



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:47 PM BST

PDB ID : 1LXF
Title : Structure of the Regulatory N-domain of Human Cardiac Troponin C in Complex with Human Cardiac Troponin-I(147-163) and Bepridil
Authors : Wang, X.; Li, M.X.; Sykes, B.D.
Deposited on : 2002-06-05

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 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

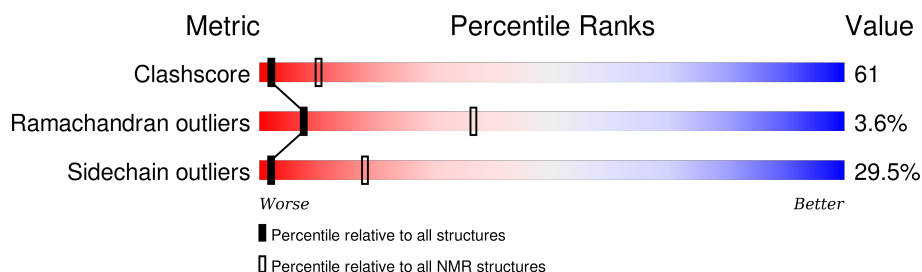
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

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



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

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

Mol	Chain	Length	Quality of chain
1	C	89	
2	I	17	

2 Ensemble composition and analysis ⓘ

This entry contains 30 models. Model 29 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	C:5-C:86, I:148-I:157 (92)	0.47	29

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 4 clusters and 7 single-model clusters were found.

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

3 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1687 atoms, of which 837 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	C	89	Total	C	H	N	O	S	0
			1364	432	666	107	150	9	

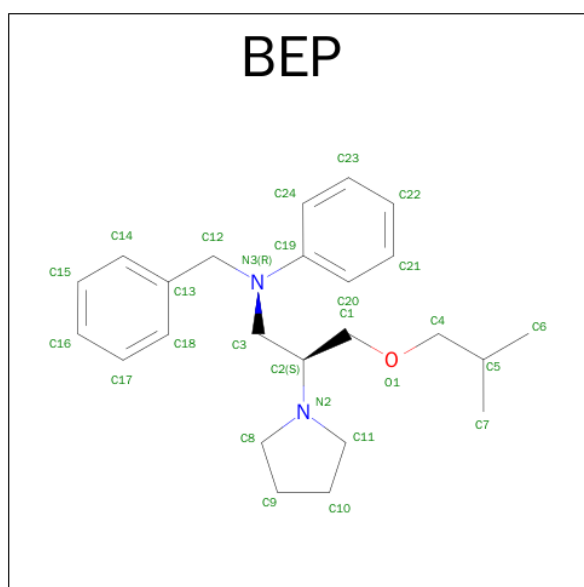
- Molecule 2 is a protein called Troponin I, cardiac muscle.

Mol	Chain	Residues	Atoms						Trace
2	I	17	Total	C	H	N	O	S	0
			261	75	137	25	22	2	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
3	C	1	Total	Ca
			1	1

- Molecule 4 is 1-ISOBUTOXY-2-PYRROLIDINO-3[N-BENZYLANILINO] PROPANE (three-letter code: BEP) (formula: C₂₄H₃₄N₂O).



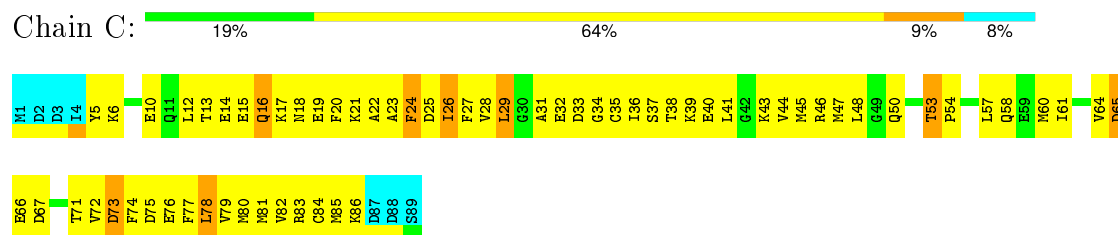
Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
4	C	1	61	24	34	2	1

4 Residue-property plots [i](#)

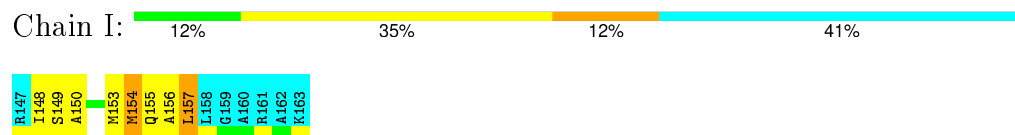
4.1 Average score per residue in the NMR ensemble

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: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



- Molecule 2: Troponin I, cardiac muscle

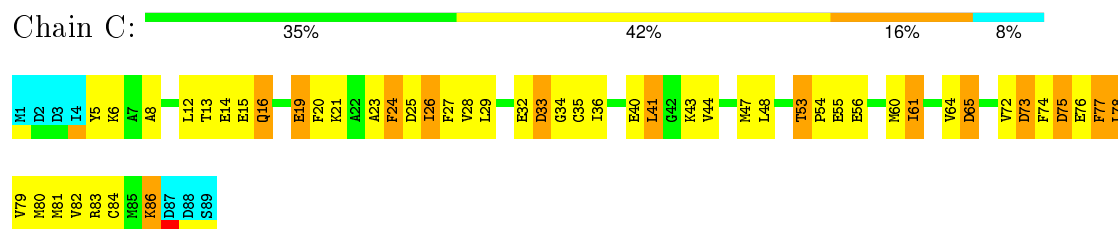


4.2 Scores per residue for each member of the ensemble

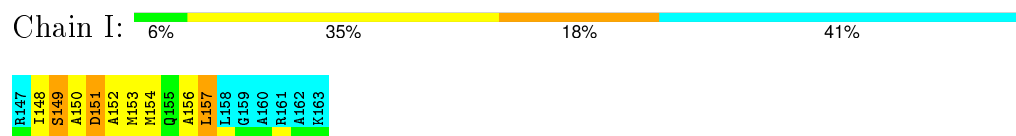
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

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

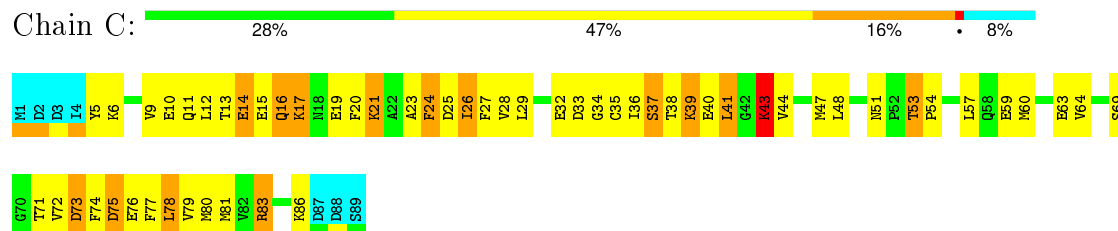


- Molecule 2: Troponin I, cardiac muscle

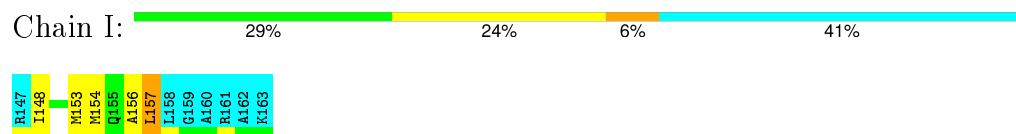


4.2.2 Score per residue for model 2

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

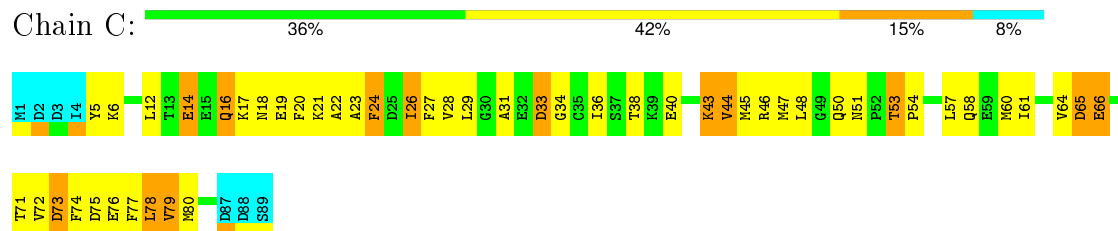


- Molecule 2: Troponin I, cardiac muscle

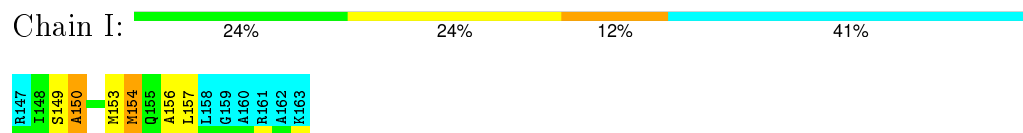


4.2.3 Score per residue for model 3

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

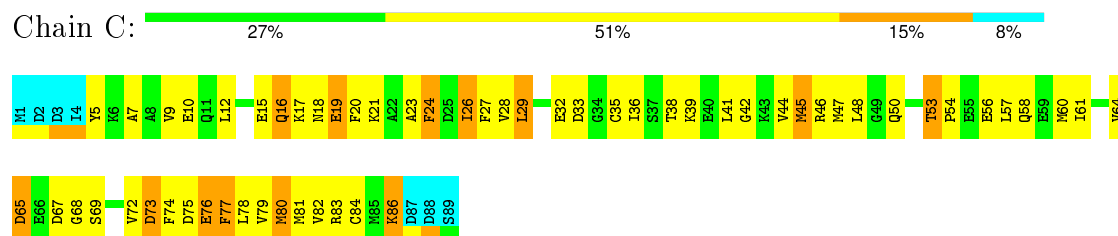


- Molecule 2: Troponin I, cardiac muscle



4.2.4 Score per residue for model 4

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

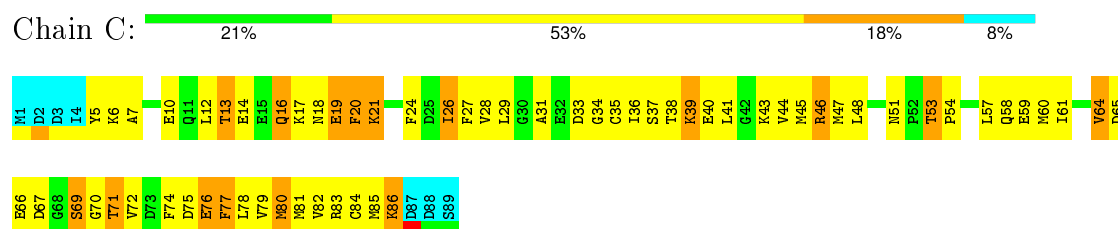


- Molecule 2: Troponin I, cardiac muscle



4.2.5 Score per residue for model 5

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

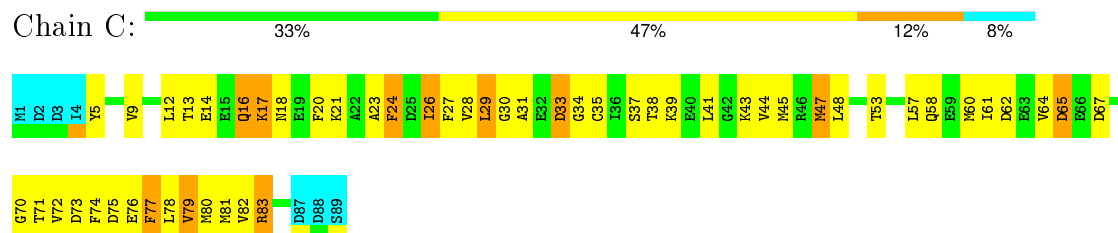


- Molecule 2: Troponin I, cardiac muscle

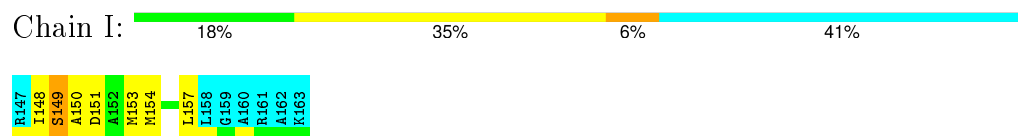


4.2.6 Score per residue for model 6

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

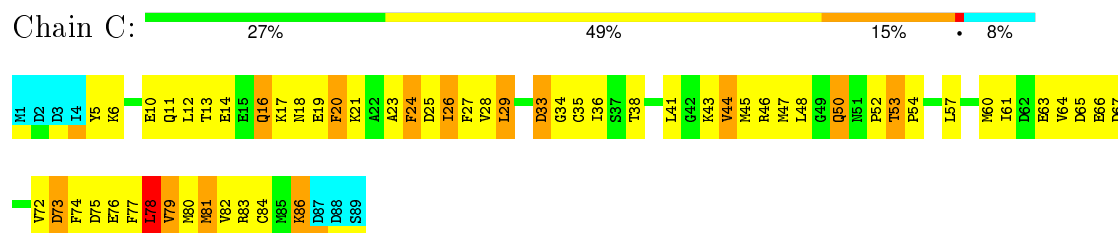


- Molecule 2: Troponin I, cardiac muscle

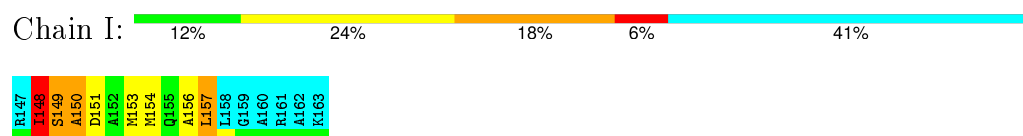


4.2.7 Score per residue for model 7

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

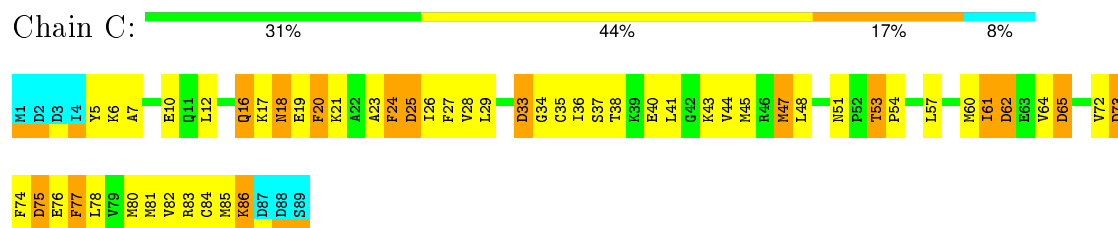


- Molecule 2: Troponin I, cardiac muscle

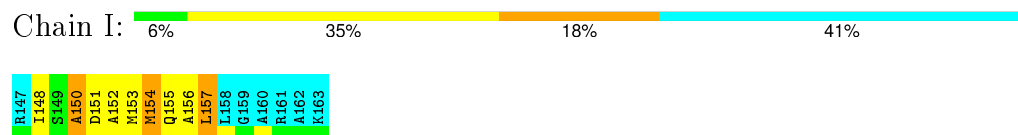


4.2.8 Score per residue for model 8

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

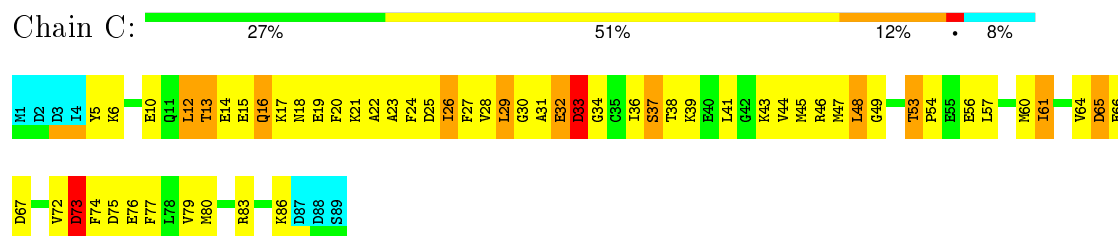


- Molecule 2: Troponin I, cardiac muscle

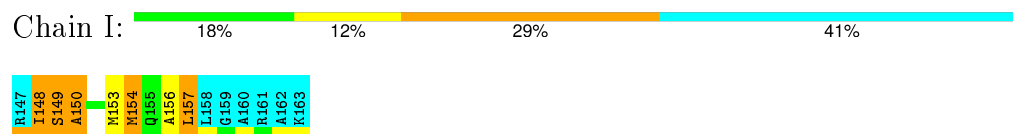


4.2.9 Score per residue for model 9

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

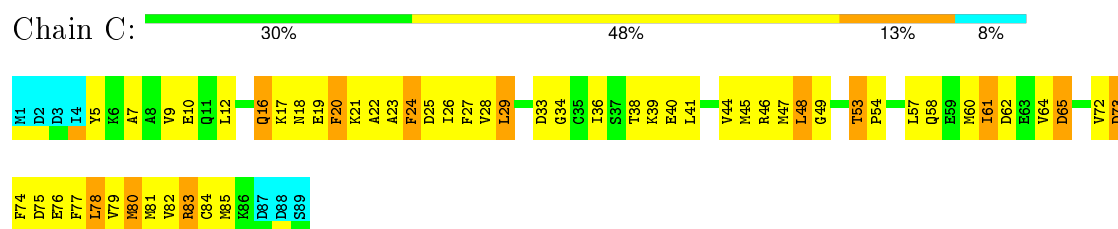


- Molecule 2: Troponin I, cardiac muscle



4.2.10 Score per residue for model 10

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

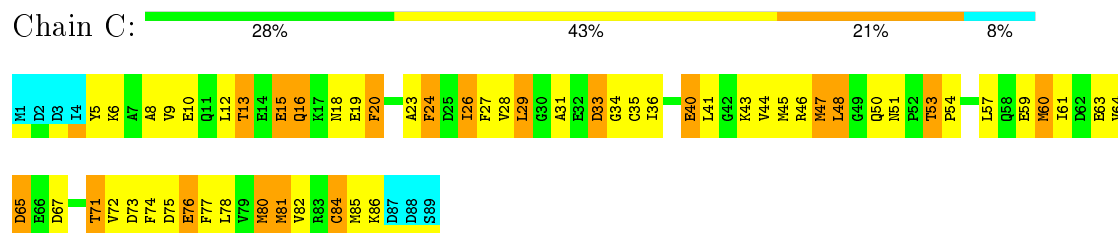


- Molecule 2: Troponin I, cardiac muscle

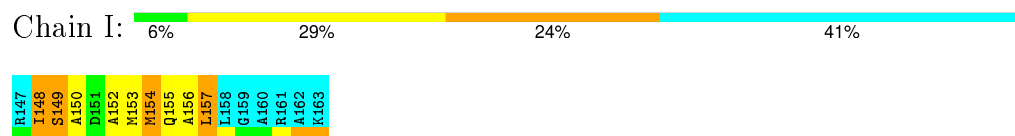


4.2.11 Score per residue for model 11

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

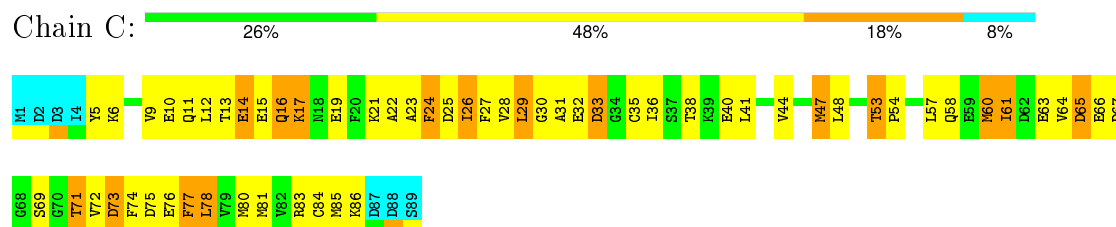


- Molecule 2: Troponin I, cardiac muscle

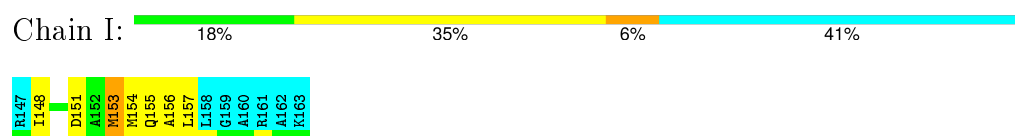


4.2.12 Score per residue for model 12

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

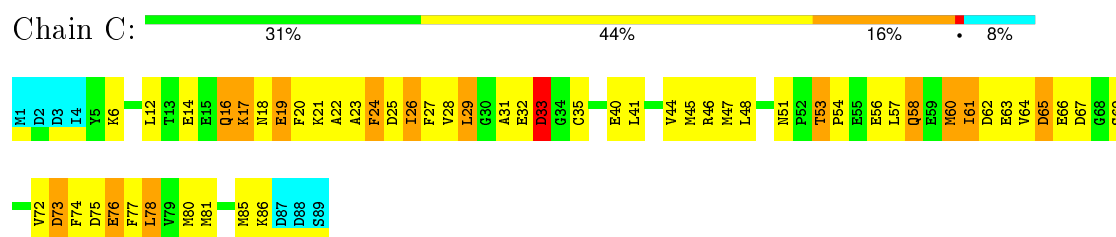


- Molecule 2: Troponin I, cardiac muscle

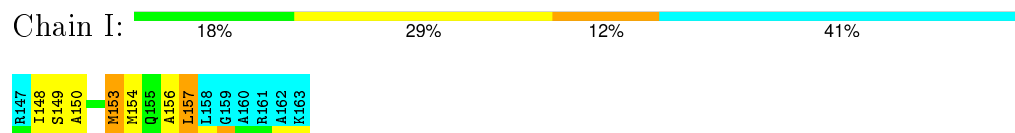


4.2.13 Score per residue for model 13

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

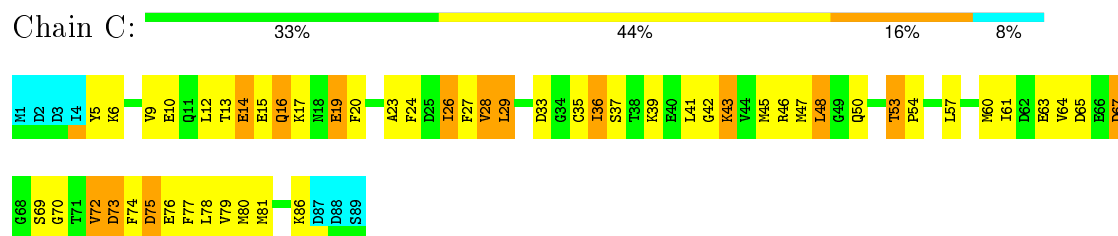


- Molecule 2: Troponin I, cardiac muscle

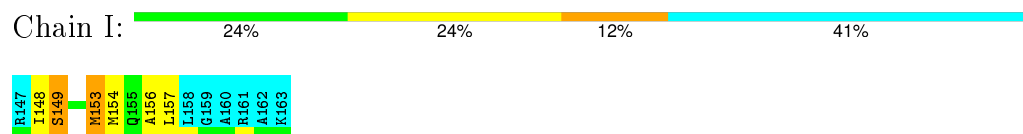


4.2.14 Score per residue for model 14

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

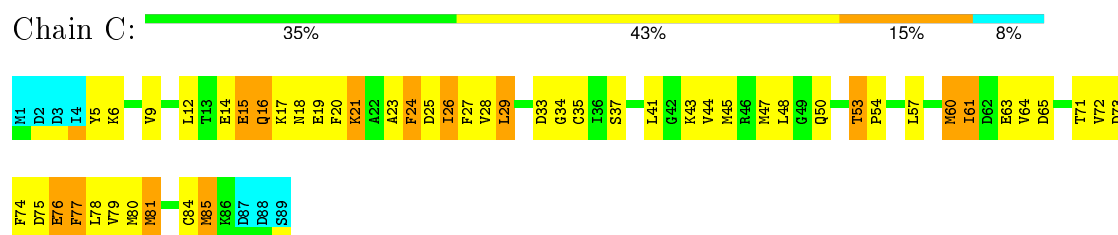


- Molecule 2: Troponin I, cardiac muscle



4.2.15 Score per residue for model 15

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

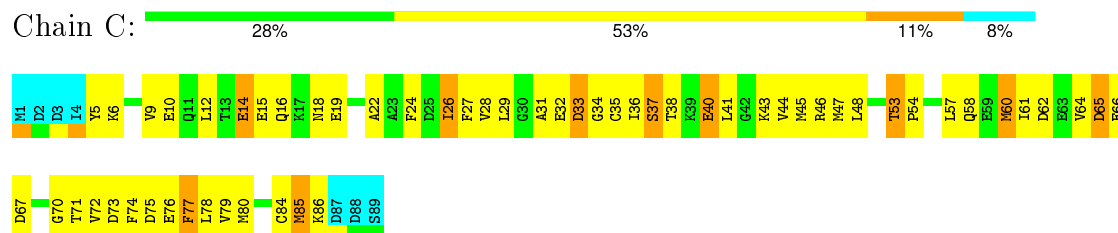


- Molecule 2: Troponin I, cardiac muscle

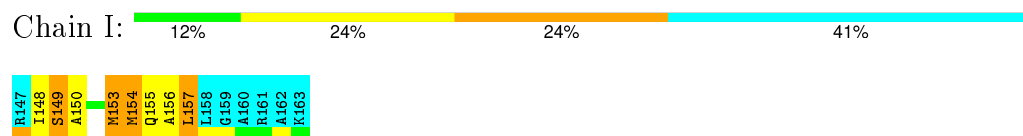


4.2.16 Score per residue for model 16

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

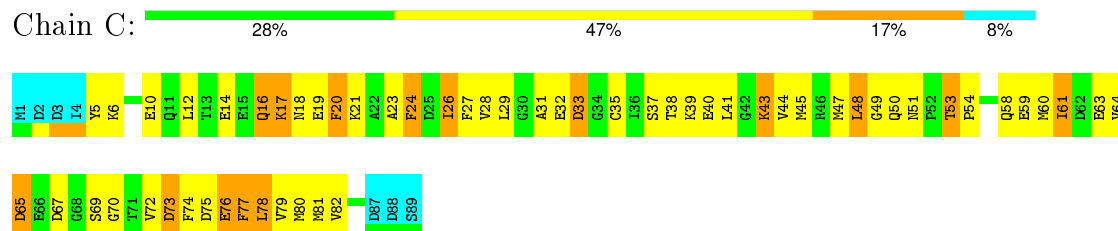


- Molecule 2: Troponin I, cardiac muscle

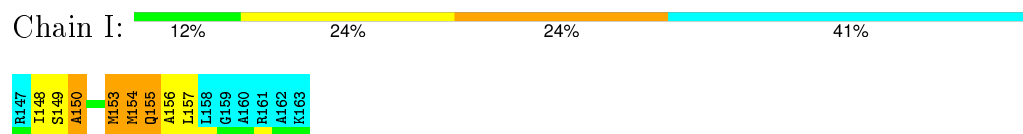


4.2.17 Score per residue for model 17

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

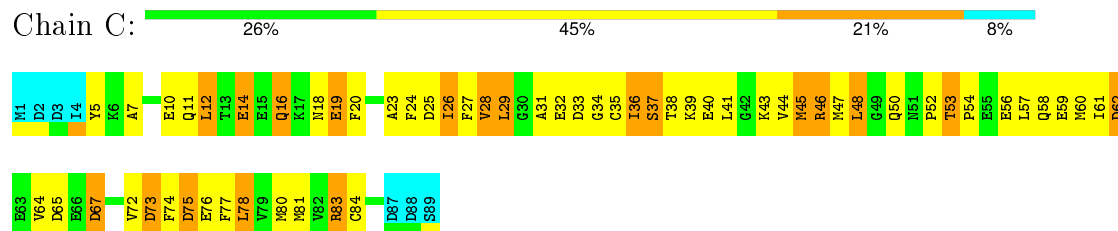


- Molecule 2: Troponin I, cardiac muscle

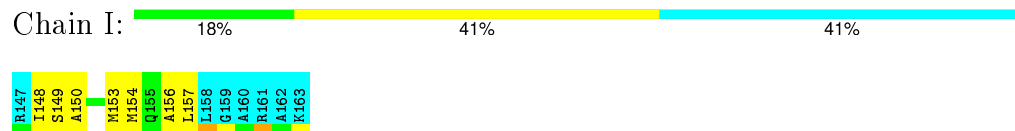


4.2.18 Score per residue for model 18

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

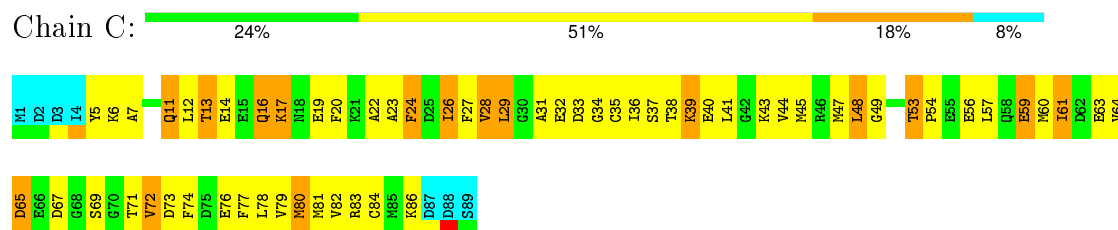


- Molecule 2: Troponin I, cardiac muscle

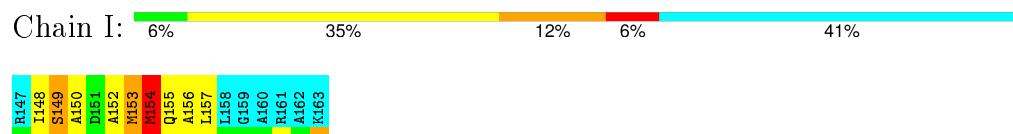


4.2.19 Score per residue for model 19

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

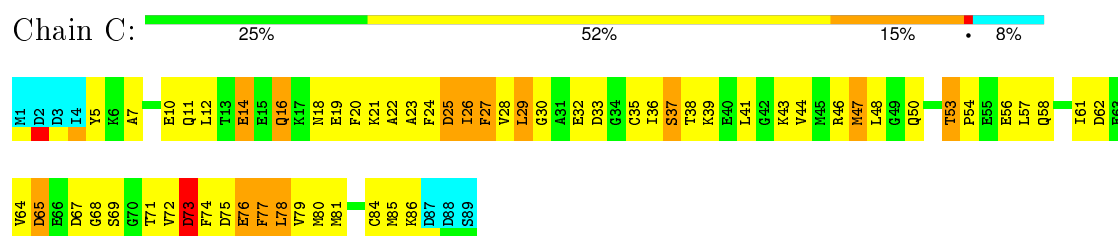


- Molecule 2: Troponin I, cardiac muscle

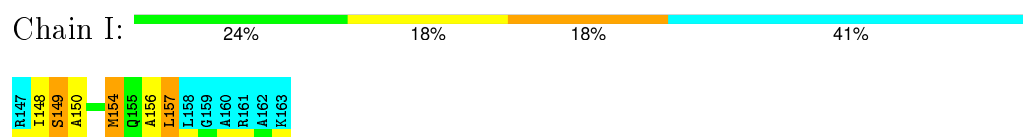


4.2.20 Score per residue for model 20

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

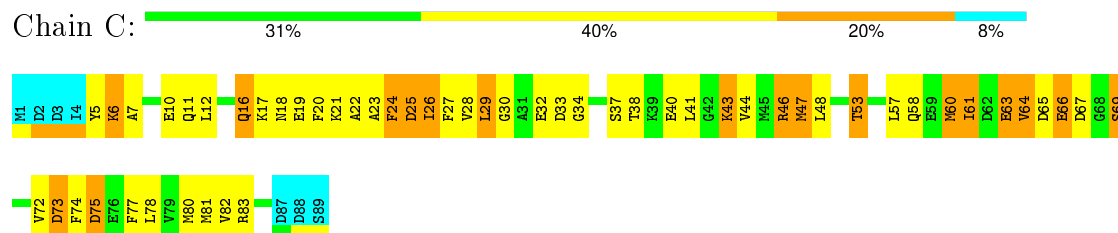


- Molecule 2: Troponin I, cardiac muscle



4.2.21 Score per residue for model 21

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

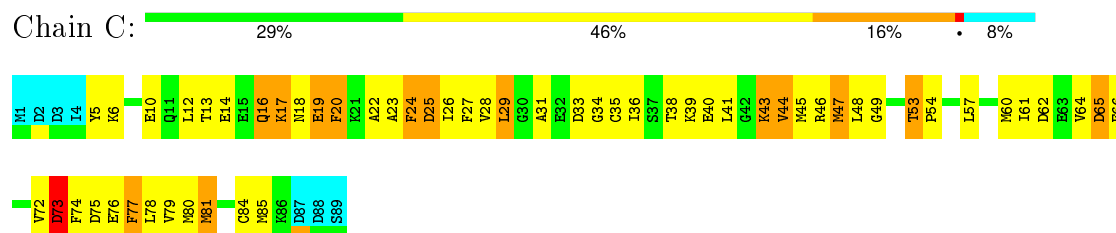


- Molecule 2: Troponin I, cardiac muscle



4.2.22 Score per residue for model 22

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

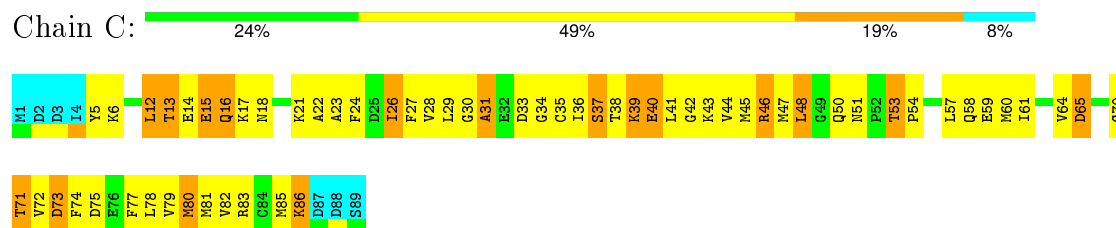


- Molecule 2: Troponin I, cardiac muscle

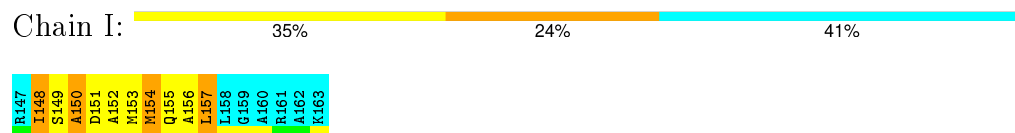


4.2.23 Score per residue for model 23

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

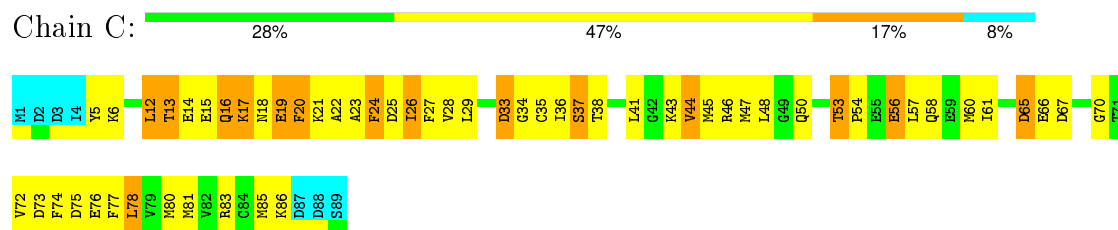


- Molecule 2: Troponin I, cardiac muscle

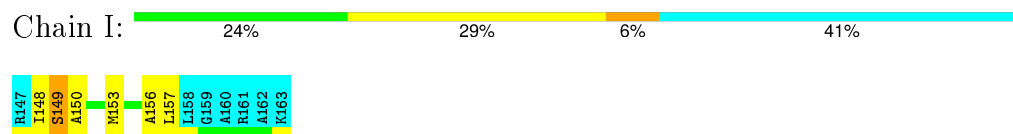


4.2.24 Score per residue for model 24

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

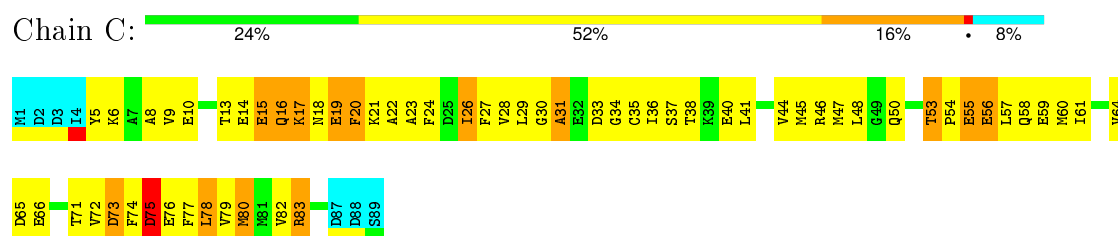


- Molecule 2: Troponin I, cardiac muscle

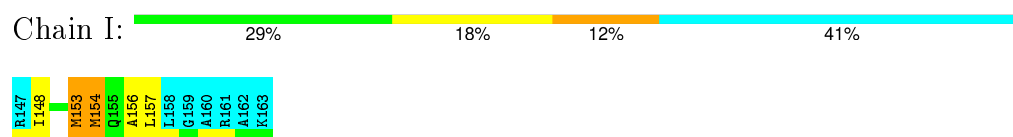


4.2.25 Score per residue for model 25

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

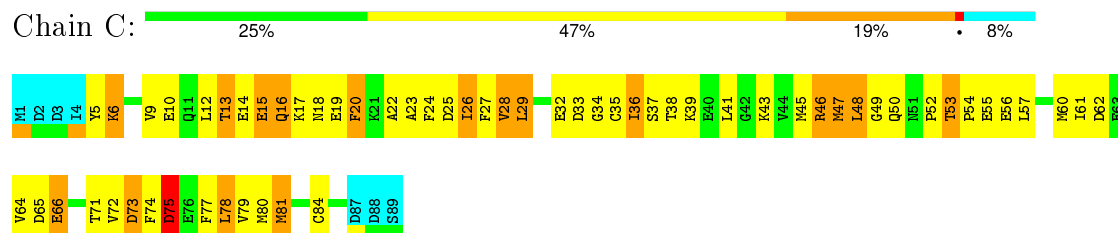


- Molecule 2: Troponin I, cardiac muscle

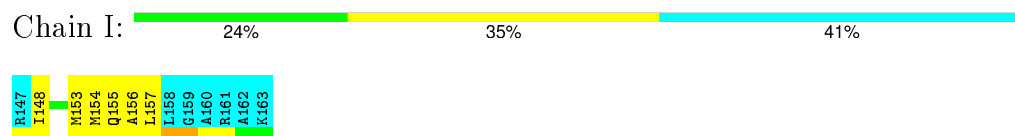


4.2.26 Score per residue for model 26

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

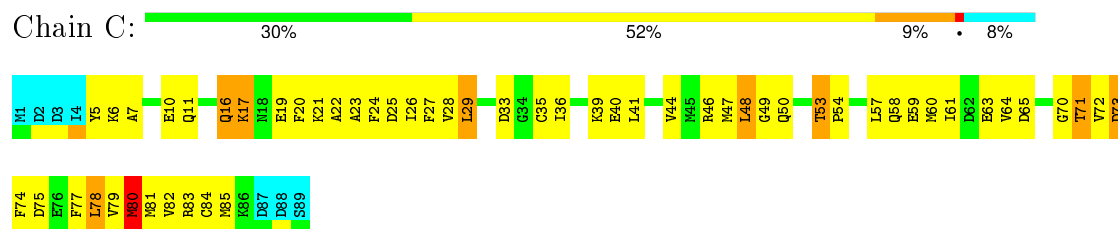


- Molecule 2: Troponin I, cardiac muscle



4.2.27 Score per residue for model 27

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

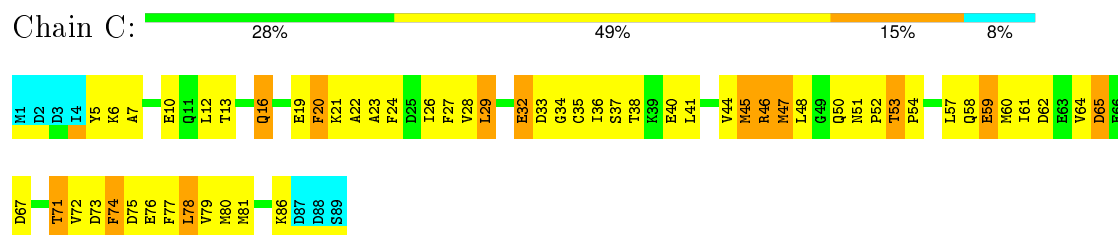


- Molecule 2: Troponin I, cardiac muscle

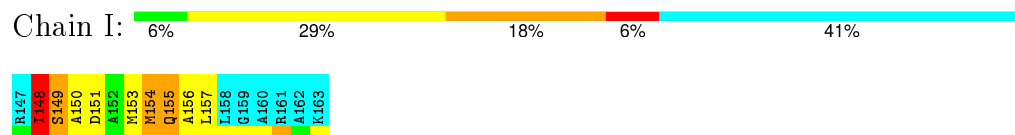


4.2.28 Score per residue for model 28

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

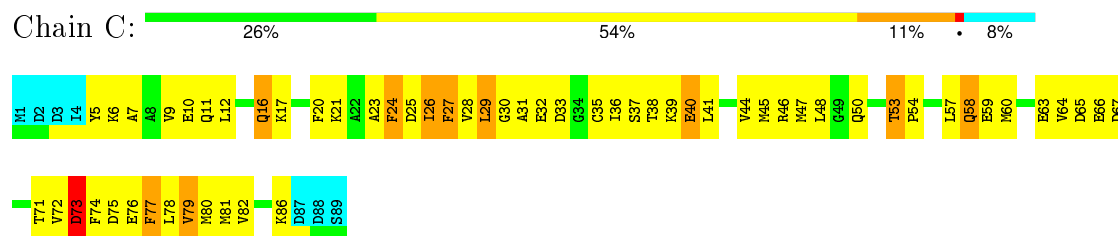


- Molecule 2: Troponin I, cardiac muscle

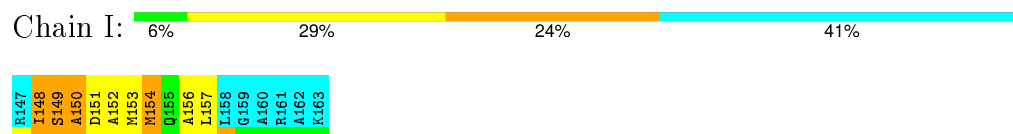


4.2.29 Score per residue for model 29 (medoid)

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

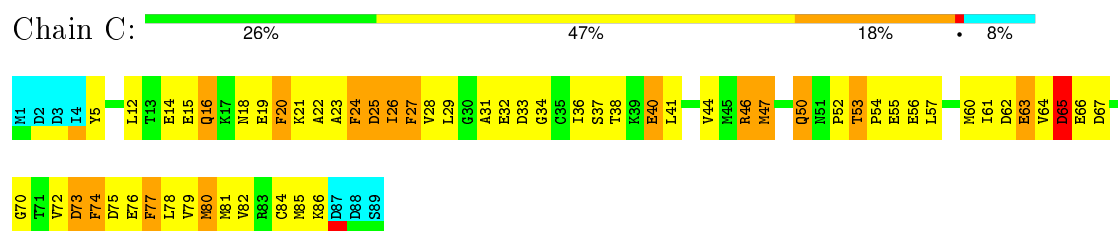


- Molecule 2: Troponin I, cardiac muscle



4.2.30 Score per residue for model 30

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



- Molecule 2: Troponin I, cardiac muscle



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	3.85

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 5386
Number of chemical shift lists	2
Total number of shifts	1007
Number of shifts mapped to atoms	1007
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

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: CA, BEP

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	C	643	623	622	78±10
2	I	70	72	72	18±5
4	C	27	34	34	12±4
All	All	22230	21870	21847	2678

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 61.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:26:ILE:HG22	1:C:44:VAL:HG22	1.09	1.10	10	4
1:C:41:LEU:HD23	1:C:57:LEU:HD22	1.05	1.11	28	19
1:C:23:ALA:HB2	2:I:157:LEU:HD21	1.00	1.24	6	13
1:C:29:LEU:HD13	1:C:30:GLY:N	1.00	1.70	29	3
1:C:41:LEU:CD2	1:C:57:LEU:HD22	0.97	1.90	14	11
1:C:27:PHE:CE1	1:C:44:VAL:HG11	0.95	1.95	11	13
1:C:26:ILE:CG2	1:C:44:VAL:HG23	0.93	1.94	22	2
1:C:38:THR:O	1:C:57:LEU:HD13	0.90	1.67	7	15
1:C:29:LEU:O	1:C:29:LEU:HD22	0.90	1.67	9	2
1:C:27:PHE:CD1	1:C:44:VAL:HG21	0.89	2.02	9	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:36:ILE:HD11	1:C:77:PHE:CE2	0.89	2.02	5	2
1:C:29:LEU:HD22	1:C:29:LEU:O	0.89	1.67	29	1
4:C:92:BEP:N2	2:I:148:ILE:HD11	0.88	1.83	5	5
1:C:29:LEU:HD12	1:C:29:LEU:O	0.88	1.69	11	5
1:C:36:ILE:HD11	1:C:77:PHE:CG	0.87	2.05	23	3
1:C:36:ILE:O	1:C:71:THR:HG22	0.86	1.70	12	3
1:C:41:LEU:HD23	1:C:57:LEU:CD2	0.86	2.00	26	9
1:C:26:ILE:HD13	2:I:157:LEU:HD21	0.86	1.45	27	1
1:C:57:LEU:HD23	1:C:60:MET:SD	0.86	2.10	11	6
1:C:36:ILE:HG21	1:C:41:LEU:HD21	0.86	1.46	16	1
1:C:26:ILE:CG2	1:C:44:VAL:HG22	0.86	2.01	27	4
1:C:64:VAL:HG13	1:C:80:MET:SD	0.86	2.10	18	8
1:C:29:LEU:O	1:C:29:LEU:HD12	0.85	1.70	27	10
1:C:28:VAL:HG11	1:C:34:GLY:C	0.85	1.92	28	16
1:C:5:TYR:O	1:C:9:VAL:HG22	0.85	1.71	25	3
1:C:48:LEU:HD23	2:I:152:ALA:O	0.85	1.71	4	1
4:C:92:BEP:H181	2:I:148:ILE:HD13	0.85	1.48	5	2
1:C:38:THR:HG22	1:C:61:ILE:HG13	0.85	1.47	4	8
2:I:156:ALA:C	2:I:157:LEU:HD13	0.84	1.92	30	6
2:I:156:ALA:C	2:I:157:LEU:HD22	0.84	1.93	27	5
1:C:48:LEU:CD2	2:I:156:ALA:HB2	0.84	2.03	17	8
1:C:23:ALA:CB	2:I:157:LEU:HD21	0.83	2.02	6	5
1:C:12:LEU:HD13	1:C:16:GLN:CD	0.83	1.92	28	12
2:I:156:ALA:O	2:I:157:LEU:HD13	0.83	1.74	8	6
1:C:27:PHE:CE2	1:C:28:VAL:HG13	0.82	2.09	18	1
2:I:157:LEU:HD13	2:I:157:LEU:N	0.82	1.89	15	4
1:C:12:LEU:HD13	1:C:16:GLN:NE2	0.82	1.89	21	15
1:C:72:VAL:HG21	4:C:92:BEP:H221	0.81	1.50	10	10
2:I:157:LEU:N	2:I:157:LEU:HD13	0.81	1.91	30	2
1:C:24:PHE:O	1:C:28:VAL:HG22	0.80	1.76	5	17
1:C:26:ILE:HD11	2:I:157:LEU:HD11	0.80	1.52	3	4
1:C:36:ILE:HD12	1:C:72:VAL:HB	0.80	1.52	30	3
1:C:26:ILE:HG13	2:I:157:LEU:HD12	0.80	1.49	30	5
1:C:41:LEU:HD11	4:C:92:BEP:C23	0.80	2.07	16	1
1:C:74:PHE:CE1	1:C:78:LEU:HD11	0.79	2.11	20	2
1:C:12:LEU:HD22	1:C:16:GLN:OE1	0.79	1.76	30	6
2:I:157:LEU:HD22	2:I:157:LEU:N	0.79	1.93	29	5
1:C:19:GLU:O	2:I:157:LEU:HD23	0.79	1.78	22	2
1:C:27:PHE:CD1	1:C:28:VAL:HG13	0.78	2.13	30	4
2:I:153:MET:O	2:I:157:LEU:HD21	0.78	1.79	30	3
1:C:74:PHE:CZ	1:C:78:LEU:HD11	0.78	2.13	20	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:I:157:LEU:N	2:I:157:LEU:HD22	0.77	1.93	24	4
1:C:48:LEU:HD11	2:I:156:ALA:HB2	0.77	1.53	15	5
1:C:47:MET:HE2	2:I:156:ALA:HB1	0.77	1.55	18	9
1:C:36:ILE:HD11	1:C:77:PHE:CD2	0.77	2.15	27	8
4:C:92:BEP:H63	4:C:92:BEP:H81	0.77	1.56	5	1
1:C:28:VAL:HB	1:C:31:ALA:HB3	0.76	1.55	16	10
1:C:48:LEU:HB3	2:I:152:ALA:HB1	0.76	1.56	11	1
2:I:153:MET:O	2:I:157:LEU:HD23	0.76	1.80	3	1
4:C:92:BEP:H73	4:C:92:BEP:H111	0.74	1.57	23	1
1:C:23:ALA:HA	2:I:157:LEU:HD11	0.74	1.57	8	6
4:C:92:BEP:C17	2:I:148:ILE:HD11	0.74	2.13	7	1
1:C:64:VAL:HG21	1:C:72:VAL:HG22	0.74	1.59	13	10
1:C:41:LEU:HD21	4:C:92:BEP:C21	0.74	2.10	1	2
1:C:26:ILE:O	1:C:29:LEU:HD22	0.74	1.81	18	3
1:C:77:PHE:CE1	1:C:81:MET:HE1	0.74	2.18	20	2
1:C:48:LEU:CD1	2:I:156:ALA:HB2	0.73	2.13	12	8
2:I:148:ILE:HG23	2:I:148:ILE:O	0.73	1.83	22	3
1:C:29:LEU:HD23	1:C:29:LEU:O	0.73	1.84	10	1
1:C:48:LEU:N	1:C:48:LEU:HD23	0.73	1.98	27	5
1:C:26:ILE:HG22	1:C:44:VAL:HG23	0.73	1.60	22	1
2:I:156:ALA:C	2:I:157:LEU:HD23	0.72	2.05	13	5
1:C:53:THR:HG22	1:C:54:PRO:CD	0.72	2.14	19	13
1:C:41:LEU:HD22	4:C:92:BEP:C21	0.72	2.15	11	3
1:C:12:LEU:HD13	1:C:16:GLN:OE1	0.72	1.85	9	4
1:C:5:TYR:CD2	1:C:79:VAL:HG13	0.72	2.20	5	6
1:C:22:ALA:HB3	2:I:157:LEU:HD13	0.72	1.60	21	3
1:C:47:MET:O	1:C:48:LEU:HD12	0.71	1.85	21	3
4:C:92:BEP:H21	2:I:148:ILE:HD11	0.71	1.61	29	6
1:C:47:MET:C	1:C:48:LEU:HD23	0.71	2.05	14	5
2:I:157:LEU:HD23	2:I:157:LEU:N	0.71	2.00	5	3
1:C:22:ALA:HB1	2:I:157:LEU:CB	0.71	2.16	27	1
1:C:78:LEU:O	1:C:82:VAL:HG23	0.71	1.86	27	8
1:C:27:PHE:CE1	1:C:28:VAL:HG13	0.71	2.20	30	4
1:C:24:PHE:CE2	1:C:77:PHE:CD2	0.71	2.79	23	11
1:C:41:LEU:HB3	1:C:57:LEU:HD22	0.71	1.62	2	1
1:C:26:ILE:CD1	2:I:157:LEU:HD21	0.70	2.15	27	1
1:C:41:LEU:HD12	1:C:57:LEU:CD2	0.70	2.15	16	1
4:C:92:BEP:H62	4:C:92:BEP:H11	0.70	1.61	18	1
1:C:28:VAL:HG12	1:C:35:CYS:O	0.70	1.87	23	19
1:C:26:ILE:HD11	2:I:157:LEU:CD1	0.70	2.16	14	5
4:C:92:BEP:H141	2:I:148:ILE:HD13	0.70	1.64	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:48:LEU:HD23	1:C:48:LEU:N	0.70	2.00	14	5
1:C:29:LEU:HD22	1:C:29:LEU:C	0.70	2.06	29	1
1:C:48:LEU:HD21	2:I:156:ALA:HB2	0.70	1.64	20	7
2:I:157:LEU:N	2:I:157:LEU:HD23	0.70	2.02	13	3
1:C:24:PHE:CD1	1:C:27:PHE:CZ	0.69	2.80	29	2
1:C:24:PHE:CZ	1:C:77:PHE:CD2	0.69	2.80	6	15
1:C:27:PHE:CE1	1:C:28:VAL:HG22	0.69	2.22	30	5
1:C:26:ILE:HG13	2:I:157:LEU:HD22	0.69	1.63	16	2
1:C:22:ALA:HB3	2:I:157:LEU:HD23	0.69	1.64	12	4
1:C:44:VAL:O	1:C:48:LEU:HD12	0.69	1.88	4	1
1:C:29:LEU:C	1:C:29:LEU:HD22	0.69	2.07	9	2
1:C:27:PHE:CD2	1:C:28:VAL:HG13	0.69	2.23	18	1
1:C:36:ILE:HD12	4:C:92:BEP:H231	0.69	1.64	4	1
1:C:29:LEU:HD13	1:C:29:LEU:C	0.69	2.09	6	1
1:C:28:VAL:HG11	1:C:34:GLY:CA	0.69	2.18	28	6
1:C:27:PHE:CE1	1:C:44:VAL:HG21	0.69	2.22	24	4
1:C:64:VAL:HG13	1:C:80:MET:HG3	0.68	1.65	2	4
1:C:26:ILE:HG22	1:C:44:VAL:CG2	0.68	2.05	10	2
4:C:92:BEP:C18	2:I:148:ILE:HD13	0.68	2.17	5	1
1:C:24:PHE:CE2	1:C:74:PHE:CE1	0.68	2.81	10	9
1:C:29:LEU:HD23	1:C:30:GLY:N	0.68	2.03	21	3
1:C:24:PHE:CE2	1:C:74:PHE:CD2	0.68	2.81	27	2
1:C:29:LEU:C	1:C:29:LEU:HD13	0.68	2.07	29	2
1:C:27:PHE:CZ	1:C:44:VAL:HG11	0.68	2.23	1	1
1:C:53:THR:O	1:C:57:LEU:HD12	0.68	1.87	26	1
4:C:92:BEP:C14	2:I:148:ILE:HD11	0.68	2.17	15	1
1:C:41:LEU:HD11	4:C:92:BEP:C15	0.68	2.19	23	2
1:C:48:LEU:HD22	2:I:156:ALA:HA	0.68	1.64	27	1
1:C:22:ALA:O	1:C:26:ILE:HD11	0.68	1.89	16	1
1:C:27:PHE:CD2	1:C:77:PHE:CZ	0.68	2.81	23	3
4:C:92:BEP:H31	2:I:148:ILE:HD11	0.67	1.65	26	3
1:C:27:PHE:CE2	1:C:77:PHE:CZ	0.67	2.81	3	7
1:C:23:ALA:HB1	1:C:27:PHE:CZ	0.67	2.24	22	5
1:C:47:MET:CE	2:I:156:ALA:HB1	0.67	2.20	22	9
1:C:60:MET:HE2	4:C:92:BEP:N3	0.67	2.04	16	2
1:C:44:VAL:HG12	1:C:48:LEU:HD13	0.67	1.64	1	2
1:C:48:LEU:HD13	2:I:153:MET:CB	0.67	2.19	14	1
1:C:48:LEU:HD13	2:I:153:MET:HA	0.67	1.67	18	2
1:C:63:GLU:OE2	4:C:92:BEP:H62	0.66	1.89	2	1
2:I:153:MET:O	2:I:157:LEU:HD11	0.66	1.90	30	2
1:C:24:PHE:CD1	1:C:77:PHE:CE2	0.66	2.83	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:26:ILE:HD11	2:I:157:LEU:HD12	0.66	1.67	8	1
1:C:12:LEU:HD13	1:C:16:GLN:CG	0.66	2.20	24	3
1:C:26:ILE:O	1:C:29:LEU:HD23	0.66	1.90	1	5
1:C:12:LEU:HD13	1:C:16:GLN:HG2	0.66	1.66	24	3
1:C:24:PHE:CZ	1:C:74:PHE:CD1	0.66	2.84	22	11
1:C:22:ALA:HB1	2:I:157:LEU:HB2	0.66	1.67	27	2
1:C:41:LEU:HD11	4:C:92:BEP:C17	0.66	2.21	22	1
1:C:27:PHE:HE1	1:C:44:VAL:HG11	0.66	1.44	13	3
4:C:92:BEP:H72	4:C:92:BEP:H111	0.66	1.65	29	1
4:C:92:BEP:H141	2:I:148:ILE:HD11	0.65	1.67	15	1
1:C:45:MET:HE3	4:C:92:BEP:H82	0.65	1.68	19	1
1:C:24:PHE:CD2	1:C:74:PHE:CE1	0.65	2.84	3	2
2:I:149:SER:O	2:I:150:ALA:HB3	0.65	1.92	17	14
1:C:26:ILE:HD12	1:C:26:ILE:N	0.65	2.06	27	2
1:C:45:MET:HE1	4:C:92:BEP:C15	0.65	2.21	5	1
1:C:23:ALA:HB1	2:I:153:MET:HE3	0.64	1.67	17	1
1:C:27:PHE:CE2	1:C:28:VAL:CG1	0.64	2.80	18	1
2:I:149:SER:O	2:I:150:ALA:HB2	0.64	1.92	4	6
1:C:27:PHE:HD1	1:C:44:VAL:HG21	0.64	1.50	20	3
1:C:12:LEU:HD22	1:C:16:GLN:NE2	0.64	2.07	12	1
1:C:29:LEU:O	1:C:29:LEU:HD23	0.64	1.92	22	2
4:C:92:BEP:C2	2:I:148:ILE:HD11	0.64	2.22	19	4
1:C:36:ILE:HD12	1:C:72:VAL:CB	0.64	2.22	30	2
1:C:47:MET:C	1:C:48:LEU:HD12	0.64	2.13	21	3
4:C:92:BEP:C4	2:I:148:ILE:HD11	0.64	2.23	6	1
1:C:36:ILE:HG21	1:C:41:LEU:CD2	0.64	2.23	16	2
1:C:77:PHE:CE1	1:C:81:MET:CE	0.63	2.81	20	3
4:C:92:BEP:H21	2:I:148:ILE:HD13	0.63	1.69	2	3
1:C:74:PHE:CE2	1:C:78:LEU:CD1	0.63	2.81	25	2
1:C:74:PHE:O	1:C:78:LEU:HD23	0.63	1.92	5	1
4:C:92:BEP:C2	2:I:148:ILE:HD13	0.63	2.23	2	2
1:C:24:PHE:CZ	1:C:74:PHE:CD2	0.63	2.87	2	1
1:C:64:VAL:HG21	1:C:72:VAL:CG1	0.63	2.23	20	3
1:C:24:PHE:CD2	1:C:74:PHE:CE2	0.63	2.87	1	4
1:C:27:PHE:CZ	1:C:28:VAL:CG2	0.63	2.82	26	3
1:C:24:PHE:CE1	1:C:74:PHE:CD1	0.63	2.86	29	1
1:C:48:LEU:HD12	2:I:156:ALA:HB2	0.62	1.69	12	2
1:C:27:PHE:HA	1:C:44:VAL:HG21	0.62	1.70	28	5
1:C:38:THR:O	1:C:57:LEU:HD12	0.62	1.94	29	1
1:C:23:ALA:N	2:I:157:LEU:HD13	0.62	2.09	2	2
1:C:38:THR:HG22	1:C:58:GLN:HA	0.62	1.70	10	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:63:GLU:OE1	4:C:92:BEP:H62	0.62	1.94	21	1
1:C:41:LEU:HD22	4:C:92:BEP:C20	0.62	2.24	7	9
2:I:157:LEU:CD1	2:I:157:LEU:N	0.62	2.62	15	8
1:C:29:LEU:HD12	1:C:29:LEU:C	0.62	2.14	11	5
1:C:24:PHE:CE1	1:C:27:PHE:CZ	0.62	2.88	29	1
1:C:24:PHE:CE1	1:C:74:PHE:CD2	0.61	2.89	2	2
1:C:44:VAL:HG12	1:C:48:LEU:CD1	0.61	2.24	1	1
1:C:53:THR:HG22	1:C:54:PRO:HD3	0.61	1.71	19	1
1:C:24:PHE:CE2	1:C:74:PHE:CD1	0.61	2.88	24	10
1:C:27:PHE:CE1	1:C:28:VAL:CG1	0.61	2.83	14	4
1:C:48:LEU:HD21	2:I:153:MET:HA	0.61	1.71	2	5
1:C:24:PHE:CZ	1:C:77:PHE:CE2	0.61	2.88	14	1
1:C:74:PHE:CG	1:C:74:PHE:O	0.61	2.53	4	12
1:C:45:MET:HE2	4:C:92:BEP:C16	0.61	2.25	28	2
1:C:26:ILE:N	1:C:26:ILE:HD12	0.61	2.09	10	2
1:C:41:LEU:HD21	1:C:57:LEU:HD22	0.61	1.72	14	1
1:C:23:ALA:HB1	1:C:27:PHE:CE1	0.61	2.30	27	1
2:I:156:ALA:CB	2:I:157:LEU:HD22	0.61	2.26	27	1
2:I:156:ALA:C	2:I:157:LEU:HD12	0.61	2.16	26	3
2:I:153:MET:O	2:I:157:LEU:HD13	0.61	1.96	22	6
1:C:64:VAL:HG21	1:C:72:VAL:HG13	0.61	1.73	15	10
1:C:60:MET:HE1	4:C:92:BEP:H32	0.61	1.73	27	1
2:I:157:LEU:N	2:I:157:LEU:CD1	0.60	2.64	26	8
2:I:148:ILE:O	2:I:148:ILE:HG23	0.60	1.95	7	2
1:C:24:PHE:CE2	1:C:78:LEU:HD12	0.60	2.31	18	2
1:C:74:PHE:CZ	1:C:78:LEU:HD13	0.60	2.31	25	1
1:C:64:VAL:CG2	1:C:72:VAL:HG22	0.60	2.27	4	9
1:C:36:ILE:CD1	1:C:77:PHE:CD2	0.60	2.85	7	3
1:C:24:PHE:O	1:C:27:PHE:CE1	0.60	2.55	18	3
1:C:74:PHE:O	1:C:74:PHE:CD2	0.60	2.55	29	8
1:C:48:LEU:HD22	2:I:153:MET:HA	0.60	1.74	14	2
1:C:53:THR:CB	1:C:54:PRO:CD	0.60	2.80	24	27
1:C:75:ASP:O	1:C:79:VAL:HG23	0.60	1.96	27	2
1:C:84:CYS:SG	4:C:92:BEP:H72	0.60	2.37	19	1
1:C:27:PHE:CE1	1:C:28:VAL:CG2	0.60	2.85	29	4
1:C:41:LEU:HD21	4:C:92:BEP:H122	0.60	1.74	27	1
1:C:23:ALA:HB1	2:I:153:MET:CE	0.60	2.26	17	1
1:C:77:PHE:CD1	1:C:81:MET:CE	0.60	2.85	23	1
1:C:80:MET:HE2	4:C:92:BEP:H32	0.60	1.71	1	2
2:I:157:LEU:HD12	2:I:157:LEU:N	0.59	2.13	17	5
1:C:61:ILE:CD1	1:C:61:ILE:N	0.59	2.65	9	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:5:TYR:CE1	1:C:79:VAL:HG13	0.59	2.31	17	1
1:C:74:PHE:CD2	1:C:74:PHE:O	0.59	2.55	13	7
1:C:74:PHE:O	1:C:78:LEU:HD12	0.59	1.97	28	1
1:C:27:PHE:CD1	1:C:44:VAL:CG2	0.59	2.84	9	5
1:C:44:VAL:CG1	1:C:45:MET:N	0.59	2.66	22	4
1:C:26:ILE:HG21	1:C:44:VAL:HG23	0.59	1.73	22	2
1:C:24:PHE:O	1:C:27:PHE:CE2	0.59	2.56	26	2
1:C:27:PHE:CZ	1:C:28:VAL:HG22	0.59	2.32	14	3
1:C:80:MET:CE	4:C:92:BEP:C23	0.59	2.81	17	4
1:C:74:PHE:O	1:C:74:PHE:CG	0.59	2.55	21	6
1:C:74:PHE:CD1	1:C:74:PHE:O	0.59	2.56	1	5
1:C:74:PHE:O	1:C:74:PHE:CD1	0.59	2.56	27	3
1:C:48:LEU:HD13	2:I:153:MET:CA	0.59	2.27	14	1
1:C:41:LEU:CD2	4:C:92:BEP:C21	0.59	2.80	11	2
1:C:41:LEU:CD2	4:C:92:BEP:C20	0.59	2.81	12	7
1:C:61:ILE:HD13	1:C:61:ILE:N	0.59	2.13	27	2
1:C:45:MET:CE	4:C:92:BEP:C16	0.59	2.81	4	3
1:C:22:ALA:CB	2:I:157:LEU:HD13	0.59	2.27	21	1
1:C:41:LEU:CD1	4:C:92:BEP:C16	0.59	2.81	18	1
1:C:24:PHE:O	1:C:27:PHE:CD1	0.58	2.56	30	2
1:C:28:VAL:HG11	1:C:34:GLY:HA2	0.58	1.74	28	5
1:C:27:PHE:CD1	1:C:27:PHE:N	0.58	2.64	20	1
4:C:92:BEP:C3	2:I:148:ILE:HD12	0.58	2.28	12	1
1:C:61:ILE:N	1:C:61:ILE:CD1	0.58	2.66	21	7
1:C:24:PHE:CE2	1:C:74:PHE:CE2	0.58	2.91	30	5
1:C:80:MET:CE	4:C:92:BEP:C21	0.58	2.81	14	1
1:C:41:LEU:CD1	4:C:92:BEP:C23	0.58	2.80	16	1
1:C:23:ALA:N	2:I:157:LEU:HD21	0.58	2.13	12	2
1:C:23:ALA:HB1	2:I:153:MET:SD	0.58	2.39	8	1
1:C:24:PHE:CD2	1:C:74:PHE:CD2	0.58	2.90	26	1
1:C:41:LEU:CD2	4:C:92:BEP:C24	0.58	2.81	20	1
4:C:92:BEP:C3	2:I:148:ILE:HD11	0.58	2.28	17	2
1:C:24:PHE:CZ	1:C:78:LEU:HD12	0.58	2.33	26	2
2:I:157:LEU:N	2:I:157:LEU:CD2	0.58	2.65	29	5
4:C:92:BEP:C15	2:I:153:MET:HE3	0.58	2.28	15	1
1:C:24:PHE:CE2	1:C:78:LEU:HD11	0.58	2.34	25	3
1:C:41:LEU:HD21	4:C:92:BEP:C12	0.58	2.29	17	2
1:C:48:LEU:HD13	2:I:152:ALA:O	0.58	1.97	23	1
1:C:41:LEU:CD2	1:C:57:LEU:CD2	0.58	2.81	26	1
1:C:19:GLU:CG	1:C:20:PHE:N	0.58	2.66	19	2
1:C:64:VAL:CG1	1:C:80:MET:CG	0.58	2.82	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:26:ILE:HG13	2:I:157:LEU:HD11	0.58	1.74	6	2
1:C:23:ALA:HB2	2:I:153:MET:SD	0.58	2.39	10	4
1:C:60:MET:CE	4:C:92:BEP:N2	0.58	2.67	29	3
1:C:36:ILE:CD1	1:C:77:PHE:CD1	0.58	2.87	23	3
1:C:24:PHE:O	1:C:24:PHE:CD1	0.58	2.57	8	2
1:C:48:LEU:HD21	2:I:153:MET:HE1	0.58	1.76	3	1
1:C:5:TYR:CE2	1:C:79:VAL:HG13	0.57	2.33	5	4
2:I:157:LEU:CD2	2:I:157:LEU:N	0.57	2.67	3	5
1:C:12:LEU:CD1	1:C:16:GLN:CG	0.57	2.81	24	1
4:C:92:BEP:C1	2:I:148:ILE:HD11	0.57	2.28	6	2
1:C:48:LEU:HD21	2:I:153:MET:SD	0.57	2.38	5	1
1:C:74:PHE:CE1	1:C:78:LEU:CD1	0.57	2.86	20	5
1:C:80:MET:CE	4:C:92:BEP:C22	0.57	2.82	9	1
1:C:24:PHE:CZ	1:C:78:LEU:CD1	0.57	2.87	26	2
1:C:36:ILE:CD1	1:C:77:PHE:CG	0.57	2.86	23	2
4:C:92:BEP:C1	2:I:148:ILE:CD1	0.57	2.82	4	1
1:C:27:PHE:CE1	1:C:44:VAL:CG1	0.57	2.87	5	3
1:C:36:ILE:HD11	1:C:77:PHE:CD1	0.57	2.35	23	3
1:C:29:LEU:C	1:C:29:LEU:HD12	0.57	2.20	15	4
4:C:92:BEP:H63	2:I:148:ILE:HB	0.57	1.77	4	1
1:C:60:MET:HE1	4:C:92:BEP:C3	0.57	2.29	27	1
1:C:36:ILE:HG22	1:C:41:LEU:HB2	0.57	1.76	30	1
1:C:53:THR:HG22	1:C:54:PRO:HD2	0.57	1.76	3	13
4:C:92:BEP:C15	2:I:153:MET:CE	0.57	2.82	15	1
1:C:48:LEU:HD22	4:C:92:BEP:H161	0.56	1.76	10	1
1:C:72:VAL:HG12	1:C:76:GLU:HG3	0.56	1.76	14	10
1:C:64:VAL:HG12	1:C:80:MET:SD	0.56	2.40	5	1
4:C:92:BEP:H91	4:C:92:BEP:H72	0.56	1.78	20	1
1:C:52:PRO:CG	1:C:57:LEU:HD21	0.56	2.31	28	1
1:C:60:MET:CE	4:C:92:BEP:C12	0.56	2.83	16	2
1:C:27:PHE:CD1	1:C:41:LEU:HD12	0.56	2.35	5	1
1:C:45:MET:HE2	4:C:92:BEP:H91	0.56	1.76	14	1
1:C:5:TYR:O	1:C:9:VAL:HG23	0.56	2.01	16	1
4:C:92:BEP:C11	2:I:148:ILE:HD11	0.56	2.31	10	1
1:C:77:PHE:CE1	1:C:81:MET:SD	0.56	2.99	4	1
1:C:12:LEU:CD2	1:C:12:LEU:N	0.56	2.68	9	2
1:C:36:ILE:HD12	1:C:77:PHE:CD2	0.56	2.36	9	1
1:C:64:VAL:HG21	1:C:72:VAL:CG2	0.56	2.31	20	10
1:C:53:THR:CG2	1:C:54:PRO:CD	0.56	2.84	19	5
1:C:23:ALA:O	1:C:27:PHE:CD2	0.56	2.59	9	2
1:C:44:VAL:HG11	2:I:153:MET:HE2	0.55	1.76	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:92:BEP:O1	4:C:92:BEP:C11	0.55	2.54	15	3
2:I:153:MET:O	2:I:157:LEU:HD22	0.55	2.01	6	2
2:I:149:SER:O	2:I:150:ALA:CB	0.55	2.54	17	19
1:C:16:GLN:O	1:C:19:GLU:N	0.55	2.40	19	2
1:C:74:PHE:CZ	1:C:78:LEU:CD1	0.55	2.89	25	4
1:C:64:VAL:CG2	1:C:72:VAL:HG21	0.55	2.30	18	1
1:C:27:PHE:CD1	1:C:36:ILE:HD13	0.55	2.37	10	1
1:C:41:LEU:HD12	1:C:57:LEU:HD22	0.55	1.78	16	1
1:C:64:VAL:HG12	1:C:80:MET:HG3	0.55	1.78	20	2
1:C:27:PHE:CD2	1:C:36:ILE:HG12	0.55	2.37	29	3
1:C:80:MET:HE3	4:C:92:BEP:C21	0.55	2.32	14	1
1:C:12:LEU:HD13	1:C:16:GLN:HE21	0.55	1.61	6	1
1:C:48:LEU:CD1	2:I:156:ALA:CB	0.55	2.84	12	2
1:C:22:ALA:O	1:C:26:ILE:CD1	0.55	2.55	22	2
1:C:61:ILE:HD13	4:C:92:BEP:H211	0.55	1.77	27	1
1:C:23:ALA:HA	2:I:157:LEU:HD22	0.54	1.78	2	5
1:C:48:LEU:CD2	1:C:48:LEU:N	0.54	2.68	18	1
1:C:64:VAL:HG12	1:C:80:MET:HB2	0.54	1.79	30	1
1:C:6:LYS:HA	1:C:9:VAL:CG2	0.54	2.31	12	5
1:C:29:LEU:CD2	1:C:29:LEU:O	0.54	2.56	22	2
1:C:61:ILE:O	1:C:65:ASP:N	0.54	2.40	19	16
2:I:148:ILE:O	2:I:149:SER:CB	0.54	2.55	10	1
1:C:19:GLU:OE2	2:I:150:ALA:HB1	0.54	2.02	16	1
1:C:27:PHE:HD2	1:C:36:ILE:HD13	0.54	1.63	11	3
1:C:19:GLU:O	2:I:157:LEU:CD1	0.54	2.56	2	1
1:C:26:ILE:N	1:C:26:ILE:HD13	0.54	2.18	3	2
1:C:53:THR:CG2	1:C:54:PRO:HD2	0.54	2.32	19	10
1:C:74:PHE:CD1	1:C:74:PHE:C	0.54	2.81	26	5
1:C:23:ALA:O	1:C:27:PHE:CE1	0.54	2.60	20	1
1:C:77:PHE:CZ	1:C:81:MET:HG3	0.54	2.38	4	1
1:C:78:LEU:HD23	1:C:81:MET:SD	0.54	2.43	7	1
4:C:92:BEP:C17	2:I:153:MET:CE	0.54	2.85	24	1
4:C:92:BEP:C3	4:C:92:BEP:C18	0.54	2.85	17	1
4:C:92:BEP:H31	2:I:148:ILE:HD12	0.54	1.80	12	1
1:C:6:LYS:O	1:C:10:GLU:CG	0.54	2.56	11	10
1:C:45:MET:HE2	4:C:92:BEP:H102	0.54	1.80	6	1
1:C:17:LYS:CD	1:C:18:ASN:N	0.54	2.71	24	1
2:I:148:ILE:CG2	2:I:148:ILE:O	0.54	2.56	18	3
1:C:16:GLN:O	1:C:19:GLU:CG	0.53	2.56	27	7
1:C:27:PHE:CE2	1:C:41:LEU:HD13	0.53	2.38	13	2
1:C:64:VAL:HG13	1:C:80:MET:CG	0.53	2.32	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:92:BEP:O1	4:C:92:BEP:C8	0.53	2.56	21	2
1:C:80:MET:CE	4:C:92:BEP:C24	0.53	2.87	24	2
1:C:23:ALA:HB1	1:C:27:PHE:CE2	0.53	2.39	9	3
2:I:153:MET:O	2:I:156:ALA:N	0.53	2.42	25	5
1:C:21:LYS:O	1:C:25:ASP:N	0.53	2.42	24	3
1:C:81:MET:O	1:C:85:MET:CE	0.53	2.57	12	1
2:I:148:ILE:O	2:I:148:ILE:HG22	0.53	2.02	24	2
1:C:48:LEU:HD21	2:I:153:MET:HB3	0.53	1.80	6	1
1:C:77:PHE:CD1	1:C:81:MET:HE2	0.53	2.39	23	1
1:C:24:PHE:O	1:C:28:VAL:CG2	0.53	2.57	27	7
1:C:74:PHE:CE2	1:C:78:LEU:HD11	0.53	2.38	23	2
2:I:153:MET:O	2:I:157:LEU:CD2	0.53	2.56	30	5
1:C:27:PHE:CD1	1:C:36:ILE:HG12	0.53	2.39	26	2
4:C:92:BEP:H12	2:I:148:ILE:HD13	0.53	1.80	15	2
1:C:15:GLU:O	1:C:19:GLU:CG	0.53	2.57	24	1
2:I:153:MET:HE3	2:I:157:LEU:HD21	0.53	1.80	5	1
1:C:42:GLY:CA	1:C:57:LEU:HD11	0.53	2.33	23	1
2:I:157:LEU:CD2	2:I:157:LEU:O	0.53	2.57	23	2
1:C:28:VAL:HG21	1:C:34:GLY:HA2	0.53	1.79	5	3
1:C:28:VAL:CG1	1:C:35:CYS:O	0.53	2.57	26	5
1:C:77:PHE:CZ	1:C:81:MET:CG	0.53	2.92	4	1
1:C:45:MET:SD	4:C:92:BEP:C16	0.53	2.97	22	2
2:I:154:MET:HA	2:I:157:LEU:HD21	0.53	1.81	20	2
2:I:157:LEU:HD23	2:I:157:LEU:O	0.53	2.03	23	2
1:C:45:MET:CE	4:C:92:BEP:C15	0.53	2.87	25	3
1:C:27:PHE:CE2	1:C:28:VAL:HG22	0.53	2.39	26	2
1:C:21:LYS:O	1:C:24:PHE:CB	0.53	2.57	3	3
1:C:19:GLU:O	1:C:22:ALA:HB3	0.53	2.03	10	3
1:C:41:LEU:HB2	1:C:57:LEU:HD22	0.53	1.80	16	1
1:C:77:PHE:C	1:C:77:PHE:CD1	0.52	2.78	28	4
1:C:77:PHE:CD1	1:C:77:PHE:C	0.52	2.80	7	4
4:C:92:BEP:H72	4:C:92:BEP:H112	0.52	1.81	7	1
1:C:26:ILE:CD1	2:I:157:LEU:HD11	0.52	2.30	3	4
4:C:92:BEP:C14	2:I:153:MET:CE	0.52	2.87	21	1
1:C:64:VAL:HG21	1:C:72:VAL:HG21	0.52	1.80	18	3
2:I:157:LEU:N	2:I:157:LEU:HD12	0.52	2.19	19	3
1:C:85:MET:HE2	2:I:148:ILE:HG22	0.52	1.80	12	1
1:C:72:VAL:HG13	1:C:76:GLU:HG3	0.52	1.81	29	4
1:C:22:ALA:HB1	2:I:157:LEU:HG	0.52	1.81	3	2
1:C:29:LEU:O	1:C:29:LEU:CD2	0.52	2.57	18	1
2:I:156:ALA:HB3	2:I:157:LEU:CD1	0.52	2.33	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:19:GLU:O	2:I:157:LEU:CD2	0.52	2.55	22	2
1:C:5:TYR:CD1	1:C:79:VAL:CG1	0.52	2.92	7	1
1:C:81:MET:HG2	1:C:82:VAL:N	0.52	2.19	7	1
1:C:41:LEU:O	1:C:44:VAL:N	0.52	2.43	11	3
1:C:73:ASP:OD1	1:C:75:ASP:N	0.52	2.41	7	17
1:C:43:LYS:O	1:C:46:ARG:CG	0.52	2.58	22	4
1:C:72:VAL:HG13	1:C:76:GLU:CD	0.52	2.25	18	1
1:C:12:LEU:CD1	1:C:16:GLN:OE1	0.52	2.57	9	2
1:C:21:LYS:O	1:C:24:PHE:N	0.52	2.43	23	7
1:C:48:LEU:HD11	4:C:92:BEP:H171	0.52	1.80	23	2
1:C:45:MET:SD	4:C:92:BEP:C18	0.52	2.98	9	1
1:C:57:LEU:O	1:C:60:MET:N	0.52	2.43	28	15
4:C:92:BEP:C1	2:I:148:ILE:HD13	0.52	2.35	2	1
1:C:53:THR:CB	1:C:54:PRO:HD2	0.52	2.35	25	26
1:C:64:VAL:CG1	1:C:80:MET:SD	0.52	2.98	8	4
1:C:29:LEU:O	1:C:29:LEU:CG	0.52	2.57	18	1
1:C:73:ASP:OD1	1:C:76:GLU:CG	0.52	2.58	13	4
1:C:82:VAL:O	1:C:85:MET:N	0.52	2.43	27	1
1:C:26:ILE:HB	1:C:44:VAL:HG22	0.52	1.82	11	3
1:C:60:MET:SD	4:C:92:BEP:C10	0.52	2.98	30	1
1:C:81:MET:O	1:C:84:CYS:N	0.52	2.43	18	2
1:C:5:TYR:CZ	1:C:83:ARG:HB3	0.52	2.40	27	1
1:C:44:VAL:O	1:C:47:MET:N	0.52	2.43	12	14
1:C:37:SER:O	1:C:40:GLU:N	0.52	2.43	18	3
1:C:23:ALA:CA	2:I:157:LEU:HD21	0.52	2.35	12	2
1:C:63:GLU:N	1:C:63:GLU:OE1	0.52	2.42	30	1
1:C:41:LEU:HD11	4:C:92:BEP:H181	0.51	1.82	28	1
1:C:34:GLY:O	1:C:74:PHE:N	0.51	2.44	18	1
1:C:24:PHE:CZ	1:C:78:LEU:HG	0.51	2.39	28	4
2:I:154:MET:HA	2:I:157:LEU:HD23	0.51	1.82	8	1
1:C:36:ILE:CG2	1:C:41:LEU:HD23	0.51	2.36	2	1
1:C:17:LYS:HD2	1:C:18:ASN:N	0.51	2.21	24	1
2:I:148:ILE:O	2:I:150:ALA:N	0.51	2.42	9	1
1:C:80:MET:SD	4:C:92:BEP:C20	0.51	2.98	23	1
1:C:48:LEU:HD22	2:I:156:ALA:CA	0.51	2.34	27	1
4:C:92:BEP:C18	4:C:92:BEP:C19	0.51	2.88	18	1
1:C:48:LEU:HD11	2:I:156:ALA:CB	0.51	2.35	12	2
1:C:26:ILE:CD1	2:I:157:LEU:CD1	0.51	2.88	14	3
1:C:26:ILE:HD13	2:I:157:LEU:CD2	0.51	2.28	27	1
1:C:27:PHE:CE1	4:C:92:BEP:H171	0.51	2.40	20	2
2:I:148:ILE:HG22	2:I:148:ILE:O	0.51	2.04	30	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:92:BEP:H41	2:I:148:ILE:HD11	0.51	1.81	6	1
1:C:26:ILE:HB	1:C:44:VAL:HG23	0.51	1.82	7	1
1:C:63:GLU:OE1	1:C:63:GLU:N	0.51	2.43	15	1
2:I:150:ALA:O	2:I:153:MET:N	0.51	2.44	17	4
1:C:17:LYS:O	1:C:20:PHE:N	0.51	2.44	22	1
1:C:84:CYS:SG	4:C:92:BEP:H62	0.51	2.46	27	1
1:C:63:GLU:CA	1:C:63:GLU:OE1	0.51	2.58	30	2
1:C:77:PHE:O	1:C:80:MET:N	0.51	2.44	4	2
1:C:6:LYS:O	1:C:10:GLU:N	0.51	2.43	2	8
1:C:7:ALA:O	1:C:10:GLU:N	0.51	2.44	20	7
1:C:41:LEU:HD22	4:C:92:BEP:C23	0.51	2.35	23	2
1:C:16:GLN:NE2	1:C:20:PHE:CD2	0.51	2.78	25	1
1:C:63:GLU:OE1	4:C:92:BEP:C6	0.51	2.58	21	1
1:C:24:PHE:HE2	1:C:78:LEU:HD11	0.51	1.66	30	1
1:C:40:GLU:O	1:C:43:LYS:N	0.51	2.43	17	1
1:C:14:GLU:O	1:C:18:ASN:ND2	0.51	2.44	13	5
1:C:9:VAL:O	1:C:17:LYS:NZ	0.51	2.44	4	1
1:C:45:MET:CE	4:C:92:BEP:C17	0.51	2.89	26	1
1:C:45:MET:HE3	4:C:92:BEP:C17	0.51	2.36	26	2
1:C:60:MET:HB3	4:C:92:BEP:C24	0.51	2.36	16	1
1:C:36:ILE:HD12	1:C:72:VAL:CG1	0.51	2.36	30	2
1:C:45:MET:O	1:C:48:LEU:N	0.51	2.43	29	4
1:C:5:TYR:O	1:C:9:VAL:N	0.51	2.43	2	2
1:C:64:VAL:CG2	1:C:72:VAL:HG13	0.51	2.35	20	2
1:C:36:ILE:O	1:C:72:VAL:HG23	0.51	2.06	19	2
2:I:153:MET:CE	2:I:157:LEU:HD21	0.51	2.36	5	1
1:C:44:VAL:CG1	2:I:153:MET:SD	0.50	2.99	17	2
1:C:23:ALA:HB2	2:I:153:MET:HG2	0.50	1.83	7	2
1:C:80:MET:O	1:C:83:ARG:CB	0.50	2.59	10	1
1:C:46:ARG:CD	1:C:51:ASN:OD1	0.50	2.59	13	1
1:C:84:CYS:SG	4:C:92:BEP:C8	0.50	2.99	26	1
1:C:27:PHE:CZ	4:C:92:BEP:H161	0.50	2.42	3	2
1:C:35:CYS:CB	1:C:72:VAL:O	0.50	2.59	15	1
1:C:29:LEU:C	1:C:29:LEU:CD2	0.50	2.76	29	3
2:I:157:LEU:HD22	2:I:157:LEU:H	0.50	1.65	30	2
1:C:12:LEU:CD2	1:C:16:GLN:OE1	0.50	2.58	28	1
1:C:80:MET:CE	4:C:92:BEP:C3	0.50	2.88	4	1
1:C:41:LEU:HD12	1:C:41:LEU:O	0.50	2.06	15	2
1:C:80:MET:HE2	4:C:92:BEP:C23	0.50	2.37	9	1
1:C:19:GLU:HG3	1:C:20:PHE:N	0.50	2.20	19	2
1:C:63:GLU:OE2	4:C:92:BEP:H61	0.50	2.05	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:21:LYS:HA	1:C:24:PHE:CD2	0.50	2.41	25	3
1:C:5:TYR:CE2	1:C:79:VAL:CG1	0.50	2.95	5	3
1:C:27:PHE:HB3	1:C:36:ILE:HG23	0.50	1.82	4	3
1:C:24:PHE:CE1	1:C:77:PHE:CE2	0.50	3.00	27	4
1:C:8:ALA:CB	1:C:82:VAL:HG13	0.50	2.36	11	1
1:C:60:MET:HE3	4:C:92:BEP:H112	0.50	1.83	5	1
1:C:67:ASP:OD1	1:C:69:SER:N	0.50	2.45	12	1
4:C:92:BEP:C18	2:I:148:ILE:HD11	0.50	2.36	7	1
1:C:36:ILE:HG22	1:C:37:SER:N	0.50	2.21	9	4
1:C:44:VAL:O	1:C:48:LEU:HD13	0.50	2.06	1	1
2:I:151:ASP:OD1	2:I:152:ALA:N	0.50	2.45	29	2
1:C:77:PHE:CD2	1:C:78:LEU:N	0.50	2.80	12	10
1:C:12:LEU:N	1:C:12:LEU:CD2	0.50	2.74	23	1
4:C:92:BEP:H12	2:I:148:ILE:CD1	0.50	2.35	4	1
1:C:23:ALA:CB	2:I:153:MET:SD	0.50	2.99	8	6
1:C:33:ASP:N	1:C:33:ASP:OD1	0.50	2.44	12	2
1:C:51:ASN:O	1:C:51:ASN:ND2	0.50	2.44	5	1
1:C:65:ASP:OD2	1:C:70:GLY:CA	0.50	2.60	24	4
1:C:80:MET:HE2	4:C:92:BEP:C24	0.50	2.36	21	1
1:C:45:MET:HE3	4:C:92:BEP:C16	0.50	2.36	4	1
1:C:27:PHE:CD2	1:C:41:LEU:HD13	0.50	2.42	11	1
1:C:27:PHE:CE2	1:C:36:ILE:HG12	0.50	2.41	18	1
2:I:154:MET:O	2:I:157:LEU:N	0.49	2.45	17	3
1:C:23:ALA:CA	2:I:157:LEU:HD11	0.49	2.36	22	1
1:C:36:ILE:CG2	1:C:41:LEU:CD2	0.49	2.89	16	2
1:C:67:ASP:N	1:C:67:ASP:OD1	0.49	2.43	17	9
1:C:78:LEU:C	1:C:81:MET:CE	0.49	2.80	7	1
1:C:20:PHE:O	1:C:24:PHE:N	0.49	2.44	2	1
1:C:27:PHE:CE1	4:C:92:BEP:C16	0.49	2.95	3	1
1:C:84:CYS:HB2	4:C:92:BEP:H72	0.49	1.84	15	1
1:C:20:PHE:CZ	1:C:81:MET:HB3	0.49	2.42	4	1
1:C:80:MET:O	1:C:83:ARG:N	0.49	2.45	25	2
1:C:77:PHE:O	1:C:77:PHE:CD1	0.49	2.65	26	2
1:C:16:GLN:OE1	1:C:20:PHE:CD2	0.49	2.65	10	1
4:C:92:BEP:C16	2:I:153:MET:SD	0.49	3.01	24	2
1:C:33:ASP:OD1	1:C:33:ASP:N	0.49	2.45	16	4
1:C:41:LEU:HD21	4:C:92:BEP:H141	0.49	1.83	23	1
1:C:60:MET:HB3	4:C:92:BEP:C20	0.49	2.38	12	3
1:C:27:PHE:CD1	1:C:44:VAL:HG11	0.49	2.42	24	2
1:C:48:LEU:HD21	2:I:153:MET:CB	0.49	2.37	6	1
1:C:85:MET:CE	2:I:148:ILE:HG22	0.49	2.38	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:41:LEU:CD2	4:C:92:BEP:H201	0.49	2.38	25	3
4:C:92:BEP:H91	4:C:92:BEP:H63	0.49	1.84	7	1
1:C:60:MET:HE3	4:C:92:BEP:H91	0.49	1.84	21	1
1:C:29:LEU:CG	1:C:29:LEU:O	0.49	2.61	15	3
2:I:153:MET:O	2:I:157:LEU:CG	0.49	2.60	21	1
1:C:61:ILE:CG2	1:C:65:ASP:CG	0.49	2.81	21	2
1:C:24:PHE:HA	1:C:27:PHE:CE2	0.49	2.42	20	3
1:C:50:GLN:OE1	4:C:92:BEP:C9	0.49	2.61	14	1
1:C:12:LEU:CD1	1:C:16:GLN:CD	0.49	2.80	24	1
1:C:60:MET:HE3	4:C:92:BEP:H11	0.49	1.83	6	1
1:C:27:PHE:CA	1:C:44:VAL:HG21	0.49	2.38	17	1
2:I:156:ALA:HB3	2:I:157:LEU:HD13	0.49	1.84	15	3
1:C:23:ALA:CB	1:C:27:PHE:CZ	0.49	2.96	22	1
1:C:59:GLU:O	1:C:63:GLU:CG	0.49	2.61	27	3
4:C:92:BEP:H11	2:I:148:ILE:HD11	0.49	1.85	1	1
1:C:27:PHE:CD1	1:C:28:VAL:N	0.49	2.81	30	2
1:C:15:GLU:O	1:C:18:ASN:N	0.49	2.46	23	4
1:C:28:VAL:O	1:C:31:ALA:N	0.49	2.46	22	1
1:C:45:MET:HE3	1:C:45:MET:HA	0.49	1.84	8	1
1:C:22:ALA:HB3	2:I:157:LEU:CD2	0.49	2.37	26	1
1:C:27:PHE:CD1	1:C:28:VAL:HG22	0.49	2.43	29	3
1:C:64:VAL:O	1:C:66:GLU:N	0.48	2.45	30	4
1:C:80:MET:HE1	4:C:92:BEP:C24	0.48	2.37	24	2
1:C:27:PHE:CE2	1:C:41:LEU:CD1	0.48	2.96	11	2
1:C:41:LEU:CB	1:C:57:LEU:HD22	0.48	2.38	16	1
1:C:51:ASN:ND2	1:C:51:ASN:O	0.48	2.46	8	1
1:C:28:VAL:HG11	1:C:35:CYS:N	0.48	2.23	26	1
1:C:5:TYR:OH	1:C:83:ARG:NH1	0.48	2.45	2	3
1:C:41:LEU:HD11	1:C:45:MET:SD	0.48	2.48	9	1
1:C:29:LEU:HD21	1:C:43:LYS:HD3	0.48	1.85	16	1
4:C:92:BEP:H181	4:C:92:BEP:C19	0.48	2.39	18	1
1:C:61:ILE:HG22	1:C:65:ASP:CG	0.48	2.29	17	2
1:C:7:ALA:O	1:C:11:GLN:CG	0.48	2.62	27	3
4:C:92:BEP:C18	4:C:92:BEP:H31	0.48	2.36	17	1
1:C:46:ARG:N	1:C:50:GLN:O	0.48	2.46	24	3
1:C:48:LEU:N	1:C:48:LEU:CD2	0.48	2.67	9	2
1:C:24:PHE:CD1	1:C:27:PHE:CE1	0.48	3.01	29	1
1:C:27:PHE:HA	1:C:44:VAL:CG2	0.48	2.38	18	5
1:C:26:ILE:CG2	1:C:47:MET:CE	0.48	2.92	19	3
1:C:78:LEU:O	1:C:81:MET:N	0.48	2.43	19	5
1:C:81:MET:O	1:C:85:MET:CG	0.48	2.62	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:24:PHE:CE2	1:C:78:LEU:HD21	0.48	2.44	5	1
1:C:48:LEU:HD23	2:I:156:ALA:HB2	0.48	1.82	17	1
1:C:80:MET:CE	4:C:92:BEP:H31	0.48	2.39	4	3
1:C:29:LEU:CD1	1:C:29:LEU:C	0.48	2.77	29	4
1:C:12:LEU:HD23	1:C:12:LEU:N	0.48	2.24	16	2
1:C:27:PHE:CD2	1:C:36:ILE:CG1	0.48	2.97	30	2
1:C:72:VAL:O	1:C:73:ASP:O	0.48	2.32	10	4
1:C:7:ALA:O	1:C:11:GLN:N	0.48	2.43	20	2
1:C:38:THR:CG2	1:C:58:GLN:HA	0.48	2.38	17	4
1:C:64:VAL:CG1	1:C:80:MET:HG3	0.48	2.39	13	7
4:C:92:BEP:H21	2:I:148:ILE:CD1	0.48	2.38	2	7
1:C:48:LEU:HD22	2:I:152:ALA:O	0.48	2.09	11	2
1:C:41:LEU:CD1	4:C:92:BEP:C15	0.48	2.91	26	1
1:C:27:PHE:CE2	1:C:77:PHE:CE2	0.48	3.01	3	1
4:C:92:BEP:C16	2:I:153:MET:CE	0.48	2.92	3	1
1:C:27:PHE:CZ	4:C:92:BEP:H171	0.48	2.44	16	1
1:C:23:ALA:HA	1:C:26:ILE:CG1	0.48	2.39	15	16
1:C:64:VAL:O	1:C:76:GLU:OE1	0.47	2.32	12	3
4:C:92:BEP:C16	2:I:148:ILE:HD11	0.47	2.39	7	1
1:C:24:PHE:HA	1:C:27:PHE:CD2	0.47	2.44	20	5
1:C:36:ILE:O	1:C:72:VAL:N	0.47	2.47	2	3
1:C:16:GLN:O	1:C:19:GLU:HG2	0.47	2.09	11	5
1:C:67:ASP:OD1	1:C:67:ASP:N	0.47	2.43	28	2
1:C:14:GLU:O	1:C:18:ASN:N	0.47	2.46	26	1
1:C:35:CYS:CB	1:C:71:THR:HB	0.47	2.39	20	2
1:C:23:ALA:HB2	2:I:153:MET:CG	0.47	2.39	13	1
1:C:60:MET:HE2	4:C:92:BEP:H31	0.47	1.86	28	1
1:C:38:THR:O	1:C:57:LEU:CD1	0.47	2.60	30	4
1:C:41:LEU:HD21	4:C:92:BEP:H241	0.47	1.87	14	1
4:C:92:BEP:H81	2:I:148:ILE:CG1	0.47	2.39	30	1
1:C:41:LEU:HD21	4:C:92:BEP:H121	0.47	1.85	17	2
1:C:61:ILE:O	1:C:64:VAL:N	0.47	2.43	11	3
1:C:16:GLN:OE1	1:C:16:GLN:O	0.47	2.32	10	1
1:C:25:ASP:C	1:C:26:ILE:HD13	0.47	2.30	30	1
1:C:27:PHE:C	1:C:27:PHE:CD1	0.47	2.88	29	2
2:I:148:ILE:O	2:I:148:ILE:CG1	0.47	2.62	28	1
1:C:16:GLN:O	1:C:19:GLU:HG3	0.47	2.10	27	11
1:C:53:THR:HB	1:C:54:PRO:HD2	0.47	1.86	5	11
2:I:156:ALA:C	2:I:157:LEU:CD1	0.47	2.79	23	2
1:C:77:PHE:CE2	1:C:81:MET:HG3	0.47	2.44	4	1
1:C:19:GLU:OE1	1:C:20:PHE:N	0.47	2.46	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:16:GLN:HG3	1:C:17:LYS:N	0.47	2.25	6	10
1:C:47:MET:CE	2:I:156:ALA:CB	0.47	2.92	22	1
1:C:25:ASP:O	1:C:29:LEU:CB	0.47	2.63	22	2
1:C:80:MET:CE	4:C:92:BEP:H12	0.47	2.40	21	3
1:C:73:ASP:OD1	1:C:76:GLU:HG3	0.47	2.10	15	2
1:C:73:ASP:OD1	1:C:76:GLU:OE2	0.47	2.33	9	2
1:C:80:MET:HE1	4:C:92:BEP:C20	0.47	2.39	30	1
1:C:58:GLN:O	1:C:58:GLN:NE2	0.47	2.47	29	1
1:C:60:MET:CE	4:C:92:BEP:C3	0.47	2.93	27	2
1:C:42:GLY:HA2	1:C:57:LEU:HD11	0.47	1.86	23	1
1:C:79:VAL:O	1:C:83:ARG:N	0.47	2.46	9	4
1:C:65:ASP:OD1	1:C:71:THR:O	0.47	2.33	29	7
2:I:157:LEU:H	2:I:157:LEU:HD22	0.47	1.70	15	2
1:C:38:THR:HG21	1:C:58:GLN:OE1	0.47	2.10	6	1
1:C:30:GLY:O	1:C:31:ALA:O	0.47	2.33	25	2
1:C:73:ASP:OD1	1:C:73:ASP:C	0.47	2.53	7	3
1:C:33:ASP:OD1	1:C:35:CYS:SG	0.47	2.73	11	3
4:C:92:BEP:H111	2:I:148:ILE:HD13	0.47	1.85	14	1
1:C:26:ILE:N	1:C:26:ILE:CD1	0.47	2.77	27	2
1:C:36:ILE:HG22	1:C:37:SER:H	0.47	1.69	16	1
1:C:36:ILE:CG2	1:C:41:LEU:HD21	0.47	2.31	16	1
4:C:92:BEP:H31	2:I:148:ILE:CD1	0.46	2.40	12	3
1:C:73:ASP:OD1	1:C:76:GLU:HG2	0.46	2.10	13	5
1:C:20:PHE:O	1:C:24:PHE:CD2	0.46	2.68	28	1
1:C:73:ASP:OD2	1:C:76:GLU:OE2	0.46	2.33	22	5
1:C:26:ILE:CG1	2:I:157:LEU:HD11	0.46	2.40	24	3
1:C:53:THR:O	1:C:57:LEU:CG	0.46	2.63	21	1
1:C:14:GLU:O	1:C:18:ASN:CB	0.46	2.64	24	1
1:C:80:MET:HE1	4:C:92:BEP:C21	0.46	2.40	27	1
1:C:22:ALA:CB	2:I:157:LEU:HB2	0.46	2.38	27	1
1:C:16:GLN:O	1:C:16:GLN:OE1	0.46	2.32	6	2
1:C:24:PHE:HE2	1:C:78:LEU:HD12	0.46	1.71	3	1
4:C:92:BEP:H63	4:C:92:BEP:H91	0.46	1.87	3	1
2:I:149:SER:OG	2:I:150:ALA:N	0.46	2.47	9	1
1:C:8:ALA:HB3	1:C:82:VAL:CG1	0.46	2.40	11	1
1:C:84:CYS:O	1:C:86:LYS:N	0.46	2.48	16	1
1:C:48:LEU:N	1:C:48:LEU:CD1	0.46	2.77	5	1
1:C:52:PRO:HG2	1:C:57:LEU:HD21	0.46	1.87	28	1
1:C:77:PHE:O	1:C:81:MET:CE	0.46	2.64	23	1
1:C:80:MET:HE1	4:C:92:BEP:H31	0.46	1.87	4	1
1:C:36:ILE:O	1:C:71:THR:CG2	0.46	2.59	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:73:ASP:CG	1:C:76:GLU:CG	0.46	2.84	11	1
4:C:92:BEP:C15	2:I:153:MET:SD	0.46	3.04	1	1
1:C:36:ILE:HG13	1:C:72:VAL:O	0.46	2.10	18	1
4:C:92:BEP:H11	2:I:148:ILE:CD1	0.46	2.40	4	1
1:C:82:VAL:O	1:C:86:LYS:N	0.46	2.44	7	1
1:C:27:PHE:CZ	1:C:28:VAL:HG21	0.46	2.45	26	2
1:C:61:ILE:HD12	1:C:61:ILE:N	0.46	2.24	9	4
1:C:77:PHE:CE1	4:C:92:BEP:H211	0.46	2.46	3	1
1:C:41:LEU:CD1	4:C:92:BEP:C24	0.46	2.94	16	1
4:C:92:BEP:H81	2:I:148:ILE:HD11	0.46	1.87	17	1
2:I:154:MET:HA	2:I:157:LEU:CD2	0.46	2.41	15	2
1:C:73:ASP:N	1:C:73:ASP:OD1	0.46	2.47	9	1
1:C:61:ILE:N	1:C:61:ILE:HD12	0.46	2.26	11	1
4:C:92:BEP:C20	4:C:92:BEP:H11	0.46	2.40	17	2
1:C:21:LYS:O	1:C:24:PHE:HB2	0.46	2.11	7	11
1:C:80:MET:CE	4:C:92:BEP:C19	0.46	2.93	1	2
1:C:48:LEU:CD1	1:C:48:LEU:N	0.46	2.78	25	1
4:C:92:BEP:H121	2:I:148:ILE:CD1	0.46	2.40	22	2
1:C:48:LEU:HD13	2:I:153:MET:HB3	0.46	1.85	14	1
1:C:24:PHE:CD1	1:C:74:PHE:CD1	0.46	3.04	29	1
1:C:28:VAL:HG12	1:C:31:ALA:CB	0.46	2.41	19	1
1:C:13:THR:O	1:C:15:GLU:N	0.46	2.48	12	2
1:C:48:LEU:HD21	2:I:153:MET:CA	0.46	2.41	6	3
1:C:26:ILE:CG2	1:C:47:MET:HE1	0.46	2.41	19	2
1:C:53:THR:HB	1:C:54:PRO:CD	0.46	2.40	5	3
1:C:5:TYR:N	1:C:5:TYR:CD1	0.46	2.83	27	1
1:C:8:ALA:CB	1:C:82:VAL:CG1	0.46	2.94	11	1
1:C:27:PHE:CG	1:C:44:VAL:HG21	0.46	2.45	1	1
1:C:80:MET:HE1	4:C:92:BEP:H42	0.46	1.88	5	1
1:C:63:GLU:HA	1:C:63:GLU:OE1	0.46	2.11	29	1
1:C:60:MET:HB3	4:C:92:BEP:C21	0.46	2.41	15	4
1:C:78:LEU:O	1:C:81:MET:SD	0.46	2.74	7	1
1:C:48:LEU:O	2:I:155:GLN:NE2	0.46	2.49	5	1
1:C:26:ILE:C	1:C:44:VAL:CG2	0.46	2.84	30	1
1:C:60:MET:CE	4:C:92:BEP:H31	0.46	2.40	15	3
1:C:77:PHE:CE1	1:C:81:MET:HE2	0.46	2.45	23	1
1:C:29:LEU:HG	1:C:29:LEU:O	0.46	2.11	23	3
1:C:64:VAL:CG1	1:C:80:MET:HB2	0.46	2.41	12	6
1:C:58:GLN:O	1:C:58:GLN:OE1	0.46	2.33	27	2
1:C:27:PHE:CE2	1:C:77:PHE:CE1	0.46	3.04	2	2
4:C:92:BEP:C14	2:I:148:ILE:HD12	0.46	2.40	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:40:GLU:O	1:C:43:LYS:CB	0.46	2.63	1	1
1:C:27:PHE:CZ	2:I:153:MET:CE	0.46	2.99	17	1
1:C:33:ASP:OD2	1:C:35:CYS:SG	0.46	2.74	17	2
1:C:64:VAL:HG12	1:C:80:MET:CB	0.46	2.41	23	1
1:C:15:GLU:O	1:C:19:GLU:OE2	0.46	2.34	25	1
1:C:60:MET:CE	4:C:92:BEP:H12	0.46	2.41	26	1
1:C:80:MET:SD	4:C:92:BEP:C23	0.46	3.04	21	1
1:C:24:PHE:CD2	1:C:74:PHE:CZ	0.46	3.04	3	1
1:C:27:PHE:O	1:C:36:ILE:HG23	0.46	2.11	11	1
1:C:61:ILE:O	1:C:64:VAL:CG2	0.46	2.64	26	2
1:C:60:MET:CE	4:C:92:BEP:H82	0.46	2.41	29	1
1:C:79:VAL:O	1:C:82:VAL:N	0.45	2.49	27	5
1:C:80:MET:SD	1:C:80:MET:O	0.45	2.74	4	1
4:C:92:BEP:C24	4:C:92:BEP:H181	0.45	2.41	22	2
1:C:41:LEU:CD1	4:C:92:BEP:H171	0.45	2.41	22	1
1:C:61:ILE:HG13	1:C:72:VAL:HG23	0.45	1.87	11	1
1:C:45:MET:SD	4:C:92:BEP:C15	0.45	3.04	5	1
4:C:92:BEP:H181	4:C:92:BEP:C3	0.45	2.40	17	1
1:C:27:PHE:CE1	1:C:36:ILE:HG12	0.45	2.46	26	2
1:C:64:VAL:CG2	1:C:64:VAL:O	0.45	2.64	21	1
1:C:15:GLU:O	1:C:19:GLU:HG3	0.45	2.10	24	1
1:C:61:ILE:O	1:C:64:VAL:HG22	0.45	2.10	15	1
1:C:45:MET:CE	4:C:92:BEP:H141	0.45	2.40	17	1
1:C:60:MET:SD	4:C:92:BEP:O1	0.45	2.74	17	2
1:C:22:ALA:CB	2:I:157:LEU:HG	0.45	2.41	28	2
1:C:58:GLN:O	1:C:61:ILE:N	0.45	2.44	4	4
2:I:156:ALA:CB	2:I:157:LEU:HD13	0.45	2.42	15	2
1:C:84:CYS:SG	1:C:85:MET:N	0.45	2.90	20	4
1:C:16:GLN:NE2	1:C:16:GLN:O	0.45	2.49	14	1
1:C:56:GLU:N	1:C:56:GLU:OE1	0.45	2.49	24	1
4:C:92:BEP:H72	4:C:92:BEP:H81	0.45	1.86	13	1
1:C:46:ARG:HG3	1:C:47:MET:N	0.45	2.26	26	5
1:C:60:MET:HE2	4:C:92:BEP:H12	0.45	1.88	10	1
1:C:60:MET:CB	4:C:92:BEP:C24	0.45	2.95	16	1
1:C:29:LEU:O	1:C:29:LEU:CD1	0.45	2.59	28	3
1:C:81:MET:HA	1:C:81:MET:CE	0.45	2.42	28	1
1:C:64:VAL:HB	1:C:76:GLU:CB	0.45	2.41	13	3
1:C:81:MET:O	1:C:85:MET:HE2	0.45	2.11	12	1
1:C:18:ASN:O	1:C:20:PHE:N	0.45	2.50	5	5
1:C:77:PHE:CD1	1:C:81:MET:HE1	0.45	2.46	23	2
1:C:44:VAL:O	1:C:48:LEU:CD1	0.45	2.65	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:48:LEU:CD2	2:I:156:ALA:HA	0.45	2.39	27	1
2:I:153:MET:O	2:I:155:GLN:N	0.45	2.50	19	2
1:C:26:ILE:HB	1:C:44:VAL:CG2	0.45	2.42	3	2
1:C:25:ASP:O	1:C:29:LEU:CA	0.45	2.64	22	1
1:C:28:VAL:HG13	1:C:36:ILE:HG12	0.45	1.89	11	1
2:I:153:MET:O	2:I:157:LEU:CD1	0.45	2.64	30	1
1:C:28:VAL:HG23	1:C:28:VAL:O	0.45	2.11	4	1
1:C:72:VAL:CG1	1:C:76:GLU:HG3	0.45	2.42	25	14
1:C:47:MET:HE1	2:I:156:ALA:HB1	0.45	1.87	25	1
4:C:92:BEP:H12	2:I:148:ILE:HD11	0.45	1.88	6	2
1:C:57:LEU:CD2	1:C:60:MET:SD	0.45	3.01	22	1
1:C:29:LEU:O	1:C:29:LEU:HG	0.45	2.10	18	1
1:C:36:ILE:HD12	4:C:92:BEP:C23	0.45	2.40	4	1
1:C:61:ILE:HA	1:C:64:VAL:CG2	0.45	2.42	14	1
1:C:43:LYS:O	1:C:46:ARG:HG3	0.45	2.12	18	2
1:C:81:MET:HB3	1:C:85:MET:CE	0.45	2.41	11	2
1:C:28:VAL:O	1:C:28:VAL:HG23	0.45	2.11	5	1
1:C:80:MET:SD	1:C:81:MET:SD	0.45	3.14	20	2
1:C:41:LEU:HD11	4:C:92:BEP:C16	0.45	2.42	18	1
1:C:43:LYS:O	1:C:47:MET:CG	0.45	2.65	6	1
1:C:86:LYS:N	1:C:86:LYS:CD	0.45	2.80	23	1
1:C:43:LYS:O	1:C:46:ARG:HG2	0.45	2.12	22	3
1:C:48:LEU:HD12	1:C:48:LEU:N	0.45	2.27	5	2
1:C:13:THR:OG1	1:C:16:GLN:CG	0.45	2.64	9	1
1:C:5:TYR:OH	1:C:83:ARG:CG	0.45	2.65	1	1
4:C:92:BEP:C16	2:I:153:MET:HG2	0.45	2.42	5	1
1:C:79:VAL:O	1:C:82:VAL:HG12	0.44	2.11	4	2
1:C:60:MET:CE	4:C:92:BEP:H122	0.44	2.42	12	3
1:C:45:MET:CB	1:C:52:PRO:HG3	0.44	2.42	7	1
1:C:64:VAL:CG2	1:C:72:VAL:CG2	0.44	2.95	26	2
1:C:80:MET:CE	4:C:92:BEP:H32	0.44	2.42	1	1
1:C:37:SER:O	1:C:39:LYS:N	0.44	2.51	5	1
1:C:24:PHE:HA	1:C:27:PHE:CD1	0.44	2.47	18	1
1:C:84:CYS:SG	4:C:92:BEP:C9	0.44	3.05	12	2
1:C:60:MET:CE	4:C:92:BEP:C8	0.44	2.95	22	2
1:C:41:LEU:HD21	4:C:92:BEP:C24	0.44	2.41	20	1
4:C:92:BEP:C2	2:I:148:ILE:CD1	0.44	2.95	13	1
1:C:77:PHE:O	1:C:78:LEU:C	0.44	2.56	12	10
1:C:70:GLY:O	1:C:71:THR:HG23	0.44	2.13	23	1
1:C:45:MET:HE2	4:C:92:BEP:C15	0.44	2.43	25	1
1:C:16:GLN:O	1:C:20:PHE:CD2	0.44	2.70	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:79:VAL:O	1:C:80:MET:C	0.44	2.56	22	12
1:C:23:ALA:N	2:I:157:LEU:CD2	0.44	2.79	12	1
1:C:27:PHE:CZ	4:C:92:BEP:C16	0.44	3.01	3	1
1:C:35:CYS:HA	1:C:72:VAL:O	0.44	2.12	15	2
1:C:26:ILE:HD11	2:I:157:LEU:HB3	0.44	1.88	20	2
1:C:72:VAL:HG13	1:C:76:GLU:CG	0.44	2.43	18	1
1:C:73:ASP:C	1:C:73:ASP:OD1	0.44	2.56	23	2
4:C:92:BEP:C19	4:C:92:BEP:H181	0.44	2.43	22	1
1:C:55:GLU:HG2	1:C:56:GLU:N	0.44	2.27	26	1
1:C:41:LEU:O	1:C:43:LYS:N	0.44	2.50	14	1
1:C:64:VAL:HG11	1:C:80:MET:SD	0.44	2.53	21	1
1:C:72:VAL:HG13	1:C:76:GLU:HB2	0.44	1.90	11	1
1:C:27:PHE:CG	1:C:28:VAL:HG13	0.44	2.48	30	2
1:C:82:VAL:HA	1:C:85:MET:CG	0.44	2.43	23	1
1:C:45:MET:C	1:C:50:GLN:O	0.44	2.55	29	8
1:C:73:ASP:N	1:C:76:GLU:OE2	0.44	2.43	12	1
1:C:16:GLN:O	1:C:19:GLU:OE2	0.44	2.35	14	1
1:C:5:TYR:OH	1:C:83:ARG:HG3	0.44	2.13	1	1
1:C:81:MET:O	1:C:83:ARG:N	0.44	2.51	5	1
1:C:13:THR:N	1:C:16:GLN:OE1	0.44	2.43	23	1
1:C:12:LEU:HB3	1:C:16:GLN:CG	0.44	2.43	22	8
1:C:48:LEU:CG	2:I:153:MET:HA	0.44	2.43	6	3
1:C:14:GLU:HG3	1:C:15:GLU:N	0.44	2.28	16	2
1:C:80:MET:HE1	4:C:92:BEP:C22	0.44	2.42	9	1
1:C:15:GLU:O	1:C:19:GLU:CD	0.44	2.56	1	1
1:C:60:MET:SD	4:C:92:BEP:C8	0.44	3.06	1	1
1:C:80:MET:HE1	4:C:92:BEP:C4	0.44	2.42	5	1
1:C:38:THR:OG1	1:C:39:LYS:N	0.44	2.51	19	4
1:C:48:LEU:HD23	4:C:92:BEP:H161	0.44	1.90	1	1
1:C:27:PHE:N	1:C:44:VAL:HG21	0.44	2.28	17	1
2:I:154:MET:O	2:I:155:GLN:C	0.44	2.56	27	2
1:C:80:MET:HE2	4:C:92:BEP:C19	0.44	2.43	26	1
1:C:81:MET:O	1:C:85:MET:HG2	0.44	2.13	15	1
1:C:29:LEU:C	1:C:29:LEU:CD1	0.44	2.86	5	1
1:C:46:ARG:HA	1:C:50:GLN:O	0.43	2.13	4	11
1:C:80:MET:HE1	4:C:92:BEP:C3	0.43	2.43	4	1
1:C:16:GLN:HA	1:C:19:GLU:CG	0.43	2.43	20	3
1:C:67:ASP:OD1	1:C:69:SER:CB	0.43	2.65	12	1
1:C:33:ASP:OD1	1:C:34:GLY:N	0.43	2.47	11	2
1:C:48:LEU:CD2	4:C:92:BEP:H161	0.43	2.43	10	3
1:C:45:MET:HE3	4:C:92:BEP:C18	0.43	2.43	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:27:PHE:CE1	1:C:44:VAL:CB	0.43	3.01	5	1
1:C:24:PHE:CD2	1:C:27:PHE:CE1	0.43	3.05	18	1
1:C:40:GLU:O	1:C:41:LEU:C	0.43	2.57	17	6
1:C:20:PHE:HB3	1:C:24:PHE:CE2	0.43	2.48	28	1
1:C:24:PHE:CZ	1:C:78:LEU:CG	0.43	3.01	28	2
1:C:77:PHE:CG	1:C:78:LEU:N	0.43	2.86	8	2
1:C:13:THR:O	1:C:14:GLU:C	0.43	2.57	12	4
1:C:9:VAL:HG22	1:C:82:VAL:HG21	0.43	1.89	6	2
1:C:73:ASP:OD1	1:C:76:GLU:N	0.43	2.42	15	1
1:C:77:PHE:O	1:C:80:MET:HG3	0.43	2.13	17	1
2:I:153:MET:O	2:I:154:MET:C	0.43	2.57	9	6
1:C:80:MET:HG3	1:C:81:MET:N	0.43	2.28	23	1
1:C:79:VAL:O	1:C:81:MET:N	0.43	2.50	27	2
1:C:18:ASN:O	1:C:21:LYS:N	0.43	2.51	4	1
4:C:92:BEP:H171	2:I:153:MET:CE	0.43	2.43	24	1
1:C:27:PHE:CB	1:C:36:ILE:HG12	0.43	2.44	9	1
1:C:24:PHE:CZ	1:C:74:PHE:HA	0.43	2.48	11	1
1:C:8:ALA:HB1	1:C:82:VAL:HG11	0.43	1.90	1	1
1:C:81:MET:CE	4:C:92:BEP:H241	0.43	2.42	6	2
1:C:36:ILE:N	1:C:72:VAL:O	0.43	2.49	28	2
1:C:77:PHE:CZ	1:C:81:MET:SD	0.43	3.11	4	1
4:C:92:BEP:H11	2:I:148:ILE:HD13	0.43	1.88	4	1
1:C:76:GLU:O	1:C:77:PHE:C	0.43	2.57	13	4
2:I:148:ILE:O	2:I:148:ILE:CG2	0.43	2.65	7	1
1:C:24:PHE:CE1	1:C:77:PHE:CD2	0.43	3.07	3	1
1:C:27:PHE:CE1	4:C:92:BEP:C17	0.43	3.02	3	1
1:C:32:GLU:OE1	1:C:33:ASP:N	0.43	2.51	9	1
4:C:92:BEP:C16	2:I:153:MET:CG	0.43	2.97	17	1
1:C:16:GLN:O	1:C:17:LYS:C	0.43	2.57	19	3
1:C:19:GLU:C	1:C:19:GLU:OE1	0.43	2.57	4	1
1:C:5:TYR:O	1:C:8:ALA:N	0.43	2.51	25	1
1:C:55:GLU:HG3	1:C:56:GLU:N	0.43	2.27	25	1
1:C:78:LEU:O	1:C:81:MET:HE2	0.43	2.13	7	1
1:C:60:MET:HE3	4:C:92:BEP:C11	0.43	2.44	22	1
1:C:14:GLU:O	1:C:18:ASN:CG	0.43	2.57	24	4
1:C:37:SER:O	1:C:41:LEU:N	0.43	2.48	20	1
1:C:11:GLN:O	1:C:12:LEU:O	0.43	2.36	18	1
1:C:26:ILE:O	1:C:44:VAL:CG2	0.43	2.67	30	1
1:C:59:GLU:N	1:C:59:GLU:OE1	0.43	2.51	28	1
1:C:12:LEU:HA	1:C:16:GLN:OE1	0.43	2.14	26	2
1:C:78:LEU:O	1:C:81:MET:CE	0.43	2.67	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:28:VAL:HB	1:C:31:ALA:CB	0.43	2.43	22	1
1:C:61:ILE:HG13	1:C:72:VAL:CG2	0.43	2.44	11	3
1:C:24:PHE:CE1	1:C:74:PHE:HA	0.43	2.49	9	1
1:C:41:LEU:CD1	1:C:57:LEU:CD2	0.43	2.95	16	1
1:C:21:LYS:O	1:C:22:ALA:C	0.43	2.57	23	3
1:C:44:VAL:O	1:C:45:MET:C	0.43	2.56	23	4
1:C:18:ASN:O	1:C:19:GLU:C	0.43	2.57	20	11
1:C:81:MET:HE1	4:C:92:BEP:H241	0.43	1.90	22	1
1:C:25:ASP:O	1:C:29:LEU:HB2	0.43	2.13	10	1
1:C:46:ARG:NH1	1:C:47:MET:HG2	0.43	2.29	3	1
1:C:77:PHE:CD1	4:C:92:BEP:C23	0.43	3.01	18	1
1:C:46:ARG:NE	1:C:51:ASN:OD1	0.43	2.52	13	1
1:C:58:GLN:NE2	1:C:62:ASP:OD2	0.43	2.52	13	1
1:C:27:PHE:CZ	4:C:92:BEP:C18	0.43	3.02	19	1
1:C:61:ILE:CD1	4:C:92:BEP:H211	0.43	2.42	27	4
1:C:37:SER:O	1:C:38:THR:C	0.43	2.57	5	6
1:C:23:ALA:O	1:C:27:PHE:CE2	0.43	2.72	3	1
4:C:92:BEP:H201	4:C:92:BEP:C14	0.43	2.44	3	1
1:C:64:VAL:HG12	1:C:80:MET:HG2	0.43	1.90	4	1
1:C:12:LEU:CD1	1:C:16:GLN:NE2	0.43	2.78	12	1
1:C:60:MET:CE	4:C:92:BEP:H201	0.43	2.44	12	1
1:C:78:LEU:O	1:C:79:VAL:C	0.43	2.57	20	6
1:C:12:LEU:HD22	1:C:16:GLN:CD	0.43	2.34	8	1
4:C:92:BEP:H111	2:I:148:ILE:HD11	0.43	1.89	10	1
1:C:56:GLU:CA	1:C:56:GLU:OE1	0.43	2.67	24	1
1:C:58:GLN:CA	1:C:58:GLN:OE1	0.43	2.67	27	1
1:C:80:MET:HE3	4:C:92:BEP:C23	0.43	2.42	17	1
1:C:65:ASP:OD2	1:C:70:GLY:N	0.43	2.52	6	4
1:C:5:TYR:O	1:C:6:LYS:C	0.43	2.57	3	4
1:C:82:VAL:O	1:C:84:CYS:N	0.43	2.52	7	1
1:C:84:CYS:O	1:C:85:MET:C	0.43	2.57	16	3
1:C:81:MET:CG	2:I:148:ILE:HG21	0.43	2.44	26	1
1:C:47:MET:HE3	2:I:156:ALA:HA	0.43	1.89	21	1
4:C:92:BEP:O1	4:C:92:BEP:H81	0.43	2.14	13	2
1:C:77:PHE:CD1	4:C:92:BEP:H231	0.43	2.49	18	1
1:C:72:VAL:HG13	1:C:76:GLU:OE1	0.43	2.14	30	1
1:C:41:LEU:CD2	4:C:92:BEP:H121	0.42	2.43	17	1
1:C:60:MET:CE	4:C:92:BEP:H32	0.42	2.44	7	1
1:C:66:GLU:OE2	1:C:83:ARG:NH1	0.42	2.52	21	1
1:C:60:MET:CG	4:C:92:BEP:H201	0.42	2.44	11	1
1:C:60:MET:CE	4:C:92:BEP:H241	0.42	2.43	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:26:ILE:O	1:C:29:LEU:CD2	0.42	2.64	18	1
4:C:92:BEP:H181	2:I:148:ILE:CD1	0.42	2.43	30	1
1:C:15:GLU:O	1:C:16:GLN:C	0.42	2.57	23	3
1:C:23:ALA:CB	2:I:153:MET:CE	0.42	2.97	19	2
4:C:92:BEP:C20	4:C:92:BEP:H181	0.42	2.43	14	1
1:C:77:PHE:O	1:C:81:MET:HG2	0.42	2.15	11	1
1:C:61:ILE:HG23	1:C:72:VAL:CG2	0.42	2.44	18	2
1:C:60:MET:CE	4:C:92:BEP:C11	0.42	2.96	18	1
1:C:40:GLU:C	1:C:40:GLU:OE1	0.42	2.58	30	1
1:C:64:VAL:HG23	1:C:76:GLU:OE1	0.42	2.13	17	1
1:C:6:LYS:O	1:C:10:GLU:CB	0.42	2.67	25	1
4:C:92:BEP:H21	4:C:92:BEP:C13	0.42	2.43	15	1
1:C:16:GLN:OE1	1:C:17:LYS:HA	0.42	2.14	29	1
4:C:92:BEP:C11	4:C:92:BEP:O1	0.42	2.67	17	1
1:C:82:VAL:O	1:C:83:ARG:C	0.42	2.56	7	1
1:C:17:LYS:O	1:C:20:PHE:HB2	0.42	2.14	24	1
1:C:5:TYR:CD2	1:C:79:VAL:CG1	0.42	3.00	27	1
2:I:153:MET:HG3	2:I:154:MET:N	0.42	2.29	9	1
1:C:41:LEU:HD11	4:C:92:BEP:C22	0.42	2.44	16	1
1:C:26:ILE:O	1:C:29:LEU:N	0.42	2.44	5	1
1:C:81:MET:O	1:C:85:MET:N	0.42	2.43	5	1
1:C:64:VAL:HG12	1:C:80:MET:CG	0.42	2.44	4	2
1:C:26:ILE:HG21	1:C:47:MET:CE	0.42	2.45	19	2
1:C:39:LYS:O	1:C:42:GLY:N	0.42	2.49	4	1
1:C:12:LEU:HD22	1:C:16:GLN:HE21	0.42	1.71	12	1
1:C:50:GLN:O	1:C:52:PRO:HD3	0.42	2.14	7	4
1:C:40:GLU:O	1:C:43:LYS:HG2	0.42	2.14	16	1
4:C:92:BEP:C19	4:C:92:BEP:C1	0.42	2.98	17	1
1:C:18:ASN:C	1:C:20:PHE:N	0.42	2.73	8	5
1:C:60:MET:HE2	4:C:92:BEP:N2	0.42	2.30	4	1
1:C:63:GLU:CB	4:C:92:BEP:H62	0.42	2.44	21	1
1:C:48:LEU:HD22	4:C:92:BEP:H171	0.42	1.90	21	1
2:I:153:MET:O	2:I:157:LEU:HG	0.42	2.14	13	3
4:C:92:BEP:C3	4:C:92:BEP:H141	0.42	2.45	3	1
1:C:17:LYS:O	1:C:21:LYS:HG3	0.42	2.15	13	1
1:C:6:LYS:O	1:C:10:GLU:HG3	0.42	2.14	26	2
1:C:48:LEU:O	2:I:155:GLN:OE1	0.42	2.38	22	1
1:C:14:GLU:O	1:C:18:ASN:HB2	0.42	2.15	24	1
1:C:80:MET:CE	4:C:92:BEP:C20	0.42	2.98	30	1
1:C:60:MET:SD	4:C:92:BEP:H111	0.42	2.54	30	1
1:C:59:GLU:O	1:C:63:GLU:HG3	0.42	2.15	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:84:CYS:SG	4:C:92:BEP:C4	0.42	3.08	19	1
1:C:26:ILE:HG13	2:I:157:LEU:CD1	0.42	2.42	12	3
1:C:29:LEU:CD1	1:C:29:LEU:O	0.42	2.67	23	1
1:C:5:TYR:CD1	1:C:5:TYR:N	0.42	2.86	25	1
1:C:17:LYS:O	1:C:18:ASN:C	0.42	2.57	22	1
4:C:92:BEP:H112	4:C:92:BEP:H73	0.42	1.90	10	1
1:C:44:VAL:HG11	2:I:153:MET:CE	0.42	2.44	17	1
1:C:60:MET:CE	4:C:92:BEP:H11	0.42	2.45	17	2
1:C:13:THR:HG22	1:C:14:GLU:N	0.42	2.30	25	1
1:C:61:ILE:O	1:C:62:ASP:C	0.42	2.58	18	2
1:C:60:MET:HE1	4:C:92:BEP:C8	0.42	2.45	14	1
1:C:61:ILE:HD13	4:C:92:BEP:H231	0.42	1.90	3	1
4:C:92:BEP:C1	4:C:92:BEP:H62	0.42	2.45	19	1
1:C:59:GLU:O	1:C:63:GLU:OE2	0.42	2.38	17	1
1:C:57:LEU:O	1:C:58:GLN:C	0.42	2.58	23	4
2:I:156:ALA:CA	2:I:157:LEU:HD13	0.42	2.45	30	2
1:C:41:LEU:HD22	4:C:92:BEP:C24	0.42	2.45	8	1
1:C:36:ILE:CG2	1:C:41:LEU:HB2	0.42	2.45	27	1
1:C:73:ASP:CG	1:C:76:GLU:HG3	0.42	2.35	11	1
1:C:48:LEU:CD2	4:C:92:BEP:C16	0.42	2.98	16	2
1:C:60:MET:HE2	4:C:92:BEP:C12	0.42	2.44	16	1
1:C:45:MET:SD	4:C:92:BEP:H151	0.42	2.54	5	2
1:C:41:LEU:HD21	4:C:92:BEP:C19	0.42	2.45	20	1
4:C:92:BEP:H12	4:C:92:BEP:H62	0.42	1.92	19	1
1:C:68:GLY:O	1:C:69:SER:C	0.41	2.59	4	1
1:C:81:MET:O	1:C:84:CYS:SG	0.41	2.75	12	1
4:C:92:BEP:C14	4:C:92:BEP:H31	0.41	2.44	12	1
1:C:16:GLN:OE1	1:C:17:LYS:HD3	0.41	2.15	5	2
1:C:72:VAL:HG12	1:C:73:ASP:H	0.41	1.75	15	1
2:I:154:MET:HA	2:I:157:LEU:CD1	0.41	2.45	11	1
1:C:14:GLU:CG	1:C:15:GLU:N	0.41	2.82	30	1
1:C:13:THR:O	1:C:17:LYS:HG2	0.41	2.14	19	1
1:C:27:PHE:CE1	2:I:153:MET:HE2	0.41	2.50	17	1
1:C:20:PHE:CE1	1:C:24:PHE:CZ	0.41	3.09	25	1
1:C:7:ALA:O	1:C:11:GLN:HG3	0.41	2.14	21	2
4:C:92:BEP:H73	4:C:92:BEP:H112	0.41	1.92	15	1
1:C:36:ILE:HD13	4:C:92:BEP:H211	0.41	1.91	20	1
1:C:80:MET:HE2	4:C:92:BEP:H31	0.41	1.92	18	1
1:C:28:VAL:O	1:C:31:ALA:CB	0.41	2.69	3	2
1:C:27:PHE:CD2	1:C:77:PHE:CE2	0.41	3.08	26	1
2:I:156:ALA:CB	2:I:157:LEU:CD2	0.41	2.96	27	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:58:GLN:OE1	1:C:58:GLN:HA	0.41	2.16	27	1
1:C:23:ALA:HA	2:I:157:LEU:HD21	0.41	1.92	3	1
1:C:37:SER:C	1:C:39:LYS:N	0.41	2.73	5	1
1:C:61:ILE:N	1:C:61:ILE:HD13	0.41	2.29	5	1
1:C:80:MET:C	1:C:80:MET:SD	0.41	2.98	23	3
1:C:23:ALA:O	1:C:26:ILE:HG12	0.41	2.15	25	4
4:C:92:BEP:C5	4:C:92:BEP:H112	0.41	2.45	10	1
1:C:45:MET:O	1:C:46:ARG:C	0.41	2.59	29	1
1:C:73:ASP:OD1	1:C:75:ASP:HB2	0.41	2.16	6	5
1:C:41:LEU:HD11	4:C:92:BEP:C20	0.41	2.45	2	1
1:C:41:LEU:CD2	4:C:92:BEP:H122	0.41	2.43	27	1
1:C:36:ILE:CG2	1:C:37:SER:N	0.41	2.83	9	1
1:C:27:PHE:CE1	1:C:44:VAL:HB	0.41	2.50	5	1
1:C:45:MET:HE3	4:C:92:BEP:H141	0.41	1.92	17	1
1:C:20:PHE:O	1:C:24:PHE:CG	0.41	2.74	28	1
1:C:6:LYS:CA	1:C:9:VAL:CG2	0.41	2.98	25	1
4:C:92:BEP:C15	2:I:153:MET:HE2	0.41	2.45	22	1
1:C:43:LYS:O	1:C:44:VAL:C	0.41	2.59	2	1
1:C:64:VAL:CB	1:C:72:VAL:HG13	0.41	2.45	14	1
4:C:92:BEP:C14	2:I:153:MET:HE1	0.41	2.45	21	1
1:C:21:LYS:HA	1:C:24:PHE:CB	0.41	2.46	24	1
1:C:81:MET:HB3	1:C:85:MET:HE2	0.41	1.93	11	1
1:C:45:MET:HE1	4:C:92:BEP:C14	0.41	2.46	16	1
1:C:44:VAL:CG1	1:C:48:LEU:CD1	0.41	2.95	1	1
1:C:45:MET:SD	4:C:92:BEP:C14	0.41	3.08	5	1
1:C:61:ILE:HD12	4:C:92:BEP:H211	0.41	1.92	17	1
1:C:60:MET:SD	4:C:92:BEP:C1	0.41	3.09	17	1
1:C:53:THR:O	1:C:57:LEU:CB	0.41	2.69	21	1
4:C:92:BEP:N2	2:I:148:ILE:HD13	0.41	2.30	21	1
1:C:36:ILE:O	1:C:71:THR:HA	0.41	2.15	3	1
1:C:85:MET:HG3	1:C:86:LYS:CG	0.41	2.46	5	1
1:C:13:THR:C	1:C:15:GLU:N	0.41	2.74	26	4
1:C:5:TYR:C	1:C:9:VAL:HG22	0.41	2.33	25	1
1:C:44:VAL:HG13	1:C:45:MET:N	0.41	2.30	22	1
1:C:32:GLU:O	1:C:33:ASP:O	0.41	2.39	9	1
1:C:16:GLN:C	1:C:18:ASN:N	0.41	2.74	11	1
1:C:60:MET:HB3	4:C:92:BEP:C23	0.41	2.45	16	1
1:C:58:GLN:CD	1:C:58:GLN:C	0.41	2.79	18	1
1:C:81:MET:HE3	4:C:92:BEP:H241	0.41	1.91	6	1
2:I:149:SER:HB3	2:I:151:ASP:OD1	0.41	2.15	6	1
1:C:20:PHE:HB3	1:C:24:PHE:CZ	0.41	2.51	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:24:PHE:CD1	1:C:24:PHE:N	0.41	2.86	28	1
1:C:27:PHE:O	1:C:40:GLU:HB3	0.41	2.15	12	1
1:C:60:MET:O	1:C:63:GLU:HG3	0.41	2.16	12	2
1:C:10:GLU:O	1:C:11:GLN:C	0.41	2.58	12	1
1:C:6:LYS:O	1:C:10:GLU:HB2	0.41	2.16	25	1
4:C:92:BEP:C18	4:C:92:BEP:H21	0.41	2.46	25	1
1:C:20:PHE:O	1:C:21:LYS:C	0.41	2.57	2	1
1:C:16:GLN:OE1	1:C:17:LYS:CE	0.41	2.69	2	1
1:C:24:PHE:CE2	1:C:74:PHE:CZ	0.41	3.09	3	1
1:C:47:MET:HE1	2:I:156:ALA:O	0.41	2.15	11	1
1:C:41:LEU:CB	1:C:57:LEU:CD2	0.41	2.99	16	1
4:C:92:BEP:H91	4:C:92:BEP:C7	0.41	2.45	20	1
4:C:92:BEP:C8	2:I:148:ILE:HD11	0.41	2.46	30	1
1:C:55:GLU:HG2	1:C:56:GLU:OE1	0.41	2.16	30	1
4:C:92:BEP:H112	4:C:92:BEP:C6	0.41	2.46	28	1
2:I:150:ALA:O	2:I:151:ASP:C	0.41	2.60	8	1
1:C:67:ASP:OD1	1:C:69:SER:OG	0.41	2.39	5	2
1:C:28:VAL:O	1:C:29:LEU:C	0.41	2.59	10	1
1:C:23:ALA:CA	2:I:157:LEU:HD22	0.41	2.46	11	1
1:C:60:MET:CB	4:C:92:BEP:H241	0.41	2.46	16	1
1:C:85:MET:HG3	1:C:86:LYS:HG3	0.41	1.91	5	1
1:C:67:ASP:OD1	1:C:68:GLY:N	0.41	2.54	20	1
1:C:77:PHE:CE1	4:C:92:BEP:C24	0.41	3.04	18	1
1:C:20:PHE:CE1	1:C:81:MET:SD	0.41	3.14	19	1
1:C:27:PHE:CD2	1:C:36:ILE:HD13	0.41	2.51	19	1
1:C:60:MET:CE	4:C:92:BEP:H91	0.40	2.46	21	1
4:C:92:BEP:H161	2:I:153:MET:SD	0.40	2.56	3	1
1:C:80:MET:SD	1:C:81:MET:HE2	0.40	2.56	15	1
1:C:84:CYS:C	1:C:86:LYS:N	0.40	2.75	16	1
1:C:48:LEU:CD2	2:I:156:ALA:CB	0.40	2.88	17	1
1:C:28:VAL:CG1	1:C:34:GLY:C	0.40	2.80	28	1
1:C:81:MET:SD	4:C:92:BEP:H51	0.40	2.56	4	1
1:C:17:LYS:O	1:C:20:PHE:HB3	0.40	2.17	25	1
1:C:48:LEU:HG	2:I:152:ALA:O	0.40	2.16	19	2
1:C:80:MET:O	1:C:83:ARG:HG2	0.40	2.16	8	1
1:C:60:MET:HE1	4:C:92:BEP:N2	0.40	2.31	2	2
2:I:149:SER:O	2:I:153:MET:SD	0.40	2.79	14	1
1:C:35:CYS:SG	1:C:73:ASP:HA	0.40	2.57	14	1
2:I:148:ILE:O	2:I:148:ILE:HG13	0.40	2.16	15	1
1:C:61:ILE:CD1	4:C:92:BEP:H231	0.40	2.47	16	1
1:C:20:PHE:CD1	1:C:24:PHE:CZ	0.40	3.09	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:23:ALA:O	1:C:26:ILE:N	0.40	2.53	22	2
1:C:25:ASP:O	1:C:29:LEU:HA	0.40	2.16	22	1
1:C:9:VAL:O	1:C:17:LYS:CE	0.40	2.69	14	1
1:C:77:PHE:O	1:C:80:MET:HB3	0.40	2.17	21	1
4:C:92:BEP:O1	4:C:92:BEP:H111	0.40	2.15	15	1
1:C:45:MET:CE	4:C:92:BEP:H151	0.40	2.47	5	1
1:C:58:GLN:O	1:C:58:GLN:CD	0.40	2.60	18	1
1:C:27:PHE:CE1	4:C:92:BEP:C18	0.40	3.05	28	1
1:C:46:ARG:HB3	1:C:51:ASN:OD1	0.40	2.16	28	1
1:C:23:ALA:HA	1:C:26:ILE:HG12	0.40	1.94	3	1
1:C:55:GLU:CG	1:C:56:GLU:N	0.40	2.85	1	2
1:C:27:PHE:CE1	2:I:153:MET:HE1	0.40	2.51	12	1
1:C:39:LYS:O	1:C:40:GLU:C	0.40	2.59	2	1
1:C:19:GLU:O	1:C:22:ALA:CB	0.40	2.70	10	1
1:C:41:LEU:HD11	4:C:92:BEP:H122	0.40	1.94	27	1
1:C:12:LEU:N	1:C:12:LEU:HD23	0.40	2.32	20	1
1:C:47:MET:HE3	2:I:156:ALA:HB1	0.40	1.92	19	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	C	82/89 (92%)	60±4 (73±5%)	19±4 (24±5%)	3±1 (3±1%)	8	40
2	I	10/17 (59%)	7±1 (74±11%)	2±1 (19±9%)	1±1 (7±9%)	3	19
All	All	2760/3180 (87%)	2024 (73%)	637 (23%)	99 (4%)	7	36

All 27 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	73	ASP	21
1	C	77	PHE	12
2	I	150	ALA	9
1	C	49	GLY	7

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Mol	Chain	Res	Type	Models (Total)
2	I	148	ILE	6
1	C	79	VAL	4
2	I	149	SER	4
1	C	33	ASP	4
1	C	31	ALA	4
1	C	78	LEU	3
1	C	48	LEU	3
1	C	80	MET	2
1	C	75	ASP	2
1	C	12	LEU	2
1	C	18	ASN	2
1	C	15	GLU	2
1	C	34	GLY	2
1	C	65	ASP	1
1	C	83	ARG	1
1	C	85	MET	1
1	C	19	GLU	1
1	C	32	GLU	1
1	C	14	GLU	1
2	I	154	MET	1
1	C	43	LYS	1
1	C	42	GLY	1
1	C	82	VAL	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	C	71/78 (91%)	51±4 (72±5%)	20±4 (28±5%)	2	19
2	I	7/11 (64%)	4±1 (60±16%)	3±1 (40±16%)	1	5
All	All	2340/2670 (88%)	1650 (71%)	690 (29%)	2	18

All 69 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	C	53	THR	30

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Mol	Chain	Res	Type	Models (Total)
1	C	33	ASP	30
1	C	16	GLN	30
2	I	154	MET	28
1	C	26	ILE	25
1	C	20	PHE	24
1	C	65	ASP	23
1	C	29	LEU	21
1	C	24	PHE	19
1	C	75	ASP	18
1	C	37	SER	18
1	C	86	LYS	17
1	C	32	GLU	16
1	C	25	ASP	16
1	C	40	GLU	15
1	C	17	LYS	15
2	I	157	LEU	15
1	C	43	LYS	14
1	C	39	LYS	14
1	C	13	THR	13
1	C	78	LEU	13
1	C	47	MET	12
1	C	14	GLU	12
1	C	66	GLU	12
2	I	149	SER	11
1	C	71	THR	11
1	C	81	MET	11
1	C	46	ARG	10
1	C	61	ILE	10
2	I	155	GLN	10
1	C	62	ASP	10
2	I	153	MET	10
1	C	80	MET	8
1	C	69	SER	8
1	C	56	GLU	8
1	C	19	GLU	8
1	C	59	GLU	8
1	C	60	MET	8
1	C	76	GLU	7
1	C	83	ARG	7
1	C	48	LEU	7
2	I	151	ASP	7
1	C	67	ASP	6

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Mol	Chain	Res	Type	Models (Total)
1	C	73	ASP	6
1	C	51	ASN	5
1	C	45	MET	5
1	C	63	GLU	4
1	C	21	LYS	4
1	C	28	VAL	4
1	C	50	GLN	4
1	C	44	VAL	4
1	C	12	LEU	3
2	I	148	ILE	3
1	C	15	GLU	3
1	C	11	GLN	3
1	C	27	PHE	3
1	C	36	ILE	3
1	C	6	LYS	3
1	C	58	GLN	3
1	C	85	MET	2
1	C	72	VAL	2
1	C	41	LEU	2
1	C	64	VAL	2
1	C	74	PHE	2
1	C	35	CYS	1
1	C	77	PHE	1
1	C	55	GLU	1
1	C	84	CYS	1
1	C	82	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is 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
4	BEP	C	92	-	28,29,29	1.15±0.02	0±0 (0±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
4	BEP	C	92	-	35,37,37	1.53±0.02	0±0 (0±0%)

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
4	BEP	C	92	-	-	0±0,22,29,29	0±0,3,3,3

There are no bond-length outliers.

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(°)	Ideal(°)	Models	
								Worst	Total
4	C	92	BEP	C8-N2-C2	5.41	118.86	113.99	21	2
4	C	92	BEP	C11-N2-C2	5.15	118.63	113.99	15	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 73% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5386

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	924
Number of shifts mapped to atoms	924
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	88	-0.30 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	82	0.03 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	85	-0.23 ± 0.31	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 74%, i.e. 805 atoms were assigned a chemical shift out of a possible 1091. 9 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	323/456 (71%)	161/182 (88%)	82/184 (45%)	80/90 (89%)
Sidechain	448/582 (77%)	277/338 (82%)	166/225 (74%)	5/19 (26%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	34/53 (64%)	20/29 (69%)	14/24 (58%)	0/0 (—%)
Overall	805/1091 (74%)	458/549 (83%)	262/433 (61%)	85/109 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 67%, i.e. 848 atoms were assigned a chemical shift out of a possible 1259. 9 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	344/526 (65%)	171/210 (81%)	88/212 (42%)	85/104 (82%)
Sidechain	470/680 (69%)	290/395 (73%)	175/259 (68%)	5/26 (19%)
Aromatic	34/53 (64%)	20/29 (69%)	14/24 (58%)	0/0 (—%)
Overall	848/1259 (67%)	481/634 (76%)	277/495 (56%)	90/130 (69%)

7.1.4 Statistically unusual chemical shifts ⓘ

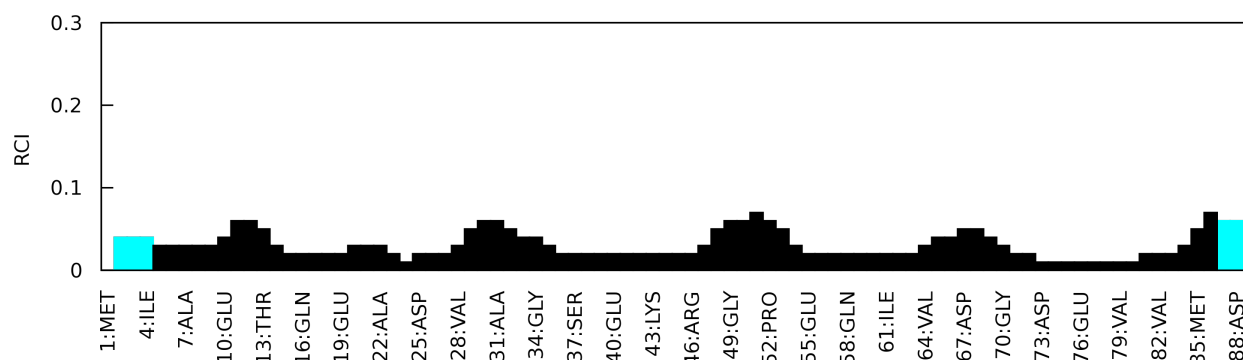
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
3	C	80	MET	CE	41.37	26.97 – 7.37	12.3

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 C:



7.2 Chemical shift list 2

File name: BMRB entry 5386

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	83
Number of shifts mapped to atoms	83
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 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 4%, i.e. 47 atoms were assigned a chemical shift out of a possible 1091. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	20/456 (4%)	20/182 (11%)	0/184 (0%)	0/90 (0%)
Sidechain	27/582 (5%)	27/338 (8%)	0/225 (0%)	0/19 (0%)
Aromatic	0/53 (0%)	0/29 (0%)	0/24 (0%)	0/0 (—%)
Overall	47/1091 (4%)	47/549 (9%)	0/433 (0%)	0/109 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 6%, i.e. 70 atoms were assigned a chemical shift out of a possible 1259. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	30/526 (6%)	30/210 (14%)	0/212 (0%)	0/104 (0%)
Sidechain	40/680 (6%)	40/395 (10%)	0/259 (0%)	0/26 (0%)
Aromatic	0/53 (0%)	0/29 (0%)	0/24 (0%)	0/0 (—%)
Overall	70/1259 (6%)	70/634 (11%)	0/495 (0%)	0/130 (0%)

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain I:

