



Full wwPDB NMR Structure Validation Report ⓘ

Feb 18, 2018 – 10:41 am GMT

PDB ID : 2KDH
Title : The Solution Structure of Human Cardiac Troponin C in complex with the
Green Tea Polyphenol; (-)-epigallocatechin-3-gallate
Authors : Robertson, I.M.; Li, M.X.; Sykes, B.D.
Deposited on : 2009-01-09

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

<https://www.wwpdb.org/validation/2017/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	:	1.7.3 (157068), CSD as539be (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk30686
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30686

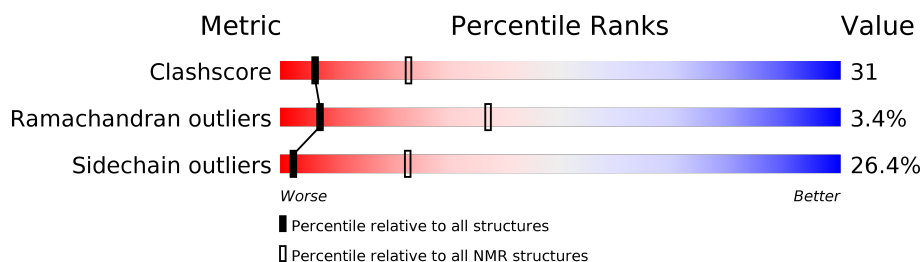
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	A	72	

2 Ensemble composition and analysis

This entry contains 30 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:92-A:158 (67)	0.56	2

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 3 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1181 atoms, of which 563 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	72	Total	C	H	N	O	S	0
			1128	360	545	88	130	5	

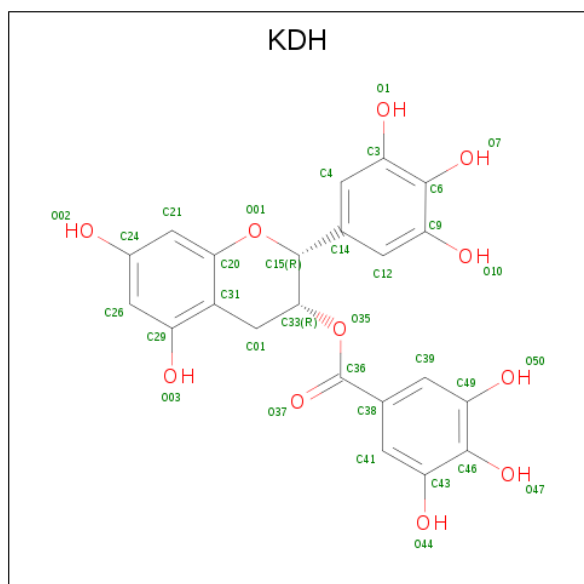
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	MET	-	INITIATING METHIONINE	UNP P63316

- 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 (2R,3R)-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-chromen-3-yl 3,4,5-trihydroxybenzoate (three-letter code: KDH) (formula: C₂₂H₁₈O₁₁).



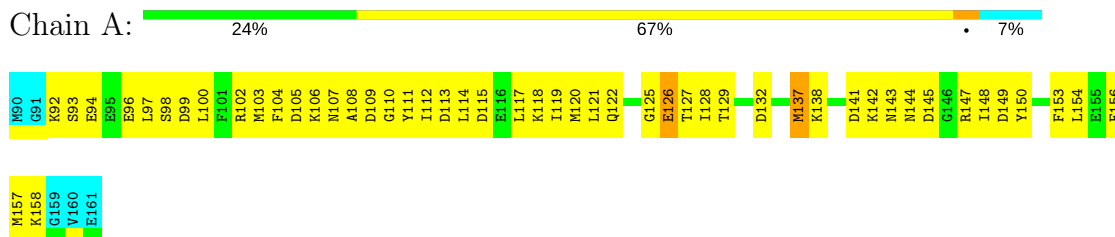
Mol	Chain	Residues	Atoms			
3	A	1	Total	C	H	O
			51	22	18	11

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

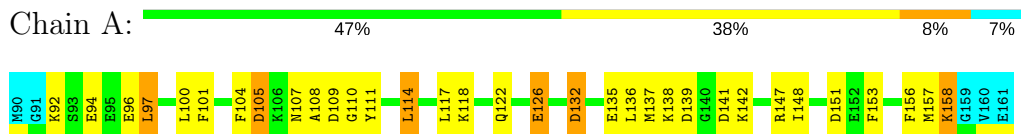


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

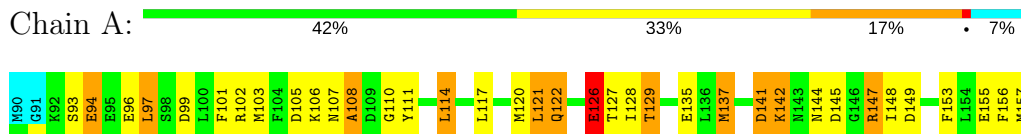
4.2.1 Score per residue for model 1

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



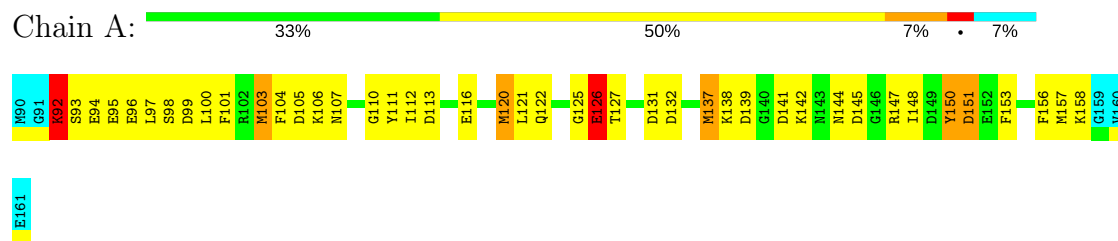
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



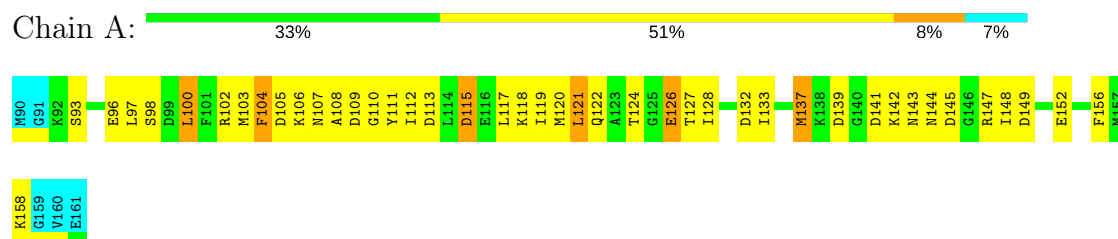
4.2.3 Score per residue for model 3

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



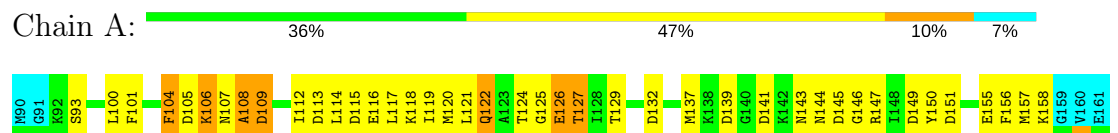
4.2.4 Score per residue for model 4

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



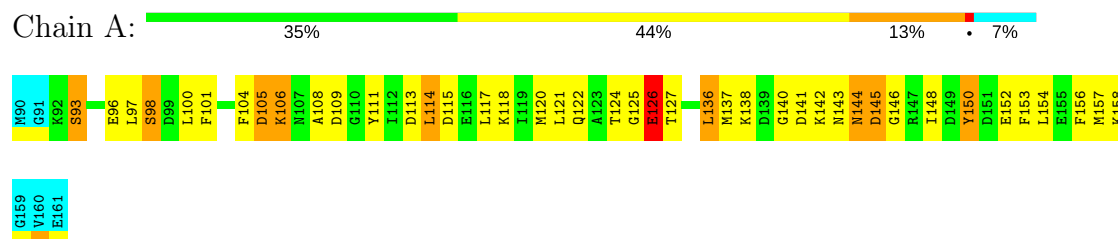
4.2.5 Score per residue for model 5

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



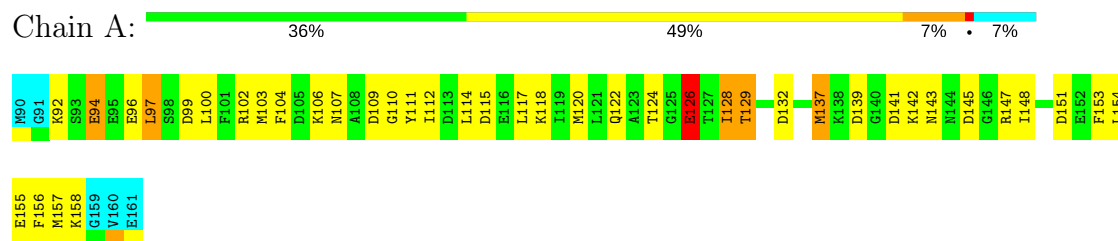
4.2.6 Score per residue for model 6

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



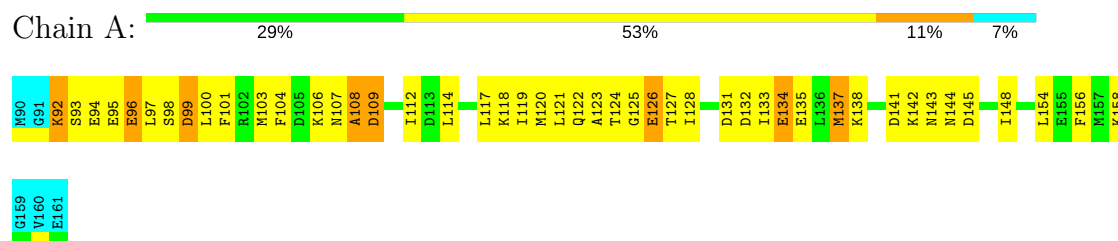
4.2.7 Score per residue for model 7

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



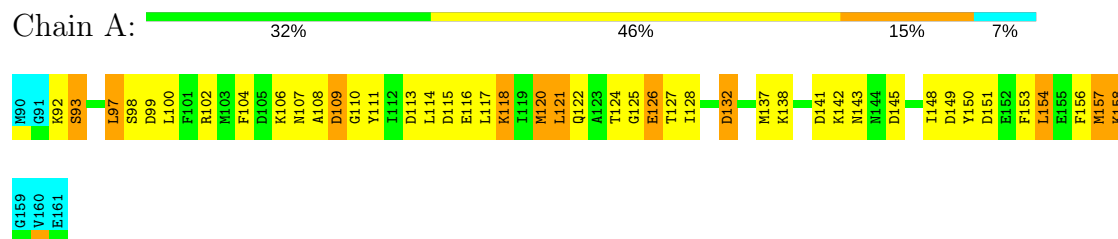
4.2.8 Score per residue for model 8

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



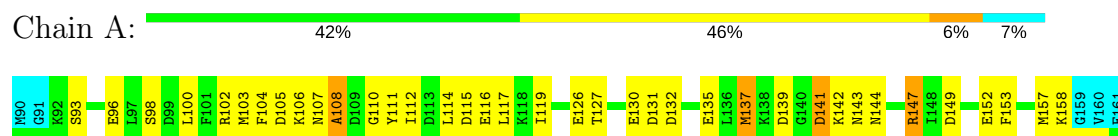
4.2.9 Score per residue for model 9

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



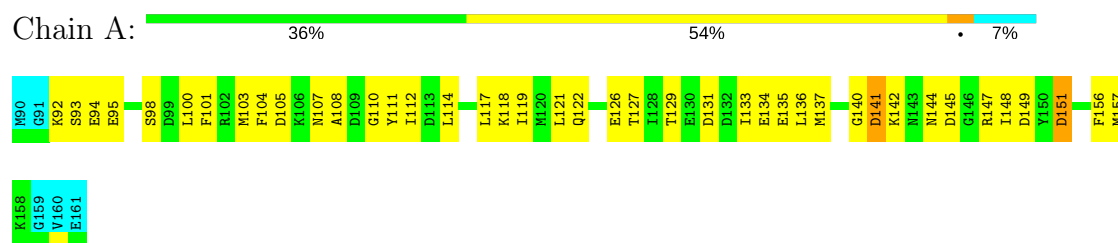
4.2.10 Score per residue for model 10

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



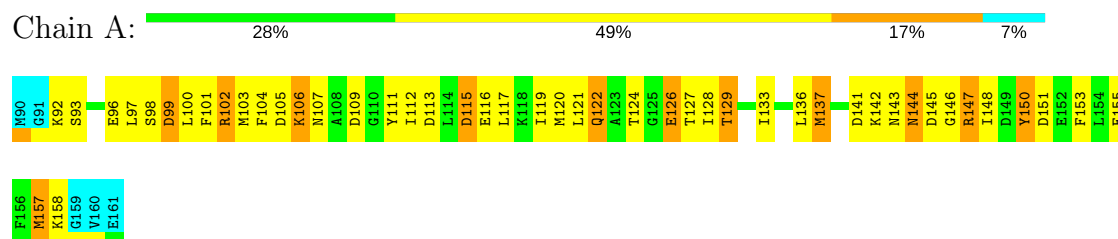
4.2.11 Score per residue for model 11

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



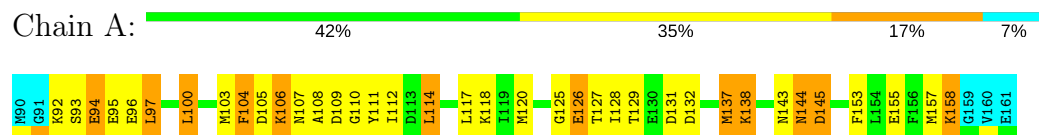
4.2.12 Score per residue for model 12

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



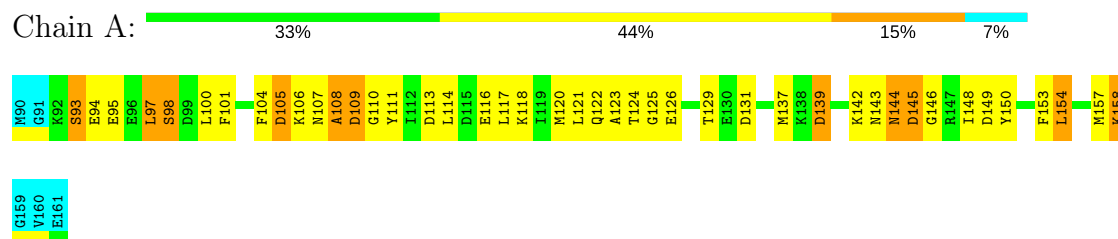
4.2.13 Score per residue for model 13

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



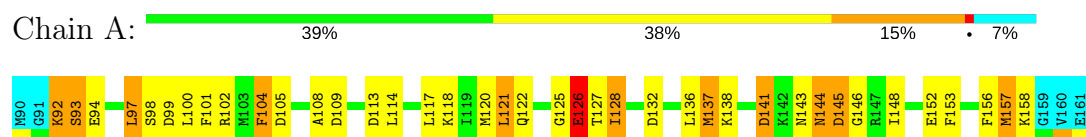
4.2.14 Score per residue for model 14

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



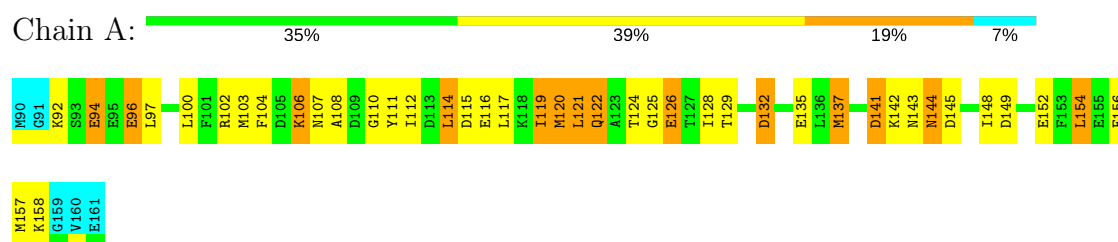
4.2.15 Score per residue for model 15

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



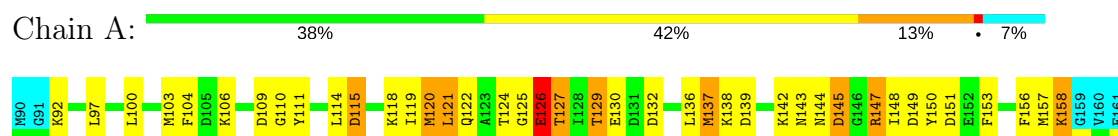
4.2.16 Score per residue for model 16

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



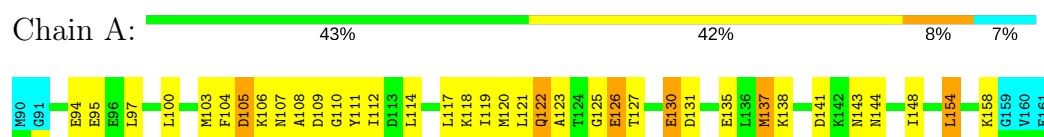
4.2.17 Score per residue for model 17

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



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

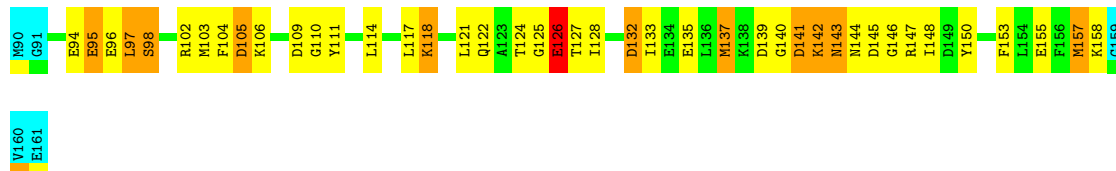
- Molecule 1: Troponin C, slow skeletal and cardiac muscles





4.2.20 Score per residue for model 20

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



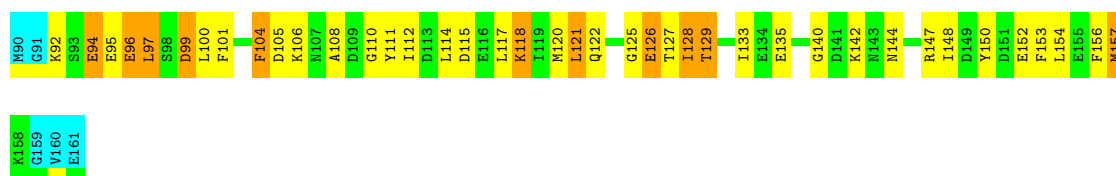
4.2.21 Score per residue for model 21

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



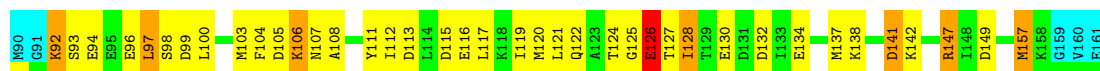
4.2.22 Score per residue for model 22

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



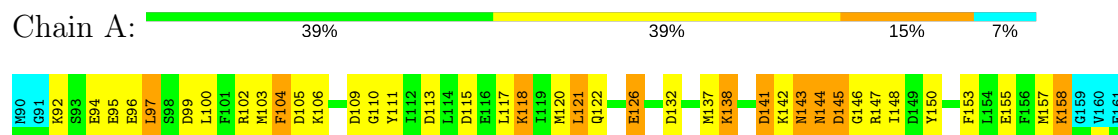
4.2.23 Score per residue for model 23

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



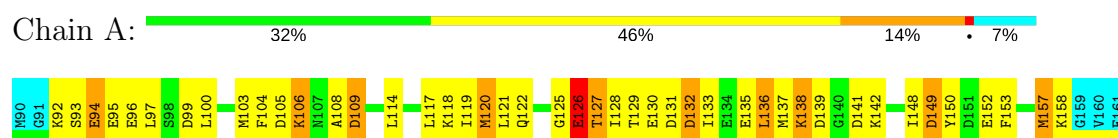
4.2.24 Score per residue for model 24

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



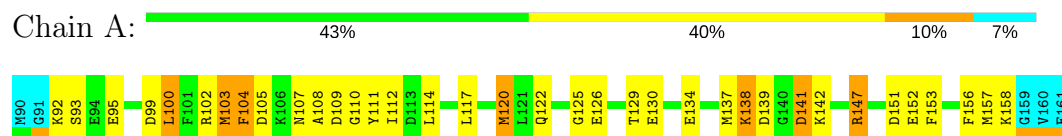
4.2.25 Score per residue for model 25

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



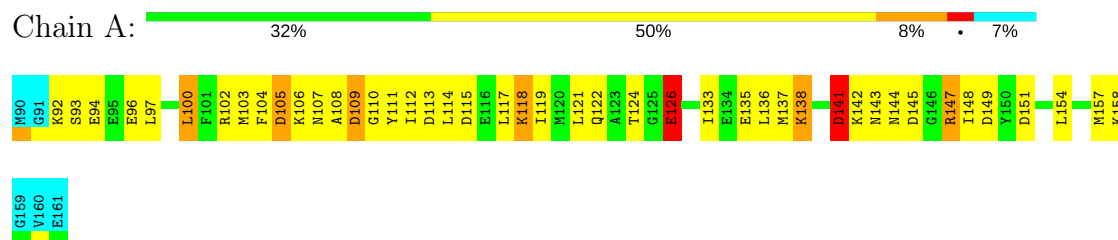
4.2.26 Score per residue for model 26

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



4.2.27 Score per residue for model 27

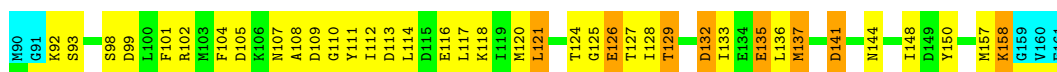
- Molecule 1: Troponin C, slow skeletal and cardiac muscles



4.2.28 Score per residue for model 28

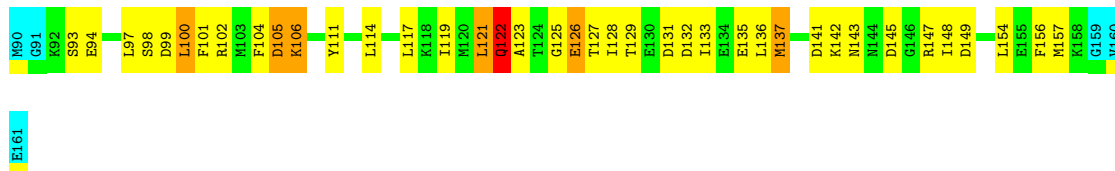
- Molecule 1: Troponin C, slow skeletal and cardiac muscles





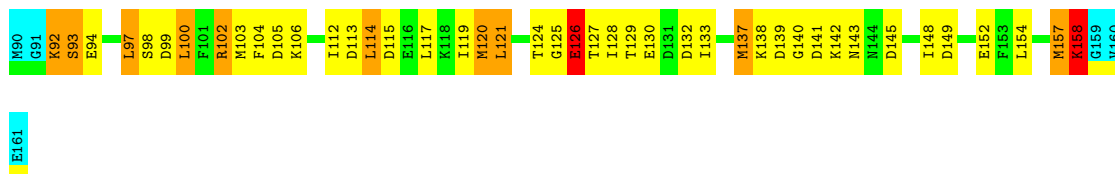
4.2.29 Score per residue for model 29

- Molecule 1: Troponin C, slow skeletal and cardiac muscles



4.2.30 Score per residue for model 30

- 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 100 calculated structures, 30 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	
X-PLOR NIH	structure solution	

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

Chemical shift file(s)	BMRB entry 17243
Number of chemical shift lists	1
Total number of shifts	756
Number of shifts mapped to atoms	756
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

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, KDH

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	550	513	513	34±6
3	A	33	18	14	2±2
All	All	17550	15930	15830	1038

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 31.

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:HD11	1:A:148:ILE:HD11	1.04	1.24	20	18
1:A:121:LEU:HD13	3:A:1:KDH:H41	1.03	1.24	6	1
1:A:100:LEU:HD11	1:A:153:PHE:CE2	0.99	1.93	7	2
1:A:117:LEU:HD11	1:A:148:ILE:CD1	0.98	1.88	24	19
1:A:121:LEU:HD22	3:A:1:KDH:H41	0.98	1.30	22	1
1:A:97:LEU:HD21	1:A:157:MET:SD	0.93	2.02	20	6
1:A:121:LEU:O	1:A:124:THR:HG22	0.87	1.70	6	8
1:A:137:MET:SD	1:A:148:ILE:HD11	0.85	2.12	14	2
1:A:128:ILE:HD13	1:A:132:ASP:HB3	0.84	1.45	20	1
1:A:100:LEU:HD11	1:A:104:PHE:CZ	0.82	2.08	6	2
1:A:104:PHE:HB3	1:A:112:ILE:HD11	0.82	1.49	26	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:LEU:HA	1:A:117:LEU:HD12	0.81	1.50	26	14
1:A:117:LEU:HD11	1:A:148:ILE:HD12	0.81	1.51	27	7
1:A:100:LEU:HD22	1:A:104:PHE:CZ	0.79	2.12	18	2
1:A:156:PHE:CE1	3:A:1:KDH:H12	0.79	2.12	8	1
1:A:156:PHE:CZ	3:A:1:KDH:H12	0.78	2.14	8	5
1:A:93:SER:O	1:A:97:LEU:HD23	0.78	1.77	4	4
1:A:121:LEU:CD2	3:A:1:KDH:H41	0.74	2.12	22	1
1:A:121:LEU:HD21	3:A:1:KDH:C36	0.73	2.13	15	1
1:A:104:PHE:CZ	1:A:117:LEU:HD23	0.73	2.18	5	1
1:A:140:GLY:O	1:A:148:ILE:HG23	0.73	1.84	11	4
1:A:125:GLY:O	1:A:127:THR:HG23	0.72	1.84	20	4
1:A:121:LEU:CD1	3:A:1:KDH:H41	0.72	2.14	3	4
1:A:118:LYS:HB3	1:A:133:ILE:HD12	0.71	1.61	22	3
1:A:112:ILE:HG21	1:A:117:LEU:CD2	0.71	2.14	30	4
1:A:117:LEU:CD1	1:A:148:ILE:HD11	0.71	2.13	20	3
1:A:112:ILE:HG21	1:A:117:LEU:HD21	0.71	1.61	30	3
1:A:115:ASP:O	1:A:119:ILE:HD12	0.71	1.86	12	7
1:A:93:SER:C	1:A:97:LEU:HD23	0.71	2.05	8	5
1:A:128:ILE:HD13	1:A:128:ILE:N	0.71	2.00	23	2
1:A:114:LEU:HD11	1:A:137:MET:SD	0.71	2.25	7	2
1:A:121:LEU:HD11	3:A:1:KDH:H41	0.70	1.64	3	1
1:A:100:LEU:HD11	1:A:153:PHE:HE2	0.69	1.44	7	1
1:A:121:LEU:HD11	3:A:1:KDH:O37	0.68	1.88	8	2
1:A:128:ILE:HD13	1:A:132:ASP:CB	0.68	2.18	20	1
1:A:128:ILE:HD12	1:A:129:THR:O	0.68	1.89	2	1
1:A:120:MET:SD	1:A:121:LEU:HD12	0.67	2.29	17	3
1:A:137:MET:HE1	1:A:148:ILE:HD11	0.67	1.67	6	2
1:A:101:PHE:CZ	1:A:112:ILE:HD12	0.67	2.24	19	1
1:A:97:LEU:HD11	1:A:157:MET:SD	0.66	2.30	30	6
1:A:117:LEU:HD21	1:A:148:ILE:HD12	0.66	1.68	11	3
1:A:128:ILE:H	1:A:128:ILE:HD13	0.66	1.51	22	1
1:A:128:ILE:HD12	1:A:132:ASP:HB3	0.65	1.68	9	4
1:A:97:LEU:HD23	1:A:100:LEU:HD12	0.65	1.67	18	1
1:A:128:ILE:HD13	1:A:128:ILE:H	0.65	1.50	15	2
1:A:114:LEU:HD21	1:A:137:MET:HG2	0.65	1.68	25	3
1:A:127:THR:O	1:A:127:THR:HG23	0.65	1.91	11	4
1:A:114:LEU:HD21	1:A:137:MET:HG3	0.65	1.69	28	4
1:A:107:ASN:O	1:A:108:ALA:HB3	0.63	1.94	9	13
1:A:156:PHE:CE2	3:A:1:KDH:H12	0.63	2.28	5	3
1:A:104:PHE:CE1	1:A:120:MET:CB	0.63	2.82	5	2
1:A:132:ASP:O	1:A:136:LEU:HD12	0.63	1.92	29	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:PHE:CD2	1:A:112:ILE:HD13	0.63	2.28	5	1
1:A:104:PHE:CB	1:A:112:ILE:HD11	0.63	2.24	26	1
1:A:106:LYS:CB	1:A:119:ILE:HG21	0.63	2.23	16	1
1:A:114:LEU:HD21	1:A:137:MET:SD	0.63	2.34	30	3
1:A:111:TYR:CD1	1:A:111:TYR:N	0.62	2.67	3	6
1:A:104:PHE:CD2	1:A:112:ILE:CD1	0.62	2.82	5	1
1:A:117:LEU:HD21	1:A:148:ILE:CD1	0.62	2.24	15	3
1:A:92:LYS:O	1:A:97:LEU:HD23	0.61	1.94	15	3
1:A:136:LEU:HD22	3:A:1:KDH:O37	0.61	1.95	17	1
1:A:128:ILE:CG2	1:A:133:ILE:HD11	0.61	2.26	29	3
1:A:104:PHE:CD2	1:A:120:MET:HE1	0.61	2.30	3	5
1:A:100:LEU:HD22	1:A:104:PHE:CE1	0.61	2.30	18	2
1:A:104:PHE:CD1	1:A:120:MET:CE	0.61	2.83	28	5
1:A:100:LEU:HD23	1:A:104:PHE:CE2	0.61	2.30	29	1
1:A:137:MET:CE	1:A:148:ILE:HD11	0.60	2.26	4	2
1:A:104:PHE:CD2	1:A:120:MET:CE	0.60	2.84	3	5
1:A:104:PHE:CG	1:A:120:MET:HE2	0.60	2.31	21	1
1:A:118:LYS:HB2	1:A:133:ILE:HG21	0.60	1.74	8	1
3:A:1:KDH:H12	3:A:1:KDH:C39	0.59	2.26	25	1
1:A:104:PHE:CD1	1:A:120:MET:HE3	0.59	2.33	13	1
3:A:1:KDH:C12	3:A:1:KDH:H41	0.59	2.28	20	1
1:A:106:LYS:NZ	1:A:119:ILE:HG21	0.59	2.12	8	1
3:A:1:KDH:H39	3:A:1:KDH:C12	0.58	2.27	10	2
1:A:121:LEU:HG	3:A:1:KDH:H41	0.58	1.73	25	3
1:A:110:GLY:O	1:A:111:TYR:CG	0.58	2.57	2	4
1:A:128:ILE:HD11	1:A:133:ILE:HD13	0.58	1.73	20	4
1:A:128:ILE:HD12	1:A:128:ILE:C	0.58	2.18	20	1
1:A:104:PHE:CE2	3:A:1:KDH:H01A	0.57	2.34	28	1
1:A:111:TYR:N	1:A:111:TYR:CD1	0.57	2.72	21	6
1:A:121:LEU:HD13	3:A:1:KDH:C41	0.57	2.29	22	2
1:A:104:PHE:CD2	1:A:120:MET:O	0.57	2.57	15	1
1:A:101:PHE:CE2	1:A:112:ILE:HD12	0.57	2.34	11	2
1:A:104:PHE:CD2	1:A:120:MET:HE2	0.56	2.35	26	2
1:A:137:MET:HE2	1:A:148:ILE:CG1	0.56	2.30	29	4
1:A:121:LEU:HD21	3:A:1:KDH:C38	0.56	2.30	15	1
1:A:104:PHE:CD1	1:A:120:MET:HE2	0.56	2.35	22	2
3:A:1:KDH:C4	3:A:1:KDH:H39	0.56	2.31	18	1
1:A:126:GLU:CG	1:A:126:GLU:O	0.56	2.53	18	11
1:A:104:PHE:CD1	1:A:112:ILE:HD13	0.55	2.37	13	3
1:A:104:PHE:CE2	1:A:120:MET:O	0.55	2.59	15	1
3:A:1:KDH:H33	3:A:1:KDH:H39	0.55	1.79	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:LEU:HD11	1:A:153:PHE:CZ	0.55	2.34	7	2
1:A:153:PHE:CE2	1:A:157:MET:SD	0.55	3.00	25	1
1:A:110:GLY:C	1:A:111:TYR:CD1	0.55	2.81	19	11
1:A:104:PHE:CD1	1:A:104:PHE:N	0.55	2.73	29	3
3:A:1:KDH:H12	3:A:1:KDH:C38	0.55	2.32	25	1
1:A:114:LEU:HD21	1:A:137:MET:CG	0.54	2.32	15	4
1:A:104:PHE:CD2	1:A:153:PHE:CE1	0.54	2.95	10	1
1:A:137:MET:HE1	1:A:148:ILE:CG1	0.54	2.32	3	1
1:A:104:PHE:CE1	1:A:120:MET:HB3	0.54	2.38	5	1
1:A:128:ILE:HG21	3:A:1:KDH:O44	0.54	2.02	13	1
1:A:118:LYS:HB3	1:A:133:ILE:HG23	0.54	1.77	27	1
1:A:126:GLU:O	1:A:126:GLU:CG	0.54	2.56	17	10
1:A:125:GLY:O	1:A:126:GLU:CG	0.54	2.56	14	2
1:A:119:ILE:O	1:A:122:GLN:CG	0.54	2.56	18	2
3:A:1:KDH:H41	3:A:1:KDH:C3	0.54	2.32	12	1
1:A:112:ILE:CG2	1:A:117:LEU:HD21	0.54	2.33	30	2
1:A:100:LEU:HG	1:A:104:PHE:CE2	0.54	2.38	6	3
1:A:110:GLY:C	1:A:111:TYR:CG	0.53	2.81	2	8
1:A:107:ASN:ND2	1:A:116:GLU:CG	0.53	2.71	9	1
1:A:97:LEU:HD12	1:A:154:LEU:HD22	0.53	1.78	7	1
1:A:125:GLY:O	1:A:127:THR:N	0.53	2.41	22	11
1:A:128:ILE:N	1:A:128:ILE:HD13	0.53	2.18	22	1
1:A:112:ILE:CG2	1:A:117:LEU:CD2	0.53	2.86	30	2
1:A:100:LEU:HD21	1:A:104:PHE:CZ	0.53	2.39	12	1
3:A:1:KDH:H39	3:A:1:KDH:C4	0.53	2.34	24	1
1:A:111:TYR:CD1	1:A:149:ASP:OD1	0.53	2.61	29	1
1:A:100:LEU:O	1:A:104:PHE:CD2	0.53	2.61	30	1
1:A:113:ASP:O	1:A:117:LEU:CD1	0.53	2.57	5	1
1:A:104:PHE:CG	1:A:120:MET:CE	0.53	2.92	26	3
1:A:119:ILE:HG23	1:A:122:GLN:OE1	0.53	2.04	29	1
1:A:97:LEU:HD12	1:A:154:LEU:HD13	0.53	1.79	29	1
3:A:1:KDH:H39	3:A:1:KDH:C3	0.52	2.34	18	1
1:A:128:ILE:HD11	1:A:133:ILE:CD1	0.52	2.34	20	1
1:A:100:LEU:HD23	1:A:153:PHE:CE2	0.52	2.40	3	1
1:A:127:THR:HG23	1:A:127:THR:O	0.52	2.04	28	2
1:A:150:TYR:O	1:A:153:PHE:N	0.52	2.42	12	4
1:A:107:ASN:CB	1:A:116:GLU:OE2	0.52	2.58	19	3
1:A:150:TYR:CE1	1:A:154:LEU:CD2	0.52	2.92	14	1
1:A:137:MET:HE1	1:A:148:ILE:HG13	0.52	1.81	18	2
1:A:137:MET:O	1:A:141:ASP:N	0.52	2.43	21	15
1:A:156:PHE:CD2	1:A:157:MET:SD	0.52	3.02	16	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:PHE:CD1	1:A:101:PHE:O	0.52	2.63	21	1
1:A:117:LEU:CD1	1:A:137:MET:SD	0.52	2.98	1	3
1:A:104:PHE:CE1	1:A:120:MET:HE3	0.52	2.39	13	1
1:A:104:PHE:O	1:A:106:LYS:N	0.52	2.42	3	11
1:A:137:MET:HE2	1:A:148:ILE:HD11	0.52	1.80	4	4
1:A:104:PHE:CE1	1:A:120:MET:CE	0.52	2.92	28	1
1:A:109:ASP:OD1	1:A:110:GLY:N	0.52	2.43	9	1
1:A:114:LEU:CD2	1:A:137:MET:SD	0.52	2.98	30	2
1:A:145:ASP:N	1:A:145:ASP:OD1	0.51	2.44	16	4
1:A:100:LEU:HD11	1:A:104:PHE:CE2	0.51	2.39	3	2
1:A:139:ASP:N	1:A:139:ASP:OD1	0.51	2.43	14	2
1:A:100:LEU:CG	1:A:104:PHE:CE2	0.51	2.92	6	1
1:A:120:MET:SD	1:A:121:LEU:CD1	0.51	2.99	30	1
1:A:113:ASP:OD1	1:A:116:GLU:CG	0.51	2.58	14	1
1:A:97:LEU:HD12	1:A:154:LEU:CD2	0.51	2.35	7	1
1:A:105:ASP:O	1:A:108:ALA:N	0.51	2.43	13	3
1:A:143:ASN:O	1:A:145:ASP:N	0.51	2.44	6	5
1:A:128:ILE:O	1:A:128:ILE:HD12	0.51	2.06	20	1
1:A:104:PHE:CE2	1:A:153:PHE:CZ	0.51	2.98	10	2
1:A:153:PHE:CZ	1:A:157:MET:SD	0.51	3.04	22	2
1:A:97:LEU:HD22	1:A:157:MET:HG3	0.51	1.82	16	1
1:A:112:ILE:HG22	1:A:117:LEU:HG	0.51	1.83	27	4
1:A:117:LEU:HD11	1:A:137:MET:SD	0.51	2.46	1	2
1:A:151:ASP:OD1	1:A:152:GLU:N	0.51	2.44	26	1
1:A:121:LEU:CD1	3:A:1:KDH:O37	0.51	2.59	8	1
1:A:122:GLN:O	1:A:125:GLY:N	0.51	2.43	8	2
1:A:121:LEU:O	1:A:123:ALA:N	0.51	2.44	29	2
1:A:97:LEU:O	1:A:101:PHE:N	0.50	2.43	6	1
1:A:104:PHE:CD1	1:A:120:MET:HB2	0.50	2.40	5	1
1:A:128:ILE:N	1:A:128:ILE:CD1	0.50	2.71	23	1
1:A:150:TYR:CE1	1:A:154:LEU:HD21	0.50	2.41	22	1
1:A:101:PHE:CD1	1:A:153:PHE:CG	0.50	3.00	1	1
1:A:113:ASP:OD1	1:A:116:GLU:N	0.50	2.44	28	1
1:A:121:LEU:CG	3:A:1:KDH:H41	0.50	2.37	25	2
1:A:93:SER:OG	1:A:94:GLU:N	0.50	2.44	19	2
1:A:100:LEU:O	1:A:104:PHE:CD1	0.50	2.65	27	1
1:A:144:ASN:O	1:A:146:GLY:N	0.50	2.43	24	4
1:A:150:TYR:C	1:A:150:TYR:CD1	0.50	2.84	3	3
1:A:110:GLY:O	1:A:111:TYR:CD1	0.50	2.64	20	4
1:A:143:ASN:O	1:A:144:ASN:ND2	0.50	2.44	16	1
1:A:104:PHE:CD2	1:A:120:MET:HE3	0.50	2.41	25	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:LYS:CE	1:A:155:GLU:OE2	0.49	2.60	20	1
1:A:109:ASP:OD2	1:A:147:ARG:NH2	0.49	2.45	17	1
1:A:97:LEU:CD1	1:A:153:PHE:CE2	0.49	2.95	20	1
1:A:145:ASP:OD1	1:A:146:GLY:N	0.49	2.45	5	3
1:A:100:LEU:HD12	1:A:100:LEU:C	0.49	2.28	7	1
1:A:143:ASN:ND2	1:A:152:GLU:OE2	0.49	2.46	10	1
1:A:143:ASN:O	1:A:144:ASN:CB	0.49	2.60	8	3
1:A:144:ASN:O	1:A:145:ASP:CB	0.49	2.59	15	4
1:A:107:ASN:ND2	1:A:116:GLU:CD	0.49	2.66	9	1
1:A:104:PHE:CE2	1:A:153:PHE:CE1	0.49	3.01	13	2
1:A:137:MET:SD	1:A:141:ASP:CB	0.49	3.00	20	2
1:A:101:PHE:O	1:A:101:PHE:CD1	0.49	2.65	29	1
1:A:104:PHE:CE2	1:A:120:MET:CE	0.49	2.96	4	2
1:A:110:GLY:C	1:A:111:TYR:CD2	0.49	2.86	22	5
1:A:128:ILE:CG1	1:A:132:ASP:HB2	0.49	2.38	7	1
1:A:100:LEU:HD23	1:A:104:PHE:CZ	0.49	2.42	30	1
1:A:100:LEU:HG	1:A:104:PHE:CZ	0.49	2.42	29	1
1:A:128:ILE:CG1	1:A:129:THR:N	0.49	2.75	12	1
1:A:104:PHE:CE1	1:A:120:MET:HG2	0.49	2.42	26	1
1:A:95:GLU:OE1	1:A:95:GLU:CA	0.49	2.60	20	1
1:A:114:LEU:HD23	1:A:137:MET:CB	0.49	2.37	10	1
1:A:125:GLY:O	1:A:126:GLU:C	0.49	2.51	29	7
3:A:1:KDH:H41	3:A:1:KDH:C4	0.49	2.38	12	1
1:A:116:GLU:O	1:A:120:MET:CB	0.49	2.60	23	1
1:A:121:LEU:HG	3:A:1:KDH:H39	0.48	1.85	14	1
1:A:96:GLU:O	1:A:100:LEU:N	0.48	2.46	22	1
1:A:104:PHE:CG	1:A:112:ILE:CD1	0.48	2.96	26	1
1:A:149:ASP:OD2	1:A:151:ASP:CB	0.48	2.61	11	1
1:A:104:PHE:CD1	1:A:120:MET:SD	0.48	3.06	30	1
1:A:128:ILE:CG1	1:A:132:ASP:HB3	0.48	2.39	28	1
1:A:114:LEU:CD1	1:A:137:MET:SD	0.48	2.99	7	1
1:A:104:PHE:CZ	3:A:1:KDH:O03	0.48	2.67	19	3
1:A:117:LEU:HD23	1:A:120:MET:SD	0.48	2.48	19	1
1:A:94:GLU:HA	1:A:97:LEU:HB2	0.48	1.85	24	8
1:A:121:LEU:CD1	1:A:121:LEU:N	0.48	2.76	14	1
1:A:113:ASP:O	1:A:117:LEU:HD12	0.48	2.07	5	2
1:A:114:LEU:CD2	1:A:137:MET:HG3	0.48	2.38	20	4
1:A:138:LYS:O	1:A:142:LYS:CG	0.48	2.61	24	1
1:A:157:MET:O	1:A:158:LYS:C	0.48	2.52	30	5
1:A:154:LEU:CD1	1:A:154:LEU:N	0.48	2.76	19	1
1:A:92:LYS:O	1:A:97:LEU:HD22	0.48	2.09	25	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:LEU:CG	1:A:137:MET:SD	0.48	3.01	21	3
1:A:104:PHE:CG	1:A:120:MET:HE1	0.48	2.44	26	3
1:A:94:GLU:CG	1:A:154:LEU:HD21	0.48	2.39	18	1
1:A:154:LEU:CD2	1:A:154:LEU:N	0.48	2.76	27	1
1:A:109:ASP:N	1:A:109:ASP:OD1	0.48	2.46	28	2
1:A:149:ASP:OD1	1:A:149:ASP:N	0.47	2.45	2	2
1:A:126:GLU:O	1:A:126:GLU:OE1	0.47	2.32	28	2
1:A:153:PHE:CE2	1:A:157:MET:HG3	0.47	2.43	10	2
1:A:121:LEU:O	1:A:124:THR:N	0.47	2.43	27	1
1:A:149:ASP:OD1	1:A:150:TYR:N	0.47	2.47	14	2
1:A:107:ASN:CB	1:A:109:ASP:OD1	0.47	2.62	7	1
1:A:157:MET:C	1:A:158:LYS:CG	0.47	2.82	30	1
1:A:100:LEU:HD11	1:A:104:PHE:CE1	0.47	2.45	15	1
1:A:100:LEU:HD23	1:A:104:PHE:HE2	0.47	1.66	29	1
1:A:156:PHE:CE2	3:A:1:KDH:H33	0.47	2.44	15	3
1:A:109:ASP:OD2	1:A:111:TYR:O	0.47	2.33	19	1
1:A:112:ILE:CG2	1:A:117:LEU:HG	0.47	2.39	16	5
1:A:109:ASP:OD1	1:A:111:TYR:O	0.47	2.33	20	6
1:A:92:LYS:O	1:A:97:LEU:HD11	0.47	2.10	12	2
1:A:150:TYR:CD1	1:A:150:TYR:C	0.47	2.86	20	1
1:A:104:PHE:CG	1:A:120:MET:HG3	0.47	2.45	7	1
1:A:154:LEU:N	1:A:154:LEU:CD2	0.47	2.78	30	1
1:A:114:LEU:CD2	1:A:137:MET:CG	0.47	2.93	20	3
1:A:118:LYS:HG3	1:A:119:ILE:N	0.47	2.24	25	2
1:A:101:PHE:CD1	1:A:101:PHE:C	0.47	2.88	3	4
1:A:104:PHE:O	1:A:105:ASP:C	0.47	2.53	23	2
1:A:124:THR:HG22	1:A:124:THR:O	0.47	2.10	8	2
1:A:105:ASP:OD1	1:A:111:TYR:O	0.47	2.33	20	7
1:A:101:PHE:HB2	1:A:153:PHE:CE2	0.47	2.45	15	1
1:A:145:ASP:OD1	1:A:147:ARG:O	0.47	2.33	11	4
1:A:100:LEU:HB3	1:A:104:PHE:CE2	0.47	2.45	25	2
1:A:105:ASP:OD2	1:A:108:ALA:CA	0.47	2.63	6	1
1:A:141:ASP:OD1	1:A:145:ASP:OD1	0.47	2.33	2	2
1:A:98:SER:O	1:A:150:TYR:OH	0.47	2.32	21	2
1:A:117:LEU:O	1:A:120:MET:N	0.47	2.46	19	1
1:A:98:SER:CB	1:A:150:TYR:OH	0.47	2.63	6	1
1:A:149:ASP:OD1	1:A:152:GLU:CG	0.47	2.63	4	1
1:A:141:ASP:OD2	1:A:147:ARG:O	0.47	2.33	2	7
1:A:141:ASP:OD1	1:A:152:GLU:OE1	0.47	2.33	6	4
1:A:156:PHE:CD1	1:A:156:PHE:C	0.47	2.88	8	1
3:A:1:KDH:C9	3:A:1:KDH:H41	0.47	2.40	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:TYR:CE1	1:A:149:ASP:OD1	0.47	2.68	29	1
1:A:137:MET:CE	1:A:141:ASP:OD2	0.46	2.63	4	1
1:A:122:GLN:N	1:A:126:GLU:HG2	0.46	2.25	18	6
1:A:117:LEU:CD1	1:A:137:MET:CG	0.46	2.93	10	1
1:A:145:ASP:OD1	1:A:147:ARG:N	0.46	2.47	5	1
1:A:114:LEU:HD23	1:A:137:MET:HG3	0.46	1.86	8	2
1:A:153:PHE:O	1:A:156:PHE:CB	0.46	2.64	2	1
1:A:157:MET:HG3	1:A:158:LYS:N	0.46	2.25	24	2
1:A:146:GLY:O	1:A:147:ARG:NH1	0.46	2.48	12	1
1:A:150:TYR:O	1:A:150:TYR:CD1	0.46	2.68	17	1
1:A:143:ASN:O	1:A:143:ASN:OD1	0.46	2.33	16	1
1:A:92:LYS:CB	1:A:92:LYS:NZ	0.46	2.78	23	1
1:A:128:ILE:HD12	1:A:132:ASP:CB	0.46	2.40	4	1
1:A:137:MET:HE2	1:A:148:ILE:CD1	0.46	2.40	4	3
1:A:107:ASN:O	1:A:108:ALA:O	0.46	2.33	10	3
1:A:143:ASN:ND2	1:A:145:ASP:HB2	0.46	2.25	13	1
1:A:97:LEU:CD2	1:A:100:LEU:HD12	0.46	2.39	18	1
1:A:112:ILE:HG23	1:A:116:GLU:HB2	0.46	1.86	23	1
1:A:145:ASP:OD1	1:A:145:ASP:N	0.46	2.49	4	1
1:A:105:ASP:OD2	1:A:111:TYR:O	0.46	2.34	10	3
1:A:112:ILE:O	1:A:148:ILE:CG1	0.46	2.63	16	1
1:A:154:LEU:O	1:A:158:LYS:N	0.46	2.49	19	1
1:A:137:MET:HE1	1:A:148:ILE:CD1	0.46	2.37	6	1
1:A:92:LYS:O	1:A:93:SER:O	0.46	2.34	15	1
1:A:154:LEU:HD22	1:A:154:LEU:N	0.46	2.26	27	1
1:A:104:PHE:CZ	1:A:120:MET:HE1	0.46	2.46	4	1
1:A:99:ASP:OD1	1:A:100:LEU:N	0.46	2.48	26	1
1:A:101:PHE:HB2	1:A:153:PHE:CD2	0.46	2.46	15	1
1:A:105:ASP:OD2	1:A:110:GLY:N	0.46	2.49	19	1
1:A:126:GLU:O	1:A:126:GLU:OE2	0.46	2.34	17	1
1:A:105:ASP:OD1	1:A:116:GLU:OE1	0.46	2.33	10	1
1:A:120:MET:SD	1:A:121:LEU:HD22	0.46	2.51	25	2
1:A:107:ASN:ND2	1:A:109:ASP:OD1	0.46	2.49	7	1
1:A:141:ASP:OD2	1:A:144:ASN:O	0.46	2.34	12	3
1:A:156:PHE:CZ	3:A:1:KDH:H4	0.46	2.46	17	1
1:A:151:ASP:OD1	1:A:151:ASP:N	0.46	2.48	26	1
1:A:132:ASP:O	1:A:135:GLU:CB	0.46	2.64	1	1
1:A:149:ASP:OD2	1:A:152:GLU:OE1	0.45	2.34	30	1
1:A:121:LEU:O	1:A:122:GLN:C	0.45	2.54	29	8
1:A:125:GLY:C	1:A:126:GLU:CG	0.45	2.84	26	2
1:A:125:GLY:O	1:A:126:GLU:HG3	0.45	2.11	26	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:SER:O	1:A:97:LEU:CD2	0.45	2.60	4	1
1:A:128:ILE:CD1	1:A:136:LEU:HD11	0.45	2.41	12	1
1:A:101:PHE:CZ	1:A:112:ILE:HG13	0.45	2.46	3	1
1:A:104:PHE:HE2	3:A:1:KDH:H01A	0.45	1.71	28	1
1:A:104:PHE:CE2	1:A:120:MET:HE3	0.45	2.47	25	2
1:A:109:ASP:OD2	1:A:111:TYR:N	0.45	2.47	14	1
1:A:145:ASP:CG	1:A:145:ASP:O	0.45	2.54	12	1
1:A:93:SER:O	1:A:95:GLU:N	0.45	2.50	13	5
1:A:118:LYS:O	1:A:126:GLU:OE2	0.45	2.35	20	3
1:A:107:ASN:O	1:A:108:ALA:CB	0.45	2.60	27	4
1:A:128:ILE:HG13	1:A:129:THR:N	0.45	2.27	7	2
1:A:142:LYS:O	1:A:144:ASN:OD1	0.45	2.35	2	1
1:A:128:ILE:HG12	1:A:129:THR:N	0.45	2.26	29	2
1:A:115:ASP:O	1:A:119:ILE:CG1	0.45	2.65	27	1
1:A:114:LEU:HD23	1:A:137:MET:CG	0.45	2.41	10	2
1:A:101:PHE:C	1:A:101:PHE:CD1	0.45	2.89	2	1
1:A:141:ASP:OD1	1:A:152:GLU:OE2	0.45	2.35	16	1
1:A:107:ASN:HB2	1:A:116:GLU:OE2	0.45	2.11	12	2
1:A:93:SER:O	1:A:94:GLU:C	0.45	2.55	13	5
1:A:113:ASP:CB	1:A:116:GLU:OE1	0.45	2.65	19	1
1:A:130:GLU:HG3	1:A:131:ASP:N	0.45	2.27	25	2
1:A:131:ASP:OD1	1:A:131:ASP:O	0.45	2.34	11	1
1:A:119:ILE:O	1:A:122:GLN:HG2	0.45	2.12	18	1
1:A:153:PHE:O	1:A:157:MET:SD	0.45	2.75	12	1
1:A:99:ASP:O	1:A:102:ARG:N	0.45	2.50	29	1
1:A:141:ASP:OD1	1:A:147:ARG:O	0.44	2.34	4	3
1:A:101:PHE:CE2	1:A:150:TYR:HA	0.44	2.47	5	1
1:A:143:ASN:O	1:A:144:ASN:CG	0.44	2.56	16	1
1:A:143:ASN:O	1:A:143:ASN:CG	0.44	2.56	14	2
1:A:105:ASP:OD2	1:A:109:ASP:OD1	0.44	2.35	1	2
1:A:137:MET:O	1:A:138:LYS:C	0.44	2.56	21	4
1:A:153:PHE:O	1:A:156:PHE:HB3	0.44	2.12	2	4
1:A:128:ILE:CD1	1:A:128:ILE:N	0.44	2.81	15	2
1:A:105:ASP:OD1	1:A:109:ASP:OD1	0.44	2.35	14	1
1:A:109:ASP:OD1	1:A:109:ASP:N	0.44	2.51	5	3
1:A:136:LEU:CD2	3:A:1:KDH:C38	0.44	2.96	25	1
1:A:119:ILE:O	1:A:122:GLN:HG3	0.44	2.13	11	1
1:A:128:ILE:HD11	1:A:132:ASP:HB3	0.44	1.89	16	1
3:A:1:KDH:C9	3:A:1:KDH:H39	0.44	2.43	17	1
1:A:143:ASN:O	1:A:144:ASN:C	0.44	2.55	16	4
1:A:106:LYS:HZ3	1:A:119:ILE:HG21	0.44	1.73	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:MET:O	1:A:120:MET:SD	0.44	2.75	28	1
1:A:109:ASP:OD1	1:A:111:TYR:N	0.44	2.46	20	2
1:A:104:PHE:CD1	1:A:120:MET:CB	0.44	3.00	5	1
1:A:98:SER:CA	1:A:150:TYR:OH	0.44	2.66	12	2
1:A:145:ASP:O	1:A:145:ASP:OD1	0.44	2.36	17	1
1:A:114:LEU:CD2	1:A:137:MET:HG2	0.44	2.43	9	2
1:A:143:ASN:C	1:A:144:ASN:ND2	0.44	2.70	16	1
3:A:1:KDH:H39	3:A:1:KDH:C9	0.44	2.42	10	1
1:A:107:ASN:O	1:A:107:ASN:OD1	0.43	2.36	12	1
1:A:104:PHE:CE1	1:A:120:MET:HE1	0.43	2.49	4	1
1:A:150:TYR:O	1:A:151:ASP:C	0.43	2.56	19	3
1:A:136:LEU:O	1:A:137:MET:C	0.43	2.57	27	2
1:A:94:GLU:HG3	1:A:154:LEU:HD21	0.43	1.90	16	1
1:A:105:ASP:O	1:A:106:LYS:C	0.43	2.57	23	3
1:A:136:LEU:CD2	3:A:1:KDH:C39	0.43	2.96	25	1
1:A:128:ILE:HG23	1:A:133:ILE:HD11	0.43	1.91	29	1
1:A:126:GLU:CD	1:A:126:GLU:O	0.43	2.57	5	6
1:A:121:LEU:HD21	3:A:1:KDH:O37	0.43	2.14	5	3
1:A:107:ASN:C	1:A:109:ASP:OD1	0.43	2.57	7	1
1:A:120:MET:HG3	1:A:121:LEU:N	0.43	2.29	2	3
1:A:122:GLN:O	1:A:123:ALA:C	0.43	2.57	14	4
1:A:102:ARG:CG	1:A:103:MET:N	0.43	2.81	26	1
1:A:113:ASP:O	1:A:117:LEU:N	0.43	2.49	15	1
1:A:96:GLU:O	1:A:99:ASP:N	0.43	2.51	22	1
1:A:114:LEU:HA	1:A:117:LEU:CD1	0.43	2.41	13	1
1:A:137:MET:HG3	1:A:141:ASP:CB	0.43	2.43	27	1
1:A:115:ASP:O	1:A:118:LYS:N	0.43	2.46	4	1
1:A:94:GLU:CA	1:A:97:LEU:HB2	0.43	2.43	13	1
1:A:118:LYS:CB	1:A:133:ILE:HD12	0.43	2.44	21	1
1:A:137:MET:CE	1:A:148:ILE:HG13	0.43	2.43	21	1
1:A:140:GLY:HA2	1:A:156:PHE:CA	0.43	2.43	6	1
1:A:153:PHE:O	1:A:156:PHE:N	0.43	2.52	9	1
1:A:122:GLN:O	1:A:124:THR:N	0.43	2.51	14	2
1:A:137:MET:SD	1:A:148:ILE:CD1	0.43	2.99	1	1
1:A:113:ASP:C	1:A:113:ASP:OD1	0.43	2.57	28	1
1:A:121:LEU:HD11	3:A:1:KDH:H39	0.43	1.91	21	1
1:A:138:LYS:HG3	1:A:139:ASP:N	0.43	2.29	26	1
1:A:117:LEU:O	1:A:119:ILE:N	0.43	2.52	19	1
1:A:137:MET:SD	1:A:141:ASP:HB2	0.43	2.54	19	1
1:A:94:GLU:OE2	1:A:154:LEU:CD1	0.43	2.67	8	1
1:A:120:MET:SD	1:A:121:LEU:CD2	0.43	3.07	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:ASN:OD1	1:A:107:ASN:O	0.43	2.37	19	2
1:A:143:ASN:ND2	1:A:145:ASP:HB3	0.43	2.29	7	2
1:A:117:LEU:HD12	1:A:137:MET:SD	0.43	2.54	9	1
1:A:157:MET:O	1:A:158:LYS:HB3	0.43	2.14	9	2
1:A:100:LEU:HD23	1:A:104:PHE:CD1	0.43	2.48	4	1
1:A:107:ASN:CG	1:A:109:ASP:OD1	0.43	2.57	7	1
1:A:126:GLU:O	1:A:126:GLU:CD	0.43	2.57	10	4
1:A:128:ILE:CD1	1:A:133:ILE:HD13	0.43	2.44	21	1
1:A:97:LEU:O	1:A:98:SER:C	0.43	2.57	3	2
1:A:105:ASP:OD2	1:A:109:ASP:CG	0.42	2.57	5	1
1:A:99:ASP:O	1:A:102:ARG:HG3	0.42	2.14	7	2
1:A:97:LEU:HA	1:A:100:LEU:HD21	0.42	1.91	7	2
1:A:145:ASP:OD2	1:A:147:ARG:HG3	0.42	2.14	21	1
1:A:129:THR:HG22	1:A:132:ASP:OD2	0.42	2.14	17	1
1:A:149:ASP:N	1:A:149:ASP:OD1	0.42	2.51	16	2
1:A:133:ILE:O	1:A:134:GLU:C	0.42	2.57	8	1
1:A:98:SER:OG	1:A:99:ASP:N	0.42	2.52	8	2
1:A:100:LEU:O	1:A:101:PHE:C	0.42	2.57	22	1
1:A:117:LEU:O	3:A:1:KDH:O47	0.42	2.36	22	1
1:A:94:GLU:HA	1:A:97:LEU:CB	0.42	2.44	13	2
1:A:109:ASP:C	1:A:109:ASP:OD1	0.42	2.56	18	1
1:A:137:MET:O	1:A:139:ASP:N	0.42	2.52	21	1
1:A:137:MET:HE2	1:A:148:ILE:HG13	0.42	1.90	17	2
1:A:100:LEU:CD1	1:A:104:PHE:CZ	0.42	2.94	6	1
1:A:117:LEU:HD11	1:A:137:MET:HE1	0.42	1.90	6	1
1:A:128:ILE:CG1	1:A:132:ASP:CB	0.42	2.97	7	1
1:A:144:ASN:O	1:A:144:ASN:ND2	0.42	2.52	10	1
1:A:122:GLN:N	1:A:126:GLU:HB3	0.42	2.29	14	1
1:A:137:MET:CE	1:A:148:ILE:CG1	0.42	2.98	6	1
1:A:96:GLU:O	1:A:97:LEU:C	0.42	2.57	22	5
1:A:106:LYS:HD2	1:A:119:ILE:HG21	0.42	1.91	12	1
1:A:99:ASP:O	1:A:100:LEU:C	0.42	2.58	26	1
1:A:104:PHE:CG	1:A:112:ILE:HD13	0.42	2.50	5	1
1:A:157:MET:O	1:A:158:LYS:HG3	0.42	2.15	30	1
1:A:143:ASN:O	1:A:144:ASN:HB3	0.42	2.15	20	3
1:A:121:LEU:CB	1:A:126:GLU:HG2	0.42	2.44	12	1
1:A:94:GLU:O	1:A:95:GLU:C	0.42	2.57	20	2
1:A:107:ASN:O	1:A:108:ALA:C	0.42	2.58	19	1
1:A:100:LEU:O	1:A:103:MET:N	0.42	2.48	3	1
1:A:107:ASN:CB	1:A:116:GLU:OE1	0.42	2.68	3	1
1:A:101:PHE:O	1:A:102:ARG:C	0.42	2.57	28	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:MET:CG	1:A:121:LEU:N	0.42	2.82	19	2
1:A:105:ASP:OD2	1:A:108:ALA:N	0.42	2.53	6	1
1:A:93:SER:O	1:A:97:LEU:HG	0.42	2.15	6	1
1:A:135:GLU:O	1:A:136:LEU:C	0.42	2.58	28	1
1:A:126:GLU:OE1	1:A:126:GLU:O	0.42	2.37	13	1
1:A:115:ASP:OD1	1:A:115:ASP:N	0.42	2.50	27	1
1:A:135:GLU:O	1:A:138:LYS:HD3	0.42	2.13	27	1
1:A:126:GLU:HG3	1:A:126:GLU:O	0.42	2.15	18	3
1:A:117:LEU:CD1	1:A:137:MET:HG2	0.42	2.44	10	1
1:A:125:GLY:O	1:A:126:GLU:CB	0.42	2.68	16	1
1:A:151:ASP:O	1:A:151:ASP:OD1	0.42	2.38	7	1
1:A:121:LEU:CD1	1:A:124:THR:HG21	0.42	2.45	12	1
1:A:99:ASP:O	1:A:102:ARG:HG2	0.42	2.15	26	2
1:A:107:ASN:HB3	1:A:116:GLU:OE2	0.42	2.14	10	1
1:A:138:LYS:CG	1:A:139:ASP:N	0.42	2.82	25	1
1:A:144:ASN:O	1:A:145:ASP:HB3	0.41	2.15	12	1
1:A:149:ASP:OD1	1:A:149:ASP:C	0.41	2.59	17	1
1:A:125:GLY:C	1:A:126:GLU:HG2	0.41	2.35	26	2
1:A:104:PHE:CE1	1:A:120:MET:HB2	0.41	2.48	5	1
1:A:113:ASP:N	1:A:116:GLU:OE1	0.41	2.50	21	1
1:A:153:PHE:O	1:A:154:LEU:C	0.41	2.58	9	2
1:A:150:TYR:CD1	1:A:150:TYR:O	0.41	2.73	20	1
1:A:117:LEU:O	1:A:118:LYS:C	0.41	2.58	19	1
1:A:130:GLU:HG3	1:A:134:GLU:OE2	0.41	2.15	23	1
1:A:124:THR:CG2	1:A:124:THR:O	0.41	2.68	27	1
1:A:126:GLU:O	1:A:126:GLU:HG3	0.41	2.14	29	3
1:A:128:ILE:HG12	1:A:132:ASP:HB2	0.41	1.92	7	1
1:A:112:ILE:CG2	1:A:117:LEU:CG	0.41	2.98	30	1
1:A:114:LEU:CG	1:A:137:MET:HG3	0.41	2.46	18	1
1:A:129:THR:O	1:A:130:GLU:C	0.41	2.59	26	1
1:A:96:GLU:O	1:A:100:LEU:HB2	0.41	2.15	23	1
1:A:97:LEU:HA	1:A:100:LEU:CD2	0.41	2.45	7	1
1:A:112:ILE:HG22	1:A:148:ILE:HD12	0.41	1.91	16	1
1:A:106:LYS:CG	1:A:119:ILE:HG21	0.41	2.46	16	1
1:A:122:GLN:HA	1:A:126:GLU:CG	0.41	2.45	16	1
1:A:137:MET:SD	1:A:141:ASP:HB3	0.41	2.55	19	1
1:A:111:TYR:HB3	1:A:147:ARG:CG	0.41	2.46	3	1
1:A:134:GLU:O	1:A:135:GLU:C	0.41	2.58	8	1
1:A:97:LEU:O	1:A:100:LEU:N	0.41	2.52	27	1
1:A:100:LEU:HD21	3:A:1:KDH:C26	0.41	2.45	4	1
1:A:107:ASN:HB3	1:A:109:ASP:OD1	0.41	2.15	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:1:KDH:H39	3:A:1:KDH:C6	0.41	2.46	17	1
1:A:143:ASN:HB2	1:A:145:ASP:OD2	0.41	2.14	9	1
1:A:107:ASN:HB3	1:A:116:GLU:OE1	0.41	2.16	28	2
1:A:147:ARG:HG2	1:A:147:ARG:NH1	0.41	2.31	23	1
1:A:109:ASP:OD1	1:A:109:ASP:C	0.41	2.58	4	1
1:A:99:ASP:O	1:A:102:ARG:HB3	0.41	2.16	2	1
1:A:127:THR:O	1:A:127:THR:CG2	0.41	2.63	11	1
1:A:157:MET:HG2	1:A:158:LYS:N	0.41	2.31	28	2
1:A:113:ASP:HB2	1:A:116:GLU:OE2	0.41	2.16	5	1
1:A:114:LEU:HG	1:A:137:MET:SD	0.41	2.56	30	2
1:A:121:LEU:CD1	3:A:1:KDH:H39	0.41	2.45	21	1
3:A:1:KDH:H39	3:A:1:KDH:C14	0.41	2.45	17	1
1:A:141:ASP:CG	1:A:147:ARG:O	0.41	2.59	26	1
1:A:118:LYS:O	1:A:126:GLU:HG3	0.41	2.16	11	1
1:A:135:GLU:O	1:A:138:LYS:CD	0.41	2.69	27	1
1:A:112:ILE:O	1:A:148:ILE:HB	0.41	2.16	7	1
1:A:149:ASP:OD1	1:A:152:GLU:OE1	0.41	2.39	21	1
1:A:125:GLY:O	1:A:126:GLU:HB2	0.41	2.15	16	1
1:A:119:ILE:O	1:A:122:GLN:HB2	0.41	2.16	5	1
1:A:111:TYR:HA	1:A:148:ILE:O	0.41	2.16	7	1
1:A:150:TYR:O	1:A:153:PHE:HB3	0.41	2.16	21	2
1:A:102:ARG:HG3	1:A:102:ARG:NH1	0.41	2.31	16	1
1:A:112:ILE:O	1:A:148:ILE:HG13	0.41	2.15	16	1
1:A:108:ALA:O	1:A:109:ASP:HB3	0.41	2.16	8	2
1:A:116:GLU:O	1:A:120:MET:N	0.41	2.53	23	1
1:A:98:SER:HB2	1:A:150:TYR:CE1	0.41	2.51	14	1
1:A:104:PHE:CD1	1:A:112:ILE:CD1	0.41	3.04	13	1
1:A:97:LEU:HD22	1:A:100:LEU:HD21	0.41	1.92	7	1
1:A:101:PHE:HB3	1:A:150:TYR:OH	0.41	2.16	19	1
1:A:96:GLU:HA	1:A:99:ASP:OD2	0.41	2.14	23	1
1:A:113:ASP:O	1:A:117:LEU:HG	0.41	2.16	6	1
1:A:100:LEU:HD23	1:A:104:PHE:HD1	0.40	1.76	4	1
1:A:138:LYS:O	1:A:142:LYS:HG3	0.40	2.16	24	1
1:A:136:LEU:HD21	3:A:1:KDH:C39	0.40	2.46	25	1
1:A:114:LEU:CA	1:A:117:LEU:HD12	0.40	2.41	13	1
1:A:140:GLY:O	1:A:152:GLU:HB3	0.40	2.16	22	1
1:A:144:ASN:CG	1:A:145:ASP:N	0.40	2.73	24	1
3:A:1:KDH:C12	3:A:1:KDH:H39	0.40	2.47	27	1
1:A:105:ASP:O	1:A:107:ASN:N	0.40	2.55	13	1
1:A:101:PHE:CE2	1:A:112:ILE:HD11	0.40	2.51	12	1
1:A:149:ASP:C	1:A:149:ASP:OD1	0.40	2.60	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:LEU:CD2	3:A:1:KDH:O37	0.40	2.69	6	1
1:A:113:ASP:OD1	1:A:116:GLU:HB2	0.40	2.16	28	1
1:A:99:ASP:O	1:A:102:ARG:HB2	0.40	2.16	12	1
1:A:149:ASP:OD1	1:A:151:ASP:N	0.40	2.55	9	1
1:A:117:LEU:HD13	1:A:137:MET:CG	0.40	2.46	10	1
1:A:96:GLU:OE1	1:A:96:GLU:O	0.40	2.39	16	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	67/72 (93%)	55±3 (82±5%)	9±3 (14±4%)	2±1 (3±2%)	7	37
All	All	2010/2160 (93%)	1657 (82%)	284 (14%)	69 (3%)	7	37

All 13 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	15
1	A	105	ASP	11
1	A	108	ALA	7
1	A	109	ASP	7
1	A	144	ASN	7
1	A	158	LYS	5
1	A	93	SER	5
1	A	92	LYS	5
1	A	129	THR	2
1	A	141	ASP	2
1	A	122	GLN	1
1	A	149	ASP	1
1	A	133	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	61/64 (95%)	45±3 (74±5%)	16±3 (26±5%)	2	23
All	All	1830/1920 (95%)	1346 (74%)	484 (26%)	2	23

All 50 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	142	LYS	24
1	A	126	GLU	21
1	A	158	LYS	21
1	A	103	MET	19
1	A	137	MET	18
1	A	106	LYS	17
1	A	132	ASP	16
1	A	122	GLN	16
1	A	97	LEU	15
1	A	92	LYS	15
1	A	138	LYS	14
1	A	118	LYS	14
1	A	121	LEU	14
1	A	96	GLU	13
1	A	98	SER	12
1	A	129	THR	12
1	A	141	ASP	10
1	A	102	ARG	10
1	A	120	MET	10
1	A	100	LEU	10
1	A	147	ARG	10
1	A	115	ASP	10
1	A	135	GLU	10
1	A	139	ASP	9
1	A	99	ASP	9
1	A	157	MET	9
1	A	114	LEU	9
1	A	104	PHE	9
1	A	94	GLU	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	151	ASP	8
1	A	113	ASP	8
1	A	131	ASP	7
1	A	93	SER	7
1	A	127	THR	6
1	A	155	GLU	6
1	A	95	GLU	6
1	A	145	ASP	6
1	A	154	LEU	6
1	A	144	ASN	5
1	A	150	TYR	5
1	A	128	ILE	4
1	A	143	ASN	4
1	A	136	LEU	4
1	A	130	GLU	4
1	A	124	THR	3
1	A	134	GLU	3
1	A	149	ASP	2
1	A	105	ASP	2
1	A	109	ASP	2
1	A	119	ILE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 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	KDH	A	1	-	36,36,36	3.29±0.01	1±0 (2±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	KDH	A	1	-	54,54,54	1.06±0.01	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
3	KDH	A	1	-	-	0±0,12,24,24	0±0,4,4,4

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	1	KDH	C14-C15	6.22	1.40	1.51	5	30

There are no bond-angle outliers.

There are no chirality outliers.

All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
3	A	1	KDH	C33-O35-C36-C38	3

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

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 17243

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 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	756
Number of shifts mapped to atoms	756
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

7.1.2 Chemical shift referencing

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 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	65	0.15 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	70	0.44 ± 0.44	None needed (< 0.5 ppm)

7.1.3 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 81%, i.e. 675 atoms were assigned a chemical shift out of a possible 830. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	268/335 (80%)	134/134 (100%)	67/134 (50%)	67/67 (100%)
Sidechain	379/443 (86%)	239/256 (93%)	140/171 (82%)	0/16 (0%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	28/52 (54%)	28/28 (100%)	0/24 (0%)	0/0 (—%)
Overall	675/830 (81%)	401/418 (96%)	207/329 (63%)	67/83 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 701 atoms were assigned a chemical shift out of a possible 876. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	281/360 (78%)	140/144 (97%)	71/144 (49%)	70/72 (97%)
Sidechain	392/464 (84%)	247/268 (92%)	145/180 (81%)	0/16 (0%)
Aromatic	28/52 (54%)	28/28 (100%)	0/24 (0%)	0/0 (—%)
Overall	701/876 (80%)	415/440 (94%)	216/348 (62%)	70/88 (80%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:

