64	1.69	15	5
1:A:128:MET:HB2	1:A:138:ILE:HD13	0.64	1.67	5	1
1:A:71:LEU:HD21	1:A:155:TYR:OH	0.64	1.92	18	3
1:A:21:ILE:HG21	1:A:158:LEU:CD1	0.64	2.22	10	2
1:A:14:TYR:CE1	1:A:18:LEU:HD11	0.64	2.27	12	1
1:A:54:ILE:HD13	1:A:58:MET:HB2	0.64	1.70	7	6
1:A:56:TYR:CE2	1:A:116:VAL:HG11	0.64	2.28	1	1
1:A:88:VAL:HG12	1:A:92:PHE:HD2	0.64	1.53	18	12
1:A:117:LEU:HD13	1:A:139:LEU:HA	0.63	1.70	16	8
1:A:32:LEU:CD1	1:A:64:ILE:HG22	0.63	2.23	3	4
1:A:141:LEU:HG	1:A:145:LEU:HD12	0.63	1.69	1	2
1:A:32:LEU:HD11	1:A:64:ILE:CG2	0.63	2.23	3	1
1:A:95:LEU:HD12	1:A:95:LEU:O	0.63	1.93	19	2
1:A:70:MET:HG3	1:A:95:LEU:HD11	0.63	1.69	9	2
1:A:117:LEU:HD11	1:A:141:LEU:HD12	0.62	1.69	6	1
1:A:61:LEU:HA	1:A:64:ILE:HD12	0.62	1.70	8	3
1:A:24:THR:HG22	1:A:151:ARG:HG2	0.62	1.70	1	2
1:A:18:LEU:HD21	1:A:162:LEU:HD21	0.62	1.71	16	2
1:A:71:LEU:HD11	1:A:155:TYR:OH	0.62	1.95	9	2
1:A:81:LEU:HD23	1:A:82:PRO:HD3	0.62	1.71	14	2
1:A:89:GLY:O	1:A:93:LEU:HD13	0.62	1.95	9	6
1:A:67:PHE:CD1	1:A:95:LEU:HD22	0.61	2.29	3	1
1:A:43:LEU:HD13	1:A:43:LEU:O	0.61	1.95	19	2
1:A:67:PHE:CZ	1:A:95:LEU:HD21	0.61	2.30	16	2
1:A:18:LEU:HD21	1:A:162:LEU:CD1	0.61	2.25	2	5
1:A:24:THR:HG22	1:A:151:ARG:CG	0.61	2.26	1	1
1:A:60:ASN:O	1:A:64:ILE:HD12	0.60	1.97	14	2
1:A:141:LEU:CD1	1:A:145:LEU:HD12	0.60	2.13	5	4
1:A:49:LEU:HD12	1:A:58:MET:CG	0.60	2.26	15	2
1:A:81:LEU:HD12	1:A:81:LEU:O	0.60	1.97	10	1
1:A:100:LYS:HG2	1:A:186:LEU:HD22	0.60	1.73	2	1
1:A:60:ASN:C	1:A:64:ILE:HD12	0.59	2.17	13	5
1:A:128:MET:SD	1:A:133:ALA:HB2	0.59	2.36	3	4
1:A:61:LEU:HD23	1:A:145:LEU:HD13	0.59	1.73	14	1
1:A:35:VAL:HG13	1:A:39:TYR:CD2	0.59	2.32	18	5
1:A:18:LEU:HD23	1:A:158:LEU:HD21	0.59	1.73	8	2
1:A:56:TYR:CE2	1:A:116:VAL:HG21	0.59	2.33	9	1
1:A:67:PHE:CZ	1:A:71:LEU:HD23	0.59	2.32	9	1
1:A:32:LEU:HD11	1:A:64:ILE:HG22	0.59	1.72	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:VAL:HG13	1:A:76:GLU:HG3	0.59	1.75	18	4
1:A:61:LEU:HD13	1:A:61:LEU:O	0.59	1.97	11	3
1:A:43:LEU:O	1:A:43:LEU:HD13	0.59	1.98	13	1
1:A:155:TYR:CE2	1:A:159:LEU:HD11	0.58	2.33	6	1
1:A:67:PHE:CE1	1:A:71:LEU:CD2	0.58	2.87	9	1
1:A:67:PHE:CE1	1:A:71:LEU:HD23	0.58	2.33	9	1
1:A:155:TYR:CE2	1:A:183:PHE:CZ	0.58	2.92	6	9
1:A:18:LEU:O	1:A:22:LEU:HD22	0.58	1.98	7	1
1:A:106:TYR:CE2	1:A:149:PHE:CE2	0.58	2.91	1	1
1:A:124:LEU:HB3	1:A:138:ILE:HD12	0.58	1.76	20	6
1:A:33:GLN:HA	1:A:36:LEU:HD12	0.58	1.75	10	1
1:A:54:ILE:HD13	1:A:58:MET:HB3	0.57	1.74	20	9
1:A:92:PHE:CZ	1:A:155:TYR:CE2	0.57	2.92	11	4
1:A:59:GLY:O	1:A:102:LEU:HD22	0.57	1.99	4	1
1:A:128:MET:CG	1:A:133:ALA:HB2	0.57	2.30	8	2
1:A:49:LEU:HD22	1:A:53:ASN:CG	0.57	2.20	20	1
1:A:92:PHE:CE1	1:A:155:TYR:CE1	0.57	2.92	3	1
1:A:155:TYR:CE1	1:A:183:PHE:CZ	0.57	2.92	5	2
1:A:57:LEU:HD11	1:A:117:LEU:HD21	0.57	1.76	17	3
1:A:155:TYR:CD2	1:A:183:PHE:CE1	0.57	2.92	8	3
1:A:96:MET:SD	1:A:182:ALA:HB1	0.57	2.40	12	2
1:A:43:LEU:HD23	1:A:58:MET:HE2	0.57	1.75	3	1
1:A:55:SER:O	1:A:105:THR:HG21	0.57	1.99	13	1
1:A:24:THR:HG22	1:A:151:ARG:HG3	0.57	1.76	17	3
1:A:19:GLN:HA	1:A:22:LEU:HD12	0.57	1.76	10	1
1:A:117:LEU:HD23	1:A:117:LEU:N	0.57	2.15	2	9
1:A:57:LEU:HD21	1:A:141:LEU:CD1	0.57	2.30	1	1
1:A:135:SER:N	1:A:136:PRO:CD	0.56	2.68	9	10
1:A:35:VAL:HG13	1:A:39:TYR:CZ	0.56	2.35	3	4
1:A:130:THR:O	1:A:130:THR:HG23	0.56	2.00	13	2
1:A:35:VAL:HG12	1:A:40:LEU:HD22	0.56	1.77	13	1
1:A:39:TYR:OH	1:A:141:LEU:HD12	0.56	1.99	4	1
1:A:164:ARG:NH1	1:A:176:ILE:HD12	0.56	2.15	20	1
1:A:17:VAL:HG21	1:A:161:GLU:OE1	0.56	1.99	11	1
1:A:57:LEU:HD11	1:A:141:LEU:HD22	0.56	1.76	9	3
1:A:67:PHE:HE1	1:A:71:LEU:HD13	0.56	1.60	3	1
1:A:61:LEU:C	1:A:61:LEU:HD13	0.55	2.20	18	4
1:A:81:LEU:O	1:A:83:GLU:N	0.55	2.39	5	18
1:A:18:LEU:HD21	1:A:162:LEU:HD13	0.55	1.77	2	2
1:A:88:VAL:HG12	1:A:92:PHE:CE2	0.55	2.37	15	7
1:A:67:PHE:CZ	1:A:71:LEU:HD13	0.55	2.35	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:LEU:HD11	1:A:76:GLU:OE2	0.55	2.01	7	1
1:A:56:TYR:CG	1:A:57:LEU:N	0.55	2.75	1	2
1:A:32:LEU:HD13	1:A:68:GLN:OE1	0.55	2.02	17	1
1:A:22:LEU:HD23	1:A:25:GLU:OE2	0.55	2.02	10	1
1:A:75:LEU:HD13	1:A:88:VAL:HG13	0.54	1.79	9	3
1:A:141:LEU:O	1:A:145:LEU:HD12	0.54	2.02	13	2
1:A:72:VAL:HG12	1:A:76:GLU:HG3	0.54	1.79	17	3
1:A:81:LEU:HD23	1:A:81:LEU:N	0.54	2.18	18	2
1:A:49:LEU:HD12	1:A:58:MET:HG2	0.54	1.80	15	2
1:A:49:LEU:HD11	1:A:124:LEU:HD21	0.54	1.80	9	1
1:A:88:VAL:CG2	1:A:162:LEU:HD22	0.54	2.33	8	4
1:A:32:LEU:HD12	1:A:68:GLN:HG3	0.54	1.78	4	3
1:A:117:LEU:HB3	1:A:139:LEU:HD12	0.54	1.79	20	1
1:A:61:LEU:HD13	1:A:145:LEU:HD21	0.54	1.79	20	1
1:A:139:LEU:N	1:A:139:LEU:HD23	0.54	2.17	17	2
1:A:162:LEU:O	1:A:162:LEU:HD13	0.54	2.03	1	3
1:A:67:PHE:CZ	1:A:95:LEU:CD2	0.54	2.91	2	1
1:A:136:PRO:O	1:A:139:LEU:HD12	0.53	2.03	4	1
1:A:81:LEU:HD12	1:A:81:LEU:C	0.53	2.22	7	2
1:A:99:MET:CE	1:A:186:LEU:HD11	0.53	2.34	19	1
1:A:117:LEU:N	1:A:117:LEU:HD23	0.53	2.17	13	5
1:A:128:MET:HB2	1:A:138:ILE:HD12	0.53	1.80	6	1
1:A:35:VAL:CG1	1:A:39:TYR:CE2	0.53	2.92	10	3
1:A:106:TYR:CD2	1:A:149:PHE:CZ	0.53	2.97	1	1
1:A:61:LEU:HD22	1:A:145:LEU:CD1	0.53	2.26	12	3
1:A:51:SER:O	1:A:52:ALA:HB2	0.53	2.04	20	2
1:A:67:PHE:CZ	1:A:95:LEU:HD22	0.53	2.39	20	2
1:A:67:PHE:CD1	1:A:95:LEU:CD2	0.53	2.92	3	1
1:A:81:LEU:CB	1:A:82:PRO:HD2	0.53	2.34	18	1
1:A:67:PHE:HE1	1:A:95:LEU:HD21	0.53	1.58	17	2
1:A:110:HIS:O	1:A:114:VAL:HG23	0.52	2.04	18	1
1:A:70:MET:SD	1:A:95:LEU:HD11	0.52	2.44	11	1
1:A:147:LYS:N	1:A:148:PRO:CD	0.52	2.72	6	8
1:A:35:VAL:CG1	1:A:40:LEU:HD13	0.52	2.34	3	5
1:A:83:GLU:O	1:A:84:ALA:HB3	0.52	2.04	17	7
1:A:81:LEU:CB	1:A:82:PRO:CD	0.52	2.88	20	4
1:A:18:LEU:HD21	1:A:79:THR:OG1	0.52	2.04	1	1
1:A:127:PHE:CZ	1:A:138:ILE:CD1	0.52	2.93	4	6
1:A:127:PHE:CD1	1:A:128:MET:N	0.52	2.77	12	4
1:A:67:PHE:CZ	1:A:71:LEU:HD22	0.52	2.40	13	1
1:A:151:ARG:NH2	1:A:155:TYR:CE2	0.52	2.78	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:LEU:HD12	1:A:61:LEU:O	0.52	2.05	8	1
1:A:17:VAL:O	1:A:21:ILE:HD12	0.51	2.05	16	2
1:A:124:LEU:HB3	1:A:138:ILE:HG21	0.51	1.78	9	1
1:A:105:THR:HG22	1:A:109:ASN:ND2	0.51	2.21	11	1
1:A:18:LEU:HD12	1:A:76:GLU:OE1	0.51	2.05	7	2
1:A:102:LEU:N	1:A:102:LEU:HD23	0.51	2.20	17	1
1:A:39:TYR:CE1	1:A:40:LEU:HD12	0.51	2.41	2	2
1:A:88:VAL:CG1	1:A:92:PHE:CD2	0.51	2.93	9	9
1:A:81:LEU:C	1:A:81:LEU:HD12	0.51	2.25	10	1
1:A:61:LEU:CD1	1:A:145:LEU:HD22	0.51	2.36	17	1
1:A:57:LEU:CD1	1:A:117:LEU:HD21	0.51	2.35	17	2
1:A:51:SER:O	1:A:52:ALA:HB3	0.50	2.06	3	5
1:A:49:LEU:HD23	1:A:53:ASN:HB3	0.50	1.83	6	1
1:A:121:SER:HA	1:A:139:LEU:HD11	0.50	1.82	9	1
1:A:96:MET:N	1:A:97:PRO:CD	0.50	2.74	17	15
1:A:157:THR:HG22	1:A:161:GLU:OE2	0.50	2.06	11	1
1:A:18:LEU:HD23	1:A:158:LEU:CD2	0.50	2.37	18	2
1:A:36:LEU:HD23	1:A:40:LEU:HD22	0.50	1.84	19	1
1:A:35:VAL:HG12	1:A:40:LEU:HD13	0.50	1.83	7	3
1:A:99:MET:CE	1:A:183:PHE:CE1	0.50	2.94	9	1
1:A:99:MET:HE1	1:A:186:LEU:HD11	0.50	1.84	19	1
1:A:103:TYR:CD1	1:A:149:PHE:CE2	0.50	2.99	9	1
1:A:43:LEU:HD23	1:A:127:PHE:CE2	0.50	2.41	16	3
1:A:127:PHE:CE2	1:A:138:ILE:CD1	0.50	2.95	16	2
1:A:17:VAL:HG12	1:A:158:LEU:CD2	0.50	2.37	1	8
1:A:49:LEU:HD13	1:A:53:ASN:CG	0.50	2.26	10	2
1:A:18:LEU:O	1:A:22:LEU:HD12	0.50	2.07	17	2
1:A:32:LEU:O	1:A:36:LEU:HD12	0.50	2.06	11	3
1:A:49:LEU:HD23	1:A:49:LEU:N	0.50	2.21	18	1
1:A:124:LEU:HD13	1:A:138:ILE:HD12	0.49	1.84	15	1
1:A:61:LEU:O	1:A:61:LEU:HD13	0.49	2.06	18	2
1:A:60:ASN:ND2	1:A:64:ILE:HD11	0.49	2.22	19	1
1:A:155:TYR:OH	1:A:183:PHE:CE2	0.49	2.65	6	1
1:A:155:TYR:CD2	1:A:183:PHE:CE2	0.49	3.00	9	2
1:A:139:LEU:CD1	1:A:139:LEU:N	0.49	2.75	9	3
1:A:28:TYR:CD2	1:A:68:GLN:OE1	0.49	2.65	13	1
1:A:28:TYR:OH	1:A:64:ILE:HG23	0.49	2.06	8	2
1:A:120:HIS:HB2	1:A:124:LEU:HD12	0.49	1.83	9	1
1:A:137:GLY:O	1:A:140:VAL:HG23	0.49	2.07	8	2
1:A:100:LYS:CD	1:A:101:THR:N	0.49	2.75	12	1
1:A:36:LEU:HD11	1:A:61:LEU:HD11	0.49	1.85	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:LEU:HD23	1:A:82:PRO:HD2	0.49	1.85	5	1
1:A:88:VAL:CG1	1:A:92:PHE:CE2	0.49	2.96	15	10
1:A:177:GLN:O	1:A:181:ALA:HB3	0.49	2.08	12	3
1:A:152:LEU:HD13	1:A:186:LEU:HB2	0.49	1.84	18	1
1:A:60:ASN:CG	1:A:64:ILE:HD11	0.49	2.29	19	1
1:A:155:TYR:CB	1:A:156:PRO:CD	0.48	2.91	9	6
1:A:110:HIS:N	1:A:111:PRO:CD	0.48	2.76	2	12
1:A:116:VAL:O	1:A:120:HIS:CG	0.48	2.66	16	3
1:A:146:SER:O	1:A:149:PHE:CE2	0.48	2.66	12	1
1:A:67:PHE:CD2	1:A:99:MET:CE	0.48	2.96	13	1
1:A:141:LEU:C	1:A:145:LEU:HD12	0.48	2.29	13	1
1:A:149:PHE:HB3	1:A:152:LEU:HD12	0.48	1.85	4	1
1:A:139:LEU:N	1:A:139:LEU:CD1	0.48	2.74	5	1
1:A:32:LEU:HD12	1:A:68:GLN:HB3	0.48	1.85	2	3
1:A:67:PHE:CE2	1:A:99:MET:CG	0.48	2.97	13	1
1:A:124:LEU:C	1:A:138:ILE:HD13	0.48	2.28	17	1
1:A:39:TYR:OH	1:A:141:LEU:HD23	0.48	2.08	19	1
1:A:32:LEU:CD1	1:A:64:ILE:CG2	0.48	2.92	9	4
1:A:70:MET:O	1:A:74:SER:CB	0.48	2.61	10	17
1:A:124:LEU:O	1:A:127:PHE:CD2	0.48	2.67	20	7
1:A:36:LEU:HD13	1:A:65:CYS:SG	0.48	2.49	9	1
1:A:103:TYR:CE2	1:A:152:LEU:HD21	0.48	2.44	12	1
1:A:146:SER:O	1:A:149:PHE:CD1	0.48	2.67	6	1
1:A:138:ILE:HG23	1:A:139:LEU:HD13	0.48	1.85	5	2
1:A:43:LEU:CD2	1:A:127:PHE:CE2	0.48	2.97	13	2
1:A:152:LEU:HD23	1:A:155:TYR:CD1	0.48	2.44	16	1
1:A:41:ARG:N	1:A:42:PRO:CD	0.47	2.77	9	8
1:A:184:LYS:HE2	1:A:188:ALA:HB2	0.47	1.85	20	1
1:A:114:VAL:HG22	1:A:142:THR:HG21	0.47	1.86	6	1
1:A:116:VAL:O	1:A:120:HIS:CD2	0.47	2.68	12	4
1:A:99:MET:O	1:A:103:TYR:CG	0.47	2.68	3	1
1:A:71:LEU:O	1:A:75:LEU:HD23	0.47	2.10	10	2
1:A:127:PHE:CD1	1:A:127:PHE:C	0.47	2.88	1	7
1:A:127:PHE:C	1:A:127:PHE:CD1	0.47	2.87	13	13
1:A:61:LEU:HD13	1:A:61:LEU:C	0.47	2.30	15	2
1:A:77:GLU:O	1:A:81:LEU:HD21	0.47	2.10	18	1
1:A:95:LEU:O	1:A:95:LEU:HD12	0.47	2.09	17	1
1:A:14:TYR:CE1	1:A:86:GLN:OE1	0.47	2.68	7	1
1:A:92:PHE:CE2	1:A:155:TYR:OH	0.47	2.65	6	1
1:A:103:TYR:CD2	1:A:186:LEU:HD13	0.47	2.45	18	1
1:A:43:LEU:HD21	1:A:49:LEU:HD12	0.46	1.87	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:PHE:CZ	1:A:71:LEU:CD2	0.46	2.99	9	1
1:A:36:LEU:HD21	1:A:65:CYS:SG	0.46	2.50	11	2
1:A:130:THR:O	1:A:131:LYS:CG	0.46	2.64	16	1
1:A:57:LEU:HD13	1:A:141:LEU:CD2	0.46	2.30	17	1
1:A:49:LEU:O	1:A:51:SER:N	0.46	2.49	9	3
1:A:104:LEU:HD23	1:A:190:CYS:SG	0.46	2.50	4	1
1:A:79:THR:HG22	1:A:86:GLN:CB	0.46	2.40	1	1
1:A:82:PRO:O	1:A:84:ALA:N	0.46	2.48	20	5
1:A:21:ILE:HD13	1:A:158:LEU:HD21	0.46	1.87	16	1
1:A:58:MET:O	1:A:62:GLU:CG	0.46	2.64	19	20
1:A:139:LEU:HD22	1:A:139:LEU:H	0.46	1.69	18	3
1:A:158:LEU:CD2	1:A:162:LEU:HD23	0.46	2.41	18	1
1:A:21:ILE:HG13	1:A:158:LEU:HD11	0.46	1.88	17	5
1:A:135:SER:CB	1:A:136:PRO:CD	0.46	2.94	16	1
1:A:120:HIS:CG	1:A:123:GLU:OE2	0.46	2.68	16	1
1:A:149:PHE:C	1:A:149:PHE:CD1	0.46	2.89	6	2
1:A:21:ILE:CG2	1:A:158:LEU:HD11	0.46	2.37	10	1
1:A:156:PRO:HA	1:A:159:LEU:CG	0.46	2.41	18	1
1:A:67:PHE:CE2	1:A:99:MET:SD	0.46	3.09	13	1
1:A:103:TYR:HE2	1:A:152:LEU:HD21	0.46	1.70	12	1
1:A:158:LEU:HD22	1:A:162:LEU:HD13	0.46	1.87	11	1
1:A:88:VAL:HG22	1:A:162:LEU:HD22	0.46	1.88	4	2
1:A:120:HIS:CB	1:A:124:LEU:HD12	0.45	2.40	9	1
1:A:52:ALA:O	1:A:53:ASN:CB	0.45	2.65	13	3
1:A:26:ASN:O	1:A:30:LYS:CG	0.45	2.64	4	10
1:A:155:TYR:CB	1:A:156:PRO:HD3	0.45	2.41	11	11
1:A:28:TYR:O	1:A:28:TYR:CD1	0.45	2.69	5	1
1:A:28:TYR:CD1	1:A:28:TYR:O	0.45	2.70	12	2
1:A:67:PHE:O	1:A:71:LEU:N	0.45	2.49	13	1
1:A:32:LEU:HD12	1:A:68:GLN:CG	0.45	2.41	4	2
1:A:40:LEU:HD11	1:A:141:LEU:HD21	0.45	1.88	20	1
1:A:58:MET:O	1:A:62:GLU:N	0.45	2.49	11	18
1:A:32:LEU:CD2	1:A:145:LEU:HD22	0.45	2.41	5	2
1:A:18:LEU:HD13	1:A:162:LEU:CD2	0.45	2.42	1	1
1:A:146:SER:O	1:A:149:PHE:CE1	0.45	2.70	6	1
1:A:73:GLN:CG	1:A:74:SER:N	0.45	2.79	10	2
1:A:81:LEU:HB3	1:A:82:PRO:CD	0.45	2.42	11	4
1:A:123:GLU:HG3	1:A:124:LEU:N	0.45	2.27	1	2
1:A:86:GLN:O	1:A:162:LEU:HD23	0.45	2.12	5	1
1:A:155:TYR:CE2	1:A:183:PHE:CE1	0.45	3.04	20	2
1:A:67:PHE:CE1	1:A:71:LEU:HG	0.45	2.47	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LEU:C	1:A:36:LEU:HD12	0.45	2.32	7	2
1:A:39:TYR:CE1	1:A:138:ILE:HD12	0.45	2.47	5	1
1:A:141:LEU:CG	1:A:145:LEU:HD12	0.45	2.41	1	1
1:A:39:TYR:CD1	1:A:128:MET:SD	0.45	3.10	9	1
1:A:75:LEU:HD22	1:A:88:VAL:HG13	0.45	1.89	15	1
1:A:26:ASN:O	1:A:30:LYS:HG2	0.45	2.12	16	2
1:A:103:TYR:OH	1:A:152:LEU:HD13	0.45	2.11	15	1
1:A:59:GLY:O	1:A:63:GLU:CG	0.44	2.65	12	5
1:A:79:THR:HG21	1:A:162:LEU:HD21	0.44	1.88	4	1
1:A:117:LEU:HD11	1:A:141:LEU:HB2	0.44	1.89	7	3
1:A:22:LEU:O	1:A:26:ASN:N	0.44	2.50	16	1
1:A:81:LEU:CB	1:A:82:PRO:HD3	0.44	2.42	20	1
1:A:18:LEU:O	1:A:22:LEU:CD1	0.44	2.65	6	5
1:A:110:HIS:CB	1:A:111:PRO:CD	0.44	2.95	6	5
1:A:177:GLN:CG	1:A:178:LYS:N	0.44	2.80	1	4
1:A:67:PHE:CE2	1:A:95:LEU:HD21	0.44	2.47	2	1
1:A:158:LEU:O	1:A:162:LEU:CB	0.44	2.65	4	13
1:A:70:MET:CE	1:A:95:LEU:HD21	0.44	2.43	15	1
1:A:128:MET:CE	1:A:133:ALA:HB3	0.44	2.41	11	1
1:A:88:VAL:HG23	1:A:162:LEU:HD12	0.44	1.88	6	1
1:A:129:GLU:O	1:A:130:THR:CG2	0.44	2.66	5	4
1:A:17:VAL:HG12	1:A:158:LEU:HD21	0.44	1.88	4	3
1:A:77:GLU:O	1:A:81:LEU:CD2	0.44	2.66	18	1
1:A:155:TYR:OH	1:A:159:LEU:HD21	0.44	2.13	6	1
1:A:155:TYR:CD2	1:A:183:PHE:CZ	0.44	3.05	3	2
1:A:106:TYR:CE2	1:A:110:HIS:CE1	0.44	3.05	4	1
1:A:155:TYR:CE1	1:A:183:PHE:CE2	0.44	3.06	5	1
1:A:32:LEU:HD12	1:A:68:GLN:CB	0.44	2.42	16	1
1:A:160:LYS:O	1:A:164:ARG:CG	0.44	2.66	4	3
1:A:32:LEU:HD11	1:A:64:ILE:HG21	0.44	1.90	4	1
1:A:77:GLU:O	1:A:81:LEU:HD23	0.44	2.13	17	1
1:A:18:LEU:HD13	1:A:80:LYS:HE3	0.44	1.88	8	1
1:A:164:ARG:CZ	1:A:176:ILE:HD12	0.44	2.43	20	1
1:A:81:LEU:HB2	1:A:82:PRO:CD	0.44	2.42	20	1
1:A:32:LEU:HD22	1:A:61:LEU:HD21	0.44	1.89	6	1
1:A:70:MET:O	1:A:74:SER:N	0.44	2.51	16	6
1:A:120:HIS:CB	1:A:124:LEU:CD1	0.44	2.95	7	1
1:A:36:LEU:O	1:A:41:ARG:N	0.44	2.51	20	9
1:A:125:GLY:O	1:A:128:MET:CG	0.44	2.66	16	1
1:A:22:LEU:O	1:A:26:ASN:ND2	0.44	2.51	1	1
1:A:120:HIS:HB3	1:A:124:LEU:CD1	0.44	2.43	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:LYS:N	1:A:148:PRO:HD2	0.44	2.28	10	4
1:A:13:TYR:O	1:A:17:VAL:N	0.44	2.51	18	1
1:A:177:GLN:O	1:A:181:ALA:CB	0.43	2.66	18	7
1:A:125:GLY:O	1:A:129:GLU:N	0.43	2.51	18	3
1:A:88:VAL:HG13	1:A:92:PHE:CE2	0.43	2.47	3	1
1:A:24:THR:HG21	1:A:154:LYS:HG3	0.43	1.89	5	1
1:A:106:TYR:CD2	1:A:149:PHE:CE1	0.43	3.06	5	1
1:A:89:GLY:O	1:A:93:LEU:CB	0.43	2.66	2	1
1:A:117:LEU:O	1:A:121:SER:N	0.43	2.52	19	12
1:A:54:ILE:HG23	1:A:59:GLY:CA	0.43	2.43	11	1
1:A:92:PHE:CZ	1:A:155:TYR:CE1	0.43	3.06	3	3
1:A:32:LEU:O	1:A:36:LEU:CG	0.43	2.67	1	5
1:A:120:HIS:CE1	1:A:123:GLU:OE1	0.43	2.71	9	1
1:A:163:GLU:CD	1:A:176:ILE:HD13	0.43	2.34	12	1
1:A:129:GLU:CG	1:A:130:THR:N	0.43	2.81	4	1
1:A:73:GLN:O	1:A:77:GLU:CG	0.43	2.66	16	2
1:A:124:LEU:CB	1:A:138:ILE:HG12	0.43	2.44	5	1
1:A:24:THR:CG2	1:A:151:ARG:NE	0.43	2.82	19	1
1:A:54:ILE:O	1:A:59:GLY:N	0.43	2.52	3	12
1:A:159:LEU:HD11	1:A:183:PHE:HD2	0.43	1.74	7	2
1:A:96:MET:O	1:A:99:MET:N	0.43	2.52	14	1
1:A:67:PHE:CD1	1:A:67:PHE:C	0.43	2.92	3	1
1:A:53:ASN:HA	1:A:56:TYR:CE2	0.43	2.48	13	1
1:A:41:ARG:N	1:A:42:PRO:HD2	0.43	2.29	2	1
1:A:159:LEU:HD11	1:A:183:PHE:CD2	0.43	2.49	20	1
1:A:128:MET:CG	1:A:129:GLU:N	0.43	2.81	1	1
1:A:39:TYR:C	1:A:39:TYR:CD1	0.43	2.92	7	3
1:A:116:VAL:O	1:A:120:HIS:N	0.43	2.52	10	7
1:A:83:GLU:OE2	1:A:86:GLN:NE2	0.43	2.52	3	1
1:A:161:GLU:O	1:A:164:ARG:CG	0.43	2.67	3	1
1:A:61:LEU:CD2	1:A:141:LEU:CD1	0.43	2.95	13	1
1:A:139:LEU:O	1:A:141:LEU:N	0.43	2.51	13	4
1:A:14:TYR:CE1	1:A:162:LEU:HD22	0.43	2.49	19	1
1:A:162:LEU:O	1:A:162:LEU:CD1	0.43	2.66	1	1
1:A:155:TYR:N	1:A:156:PRO:CD	0.43	2.82	6	3
1:A:49:LEU:O	1:A:53:ASN:ND2	0.43	2.51	9	1
1:A:28:TYR:OH	1:A:64:ILE:CG2	0.43	2.67	14	4
1:A:60:ASN:O	1:A:64:ILE:CD1	0.43	2.66	14	1
1:A:96:MET:CB	1:A:97:PRO:CD	0.43	2.97	14	2
1:A:178:LYS:O	1:A:182:ALA:HB2	0.43	2.13	3	2
1:A:96:MET:N	1:A:97:PRO:HD2	0.43	2.29	17	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:LEU:HB3	1:A:82:PRO:HD2	0.43	1.91	18	1
1:A:128:MET:HG2	1:A:133:ALA:HB2	0.43	1.89	4	1
1:A:117:LEU:O	1:A:120:HIS:N	0.43	2.52	7	9
1:A:135:SER:N	1:A:136:PRO:HD2	0.43	2.29	9	1
1:A:22:LEU:O	1:A:26:ASN:CB	0.43	2.67	10	2
1:A:39:TYR:CE1	1:A:128:MET:HB2	0.43	2.49	12	1
1:A:50:SER:O	1:A:52:ALA:N	0.43	2.51	12	1
1:A:95:LEU:CD2	1:A:98:GLN:OE1	0.43	2.65	11	1
1:A:66:SER:O	1:A:70:MET:CG	0.43	2.67	1	2
1:A:124:LEU:HB3	1:A:138:ILE:HD13	0.43	1.88	9	2
1:A:53:ASN:OD1	1:A:120:HIS:CE1	0.43	2.72	13	1
1:A:18:LEU:HD21	1:A:162:LEU:HD11	0.43	1.90	4	1
1:A:106:TYR:O	1:A:110:HIS:N	0.43	2.52	4	2
1:A:159:LEU:O	1:A:176:ILE:HG23	0.43	2.13	20	1
1:A:17:VAL:CG1	1:A:158:LEU:HD23	0.43	2.44	1	1
1:A:155:TYR:CZ	1:A:159:LEU:HD21	0.42	2.48	6	1
1:A:18:LEU:HD12	1:A:76:GLU:OE2	0.42	2.14	4	2
1:A:110:HIS:O	1:A:113:ALA:HB3	0.42	2.13	9	2
1:A:34:THR:O	1:A:38:THR:CB	0.42	2.68	9	1
1:A:18:LEU:HD23	1:A:80:LYS:CE	0.42	2.43	11	1
1:A:49:LEU:O	1:A:53:ASN:CB	0.42	2.67	7	1
1:A:26:ASN:O	1:A:30:LYS:CB	0.42	2.68	9	3
1:A:140:VAL:O	1:A:144:GLY:N	0.42	2.52	17	3
1:A:105:THR:O	1:A:109:ASN:N	0.42	2.52	13	2
1:A:158:LEU:O	1:A:162:LEU:N	0.42	2.51	14	1
1:A:121:SER:OG	1:A:139:LEU:HD21	0.42	2.14	3	1
1:A:81:LEU:N	1:A:81:LEU:HD23	0.42	2.29	2	1
1:A:69:GLN:O	1:A:73:GLN:CG	0.42	2.67	2	1
1:A:181:ALA:O	1:A:185:ASN:ND2	0.42	2.52	16	1
1:A:54:ILE:HG23	1:A:59:GLY:HA2	0.42	1.90	8	2
1:A:14:TYR:CE1	1:A:18:LEU:CD1	0.42	3.01	12	1
1:A:14:TYR:CZ	1:A:83:GLU:OE2	0.42	2.73	12	1
1:A:35:VAL:O	1:A:39:TYR:CB	0.42	2.68	18	1
1:A:32:LEU:HD12	1:A:68:GLN:OE1	0.42	2.15	4	1
1:A:57:LEU:HD11	1:A:141:LEU:HD11	0.42	1.91	5	1
1:A:83:GLU:CG	1:A:84:ALA:N	0.42	2.82	5	1
1:A:85:GLN:O	1:A:87:ARG:N	0.42	2.53	19	1
1:A:72:VAL:O	1:A:76:GLU:CG	0.42	2.67	9	3
1:A:141:LEU:O	1:A:145:LEU:N	0.42	2.51	1	3
1:A:139:LEU:H	1:A:139:LEU:HD22	0.42	1.74	5	3
1:A:43:LEU:HG	1:A:127:PHE:CE2	0.42	2.49	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:VAL:HG13	1:A:39:TYR:HD2	0.42	1.74	14	2
1:A:40:LEU:HD21	1:A:61:LEU:HD21	0.42	1.91	13	1
1:A:60:ASN:ND2	1:A:102:LEU:O	0.42	2.53	1	2
1:A:57:LEU:HD11	1:A:117:LEU:CD2	0.42	2.45	3	1
1:A:37:SER:O	1:A:41:ARG:CB	0.42	2.68	18	1
1:A:106:TYR:CE2	1:A:149:PHE:CD1	0.42	3.08	5	1
1:A:105:THR:CG2	1:A:109:ASN:OD1	0.42	2.68	8	1
1:A:25:GLU:OE1	1:A:72:VAL:HG22	0.42	2.14	10	1
1:A:110:HIS:N	1:A:111:PRO:HD2	0.42	2.30	14	2
1:A:18:LEU:HD23	1:A:80:LYS:HE2	0.42	1.92	11	1
1:A:92:PHE:O	1:A:96:MET:N	0.42	2.52	17	1
1:A:43:LEU:HB2	1:A:127:PHE:CZ	0.42	2.50	16	1
1:A:131:LYS:CG	1:A:131:LYS:O	0.42	2.67	16	1
1:A:123:GLU:CG	1:A:124:LEU:N	0.42	2.82	1	1
1:A:39:TYR:CD1	1:A:39:TYR:C	0.42	2.92	6	3
1:A:152:LEU:HD12	1:A:155:TYR:CD1	0.42	2.49	19	1
1:A:56:TYR:O	1:A:109:ASN:ND2	0.42	2.53	7	1
1:A:26:ASN:O	1:A:30:LYS:N	0.42	2.51	9	1
1:A:55:SER:O	1:A:109:ASN:ND2	0.42	2.53	20	1
1:A:18:LEU:HD13	1:A:162:LEU:HD21	0.42	1.90	1	1
1:A:148:PRO:HA	1:A:151:ARG:NH2	0.42	2.30	13	1
1:A:112:SER:O	1:A:115:ASN:N	0.42	2.53	4	1
1:A:103:TYR:CE2	1:A:152:LEU:HD11	0.42	2.50	16	1
1:A:155:TYR:CZ	1:A:183:PHE:CZ	0.42	3.08	20	1
1:A:75:LEU:HD22	1:A:92:PHE:CE2	0.41	2.50	7	1
1:A:115:ASN:O	1:A:119:GLU:CG	0.41	2.68	9	1
1:A:49:LEU:HD13	1:A:53:ASN:ND2	0.41	2.30	10	1
1:A:130:THR:O	1:A:131:LYS:CB	0.41	2.68	12	3
1:A:55:SER:O	1:A:105:THR:CG2	0.41	2.68	4	1
1:A:99:MET:HG3	1:A:103:TYR:CD1	0.41	2.50	16	1
1:A:21:ILE:HG22	1:A:25:GLU:HG2	0.41	1.92	10	1
1:A:41:ARG:CB	1:A:42:PRO:HD3	0.41	2.45	19	2
1:A:75:LEU:CD2	1:A:76:GLU:N	0.41	2.83	20	1
1:A:56:TYR:CD1	1:A:109:ASN:OD1	0.41	2.73	9	1
1:A:14:TYR:CE1	1:A:162:LEU:HD21	0.41	2.50	10	1
1:A:25:GLU:OE1	1:A:72:VAL:CG2	0.41	2.69	4	1
1:A:117:LEU:CD2	1:A:117:LEU:N	0.41	2.83	2	1
1:A:159:LEU:O	1:A:176:ILE:CG2	0.41	2.68	19	1
1:A:51:SER:O	1:A:52:ALA:CB	0.41	2.68	20	1
1:A:56:TYR:HE2	1:A:116:VAL:HG11	0.41	1.69	1	1
1:A:17:VAL:O	1:A:21:ILE:CD1	0.41	2.69	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:TYR:CD1	1:A:148:PRO:HB3	0.41	2.50	10	1
1:A:73:GLN:HG3	1:A:74:SER:N	0.41	2.31	10	1
1:A:21:ILE:HG23	1:A:25:GLU:OE1	0.41	2.16	12	1
1:A:75:LEU:HD12	1:A:76:GLU:N	0.41	2.31	14	1
1:A:25:GLU:O	1:A:28:TYR:N	0.41	2.53	3	1
1:A:163:GLU:HB2	1:A:176:ILE:CD1	0.41	2.46	6	1
1:A:135:SER:H	1:A:136:PRO:CD	0.41	2.29	13	2
1:A:32:LEU:O	1:A:36:LEU:N	0.41	2.52	3	1
1:A:117:LEU:HD11	1:A:141:LEU:CB	0.41	2.46	5	1
1:A:83:GLU:O	1:A:85:GLN:N	0.41	2.51	5	1
1:A:50:SER:O	1:A:51:SER:CB	0.41	2.68	7	1
1:A:147:LYS:O	1:A:151:ARG:NH1	0.41	2.54	15	1
1:A:96:MET:HB3	1:A:97:PRO:CD	0.41	2.46	14	1
1:A:21:ILE:HG21	1:A:158:LEU:HD12	0.41	1.91	18	1
1:A:86:GLN:NE2	1:A:162:LEU:HD13	0.41	2.30	16	1
1:A:110:HIS:HB3	1:A:111:PRO:CD	0.41	2.45	6	1
1:A:185:ASN:O	1:A:189:GLN:NE2	0.41	2.54	4	1
1:A:163:GLU:OE1	1:A:176:ILE:HD13	0.41	2.16	17	1
1:A:39:TYR:CG	1:A:128:MET:SD	0.41	3.14	9	1
1:A:155:TYR:CE2	1:A:183:PHE:CE2	0.41	3.09	9	1
1:A:21:ILE:CG2	1:A:25:GLU:OE1	0.41	2.69	12	1
1:A:67:PHE:CD1	1:A:71:LEU:HD22	0.41	2.49	4	1
1:A:114:VAL:HG22	1:A:142:THR:CG2	0.41	2.46	19	1
1:A:117:LEU:N	1:A:117:LEU:CD2	0.41	2.83	20	1
1:A:78:CYS:O	1:A:83:GLU:N	0.41	2.53	20	1
1:A:51:SER:OG	1:A:52:ALA:N	0.41	2.54	6	1
1:A:67:PHE:CE1	1:A:95:LEU:HG	0.41	2.51	10	2
1:A:67:PHE:CZ	1:A:71:LEU:CD1	0.41	3.03	18	1
1:A:138:ILE:CG1	1:A:138:ILE:O	0.41	2.69	18	1
1:A:21:ILE:HG13	1:A:158:LEU:HD21	0.41	1.92	5	1
1:A:79:THR:O	1:A:81:LEU:O	0.41	2.38	19	1
1:A:43:LEU:HB2	1:A:127:PHE:CE1	0.41	2.51	19	1
1:A:122:GLU:O	1:A:126:GLU:CB	0.41	2.69	10	1
1:A:147:LYS:N	1:A:148:PRO:HD3	0.41	2.31	14	2
1:A:124:LEU:O	1:A:127:PHE:CE2	0.41	2.73	4	1
1:A:29:SER:OG	1:A:68:GLN:NE2	0.40	2.54	7	1
1:A:156:PRO:HA	1:A:159:LEU:HG	0.40	1.93	18	1
1:A:42:PRO:HB2	1:A:127:PHE:CD1	0.40	2.51	6	1
1:A:87:ARG:NH1	1:A:175:ASP:OD2	0.40	2.54	6	1
1:A:109:ASN:O	1:A:112:SER:N	0.40	2.52	14	1
1:A:35:VAL:O	1:A:39:TYR:HB2	0.40	2.16	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:GLU:CD	1:A:86:GLN:CG	0.40	2.90	5	1
1:A:105:THR:O	1:A:109:ASN:ND2	0.40	2.54	19	1
1:A:124:LEU:CD1	1:A:138:ILE:HD12	0.40	2.46	15	1
1:A:158:LEU:HD22	1:A:162:LEU:HD23	0.40	1.92	14	1
1:A:83:GLU:HG2	1:A:86:GLN:CG	0.40	2.46	11	1
1:A:83:GLU:HG3	1:A:84:ALA:N	0.40	2.32	5	1
1:A:14:TYR:OH	1:A:86:GLN:CG	0.40	2.69	16	1
1:A:188:ALA:O	1:A:191:GLN:CG	0.40	2.69	8	1
1:A:64:ILE:O	1:A:68:GLN:N	0.40	2.49	20	1
1:A:103:TYR:CD2	1:A:186:LEU:HB3	0.40	2.51	1	1
1:A:133:ALA:HB1	1:A:137:GLY:O	0.40	2.17	7	1
1:A:100:LYS:HD3	1:A:101:THR:N	0.40	2.31	12	1
1:A:67:PHE:CZ	1:A:95:LEU:HG	0.40	2.51	15	1
1:A:41:ARG:CB	1:A:42:PRO:CD	0.40	2.99	13	1
1:A:117:LEU:HD12	1:A:142:THR:OG1	0.40	2.16	4	1
1:A:134:SER:OG	1:A:140:VAL:HG21	0.40	2.16	5	1
1:A:14:TYR:OH	1:A:86:GLN:CB	0.40	2.70	16	1
1:A:58:MET:O	1:A:62:GLU:CB	0.40	2.69	6	1
1:A:39:TYR:CB	1:A:132:GLY:O	0.40	2.69	15	1
1:A:128:MET:SD	1:A:133:ALA:CB	0.40	3.09	3	1
1:A:141:LEU:O	1:A:145:LEU:CG	0.40	2.69	17	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	165/209 (79%)	129±4 (78±3%)	28±4 (17±3%)	8±2 (5±1%)	5	28
All	All	3300/4180 (79%)	2576 (78%)	566 (17%)	158 (5%)	5	28

All 32 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	83	GLU	14

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Mol	Chain	Res	Type	Models (Total)
1	A	82	PRO	13
1	A	134	SER	11
1	A	51	SER	11
1	A	140	VAL	10
1	A	135	SER	10
1	A	50	SER	9
1	A	148	PRO	8
1	A	141	LEU	7
1	A	133	ALA	6
1	A	146	SER	6
1	A	81	LEU	6
1	A	59	GLY	5
1	A	129	GLU	4
1	A	142	THR	4
1	A	132	GLY	4
1	A	86	GLN	4
1	A	52	ALA	3
1	A	87	ARG	3
1	A	84	ALA	3
1	A	131	LYS	3
1	A	49	LEU	2
1	A	34	THR	2
1	A	74	SER	2
1	A	191	GLN	1
1	A	57	LEU	1
1	A	42	PRO	1
1	A	55	SER	1
1	A	54	ILE	1
1	A	36	LEU	1
1	A	38	THR	1
1	A	53	ASN	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	150/191 (79%)	109±5 (72±3%)	41±5 (28±3%)	<b>2</b> <b>21</b>

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3000/3820 (79%)	2172 (72%)	828 (28%)	<b>2</b> <b>21</b>

All 108 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	139	LEU	20
1	A	183	PHE	20
1	A	62	GLU	20
1	A	162	LEU	19
1	A	117	LEU	19
1	A	67	PHE	17
1	A	110	HIS	17
1	A	95	LEU	17
1	A	33	GLN	17
1	A	71	LEU	17
1	A	155	TYR	16
1	A	80	LYS	16
1	A	126	GLU	15
1	A	30	LYS	14
1	A	68	GLN	14
1	A	143	THR	14
1	A	96	MET	14
1	A	178	LYS	13
1	A	127	PHE	13
1	A	135	SER	13
1	A	81	LEU	13
1	A	141	LEU	12
1	A	13	TYR	12
1	A	187	SER	12
1	A	41	ARG	12
1	A	151	ARG	12
1	A	66	SER	11
1	A	129	GLU	11
1	A	142	THR	11
1	A	100	LYS	10
1	A	147	LYS	10
1	A	179	SER	10
1	A	160	LYS	10
1	A	40	LEU	10
1	A	138	ILE	10
1	A	184	LYS	10

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Mol	Chain	Res	Type	Models (Total)
1	A	153	ASP	10
1	A	150	MET	10
1	A	163	GLU	10
1	A	131	LYS	10
1	A	107	CYS	9
1	A	51	SER	9
1	A	91	CYS	9
1	A	56	TYR	9
1	A	146	SER	9
1	A	31	GLU	8
1	A	55	SER	8
1	A	128	MET	8
1	A	77	GLU	8
1	A	191	GLN	8
1	A	154	LYS	8
1	A	134	SER	7
1	A	57	LEU	7
1	A	53	ASN	7
1	A	103	TYR	7
1	A	58	MET	7
1	A	37	SER	6
1	A	149	PHE	6
1	A	50	SER	6
1	A	83	GLU	6
1	A	98	GLN	6
1	A	99	MET	6
1	A	15	ASN	5
1	A	121	SER	5
1	A	70	MET	5
1	A	94	ASN	5
1	A	78	CYS	5
1	A	69	GLN	4
1	A	180	MET	4
1	A	73	GLN	4
1	A	130	THR	4
1	A	20	ASN	4
1	A	115	ASN	4
1	A	19	GLN	4
1	A	177	GLN	3
1	A	75	LEU	3
1	A	22	LEU	3
1	A	161	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	189	GLN	3
1	A	123	GLU	3
1	A	86	GLN	3
1	A	28	TYR	3
1	A	109	ASN	3
1	A	176	ILE	3
1	A	106	TYR	3
1	A	112	SER	3
1	A	185	ASN	3
1	A	152	LEU	3
1	A	26	ASN	2
1	A	25	GLU	2
1	A	175	ASP	2
1	A	43	LEU	2
1	A	39	TYR	2
1	A	54	ILE	2
1	A	65	CYS	2
1	A	192	GLU	2
1	A	60	ASN	1
1	A	61	LEU	1
1	A	92	PHE	1
1	A	24	THR	1
1	A	18	LEU	1
1	A	87	ARG	1
1	A	164	ARG	1
1	A	35	VAL	1
1	A	122	GLU	1
1	A	190	CYS	1
1	A	14	TYR	1
1	A	29	SER	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no 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

No chemical shift data were provided