



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:19 PM BST

PDB ID : 1IH0  
Title : Structure of the C-domain of Human Cardiac Troponin C in Complex with Ca<sup>2+</sup> Sensitizer EMD 57033  
Authors : Wang, X.; Li, M.X.; Spyropoulos, L.; Beier, N.; Chandra, M.; Solaro, R.J.; Sykes, B.D.  
Deposited on : 2001-04-18

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 : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

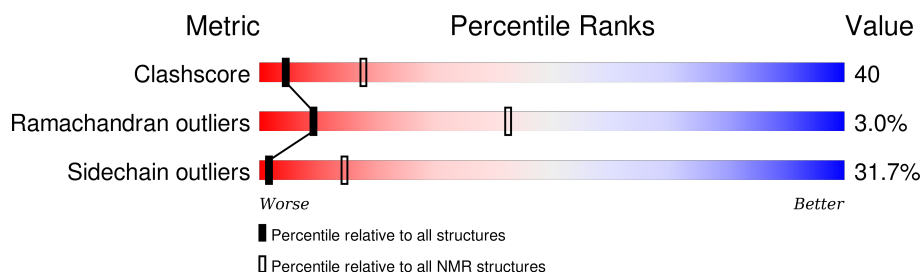
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 82%.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	71	

## 2 Ensemble composition and analysis ⓘ

This entry contains 30 models. Model 30 is the overall representative, medoid model (most similar to other models). The authors have identified model 11 as representative, based on the following criterion: *closest to the minimized average structure*.

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:93-A:161 (69)	0.53	30

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 5 single-model clusters were found.

Cluster number	Models
1	1, 3, 6, 7, 8, 11, 14, 15, 16, 20, 22, 25, 26, 30
2	2, 4, 5, 18, 27
3	9, 21
4	12, 29
5	13, 24
Single-model clusters	10; 17; 19; 23; 28

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

There are 3 unique types of molecules in this entry. The entry contains 1167 atoms, of which 559 are hydrogens and 0 are deuteriums.

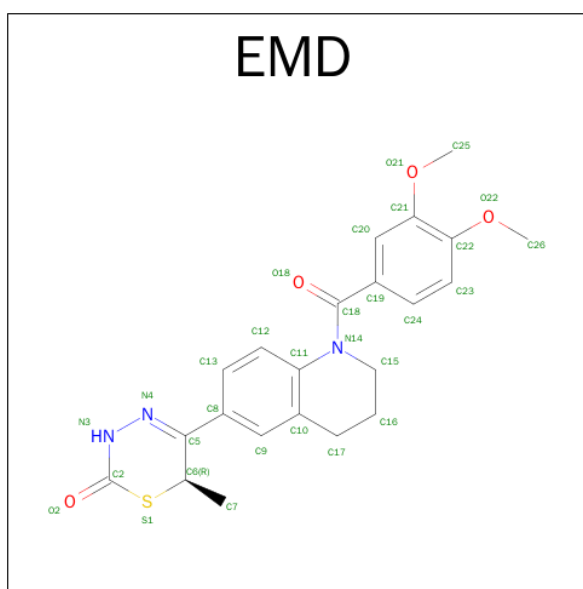
- Molecule 1 is a protein called TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES.

Mol	Chain	Residues	Atoms						Trace
1	A	71	Total	C	H	N	O	S	0
			1112	356	536	87	129	4	

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

Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

- Molecule 3 is 5-[1-(3,4-DIMETHOXY-BENZOYL)-1,2,3,4-TETRAHYDRO-QUINOLIN-6-YL]-6-METHYL-3,6-DIHYDRO-[1,3,4]THIADIAZIN-2-ONE (three-letter code: EMD) (formula: C<sub>22</sub>H<sub>23</sub>N<sub>3</sub>O<sub>4</sub>S).



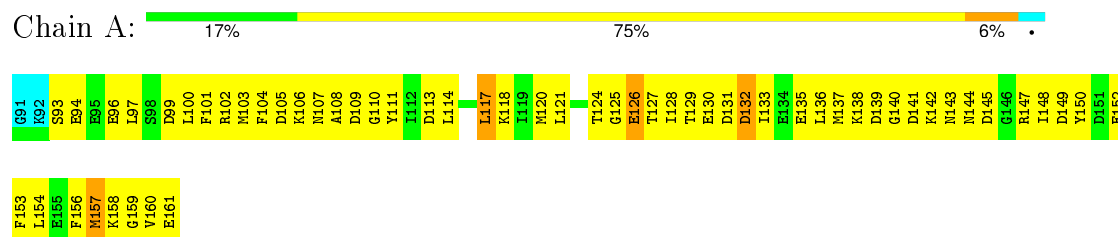
Mol	Chain	Residues	Atoms					
3	A	1	Total	C	H	N	O	S
			53	22	23	3	4	1

## 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: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES

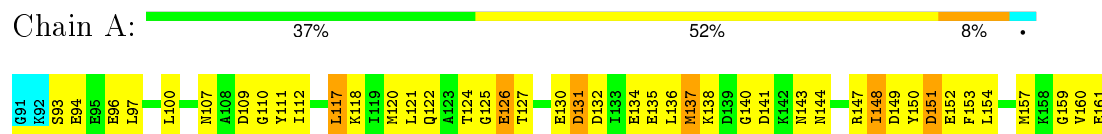


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

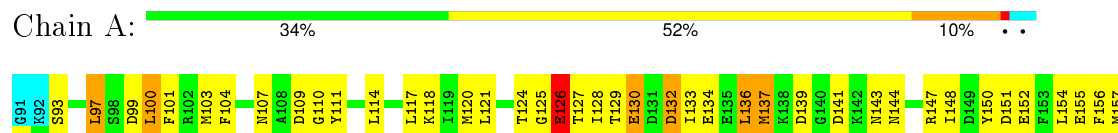
#### 4.2.1 Score per residue for model 1

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



#### 4.2.2 Score per residue for model 2

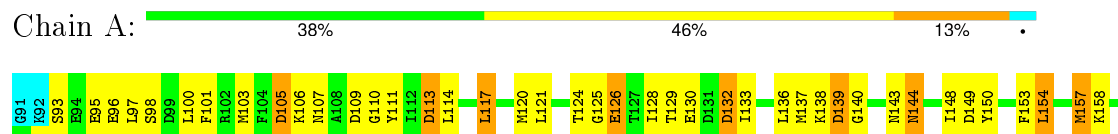
- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



K158  
G159  
V160  
E161

### 4.2.3 Score per residue for model 3

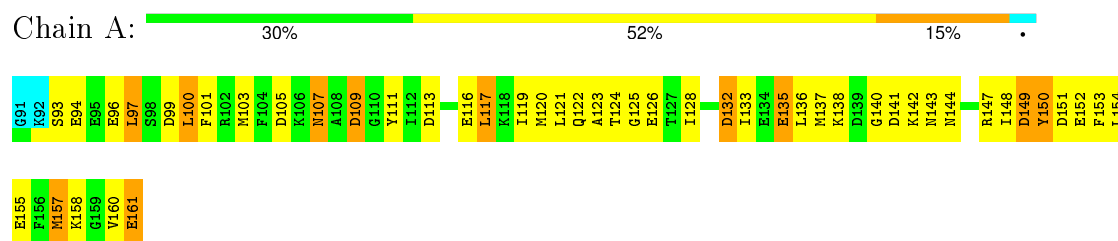
- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



E161

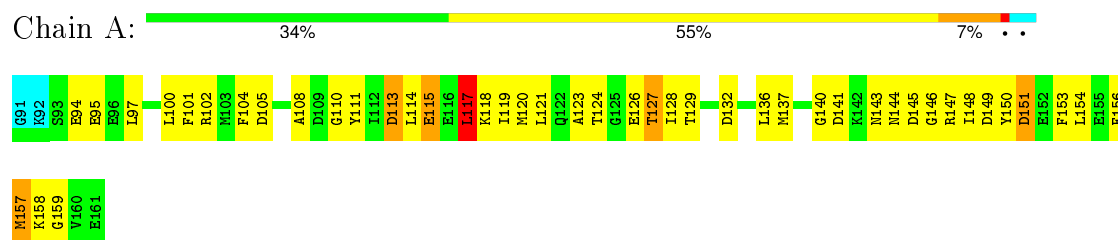
### 4.2.4 Score per residue for model 4

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



### 4.2.5 Score per residue for model 5

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



### 4.2.6 Score per residue for model 6

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES





#### 4.2.7 Score per residue for model 7

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES

Chain A: 38% 41% 18%



#### 4.2.8 Score per residue for model 8

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES

Chain A: 28% 58% 11%



#### 4.2.9 Score per residue for model 9

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES

Chain A: 28% 58% 10%

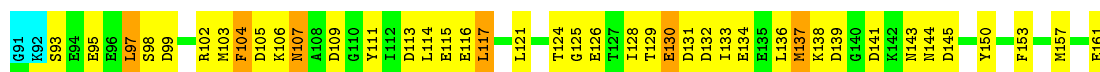


#### 4.2.10 Score per residue for model 10

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES

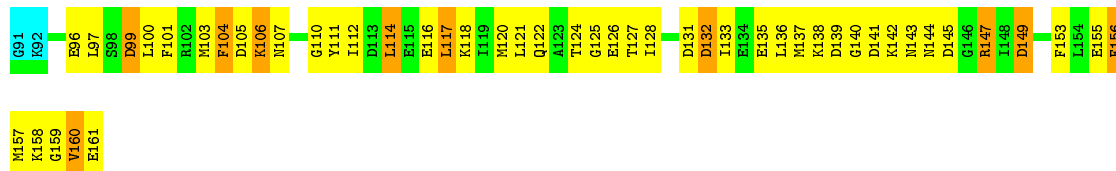
Chain A: 39% 49% 8%





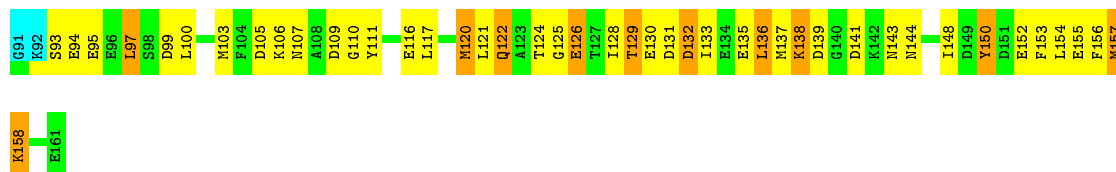
#### 4.2.11 Score per residue for model 11

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



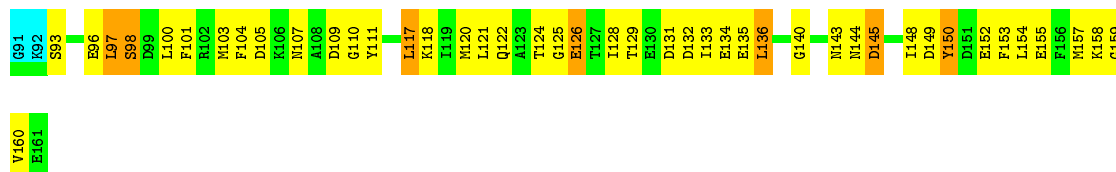
#### 4.2.12 Score per residue for model 12

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



#### 4.2.13 Score per residue for model 13

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES

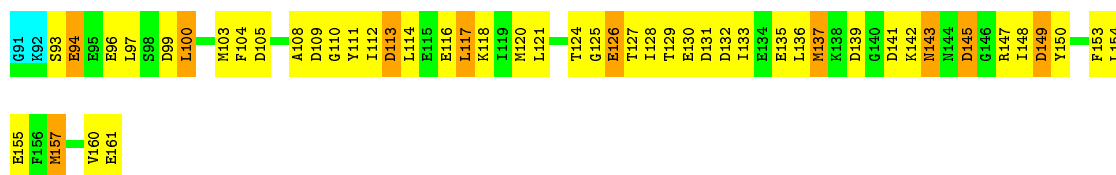


#### 4.2.14 Score per residue for model 14

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



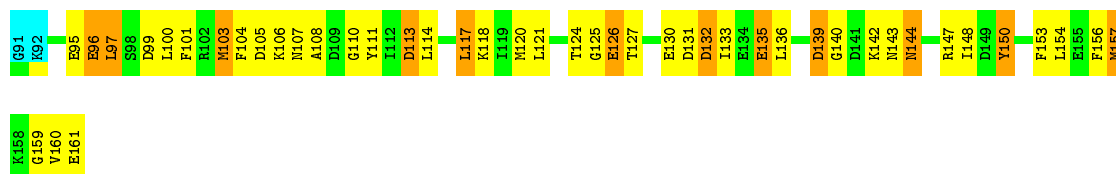




#### 4.2.15 Score per residue for model 15

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES

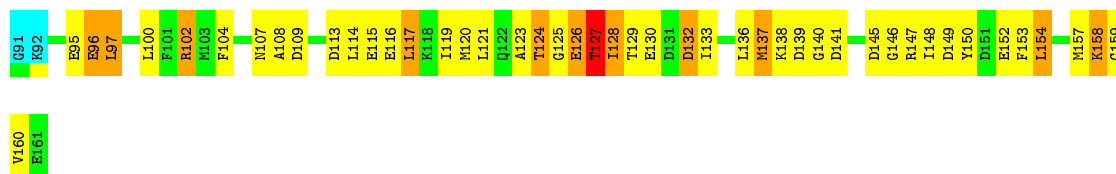
Chain A: 34% 46% 17%



#### 4.2.16 Score per residue for model 16

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES

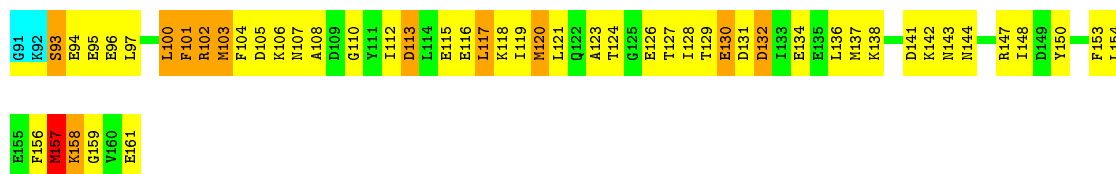
Chain A: 32% 48% 15%



#### 4.2.17 Score per residue for model 17

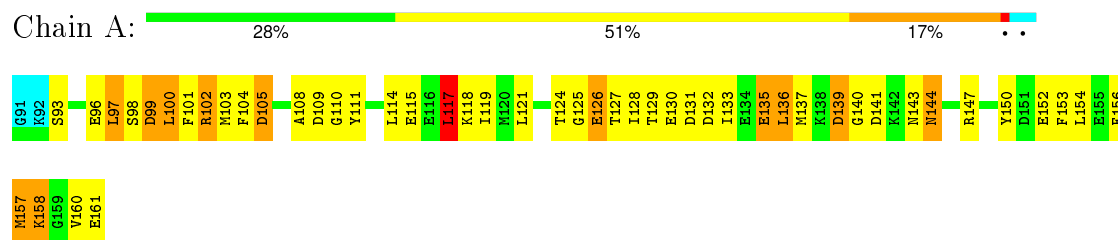
- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES

Chain A: 25% 55% 15%



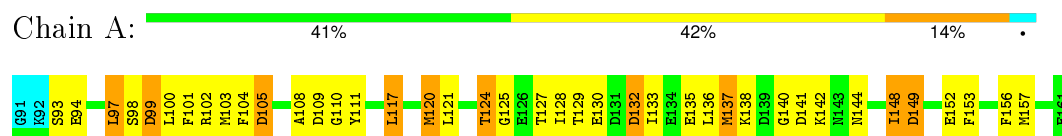
#### 4.2.18 Score per residue for model 18

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



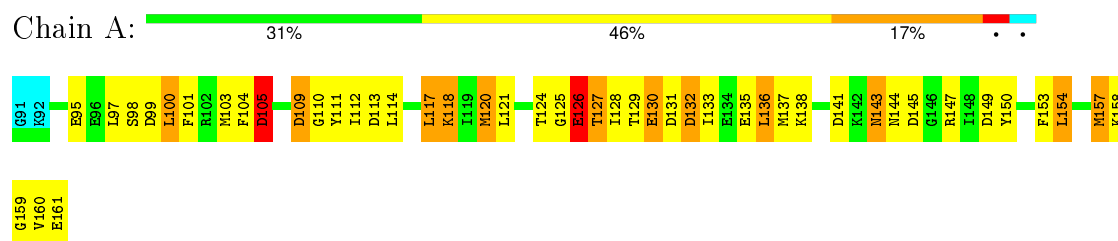
#### 4.2.19 Score per residue for model 19

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



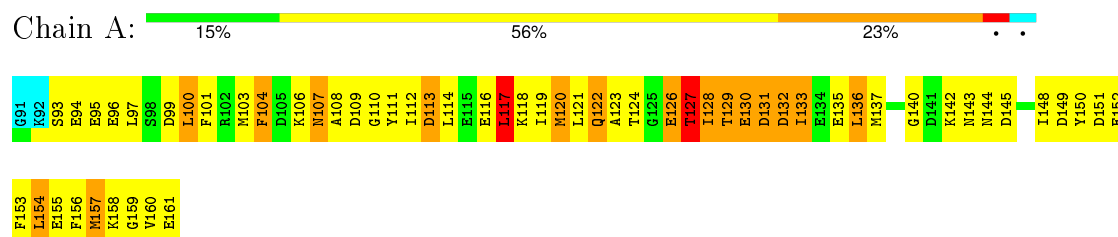
#### 4.2.20 Score per residue for model 20

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



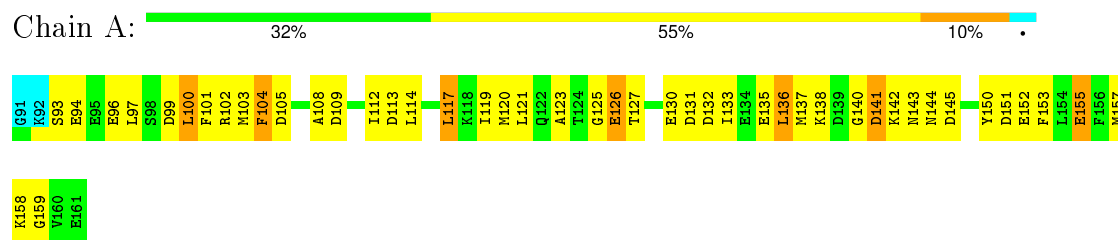
#### 4.2.21 Score per residue for model 21

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



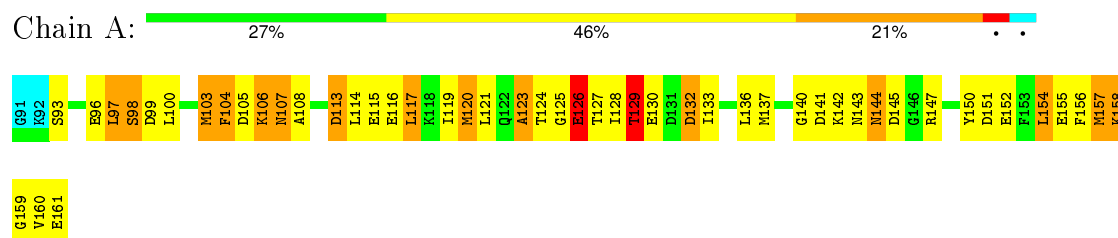
#### 4.2.22 Score per residue for model 22

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



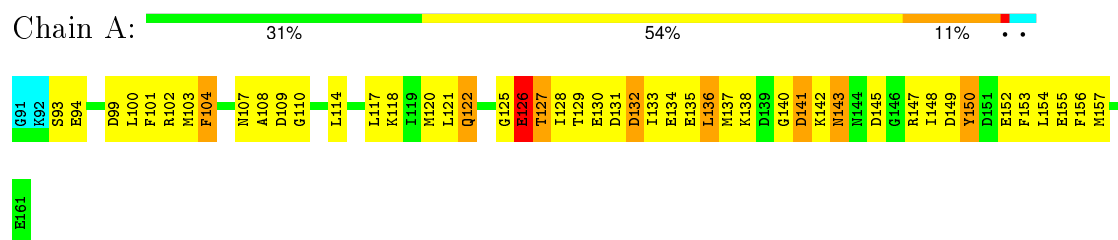
#### 4.2.23 Score per residue for model 23

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



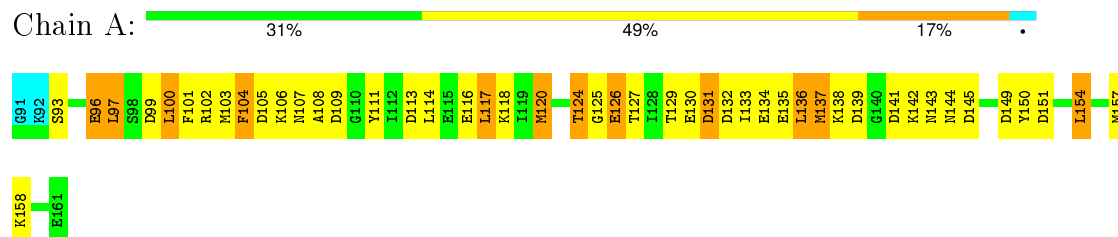
#### 4.2.24 Score per residue for model 24

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



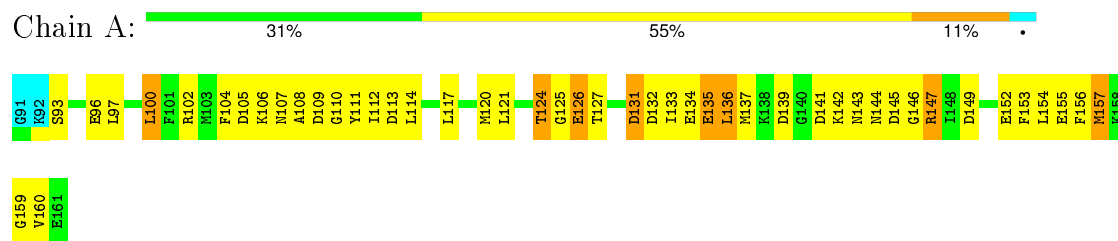
#### 4.2.25 Score per residue for model 25

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



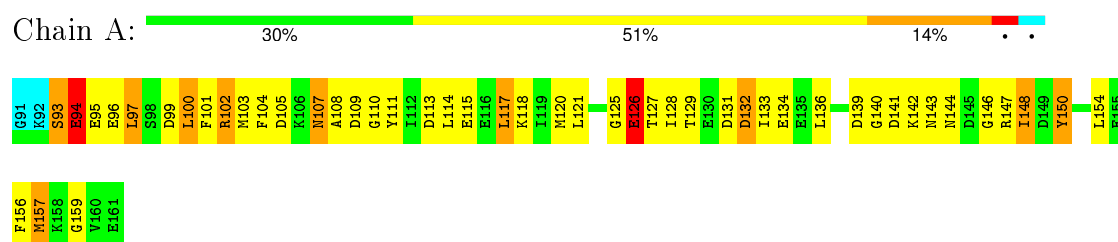
### 4.2.26 Score per residue for model 26

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



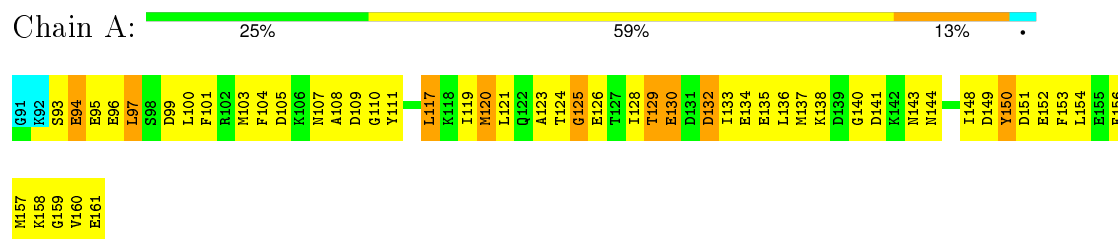
### 4.2.27 Score per residue for model 27

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



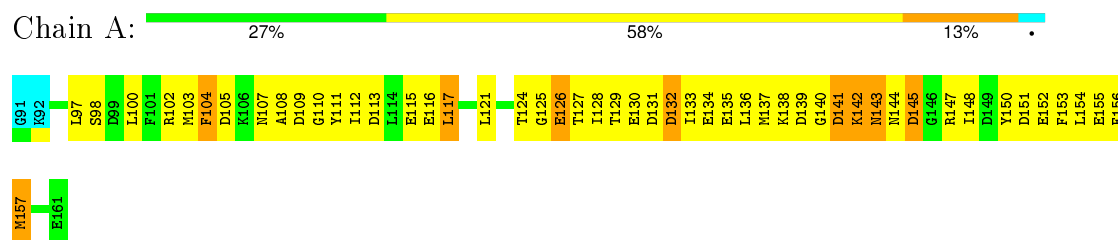
### 4.2.28 Score per residue for model 28

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



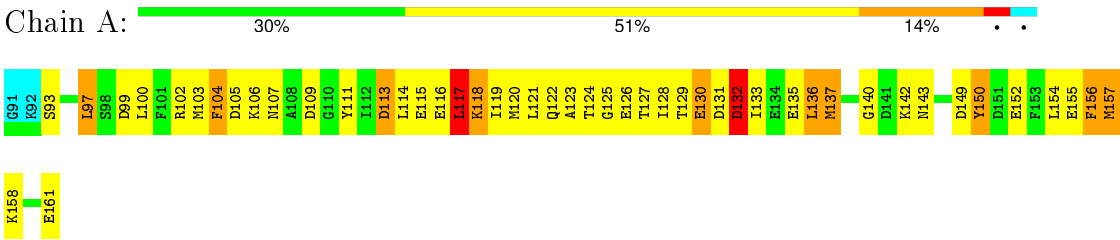
### 4.2.29 Score per residue for model 29

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



4.2.30 Score per residue for model 30 (medoid)

- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



## 5 Refinement protocol and experimental data overview

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

Of the 30 calculated structures, 30 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851

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

Chemical shift file(s)	BMRB entry 4994
Number of chemical shift lists	2
Total number of shifts	806
Number of shifts mapped to atoms	788
Number of unparsed shifts	0
Number of shifts with mapping errors	18
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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

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	563	520	520	44±9
3	A	30	23	23	8±4
All	All	17850	16290	16290	1367

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 40.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LEU:HD23	1:A:136:LEU:HD23	0.99	1.28	19	1
1:A:117:LEU:HD22	1:A:136:LEU:HD23	0.93	1.40	28	1
1:A:97:LEU:HD13	1:A:154:LEU:CD2	0.92	1.95	26	5
1:A:119:ILE:O	1:A:123:ALA:HB3	0.90	1.66	21	6
1:A:136:LEU:HD11	3:A:1:EMD:C12	0.90	1.96	17	3
1:A:97:LEU:HD13	1:A:154:LEU:HD23	0.89	1.42	6	6
1:A:100:LEU:HD22	1:A:157:MET:SD	0.89	2.08	8	4
1:A:100:LEU:HD11	1:A:160:VAL:O	0.89	1.67	20	8
1:A:97:LEU:HD11	1:A:157:MET:O	0.89	1.67	28	5
1:A:97:LEU:HD13	1:A:154:LEU:HD13	0.88	1.46	15	4
1:A:114:LEU:HD11	1:A:133:ILE:HG22	0.88	1.41	20	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:LEU:HD13	1:A:157:MET:SD	0.88	2.09	17	2
1:A:117:LEU:CD2	1:A:136:LEU:HD22	0.86	2.00	6	3
1:A:136:LEU:HD21	3:A:1:EMD:C13	0.85	2.00	28	5
1:A:117:LEU:CD2	1:A:136:LEU:HD23	0.84	2.01	19	2
1:A:117:LEU:HD11	3:A:1:EMD:C7	0.83	2.02	6	6
1:A:136:LEU:HD22	3:A:1:EMD:C13	0.83	2.04	26	11
1:A:136:LEU:HD11	3:A:1:EMD:C13	0.82	2.04	17	3
1:A:114:LEU:CD1	1:A:133:ILE:HG22	0.82	2.04	20	1
1:A:97:LEU:CD1	1:A:154:LEU:HD23	0.81	2.06	6	1
1:A:104:PHE:CE2	3:A:1:EMD:H71	0.79	2.13	10	2
1:A:127:THR:C	1:A:128:ILE:HD12	0.79	1.99	5	2
1:A:97:LEU:HD21	1:A:157:MET:O	0.78	1.78	7	15
1:A:93:SER:C	1:A:97:LEU:HD23	0.77	2.00	28	1
1:A:121:LEU:HB3	1:A:128:ILE:HD13	0.77	1.55	24	2
1:A:136:LEU:HD21	3:A:1:EMD:C12	0.77	2.08	19	1
1:A:124:THR:HG21	3:A:1:EMD:C23	0.77	2.10	8	2
1:A:112:ILE:HD13	1:A:153:PHE:CE2	0.76	2.16	26	2
1:A:136:LEU:HD22	3:A:1:EMD:H13	0.75	1.56	26	6
1:A:117:LEU:HD21	1:A:136:LEU:HD22	0.75	1.59	23	2
1:A:128:ILE:HG22	1:A:129:THR:N	0.74	1.98	21	7
1:A:154:LEU:O	1:A:154:LEU:HD13	0.74	1.82	23	1
1:A:121:LEU:O	1:A:124:THR:HG22	0.73	1.83	5	8
1:A:136:LEU:HD23	1:A:136:LEU:O	0.73	1.82	16	3
1:A:137:MET:HG2	1:A:148:ILE:HD11	0.73	1.61	28	1
1:A:100:LEU:HD22	1:A:157:MET:CE	0.72	2.14	5	2
1:A:120:MET:O	1:A:124:THR:HG23	0.72	1.84	26	4
1:A:160:VAL:O	1:A:160:VAL:HG12	0.71	1.86	6	1
1:A:121:LEU:HD13	1:A:128:ILE:CD1	0.71	2.15	12	1
1:A:121:LEU:HD22	1:A:128:ILE:HD13	0.71	1.61	18	2
1:A:150:TYR:CE1	1:A:154:LEU:HD23	0.70	2.21	23	1
1:A:136:LEU:HD21	1:A:156:PHE:CE1	0.70	2.21	12	1
1:A:112:ILE:HD13	1:A:153:PHE:CE1	0.70	2.21	17	1
1:A:114:LEU:HD11	1:A:133:ILE:CG2	0.70	2.16	18	7
1:A:136:LEU:HD22	3:A:1:EMD:N4	0.69	2.03	7	6
1:A:136:LEU:HD13	1:A:136:LEU:C	0.69	2.08	8	1
1:A:101:PHE:CD1	1:A:153:PHE:CG	0.69	2.81	22	1
1:A:128:ILE:HD13	1:A:132:ASP:OD2	0.68	1.88	17	1
1:A:136:LEU:HD11	3:A:1:EMD:H13	0.68	1.65	8	3
1:A:97:LEU:HD21	1:A:159:GLY:N	0.68	2.02	28	3
1:A:121:LEU:HD12	1:A:133:ILE:HG13	0.68	1.65	21	1
1:A:126:GLU:OE1	1:A:128:ILE:HD12	0.68	1.89	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:PHE:CZ	3:A:1:EMD:H71	0.68	2.22	7	2
1:A:136:LEU:HD21	3:A:1:EMD:H13	0.67	1.64	23	4
1:A:97:LEU:CD1	1:A:154:LEU:HD13	0.67	2.18	3	3
1:A:130:GLU:HA	1:A:133:ILE:HD12	0.67	1.67	20	5
1:A:117:LEU:HD11	3:A:1:EMD:H73	0.66	1.66	13	9
1:A:157:MET:HB2	1:A:160:VAL:HG22	0.65	1.68	20	1
1:A:124:THR:HG21	3:A:1:EMD:H24	0.65	1.66	26	1
1:A:101:PHE:CE1	1:A:112:ILE:HD12	0.65	2.26	22	1
1:A:97:LEU:HD22	1:A:154:LEU:HD22	0.65	1.67	30	3
1:A:97:LEU:HD13	1:A:154:LEU:HD22	0.65	1.69	13	1
1:A:121:LEU:HD12	1:A:133:ILE:HD11	0.64	1.67	10	1
1:A:114:LEU:HD13	1:A:137:MET:SD	0.64	2.32	22	2
1:A:150:TYR:O	1:A:154:LEU:HD12	0.64	1.92	4	4
1:A:124:THR:HG23	1:A:124:THR:O	0.64	1.93	13	3
1:A:124:THR:HG21	3:A:1:EMD:C24	0.63	2.24	26	3
1:A:107:ASN:O	1:A:108:ALA:HB3	0.62	1.93	7	11
1:A:156:PHE:CE2	3:A:1:EMD:N4	0.62	2.66	6	1
1:A:114:LEU:HD11	1:A:133:ILE:HG23	0.62	1.71	18	1
1:A:104:PHE:CE1	1:A:112:ILE:HG21	0.62	2.30	22	3
1:A:160:VAL:HG12	1:A:161:GLU:OE1	0.62	1.93	4	1
1:A:150:TYR:O	1:A:154:LEU:HD23	0.62	1.94	16	4
1:A:97:LEU:HD22	1:A:154:LEU:HD23	0.62	1.71	13	2
1:A:118:LYS:CG	1:A:133:ILE:HD13	0.62	2.25	8	1
1:A:121:LEU:HD13	1:A:128:ILE:HD13	0.61	1.72	12	1
1:A:132:ASP:O	1:A:136:LEU:HD12	0.61	1.95	3	1
1:A:136:LEU:HD21	1:A:156:PHE:CZ	0.61	2.31	15	1
1:A:100:LEU:HD21	1:A:161:GLU:O	0.60	1.94	21	1
1:A:117:LEU:HD22	1:A:136:LEU:HD22	0.60	1.73	6	1
1:A:117:LEU:HD21	3:A:1:EMD:H71	0.60	1.72	28	1
1:A:121:LEU:HD12	1:A:133:ILE:HG12	0.60	1.73	27	3
1:A:120:MET:O	1:A:124:THR:HG22	0.59	1.97	13	4
1:A:128:ILE:HG21	1:A:132:ASP:HB2	0.59	1.73	17	1
1:A:136:LEU:HD13	3:A:1:EMD:C12	0.59	2.28	12	2
1:A:121:LEU:HD13	1:A:128:ILE:HG21	0.59	1.73	11	3
1:A:97:LEU:CD2	1:A:159:GLY:CA	0.59	2.81	22	2
1:A:117:LEU:HD23	1:A:121:LEU:HD11	0.59	1.72	23	1
1:A:115:GLU:O	1:A:119:ILE:HD12	0.59	1.98	18	2
1:A:100:LEU:HD11	1:A:161:GLU:N	0.59	2.13	6	1
1:A:127:THR:HG22	1:A:127:THR:O	0.58	1.97	19	4
1:A:117:LEU:CD2	1:A:136:LEU:CD2	0.58	2.81	6	1
1:A:114:LEU:HD21	1:A:133:ILE:O	0.58	1.98	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:LEU:CD2	3:A:1:EMD:N4	0.58	2.66	7	9
1:A:94:GLU:HG2	1:A:154:LEU:HD22	0.58	1.75	17	1
1:A:148:ILE:HG21	3:A:1:EMD:S1	0.58	2.38	15	3
1:A:156:PHE:CD1	3:A:1:EMD:N3	0.58	2.71	19	1
1:A:148:ILE:HD12	3:A:1:EMD:S1	0.57	2.39	15	4
1:A:97:LEU:HD21	1:A:159:GLY:H	0.57	1.57	28	1
1:A:100:LEU:HD11	1:A:157:MET:HE3	0.57	1.77	18	1
1:A:97:LEU:HD21	1:A:159:GLY:CA	0.57	2.30	27	5
1:A:136:LEU:O	1:A:136:LEU:HD23	0.57	1.99	11	4
1:A:121:LEU:HD22	3:A:1:EMD:O18	0.57	1.99	30	2
1:A:97:LEU:HD13	1:A:154:LEU:CD1	0.57	2.26	15	2
1:A:114:LEU:HD11	1:A:137:MET:SD	0.57	2.40	10	2
1:A:143:ASN:O	1:A:144:ASN:CB	0.57	2.52	15	3
1:A:136:LEU:HD21	3:A:1:EMD:C5	0.57	2.29	6	1
1:A:104:PHE:CE1	1:A:120:MET:SD	0.57	2.98	25	3
1:A:153:PHE:CD1	1:A:157:MET:SD	0.57	2.98	20	2
1:A:153:PHE:CZ	1:A:157:MET:SD	0.56	2.98	3	8
1:A:153:PHE:CE1	1:A:157:MET:SD	0.56	2.98	20	6
1:A:153:PHE:CE2	1:A:157:MET:SD	0.56	2.98	13	3
1:A:153:PHE:CZ	1:A:157:MET:CG	0.56	2.88	15	3
1:A:150:TYR:CD2	1:A:154:LEU:HD11	0.56	2.35	27	2
1:A:128:ILE:CG2	1:A:132:ASP:CB	0.56	2.83	3	5
1:A:129:THR:HG23	1:A:129:THR:O	0.56	2.00	9	1
1:A:121:LEU:HD12	1:A:133:ILE:HD13	0.56	1.77	6	1
1:A:150:TYR:O	1:A:150:TYR:CD2	0.56	2.59	29	1
1:A:124:THR:HG21	3:A:1:EMD:H23	0.55	1.77	8	1
1:A:136:LEU:HD21	3:A:1:EMD:N4	0.55	2.17	6	2
1:A:125:GLY:O	1:A:127:THR:HG23	0.55	2.01	22	1
1:A:153:PHE:CE1	1:A:157:MET:CG	0.55	2.90	5	2
1:A:119:ILE:O	1:A:123:ALA:HB2	0.54	2.02	6	2
1:A:110:GLY:C	1:A:111:TYR:CD1	0.54	2.81	18	13
1:A:111:TYR:CZ	1:A:149:ASP:OD1	0.54	2.61	21	1
1:A:97:LEU:HD23	1:A:153:PHE:CE2	0.54	2.37	19	1
1:A:118:LYS:HE2	1:A:133:ILE:HG21	0.54	1.79	18	1
1:A:150:TYR:CE1	1:A:154:LEU:CD2	0.54	2.91	21	1
1:A:153:PHE:CE1	1:A:157:MET:HE2	0.54	2.38	19	4
1:A:104:PHE:CZ	1:A:120:MET:SD	0.54	3.01	9	2
1:A:110:GLY:O	1:A:111:TYR:CD1	0.54	2.61	28	9
1:A:150:TYR:CG	1:A:150:TYR:O	0.54	2.60	29	1
1:A:126:GLU:O	1:A:128:ILE:CD1	0.54	2.56	16	1
1:A:104:PHE:CD1	1:A:120:MET:SD	0.54	3.00	23	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:THR:OG1	1:A:130:GLU:N	0.54	2.41	21	5
1:A:119:ILE:O	1:A:123:ALA:CB	0.54	2.56	6	4
1:A:101:PHE:CZ	1:A:110:GLY:O	0.54	2.61	24	5
1:A:143:ASN:OD1	1:A:145:ASP:CB	0.53	2.56	24	2
1:A:122:GLN:N	1:A:126:GLU:OE2	0.53	2.40	21	1
1:A:128:ILE:CG2	1:A:129:THR:N	0.53	2.71	9	8
1:A:112:ILE:CG2	1:A:113:ASP:N	0.53	2.71	21	1
1:A:104:PHE:CZ	1:A:120:MET:CB	0.53	2.92	17	2
1:A:131:ASP:O	1:A:135:GLU:CB	0.53	2.56	18	8
1:A:132:ASP:O	1:A:136:LEU:CB	0.53	2.57	25	9
1:A:150:TYR:O	1:A:154:LEU:CD1	0.53	2.57	13	2
1:A:99:ASP:O	1:A:103:MET:N	0.53	2.41	23	5
1:A:137:MET:CE	1:A:146:GLY:O	0.53	2.57	9	2
1:A:126:GLU:O	1:A:127:THR:CG2	0.53	2.56	1	1
1:A:153:PHE:O	1:A:157:MET:CB	0.53	2.57	12	6
1:A:104:PHE:CZ	1:A:120:MET:HB2	0.53	2.39	28	2
1:A:125:GLY:O	1:A:127:THR:N	0.53	2.42	20	7
1:A:140:GLY:CA	3:A:1:EMD:O2	0.53	2.56	13	10
1:A:121:LEU:CD2	3:A:1:EMD:O18	0.53	2.57	14	14
1:A:107:ASN:O	1:A:108:ALA:CB	0.53	2.56	7	5
1:A:136:LEU:HD13	1:A:136:LEU:O	0.53	2.04	8	1
1:A:101:PHE:CA	1:A:153:PHE:CE2	0.53	2.92	19	2
1:A:137:MET:O	1:A:141:ASP:CB	0.52	2.57	10	2
1:A:121:LEU:O	1:A:125:GLY:N	0.52	2.42	19	4
1:A:117:LEU:O	1:A:120:MET:N	0.52	2.42	6	8
1:A:107:ASN:ND2	1:A:116:GLU:OE2	0.52	2.42	4	3
1:A:109:ASP:OD1	1:A:110:GLY:N	0.52	2.43	18	7
1:A:158:LYS:O	1:A:158:LYS:CG	0.52	2.57	12	3
1:A:150:TYR:O	1:A:154:LEU:N	0.52	2.42	20	7
1:A:107:ASN:OD1	1:A:108:ALA:N	0.52	2.43	7	2
1:A:100:LEU:HD22	1:A:157:MET:CG	0.52	2.35	2	1
1:A:107:ASN:CB	1:A:116:GLU:OE2	0.52	2.57	11	2
1:A:128:ILE:CG2	1:A:132:ASP:HB2	0.52	2.34	19	9
1:A:117:LEU:HD13	1:A:137:MET:HG3	0.52	1.82	25	1
1:A:143:ASN:ND2	1:A:152:GLU:OE2	0.52	2.43	26	8
1:A:100:LEU:HD22	1:A:157:MET:HE2	0.52	1.81	5	1
1:A:101:PHE:HA	1:A:153:PHE:CE2	0.52	2.40	13	3
1:A:101:PHE:HE1	1:A:112:ILE:HD12	0.52	1.63	22	1
1:A:101:PHE:N	1:A:153:PHE:CE2	0.52	2.78	19	1
1:A:154:LEU:O	1:A:154:LEU:CD1	0.52	2.57	23	1
1:A:113:ASP:OD1	1:A:115:GLU:N	0.52	2.43	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:GLU:O	1:A:128:ILE:HD12	0.52	2.03	16	2
1:A:160:VAL:HG12	1:A:161:GLU:N	0.52	2.19	9	2
1:A:137:MET:O	1:A:140:GLY:N	0.52	2.43	8	1
1:A:137:MET:O	1:A:141:ASP:N	0.52	2.43	28	5
1:A:136:LEU:HD23	1:A:136:LEU:C	0.52	2.25	6	4
1:A:97:LEU:HD11	1:A:158:LYS:HA	0.52	1.80	16	2
1:A:143:ASN:OD1	1:A:144:ASN:N	0.52	2.43	2	3
1:A:120:MET:O	1:A:124:THR:CG2	0.52	2.58	23	2
1:A:112:ILE:O	1:A:147:ARG:CG	0.52	2.58	6	2
1:A:133:ILE:O	1:A:137:MET:CB	0.52	2.57	4	3
1:A:96:GLU:O	1:A:99:ASP:N	0.52	2.43	28	6
1:A:101:PHE:HA	1:A:153:PHE:CZ	0.52	2.40	19	6
1:A:148:ILE:HD12	3:A:1:EMD:O2	0.52	2.05	15	2
1:A:145:ASP:OD2	1:A:147:ARG:NH1	0.52	2.43	29	1
1:A:114:LEU:CD1	1:A:133:ILE:O	0.52	2.58	20	1
1:A:114:LEU:O	1:A:117:LEU:N	0.52	2.43	5	1
1:A:119:ILE:N	1:A:119:ILE:HD13	0.52	2.19	22	1
1:A:99:ASP:O	1:A:102:ARG:CG	0.52	2.58	25	1
1:A:153:PHE:O	1:A:157:MET:N	0.51	2.43	7	4
1:A:101:PHE:CD2	1:A:153:PHE:CG	0.51	2.99	4	1
1:A:135:GLU:O	1:A:138:LYS:N	0.51	2.43	11	1
1:A:114:LEU:HD22	1:A:133:ILE:HG22	0.51	1.79	23	1
1:A:141:ASP:O	1:A:144:ASN:N	0.51	2.44	22	13
1:A:153:PHE:CZ	1:A:157:MET:CE	0.51	2.94	4	2
1:A:128:ILE:CG2	1:A:132:ASP:HB3	0.51	2.35	3	1
1:A:109:ASP:OD1	1:A:109:ASP:N	0.51	2.44	24	5
1:A:153:PHE:CE1	1:A:157:MET:HG2	0.51	2.40	5	2
1:A:105:ASP:OD2	1:A:111:TYR:N	0.51	2.44	28	2
1:A:114:LEU:CG	1:A:133:ILE:HG22	0.51	2.35	20	1
1:A:153:PHE:CE1	1:A:157:MET:HB3	0.51	2.41	12	2
1:A:127:THR:O	1:A:127:THR:HG22	0.51	2.05	14	2
1:A:129:THR:HG23	1:A:130:GLU:N	0.51	2.21	2	2
1:A:124:THR:OG1	1:A:125:GLY:N	0.51	2.42	29	1
1:A:121:LEU:CD1	1:A:133:ILE:CD1	0.51	2.88	13	1
1:A:143:ASN:ND2	1:A:145:ASP:OD2	0.51	2.44	13	1
1:A:156:PHE:CD2	3:A:1:EMD:N4	0.51	2.78	6	1
1:A:112:ILE:HG22	1:A:117:LEU:HD12	0.51	1.80	8	2
1:A:121:LEU:O	1:A:124:THR:N	0.51	2.44	29	6
1:A:160:VAL:O	1:A:160:VAL:CG1	0.51	2.58	6	1
1:A:129:THR:O	1:A:133:ILE:HD12	0.51	2.04	2	1
1:A:135:GLU:O	1:A:139:ASP:N	0.51	2.44	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:GLU:O	1:A:133:ILE:N	0.51	2.44	12	2
1:A:147:ARG:CG	1:A:148:ILE:N	0.51	2.74	2	3
1:A:126:GLU:N	1:A:126:GLU:OE1	0.51	2.42	21	1
1:A:128:ILE:HG22	1:A:129:THR:H	0.51	1.66	17	1
1:A:157:MET:CE	1:A:160:VAL:O	0.51	2.59	16	1
1:A:149:ASP:OD1	1:A:149:ASP:N	0.51	2.44	13	2
1:A:93:SER:O	1:A:95:GLU:N	0.51	2.44	27	3
1:A:99:ASP:O	1:A:103:MET:CG	0.51	2.59	15	3
1:A:102:ARG:O	1:A:105:ASP:N	0.50	2.43	27	4
1:A:97:LEU:O	1:A:100:LEU:N	0.50	2.43	21	4
1:A:114:LEU:HD11	1:A:133:ILE:O	0.50	2.06	20	1
1:A:150:TYR:CD2	1:A:154:LEU:CD2	0.50	2.94	15	1
1:A:143:ASN:N	1:A:152:GLU:OE2	0.50	2.44	1	6
1:A:126:GLU:OE1	1:A:127:THR:N	0.50	2.45	21	1
1:A:156:PHE:CD2	3:A:1:EMD:N3	0.50	2.79	28	2
1:A:93:SER:O	1:A:97:LEU:HD23	0.50	2.06	28	1
1:A:153:PHE:CD1	1:A:157:MET:HB2	0.50	2.42	6	1
1:A:121:LEU:O	1:A:124:THR:CG2	0.50	2.59	2	2
1:A:118:LYS:HG3	1:A:133:ILE:HD13	0.50	1.82	8	1
1:A:136:LEU:HD13	3:A:1:EMD:H12	0.50	1.82	22	1
1:A:114:LEU:HD13	1:A:137:MET:HG3	0.50	1.83	2	2
1:A:120:MET:O	1:A:123:ALA:HB3	0.50	2.07	16	1
1:A:136:LEU:HD23	1:A:139:ASP:HB2	0.50	1.83	2	1
1:A:148:ILE:CG2	3:A:1:EMD:S1	0.50	2.99	15	1
1:A:107:ASN:ND2	1:A:109:ASP:OD1	0.50	2.45	16	2
1:A:114:LEU:HD12	1:A:114:LEU:H	0.50	1.67	21	1
1:A:106:LYS:HE2	1:A:119:ILE:HD13	0.50	1.81	23	1
1:A:151:ASP:N	1:A:151:ASP:OD1	0.50	2.44	5	1
1:A:136:LEU:HD22	1:A:136:LEU:O	0.50	2.06	8	1
1:A:129:THR:O	1:A:130:GLU:CB	0.50	2.59	12	2
1:A:153:PHE:CD1	1:A:153:PHE:O	0.50	2.64	11	1
1:A:120:MET:C	1:A:124:THR:HG22	0.50	2.27	23	1
1:A:128:ILE:HD12	1:A:128:ILE:N	0.49	2.22	5	1
1:A:148:ILE:HD12	3:A:1:EMD:C2	0.49	2.37	15	2
1:A:94:GLU:O	1:A:97:LEU:N	0.49	2.45	14	1
1:A:107:ASN:ND2	1:A:109:ASP:OD2	0.49	2.44	27	1
1:A:117:LEU:HD11	3:A:1:EMD:H71	0.49	1.83	15	1
1:A:153:PHE:CZ	1:A:157:MET:CB	0.49	2.95	16	1
1:A:100:LEU:HD13	1:A:157:MET:CG	0.49	2.38	22	2
3:A:1:EMD:C15	3:A:1:EMD:C24	0.49	2.91	5	6
1:A:113:ASP:OD1	1:A:113:ASP:N	0.49	2.45	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:LEU:O	1:A:103:MET:N	0.49	2.46	23	2
1:A:153:PHE:CE1	1:A:157:MET:HB2	0.49	2.43	29	3
1:A:121:LEU:CD1	1:A:133:ILE:HG12	0.49	2.38	26	1
1:A:136:LEU:CD2	3:A:1:EMD:C13	0.49	2.90	19	2
1:A:128:ILE:CG2	1:A:132:ASP:CG	0.49	2.81	23	1
1:A:153:PHE:CZ	1:A:157:MET:HG2	0.49	2.43	5	5
1:A:150:TYR:O	1:A:154:LEU:CG	0.49	2.61	27	4
1:A:124:THR:CG2	3:A:1:EMD:C23	0.49	2.88	8	1
1:A:112:ILE:O	1:A:147:ARG:CB	0.48	2.61	1	1
1:A:127:THR:O	1:A:127:THR:OG1	0.48	2.31	16	1
1:A:100:LEU:HD23	1:A:103:MET:SD	0.48	2.48	29	2
1:A:128:ILE:C	1:A:129:THR:HG22	0.48	2.29	23	1
1:A:125:GLY:C	1:A:126:GLU:CG	0.48	2.81	6	7
3:A:1:EMD:C24	3:A:1:EMD:H151	0.48	2.38	5	2
1:A:118:LYS:CG	1:A:133:ILE:CD1	0.48	2.92	24	1
1:A:121:LEU:HD21	3:A:1:EMD:O18	0.48	2.08	15	4
1:A:128:ILE:HG21	1:A:133:ILE:CD1	0.48	2.38	16	1
1:A:111:TYR:CD1	1:A:147:ARG:HD2	0.48	2.43	8	2
1:A:102:ARG:HG3	1:A:103:MET:N	0.48	2.22	30	3
1:A:157:MET:SD	1:A:160:VAL:CG2	0.48	3.02	28	1
1:A:117:LEU:HD21	3:A:1:EMD:N4	0.48	2.23	21	4
1:A:112:ILE:HG22	1:A:113:ASP:N	0.48	2.23	21	1
1:A:124:THR:O	3:A:1:EMD:C24	0.48	2.62	12	1
1:A:160:VAL:CG1	1:A:161:GLU:N	0.48	2.75	9	1
1:A:136:LEU:O	1:A:139:ASP:OD2	0.48	2.31	18	1
1:A:121:LEU:O	1:A:126:GLU:CB	0.48	2.62	28	1
1:A:156:PHE:CE1	3:A:1:EMD:N4	0.48	2.81	19	1
1:A:131:ASP:N	1:A:131:ASP:OD1	0.48	2.46	10	1
1:A:112:ILE:O	1:A:148:ILE:N	0.48	2.44	29	2
1:A:112:ILE:N	1:A:112:ILE:HD13	0.48	2.23	20	2
1:A:101:PHE:C	1:A:101:PHE:CD1	0.48	2.87	11	5
1:A:100:LEU:O	1:A:103:MET:CG	0.48	2.61	21	1
1:A:153:PHE:CE1	1:A:157:MET:CB	0.47	2.97	6	4
3:A:1:EMD:H151	3:A:1:EMD:C24	0.47	2.39	12	7
1:A:132:ASP:O	1:A:136:LEU:N	0.47	2.45	23	3
1:A:105:ASP:OD1	1:A:108:ALA:HB3	0.47	2.09	19	1
1:A:149:ASP:N	1:A:152:GLU:OE1	0.47	2.47	26	2
1:A:147:ARG:C	1:A:148:ILE:HD13	0.47	2.30	4	1
1:A:136:LEU:O	1:A:139:ASP:N	0.47	2.47	3	3
1:A:148:ILE:HG21	1:A:153:PHE:HD1	0.47	1.69	17	1
1:A:100:LEU:HD12	1:A:159:GLY:HA2	0.47	1.84	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:MET:HE1	3:A:1:EMD:C17	0.47	2.40	8	1
1:A:111:TYR:CD2	1:A:147:ARG:HD3	0.47	2.44	5	2
1:A:97:LEU:CD2	1:A:159:GLY:N	0.47	2.77	5	2
3:A:1:EMD:C24	3:A:1:EMD:C15	0.47	2.92	13	3
1:A:150:TYR:CE2	1:A:154:LEU:HD11	0.47	2.44	27	1
1:A:132:ASP:O	1:A:136:LEU:HB2	0.47	2.10	25	13
1:A:145:ASP:OD1	1:A:146:GLY:N	0.47	2.47	26	2
1:A:121:LEU:O	1:A:126:GLU:N	0.47	2.46	23	1
1:A:136:LEU:CD1	3:A:1:EMD:H13	0.47	2.38	23	1
1:A:153:PHE:O	1:A:157:MET:CG	0.47	2.63	24	1
1:A:109:ASP:OD2	1:A:111:TYR:O	0.47	2.33	14	6
1:A:121:LEU:N	1:A:121:LEU:HD23	0.47	2.24	5	1
1:A:126:GLU:HG3	1:A:127:THR:N	0.47	2.25	1	2
1:A:110:GLY:O	1:A:111:TYR:CG	0.47	2.67	8	5
1:A:143:ASN:ND2	1:A:152:GLU:CD	0.47	2.68	12	4
1:A:149:ASP:N	1:A:149:ASP:OD1	0.47	2.47	11	1
1:A:109:ASP:N	1:A:109:ASP:OD1	0.47	2.48	19	5
1:A:143:ASN:CB	1:A:152:GLU:OE2	0.47	2.63	13	2
1:A:121:LEU:O	1:A:123:ALA:N	0.47	2.48	7	1
1:A:150:TYR:CE1	1:A:154:LEU:HD21	0.47	2.45	21	1
1:A:144:ASN:ND2	1:A:144:ASN:O	0.47	2.47	8	1
1:A:128:ILE:HG23	1:A:132:ASP:HB2	0.47	1.86	12	1
1:A:149:ASP:O	1:A:153:PHE:CB	0.47	2.63	1	3
1:A:121:LEU:HD12	1:A:133:ILE:CD1	0.47	2.40	13	2
1:A:143:ASN:O	1:A:144:ASN:ND2	0.47	2.48	3	1
1:A:97:LEU:CD2	1:A:159:GLY:HA2	0.47	2.39	21	1
1:A:121:LEU:HD13	1:A:128:ILE:HD12	0.47	1.84	12	1
1:A:97:LEU:CD1	1:A:154:LEU:CD2	0.47	2.92	9	1
1:A:111:TYR:CD1	1:A:147:ARG:HD3	0.47	2.45	14	1
1:A:143:ASN:O	1:A:144:ASN:OD1	0.47	2.33	15	1
1:A:154:LEU:O	1:A:157:MET:N	0.47	2.47	13	1
1:A:104:PHE:CD1	1:A:112:ILE:HG12	0.47	2.45	22	1
1:A:99:ASP:N	1:A:99:ASP:OD1	0.47	2.45	19	1
1:A:118:LYS:HG2	1:A:133:ILE:CD1	0.47	2.40	24	1
1:A:118:LYS:O	1:A:121:LEU:N	0.47	2.44	27	2
1:A:118:LYS:HE3	1:A:133:ILE:HG21	0.47	1.87	6	1
1:A:136:LEU:HD11	3:A:1:EMD:H12	0.47	1.79	17	1
1:A:104:PHE:CG	1:A:120:MET:SD	0.47	3.08	19	2
1:A:118:LYS:HE2	1:A:133:ILE:HD13	0.47	1.86	20	1
1:A:144:ASN:O	1:A:144:ASN:OD1	0.47	2.33	20	1
1:A:114:LEU:HD22	1:A:133:ILE:CG2	0.47	2.40	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:ASP:OD2	1:A:109:ASP:OD1	0.46	2.33	26	6
1:A:148:ILE:CG2	1:A:149:ASP:N	0.46	2.78	19	1
1:A:105:ASP:OD1	1:A:109:ASP:OD1	0.46	2.32	8	2
1:A:149:ASP:OD1	1:A:150:TYR:N	0.46	2.46	5	2
1:A:113:ASP:OD1	1:A:116:GLU:OE2	0.46	2.34	6	3
1:A:101:PHE:CE1	1:A:110:GLY:C	0.46	2.88	17	1
1:A:157:MET:CE	3:A:1:EMD:H171	0.46	2.40	8	2
1:A:128:ILE:CG2	1:A:133:ILE:CD1	0.46	2.93	16	1
1:A:137:MET:CE	1:A:146:GLY:C	0.46	2.84	5	1
1:A:100:LEU:HD22	1:A:157:MET:HG2	0.46	1.88	2	2
1:A:97:LEU:HD11	1:A:159:GLY:N	0.46	2.25	23	1
1:A:141:ASP:OD1	1:A:143:ASN:OD1	0.46	2.33	2	2
1:A:97:LEU:HD12	1:A:154:LEU:CD2	0.46	2.41	9	2
1:A:144:ASN:OD1	1:A:144:ASN:O	0.46	2.33	1	1
1:A:147:ARG:HG2	1:A:148:ILE:N	0.46	2.25	2	1
1:A:125:GLY:O	1:A:126:GLU:C	0.46	2.54	2	18
1:A:141:ASP:OD1	1:A:147:ARG:O	0.46	2.33	29	5
1:A:157:MET:O	1:A:157:MET:CG	0.46	2.62	4	2
1:A:126:GLU:OE1	3:A:1:EMD:C26	0.46	2.64	28	1
1:A:111:TYR:CE2	1:A:149:ASP:OD2	0.46	2.69	30	1
1:A:145:ASP:OD1	1:A:145:ASP:N	0.46	2.49	23	1
1:A:122:GLN:O	1:A:126:GLU:CG	0.46	2.63	24	1
1:A:150:TYR:CD2	1:A:154:LEU:HD21	0.46	2.45	15	1
1:A:126:GLU:C	1:A:127:THR:HG22	0.46	2.31	1	1
1:A:153:PHE:CZ	1:A:157:MET:HE3	0.46	2.45	22	1
1:A:116:GLU:O	1:A:119:ILE:N	0.46	2.49	16	1
1:A:113:ASP:O	1:A:117:LEU:HD12	0.46	2.10	22	2
1:A:136:LEU:CD2	3:A:1:EMD:H13	0.46	2.41	6	2
1:A:121:LEU:HD11	1:A:136:LEU:HD22	0.46	1.87	28	1
1:A:136:LEU:HD13	3:A:1:EMD:C13	0.46	2.41	12	1
1:A:121:LEU:CD1	1:A:133:ILE:HG13	0.46	2.41	16	2
1:A:140:GLY:O	3:A:1:EMD:O2	0.46	2.33	5	2
1:A:107:ASN:OD1	1:A:109:ASP:OD1	0.46	2.34	1	2
1:A:136:LEU:CG	3:A:1:EMD:H13	0.46	2.40	6	1
1:A:140:GLY:O	1:A:141:ASP:C	0.46	2.54	22	1
1:A:104:PHE:O	1:A:106:LYS:N	0.46	2.49	11	1
3:A:1:EMD:H12	3:A:1:EMD:O18	0.46	2.11	13	17
1:A:121:LEU:CD1	1:A:133:ILE:HD11	0.46	2.41	10	1
3:A:1:EMD:O18	3:A:1:EMD:H12	0.46	2.11	23	13
1:A:125:GLY:O	1:A:126:GLU:O	0.46	2.34	26	2
1:A:153:PHE:O	1:A:157:MET:HB3	0.45	2.11	21	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:THR:O	1:A:131:ASP:N	0.45	2.47	25	3
1:A:103:MET:HG3	1:A:104:PHE:N	0.45	2.26	29	4
1:A:111:TYR:CD2	1:A:148:ILE:O	0.45	2.68	21	1
1:A:103:MET:SD	1:A:104:PHE:N	0.45	2.89	30	1
1:A:156:PHE:CD1	1:A:156:PHE:O	0.45	2.70	29	1
1:A:157:MET:SD	1:A:160:VAL:HG21	0.45	2.51	9	1
1:A:126:GLU:O	1:A:128:ILE:N	0.45	2.50	20	4
1:A:107:ASN:OD1	1:A:109:ASP:CB	0.45	2.64	6	1
1:A:113:ASP:N	1:A:113:ASP:OD1	0.45	2.49	21	1
1:A:137:MET:O	1:A:141:ASP:HB2	0.45	2.11	10	7
1:A:136:LEU:CD1	3:A:1:EMD:C12	0.45	2.94	22	1
1:A:148:ILE:HG21	1:A:153:PHE:CD1	0.45	2.47	16	1
1:A:140:GLY:HA2	1:A:156:PHE:CE2	0.45	2.46	11	1
1:A:128:ILE:O	1:A:129:THR:CB	0.45	2.64	23	1
1:A:128:ILE:CG1	1:A:132:ASP:HB2	0.45	2.42	24	1
1:A:126:GLU:O	1:A:127:THR:C	0.45	2.55	18	4
1:A:120:MET:O	1:A:124:THR:HG21	0.45	2.12	21	1
1:A:151:ASP:CG	1:A:152:GLU:N	0.45	2.70	2	1
1:A:152:GLU:O	1:A:155:GLU:N	0.45	2.50	22	1
1:A:127:THR:HG23	1:A:127:THR:O	0.45	2.11	25	1
1:A:143:ASN:O	1:A:144:ASN:CG	0.45	2.55	15	2
1:A:128:ILE:HG12	1:A:132:ASP:CB	0.45	2.42	24	1
1:A:131:ASP:O	1:A:135:GLU:HB3	0.45	2.12	18	5
1:A:139:ASP:OD1	1:A:139:ASP:C	0.45	2.55	18	1
1:A:160:VAL:O	1:A:161:GLU:O	0.45	2.35	18	1
1:A:101:PHE:CD1	1:A:101:PHE:O	0.45	2.70	27	1
1:A:160:VAL:HG12	1:A:160:VAL:O	0.45	2.11	21	1
1:A:126:GLU:C	1:A:127:THR:CG2	0.45	2.85	16	2
1:A:153:PHE:CD2	1:A:157:MET:SD	0.45	3.10	4	1
1:A:143:ASN:O	1:A:143:ASN:OD1	0.45	2.35	5	1
1:A:117:LEU:HD21	1:A:136:LEU:CD2	0.45	2.37	23	2
1:A:153:PHE:CE1	1:A:157:MET:CE	0.45	2.99	19	3
1:A:101:PHE:O	1:A:105:ASP:N	0.45	2.45	13	1
1:A:128:ILE:HG23	1:A:132:ASP:OD2	0.45	2.11	13	1
1:A:157:MET:CE	3:A:1:EMD:C17	0.45	2.95	8	2
1:A:121:LEU:O	1:A:126:GLU:HA	0.44	2.12	23	1
1:A:121:LEU:CD1	1:A:133:ILE:HD13	0.44	2.42	22	2
1:A:157:MET:SD	1:A:160:VAL:HG23	0.44	2.53	11	1
1:A:96:GLU:O	1:A:97:LEU:C	0.44	2.56	23	9
1:A:156:PHE:CB	3:A:1:EMD:O2	0.44	2.65	5	1
1:A:125:GLY:O	1:A:126:GLU:HG3	0.44	2.12	11	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:SER:O	1:A:94:GLU:C	0.44	2.55	27	6
1:A:114:LEU:HG	1:A:133:ILE:CG2	0.44	2.43	11	2
1:A:114:LEU:HD23	1:A:133:ILE:CG2	0.44	2.41	10	1
1:A:153:PHE:O	1:A:157:MET:HB2	0.44	2.12	17	3
1:A:141:ASP:OD2	1:A:146:GLY:N	0.44	2.50	27	1
1:A:107:ASN:CG	1:A:108:ALA:N	0.44	2.70	17	1
1:A:136:LEU:CD1	1:A:136:LEU:C	0.44	2.80	8	1
1:A:114:LEU:HD23	1:A:133:ILE:HG22	0.44	1.88	10	1
1:A:118:LYS:HG2	1:A:133:ILE:HD13	0.44	1.89	8	2
1:A:107:ASN:OD1	1:A:109:ASP:N	0.44	2.51	2	1
1:A:94:GLU:HG3	1:A:154:LEU:HD22	0.44	1.89	24	1
1:A:153:PHE:CD1	1:A:157:MET:HB3	0.44	2.47	12	2
1:A:153:PHE:CE2	1:A:157:MET:CE	0.44	3.00	4	1
1:A:125:GLY:O	1:A:126:GLU:HG2	0.44	2.13	8	1
1:A:143:ASN:OD1	1:A:143:ASN:C	0.44	2.56	2	2
1:A:129:THR:O	1:A:130:GLU:HB2	0.44	2.12	12	1
1:A:114:LEU:CD1	1:A:137:MET:HB2	0.44	2.43	6	1
1:A:102:ARG:CG	1:A:103:MET:N	0.44	2.81	30	1
1:A:148:ILE:CD1	3:A:1:EMD:S1	0.44	3.06	4	2
1:A:101:PHE:CD2	1:A:153:PHE:CD2	0.44	3.06	13	1
1:A:107:ASN:OD1	1:A:109:ASP:CG	0.44	2.56	6	2
1:A:107:ASN:O	1:A:107:ASN:OD1	0.44	2.36	9	3
1:A:124:THR:CG2	1:A:125:GLY:N	0.44	2.80	28	1
1:A:107:ASN:HB2	1:A:116:GLU:OE2	0.44	2.13	8	2
1:A:113:ASP:O	1:A:116:GLU:N	0.44	2.50	25	2
1:A:157:MET:O	1:A:157:MET:HG2	0.44	2.13	4	2
1:A:94:GLU:CA	1:A:94:GLU:OE1	0.44	2.63	27	1
1:A:133:ILE:O	1:A:137:MET:HB2	0.44	2.13	25	4
1:A:121:LEU:O	1:A:122:GLN:C	0.44	2.56	7	2
1:A:150:TYR:O	1:A:154:LEU:CB	0.43	2.66	27	2
1:A:143:ASN:OD1	1:A:145:ASP:N	0.43	2.51	26	2
1:A:114:LEU:O	1:A:114:LEU:HD12	0.43	2.12	3	1
1:A:113:ASP:C	1:A:137:MET:CE	0.43	2.86	6	1
1:A:114:LEU:O	1:A:115:GLU:C	0.43	2.57	5	1
1:A:126:GLU:O	1:A:127:THR:HB	0.43	2.13	17	3
1:A:105:ASP:OD1	1:A:116:GLU:OE2	0.43	2.36	12	1
1:A:101:PHE:CD1	1:A:101:PHE:C	0.43	2.91	19	1
1:A:112:ILE:O	1:A:147:ARG:HG2	0.43	2.11	6	1
1:A:132:ASP:OD1	1:A:136:LEU:HD12	0.43	2.13	15	1
1:A:122:GLN:HA	1:A:126:GLU:CB	0.43	2.43	13	1
1:A:128:ILE:O	1:A:129:THR:HB	0.43	2.13	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:PHE:CE1	1:A:112:ILE:CD1	0.43	3.00	22	1
1:A:94:GLU:CA	1:A:97:LEU:HB2	0.43	2.42	12	1
1:A:140:GLY:HA3	3:A:1:EMD:O2	0.43	2.13	28	6
1:A:100:LEU:O	1:A:103:MET:HG2	0.43	2.13	22	1
1:A:153:PHE:O	1:A:157:MET:HG2	0.43	2.13	24	1
1:A:143:ASN:C	1:A:143:ASN:OD1	0.43	2.57	4	1
1:A:149:ASP:OD1	1:A:152:GLU:CG	0.43	2.67	1	1
1:A:125:GLY:O	1:A:126:GLU:CD	0.43	2.56	27	1
1:A:93:SER:C	1:A:95:GLU:N	0.43	2.71	28	1
1:A:111:TYR:CD2	1:A:147:ARG:HD2	0.43	2.49	2	1
1:A:107:ASN:N	1:A:107:ASN:OD1	0.43	2.51	16	1
1:A:149:ASP:OD2	1:A:152:GLU:OE2	0.43	2.37	4	1
1:A:121:LEU:O	1:A:124:THR:OG1	0.43	2.33	4	1
1:A:117:LEU:O	1:A:118:LYS:C	0.43	2.57	21	6
1:A:112:ILE:O	1:A:147:ARG:CA	0.43	2.67	1	1
1:A:131:ASP:O	1:A:135:GLU:HB2	0.43	2.13	12	3
1:A:97:LEU:O	1:A:98:SER:C	0.43	2.57	29	4
1:A:140:GLY:O	1:A:148:ILE:CD1	0.43	2.66	13	1
1:A:97:LEU:CD2	1:A:157:MET:O	0.43	2.62	3	1
1:A:106:LYS:HE2	1:A:119:ILE:CD1	0.43	2.44	6	1
1:A:115:GLU:O	1:A:119:ILE:CD1	0.43	2.66	17	1
1:A:106:LYS:N	1:A:116:GLU:OE2	0.43	2.47	30	1
1:A:157:MET:SD	1:A:160:VAL:O	0.43	2.76	11	1
1:A:121:LEU:HD22	1:A:128:ILE:CD1	0.43	2.43	23	1
1:A:114:LEU:O	1:A:116:GLU:N	0.43	2.52	9	1
1:A:114:LEU:CD1	1:A:137:MET:HG3	0.43	2.44	16	1
1:A:100:LEU:O	1:A:101:PHE:C	0.43	2.57	18	2
1:A:143:ASN:CG	1:A:152:GLU:OE2	0.43	2.57	18	2
1:A:153:PHE:CG	1:A:157:MET:SD	0.43	3.12	4	1
1:A:160:VAL:O	1:A:161:GLU:OXT	0.43	2.36	6	1
1:A:141:ASP:OD1	1:A:144:ASN:N	0.43	2.50	19	1
1:A:143:ASN:O	1:A:144:ASN:C	0.43	2.57	3	1
1:A:127:THR:CG2	1:A:127:THR:O	0.43	2.67	19	1
1:A:134:GLU:O	1:A:138:LYS:N	0.42	2.50	25	1
1:A:110:GLY:C	1:A:111:TYR:CG	0.42	2.92	14	1
1:A:140:GLY:C	3:A:1:EMD:O2	0.42	2.57	27	5
1:A:148:ILE:C	1:A:149:ASP:OD1	0.42	2.57	14	2
1:A:132:ASP:O	1:A:136:LEU:HD13	0.42	2.13	28	1
1:A:156:PHE:CG	3:A:1:EMD:C2	0.42	3.02	8	1
1:A:145:ASP:OD2	1:A:147:ARG:NE	0.42	2.51	20	2
1:A:94:GLU:HA	1:A:97:LEU:HB2	0.42	1.91	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:ASP:OD2	1:A:152:GLU:OE1	0.42	2.37	19	1
1:A:102:ARG:NH1	1:A:102:ARG:HB2	0.42	2.29	16	1
1:A:149:ASP:O	1:A:150:TYR:C	0.42	2.57	28	3
1:A:107:ASN:CG	1:A:107:ASN:O	0.42	2.57	8	2
1:A:100:LEU:O	1:A:103:MET:HG3	0.42	2.13	21	3
1:A:109:ASP:OD1	1:A:111:TYR:N	0.42	2.47	21	1
1:A:143:ASN:ND2	1:A:152:GLU:OE1	0.42	2.51	21	1
1:A:117:LEU:HD21	3:A:1:EMD:C7	0.42	2.42	28	1
1:A:156:PHE:CD2	3:A:1:EMD:C2	0.42	3.03	28	1
1:A:131:ASP:O	1:A:132:ASP:CB	0.42	2.67	30	1
1:A:99:ASP:O	1:A:102:ARG:HG2	0.42	2.12	25	1
1:A:114:LEU:HD11	1:A:133:ILE:C	0.42	2.35	20	1
1:A:107:ASN:OD1	1:A:107:ASN:C	0.42	2.57	2	1
1:A:93:SER:O	1:A:96:GLU:N	0.42	2.49	22	1
1:A:129:THR:O	1:A:129:THR:HG23	0.42	2.14	24	1
1:A:125:GLY:O	1:A:126:GLU:CG	0.42	2.68	26	2
1:A:143:ASN:O	1:A:144:ASN:HB3	0.42	2.15	27	1
1:A:128:ILE:HG23	1:A:132:ASP:CB	0.42	2.45	3	1
1:A:115:GLU:O	1:A:118:LYS:HG2	0.42	2.15	30	1
1:A:140:GLY:HA2	1:A:156:PHE:CD1	0.42	2.50	30	1
1:A:140:GLY:O	1:A:148:ILE:HG12	0.42	2.14	19	1
1:A:105:ASP:OD2	1:A:109:ASP:N	0.42	2.44	29	1
1:A:122:GLN:HA	1:A:126:GLU:CA	0.42	2.44	1	1
1:A:107:ASN:C	1:A:107:ASN:OD1	0.42	2.58	7	1
1:A:97:LEU:HG	1:A:154:LEU:HD23	0.42	1.91	28	1
1:A:134:GLU:O	1:A:138:LYS:CB	0.42	2.68	25	1
1:A:143:ASN:OD1	1:A:145:ASP:HB2	0.42	2.13	24	2
1:A:117:LEU:HD21	3:A:1:EMD:H13	0.42	1.91	18	1
1:A:136:LEU:O	1:A:140:GLY:N	0.42	2.52	21	1
1:A:105:ASP:OD2	1:A:110:GLY:N	0.42	2.51	6	1
1:A:105:ASP:OD1	1:A:108:ALA:C	0.42	2.57	17	1
1:A:134:GLU:O	1:A:138:LYS:HB2	0.42	2.14	17	1
1:A:158:LYS:O	1:A:159:GLY:C	0.42	2.57	17	1
1:A:114:LEU:HG	1:A:133:ILE:HG21	0.42	1.91	9	1
1:A:157:MET:CE	1:A:160:VAL:HB	0.42	2.45	15	1
1:A:124:THR:CG2	1:A:124:THR:O	0.42	2.64	13	1
1:A:105:ASP:HB2	1:A:112:ILE:CD1	0.42	2.45	8	1
1:A:126:GLU:O	1:A:128:ILE:HG12	0.42	2.15	20	1
1:A:138:LYS:O	1:A:138:LYS:CG	0.41	2.68	16	1
1:A:143:ASN:OD1	1:A:145:ASP:CG	0.41	2.58	14	2
1:A:107:ASN:OD1	1:A:109:ASP:HB3	0.41	2.15	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:ASN:CG	1:A:144:ASN:O	0.41	2.57	15	2
1:A:129:THR:CG2	1:A:132:ASP:OD1	0.41	2.68	23	1
1:A:112:ILE:O	1:A:147:ARG:HA	0.41	2.15	1	1
1:A:153:PHE:CD1	3:A:1:EMD:S1	0.41	3.13	17	1
1:A:154:LEU:HD22	1:A:154:LEU:HA	0.41	1.75	25	2
1:A:141:ASP:O	1:A:142:LYS:C	0.41	2.59	27	3
1:A:139:ASP:OD1	1:A:156:PHE:CE1	0.41	2.73	27	1
1:A:121:LEU:C	1:A:123:ALA:N	0.41	2.72	7	1
1:A:111:TYR:HB3	1:A:147:ARG:CD	0.41	2.45	6	1
1:A:153:PHE:CZ	1:A:157:MET:HG3	0.41	2.50	17	1
1:A:137:MET:O	1:A:138:LYS:C	0.41	2.59	12	1
1:A:140:GLY:HA2	3:A:1:EMD:O2	0.41	2.15	29	1
1:A:95:GLU:HG3	1:A:96:GLU:N	0.41	2.30	9	1
1:A:152:GLU:O	1:A:156:PHE:HB2	0.41	2.15	24	1
1:A:99:ASP:OD1	1:A:99:ASP:N	0.41	2.51	14	1
1:A:121:LEU:HD13	1:A:128:ILE:CG2	0.41	2.45	10	1
1:A:126:GLU:O	1:A:127:THR:HG22	0.41	2.15	1	1
1:A:121:LEU:O	1:A:126:GLU:HB2	0.41	2.15	28	1
1:A:131:ASP:OD1	1:A:135:GLU:OE2	0.41	2.37	30	1
1:A:128:ILE:HD13	1:A:132:ASP:HB3	0.41	1.93	12	1
1:A:149:ASP:OD1	1:A:149:ASP:C	0.41	2.58	24	1
1:A:125:GLY:C	1:A:126:GLU:HG2	0.41	2.35	6	2
1:A:150:TYR:O	1:A:151:ASP:C	0.41	2.58	5	1
1:A:143:ASN:HB3	1:A:152:GLU:OE2	0.41	2.16	13	1
1:A:126:GLU:O	1:A:127:THR:CB	0.41	2.68	8	1
1:A:133:ILE:O	1:A:137:MET:HB3	0.41	2.14	4	1
1:A:149:ASP:OD1	1:A:152:GLU:HG3	0.41	2.16	1	1
1:A:130:GLU:HG3	1:A:130:GLU:O	0.41	2.16	1	1
1:A:118:LYS:HE3	1:A:133:ILE:CG2	0.41	2.45	6	1
1:A:113:ASP:HA	1:A:137:MET:CE	0.41	2.45	23	1
1:A:140:GLY:HA3	3:A:1:EMD:C2	0.41	2.45	3	1
1:A:131:ASP:O	1:A:132:ASP:C	0.41	2.59	21	1
1:A:149:ASP:O	1:A:153:PHE:HB2	0.41	2.15	11	2
1:A:130:GLU:O	1:A:131:ASP:C	0.41	2.59	12	2
1:A:104:PHE:CE1	1:A:120:MET:HB2	0.41	2.50	11	1
1:A:121:LEU:HA	1:A:124:THR:OG1	0.41	2.16	11	1
1:A:99:ASP:O	1:A:102:ARG:N	0.41	2.54	9	1
1:A:97:LEU:CD2	1:A:153:PHE:CD2	0.41	3.04	19	1
1:A:153:PHE:CE2	1:A:157:MET:HG2	0.41	2.50	16	1
1:A:151:ASP:O	1:A:154:LEU:HB2	0.41	2.16	21	1
1:A:104:PHE:CD1	1:A:112:ILE:HG21	0.41	2.51	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:ASP:OD2	1:A:116:GLU:OE2	0.41	2.39	23	1
1:A:100:LEU:HB3	1:A:153:PHE:CE2	0.41	2.51	15	1
1:A:121:LEU:HD12	1:A:133:ILE:CG1	0.41	2.46	16	1
1:A:97:LEU:CD2	1:A:154:LEU:HD23	0.41	2.42	13	1
1:A:99:ASP:O	1:A:103:MET:HG3	0.41	2.16	27	1
1:A:109:ASP:C	1:A:109:ASP:OD1	0.41	2.58	21	1
1:A:136:LEU:O	1:A:139:ASP:HB2	0.41	2.15	6	1
1:A:114:LEU:O	1:A:118:LYS:CD	0.41	2.69	30	1
1:A:104:PHE:CD2	1:A:120:MET:SD	0.41	3.14	19	1
1:A:100:LEU:HA	1:A:103:MET:CG	0.41	2.46	9	1
1:A:157:MET:O	1:A:159:GLY:N	0.40	2.53	13	2
1:A:128:ILE:HG23	1:A:132:ASP:CG	0.40	2.37	13	1
1:A:144:ASN:N	1:A:144:ASN:OD1	0.40	2.52	13	1
1:A:105:ASP:OD1	1:A:108:ALA:N	0.40	2.54	17	1
1:A:97:LEU:O	1:A:99:ASP:N	0.40	2.54	11	1
1:A:114:LEU:CD1	1:A:133:ILE:CG2	0.40	2.91	20	1
1:A:122:GLN:O	1:A:126:GLU:HG3	0.40	2.14	24	1
1:A:157:MET:HG3	1:A:157:MET:O	0.40	2.16	10	2
1:A:119:ILE:O	1:A:123:ALA:N	0.40	2.49	5	1
1:A:137:MET:SD	1:A:148:ILE:HD11	0.40	2.55	1	1
1:A:139:ASP:O	1:A:156:PHE:CD1	0.40	2.73	2	1
1:A:161:GLU:O	1:A:161:GLU:OE1	0.40	2.40	2	1
1:A:114:LEU:N	1:A:137:MET:HE3	0.40	2.31	22	1
1:A:107:ASN:ND2	1:A:109:ASP:HB3	0.40	2.30	13	1
1:A:107:ASN:OD1	1:A:116:GLU:OE2	0.40	2.39	21	1
1:A:105:ASP:CG	1:A:108:ALA:C	0.40	2.80	17	1
1:A:97:LEU:HD23	1:A:153:PHE:CD2	0.40	2.51	19	1
1:A:113:ASP:OD1	1:A:115:GLU:HB2	0.40	2.17	9	1
1:A:145:ASP:O	1:A:145:ASP:OD1	0.40	2.40	10	1
1:A:128:ILE:HG12	1:A:132:ASP:HB3	0.40	1.93	16	1
1:A:149:ASP:OD2	1:A:151:ASP:HB2	0.40	2.16	1	1
1:A:140:GLY:O	1:A:148:ILE:HD13	0.40	2.16	13	1
1:A:146:GLY:O	1:A:147:ARG:HB3	0.40	2.17	26	1
1:A:101:PHE:CD1	1:A:153:PHE:CD2	0.40	3.09	22	1
1:A:130:GLU:O	1:A:133:ILE:HB	0.40	2.17	16	1
1:A:99:ASP:O	1:A:103:MET:HB2	0.40	2.17	18	1
1:A:125:GLY:C	1:A:127:THR:N	0.40	2.75	7	1
1:A:150:TYR:CE2	1:A:154:LEU:HD21	0.40	2.52	15	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	68/71 (96%)	51±4 (75±5%)	15±4 (22±6%)	2±1 (3±2%)	9	42
All	All	2040/2130 (96%)	1527 (75%)	452 (22%)	61 (3%)	9	42

All 24 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	126	GLU	14
1	A	108	ALA	8
1	A	105	ASP	5
1	A	117	LEU	4
1	A	127	THR	3
1	A	129	THR	3
1	A	124	THR	2
1	A	133	ILE	2
1	A	144	ASN	2
1	A	94	GLU	2
1	A	147	ARG	2
1	A	159	GLY	2
1	A	158	LYS	1
1	A	95	GLU	1
1	A	115	GLU	1
1	A	122	GLN	1
1	A	157	MET	1
1	A	155	GLU	1
1	A	132	ASP	1
1	A	125	GLY	1
1	A	156	PHE	1
1	A	123	ALA	1
1	A	135	GLU	1
1	A	128	ILE	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	62/63 (98%)	42±3 (68±6%)	20±3 (32±6%)	1	14
All	All	1860/1890 (98%)	1270 (68%)	590 (32%)	1	14

All 54 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	117	LEU	30
1	A	132	ASP	25
1	A	104	PHE	21
1	A	120	MET	19
1	A	100	LEU	17
1	A	93	SER	17
1	A	158	LYS	16
1	A	142	LYS	16
1	A	136	LEU	16
1	A	137	MET	15
1	A	97	LEU	15
1	A	161	GLU	15
1	A	157	MET	15
1	A	150	TYR	15
1	A	113	ASP	14
1	A	130	GLU	14
1	A	106	LYS	14
1	A	96	GLU	13
1	A	103	MET	13
1	A	138	LYS	13
1	A	155	GLU	12
1	A	139	ASP	12
1	A	126	GLU	12
1	A	105	ASP	12
1	A	134	GLU	11
1	A	135	GLU	11
1	A	129	THR	11
1	A	99	ASP	11
1	A	145	ASP	10

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Mol	Chain	Res	Type	Models (Total)
1	A	127	THR	10
1	A	102	ARG	10
1	A	151	ASP	10
1	A	95	GLU	9
1	A	94	GLU	9
1	A	118	LYS	9
1	A	131	ASP	9
1	A	122	GLN	7
1	A	115	GLU	7
1	A	98	SER	7
1	A	156	PHE	7
1	A	143	ASN	7
1	A	149	ASP	6
1	A	114	LEU	6
1	A	144	ASN	6
1	A	154	LEU	6
1	A	124	THR	5
1	A	147	ARG	5
1	A	107	ASN	5
1	A	141	ASP	4
1	A	148	ILE	4
1	A	160	VAL	2
1	A	109	ASP	2
1	A	101	PHE	2
1	A	128	ILE	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 ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	EMD	A	1	-	30,33,33	2.09±0.01	2±0 (6±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	EMD	A	1	-	38,47,47	2.09±0.01	1±1 (2±1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EMD	A	1	-	-	0±0,16,39,39	0±0,3,4,4

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	1	EMD	C8-C5	6.42	1.57	1.48	10	30
3	A	1	EMD	C11-N14	6.21	1.52	1.41	30	30

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst

occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )	Models	
								Worst	Total
3	A	1	EMD	O22-C22-C21	5.28	122.52	115.41	13	21
3	A	1	EMD	O21-C21-C22	5.06	122.23	115.41	23	5

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 82% for the well-defined parts and 82% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 4994

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	788
Number of shifts mapped to atoms	788
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	71	$-0.07 \pm 0.17$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	65	$0.18 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	—
$^{15}\text{N}$	70	$0.57 \pm 0.40$	None needed (imprecise)

#### 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 82%, i.e. 688 atoms were assigned a chemical shift out of a possible 843. 8 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	276/345 (80%)	138/138 (100%)	69/138 (50%)	69/69 (100%)
Sidechain	385/446 (86%)	242/257 (94%)	139/174 (80%)	4/15 (27%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	27/52 (52%)	27/28 (96%)	0/24 (0%)	0/0 (—%)
Overall	688/843 (82%)	407/423 (96%)	208/336 (62%)	73/84 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 706 atoms were assigned a chemical shift out of a possible 866. 8 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	282/355 (79%)	141/142 (99%)	71/142 (50%)	70/71 (99%)
Sidechain	397/459 (86%)	250/265 (94%)	143/178 (80%)	4/16 (25%)
Aromatic	27/52 (52%)	27/28 (96%)	0/24 (0%)	0/0 (—%)
Overall	706/866 (82%)	418/435 (96%)	214/344 (62%)	74/87 (85%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

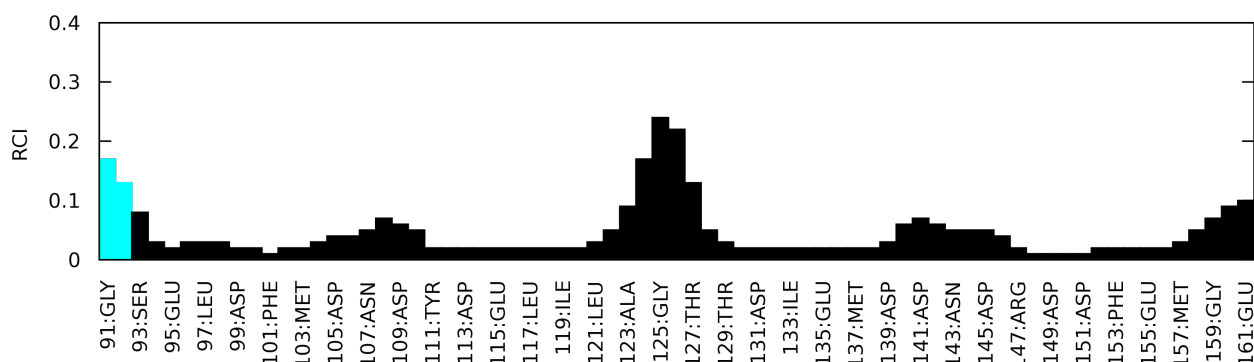
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	115	GLU	CB	40.60	38.65 – 21.35	6.1
1	A	116	GLU	CG	29.40	42.24 – 29.94	-5.4

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

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

Random coil index (RCI) for chain A:



## 7.2 Chemical shift list 2

File name: BMRB entry 4994

Chemical shift list name: *assigned\_chem\_shift\_list\_2*

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

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

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

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	EMD	H23	6.86	0.02	1
UNMAPPED	1	EMD	H262	3.79	0.02	1
UNMAPPED	1	EMD	H72	1.24	0.02	1
UNMAPPED	1	EMD	H261	3.79	0.02	1
UNMAPPED	1	EMD	H172	2.96	0.02	2
UNMAPPED	1	EMD	H13	7.24	0.02	1
UNMAPPED	1	EMD	H253	3.69	0.02	1
UNMAPPED	1	EMD	H263	3.79	0.02	1
UNMAPPED	1	EMD	H73	1.24	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	EMD	H252	3.69	0.02	1
UNMAPPED	1	EMD	H6	4.11	0.02	1
UNMAPPED	1	EMD	H24	6.95	0.02	1
UNMAPPED	1	EMD	H71	1.24	0.02	1
UNMAPPED	1	EMD	H251	3.69	0.02	1
UNMAPPED	1	EMD	H20	6.94	0.02	1
UNMAPPED	1	EMD	H12	6.64	0.02	1
UNMAPPED	1	EMD	H9	7.6	0.02	1
UNMAPPED	1	EMD	H171	2.96	0.02	2

### 7.2.2 Chemical shift referencing ⓘ

No chemical shift referencing corrections were calculated (not enough data).

### 7.2.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 843. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/345 (0%)	0/138 (0%)	0/138 (0%)	0/69 (0%)
Sidechain	0/446 (0%)	0/257 (0%)	0/174 (0%)	0/15 (0%)
Aromatic	0/52 (0%)	0/28 (0%)	0/24 (0%)	0/0 (—%)
Overall	0/843 (0%)	0/423 (0%)	0/336 (0%)	0/84 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 866. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/355 (0%)	0/142 (0%)	0/142 (0%)	0/71 (0%)
Sidechain	0/459 (0%)	0/265 (0%)	0/178 (0%)	0/16 (0%)
Aromatic	0/52 (0%)	0/28 (0%)	0/24 (0%)	0/0 (—%)
Overall	0/866 (0%)	0/435 (0%)	0/344 (0%)	0/87 (0%)

### 7.2.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

### 7.2.5 Random Coil Index (RCI) plots

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned\_chem\_shift\_list\_2). RCI is only applicable to proteins.