Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2022 – 09:25 AM EST

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 (i) symbol.

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

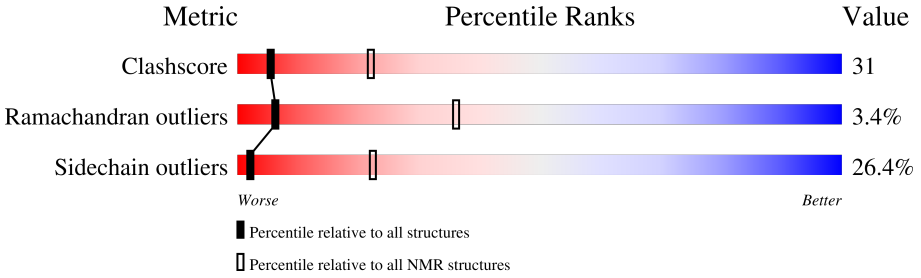
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

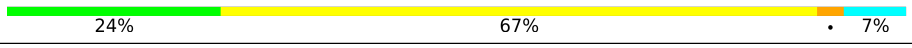
The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	72	

2 Ensemble composition and analysis (i)

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
			Total	C	H	N	O	S	
1	A	72	1128	360	545	88	130	5	0

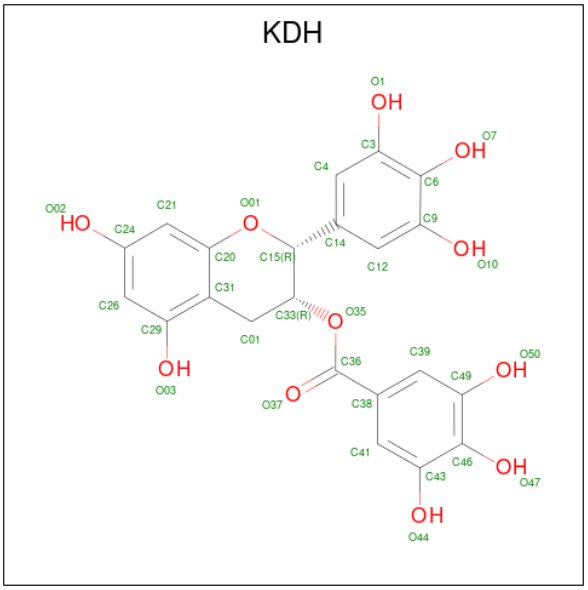
There is a discrepancy between the modelled and reference sequences:

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	
			Total	Ca
2	A	2	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: $C_{22}H_{18}O_{11}$).



Mol	Chain	Residues	Atoms			
			Total	C	H	O
3	A	1	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, DNA and oligosaccharide 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

Chain A: 24% 67% • 7%

M90 G91 K92 S93 E94 E95 E96 L97 S98 D99 L100 F101 R102 M103 F104 D105 K106 N107 A108 D109 G110 Y111 I112 D113 L114 D115 E116 L117 K118 I119 M120 L121 Q122 G125 E126 T127 I128 T129 D132 M137 K138 D141 K142 N143 N144 D145 G146 R147 I148 D149 Y150 F153 L154 E155 F156

M157 K158 G159 V160 E161

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

Chain A: 47% 38% 8% 7%

M90 G91 K92 S93 E94 E95 E96 L97 L100 F101 F104 D105 K106 N107 A108 D109 G110 Y111 L114 L117 K118 Q122 E126 D132 E135 L136 M137 K138 D139 G140 D141 K142 R147 I148 D151 E152 F153 F156 M157 K158 G159 V160 E161

4.2.2 Score per residue for model 2 (medoid)

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

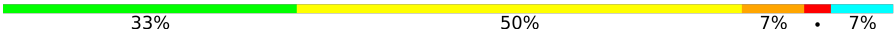
Chain A: 42% 33% 17% • 7%

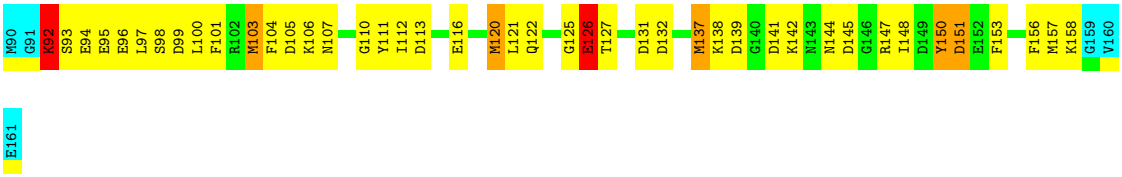
M90 G91 K92 S93 E94 E95 E96 L97 S98 D99 L100 F101 R102 M103 F104 D105 K106 N107 A108 D109 G110 Y111 L114 L117 M120 L121 Q122 E126 T127 I128 T129 E135 L136 M137 D141 K142 N143 N144 D145 G146 R147 I148 D149 F153 L154 E155 F156 M157 K158 G159 V160 E161

4.2.3 Score per residue for model 3

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

Chain A:

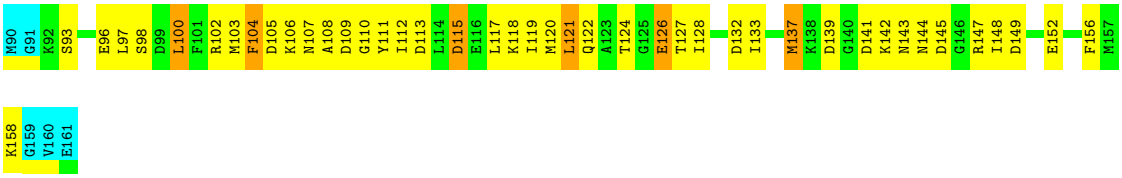




4.2.4 Score per residue for model 4

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

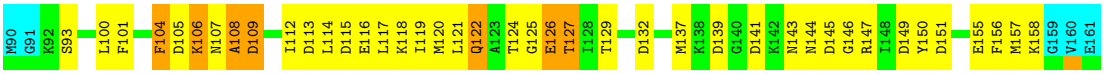
Chain A:



4.2.5 Score per residue for model 5

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

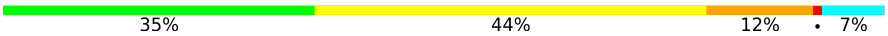
Chain A:

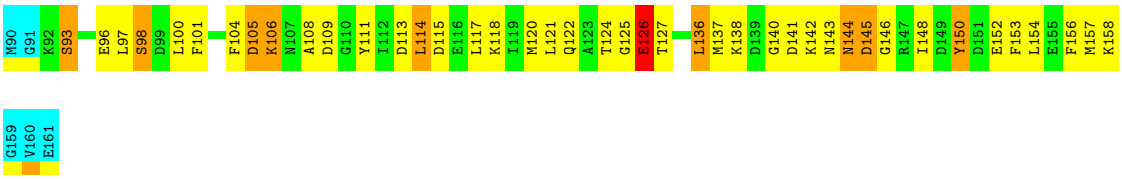


4.2.6 Score per residue for model 6

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

Chain A:

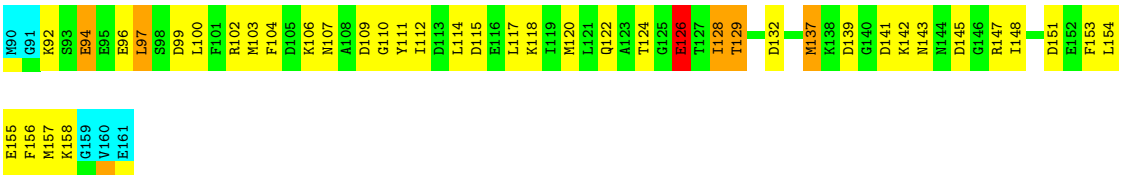




4.2.7 Score per residue for model 7

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

Chain A: 36% 49% 7% • 7%



4.2.8 Score per residue for model 8

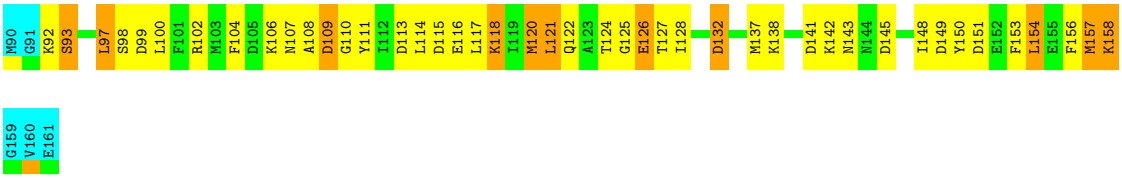
• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A: 29% 53% 11% 7%

4.2.9 Score per residue for model 9

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

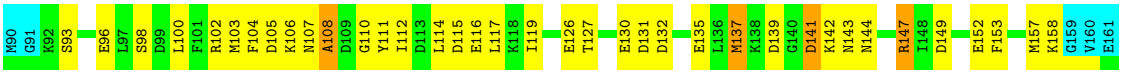
Chain A: 32% 46% 15% 7%



4.2.10 Score per residue for model 10

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

Chain A: 42% 46% 6% 7%



4.2.11 Score per residue for model 11

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

Chain A: 36% 54% • 7%

M90 G91 K92 S93 E94 E95 S98 D99 L100 F101 R102 M103 F104 D105 K106 N107 A108 D109 G110 Y111 I112 D113 L114 L117 K118 I119 M120 L121 Q122 E126 T127 I128 T129 E130 D131 D132 I133 E134 E135 L136 M137 G140 D141 K142 N143 N144 D145 G146 R147 I148 D149 Y150 D151 F156 M157

K158 G159 V160 E161

4.2.12 Score per residue for model 12

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

Chain A: 28% 49% 17% 7%

M90 G91 K92 S93 E96 L97 S98 D99 L100 F101 R102 M103 F104 D105 K106 N107 A108 D109 G110 Y111 I112 D113 L114 D115 E116 L117 K118 I119 M120 L121 Q122 A123 T124 G125 E126 T127 I128 T129 I133 L136 M137 D141 K142 N143 N144 D145 G146 R147 I148 D149 Y150 D151 E152 F153 L154 E155

F156 M157 K158 G159 V160 E161

4.2.13 Score per residue for model 13

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

Chain A: 42% 35% 17% 7%

M90 G91 K92 S93 E94 E95 E96 L97 L100 M103 F104 D105 K106 N107 A108 D109 G110 Y111 I112 D113 L114 L117 K118 I119 M120 G125 E126 T127 I128 T129 E130 D131 D132 M137 K138 N143 N144 D145 F153 L154 E155 F156 M157 K158 G159 V160 E161

4.2.14 Score per residue for model 14

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

Chain A: 33% 44% 15% 7%

M90 G91 K92 S93 E94 E95 E96 L97 S98 D99 L100 F101 F104 D105 K106 N107 A108 D109 G110 Y111 I112 D113 L114 D115 E116 L117 K118 I119 M120 L121 Q122 A123 T124 G125 E126 T129 E130 D131 M137 K138 D139 K142 N143 N144 D145 G146 R147 I148 D149 Y150 F153 L154 M157 K158

G159 V160 E161

4.2.15 Score per residue for model 15

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

Chain A: 39% 38% 15% • 7%

M90 G91 K92 S93 E94 L97 S98 D99 L100 F101 R102 M103 F104 D105 A108 D109 D113 L114 L117 K118 I119 M120 L121 Q122 G125 E126 T127 I128 D132 L136 M137 K138 D141 K142 N143 N144 D145 G146 R147 I148 E152 F153 F156 M157 K158 G159 V160 E161

4.2.16 Score per residue for model 16

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

Chain A: 35% 39% 19% 7%

M90 G91 K92 S93 E94 E95 E96 L97 L100 F101 R102 M103 F104 D105 K106 N107 A108 D109 G110 Y111 I112 D113 L114 D115 E116 L117 K118 I119 M120 L121 Q122 A123 T124 G125 E126 T127 I128 T129 D132 E135 L136 M137 D141 K142 N143 N144 D145 I148 D149 E152 F153 L154 E155 F156 M157 K158 G159 V160 E161

4.2.17 Score per residue for model 17

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

Chain A: 38% 42% 12% • 7%

M90 G91 K92 L97 L100 M103 F104 D105 K106 D109 G110 Y111 L114 D115 K118 I119 M120 L121 Q122 A123 T124 G125 E126 T127 I128 T129 E130 D131 D132 L136 M137 K138 D139 K142 N143 N144 D145 G146 R147 I148 D149 Y150 D151 E152 F153 F156 M157 K158 G159 V160 E161

4.2.18 Score per residue for model 18

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

Chain A: 43% 42% 8% 7%

M90 G91 E94 E95 E96 L97 L100 M103 F104 D105 K106 N107 A108 D109 G110 Y111 I112 D113 L114 L117 K118 I119 M120 L121 Q122 A123 T124 G125 E126 T127 E130 D131 E135 L136 M137 K138 D141 K142 N143 N144 I148 L154 K158 G159 V160 E161

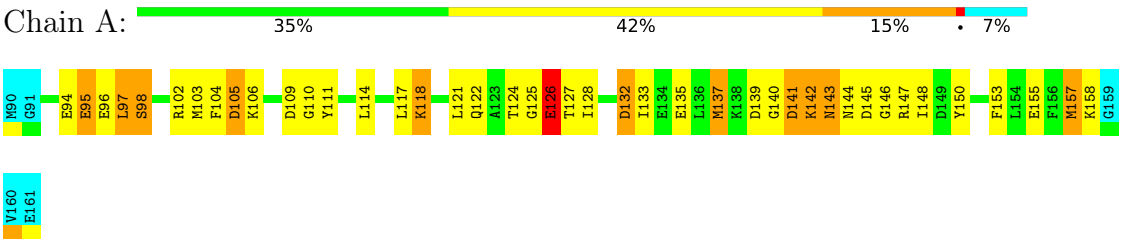
4.2.19 Score per residue for model 19

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

Chain A: 38% 43% 12% 7%

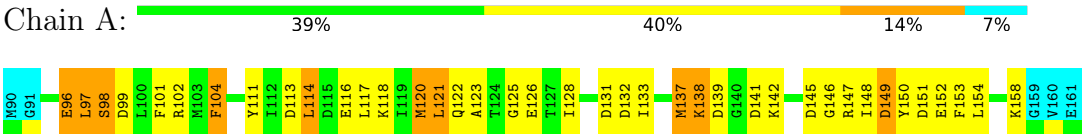
4.2.20 Score per residue for model 20

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



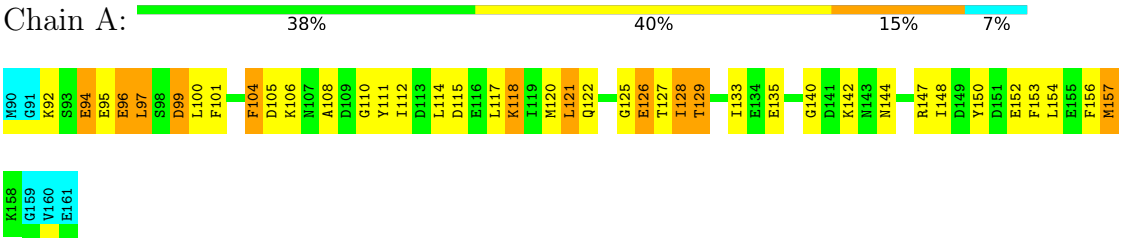
4.2.21 Score per residue for model 21

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



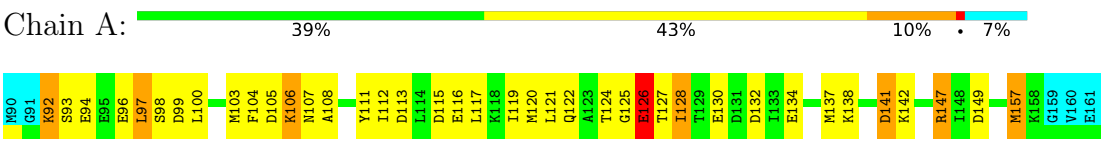
4.2.22 Score per residue for model 22

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



4.2.23 Score per residue for model 23

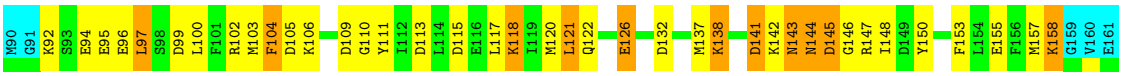
• Molecule 1: Troponin C, slow skeletal and cardiac muscles



4.2.24 Score per residue for model 24

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

Chain A: 39% 39% 15% 7%



4.2.25 Score per residue for model 25

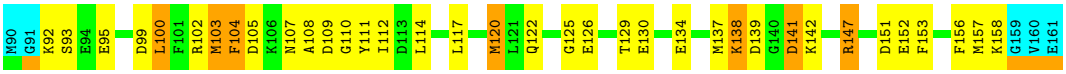
- Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A: 32% 46% 14% • 7%

4.2.26 Score per residue for model 26

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

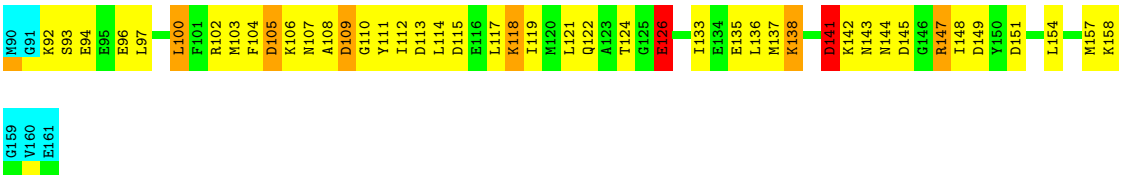
Chain A: 43% 40% 10% 7%



4.2.27 Score per residue for model 27

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

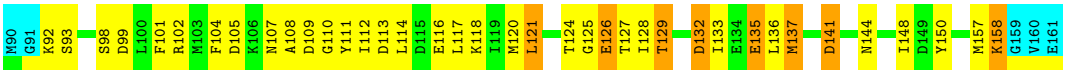
Chain A: 32% 50% 8% • 7%



4.2.28 Score per residue for model 28

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

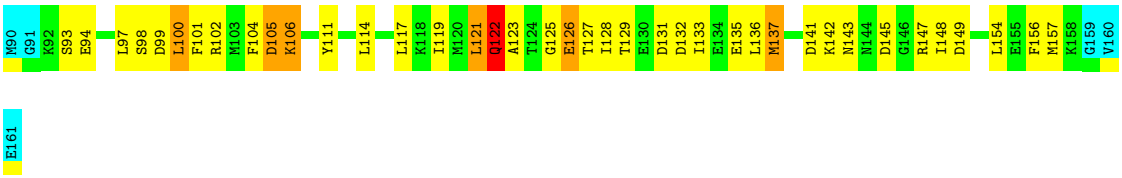
Chain A: 40% 42% 11% 7%



4.2.29 Score per residue for model 29

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

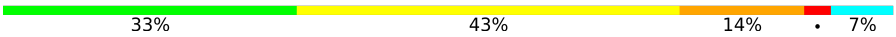
Chain A:

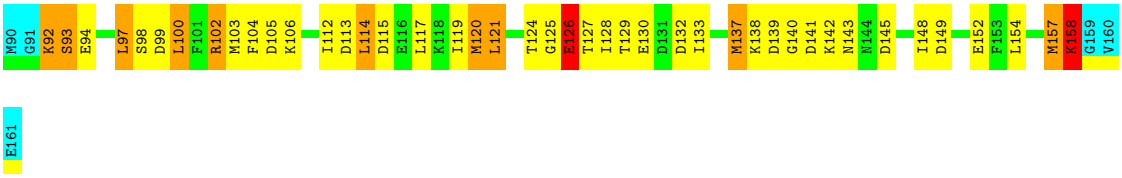


4.2.30 Score per residue for model 30

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

Chain A:





5 Refinement protocol and experimental data overview (i)

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	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (i)

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:N	1:A:128:ILE:HD13	0.71	2.00	23	1
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:137:MET:HE1	1:A:148:ILE:HD11	0.67	1.67	6	2
1:A:120:MET:SD	1:A:121:LEU:HD12	0.67	2.29	17	3
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	2
1:A:128:ILE:HD12	1:A:132:ASP:HB3	0.65	1.68	9	4
1:A:114:LEU:HD21	1:A:137:MET:HG2	0.65	1.68	25	3
1:A:97:LEU:HD23	1:A:100:LEU:HD12	0.65	1.67	18	1
1:A:127:THR:HG23	1:A:127:THR:O	0.65	1.91	11	6
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
1:A:104:PHE:CD2	1:A:112:ILE:HD13	0.63	2.28	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:LYS:CB	1:A:119:ILE:HG21	0.63	2.23	16	1
1:A:104:PHE:CB	1:A:112:ILE:HD11	0.63	2.24	26	1
1:A:114:LEU:HD21	1:A:137:MET:SD	0.63	2.34	30	3
1:A:111:TYR:N	1:A:111:TYR:CD1	0.62	2.67	3	9
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:118:LYS:HB2	1:A:133:ILE:HG21	0.60	1.74	8	1
1:A:104:PHE:CG	1:A:120:MET:HE2	0.60	2.31	21	1
3:A:1:KDH:C39	3:A:1:KDH:H12	0.59	2.26	25	1
1:A:128:ILE:HD13	1:A:128:ILE:H	0.59	1.54	23	1
1:A:104:PHE:CD1	1:A:120:MET:HE3	0.59	2.33	13	1
1:A:106:LYS:NZ	1:A:119:ILE:HG21	0.59	2.12	8	1
3:A:1:KDH:C12	3:A:1:KDH:H41	0.59	2.28	20	1
3:A:1:KDH:H39	3:A:1:KDH:C12	0.58	2.27	10	3
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:C	1:A:128:ILE:HD12	0.58	2.18	20	1
1:A:104:PHE:CE2	3:A:1:KDH:H01A	0.57	2.34	28	1
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:H39	3:A:1:KDH:C4	0.56	2.31	18	2
1:A:126:GLU:O	1:A:126:GLU:CG	0.56	2.53	18	20
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:H39	3:A:1:KDH:H33	0.55	1.79	4	1
1:A:100:LEU:HD11	1:A:153:PHE:CZ	0.55	2.34	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:128:ILE:HD13	1:A:128:ILE:N	0.54	2.17	15	2
1:A:137:MET:HE1	1:A:148:ILE:CG1	0.54	2.32	3	1
1:A:104:PHE:CD2	1:A:153:PHE:CE1	0.54	2.95	10	1
1:A:114:LEU:HD21	1:A:137:MET:CG	0.54	2.32	15	4
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: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:C3	3:A:1:KDH:H41	0.54	2.32	12	1
1:A:100:LEU:HG	1:A:104:PHE:CE2	0.54	2.38	6	3
1:A:112:ILE:CG2	1:A:117:LEU:HD21	0.54	2.33	30	2
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:100:LEU:HD21	1:A:104:PHE:CZ	0.53	2.39	12	1
1:A:112:ILE:CG2	1:A:117:LEU:CD2	0.53	2.86	30	2
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:97:LEU:HD12	1:A:154:LEU:HD13	0.53	1.79	29	1
1:A:119:ILE:HG23	1:A:122:GLN:OE1	0.53	2.04	29	1
1:A:100:LEU:HD23	1:A:153:PHE:CE2	0.52	2.40	3	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: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
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:101:PHE:O	1:A:101:PHE:CD1	0.52	2.63	21	2
1:A:104:PHE:O	1:A:106:LYS:N	0.52	2.42	3	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:145:ASP:OD1	1:A:145:ASP:N	0.51	2.44	16	2
1:A:113:ASP:OD1	1:A:116:GLU:CG	0.51	2.58	14	1
1:A:120:MET:SD	1:A:121:LEU:CD1	0.51	2.99	30	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:HD12	1:A:128:ILE:O	0.51	2.06	20	1
1:A:104:PHE:CE2	1:A:153:PHE:CZ	0.51	2.98	10	2
1:A:117:LEU:HD11	1:A:137:MET:SD	0.51	2.46	1	2
1:A:112:ILE:HG22	1:A:117:LEU:HG	0.51	1.83	27	4
1:A:97:LEU:HD22	1:A:157:MET:HG3	0.51	1.82	16	1
1:A:153:PHE:CZ	1:A:157:MET:SD	0.51	3.04	22	2
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:151:ASP:OD1	1:A:152:GLU:N	0.51	2.44	26	1
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	3
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:121:LEU:CG	3:A:1:KDH:H41	0.50	2.37	25	2
1:A:113:ASP:OD1	1:A:116:GLU:N	0.50	2.44	28	1
1:A:93:SER:OG	1:A:94:GLU:N	0.50	2.44	19	2
1:A:111:TYR:CD1	1:A:111:TYR:N	0.50	2.79	28	3
1:A:100:LEU:O	1:A:104:PHE:CD1	0.50	2.65	27	1
1:A:150:TYR:C	1:A:150:TYR:CD1	0.50	2.84	3	4
1:A:144:ASN:O	1:A:146:GLY:N	0.50	2.43	24	4
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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	19	2
1:A:110:GLY:C	1:A:111:TYR:CD2	0.49	2.86	22	5
1:A:104:PHE:CE2	1:A:120:MET:CE	0.49	2.96	4	2
1:A:128:ILE:CG1	1:A:132:ASP:HB2	0.49	2.38	7	1
1:A:100:LEU:HG	1:A:104:PHE:CZ	0.49	2.42	29	1
1:A:100:LEU:HD23	1:A:104:PHE:CZ	0.49	2.42	30	1
1:A:114:LEU:HD23	1:A:137:MET:CB	0.49	2.37	10	1
1:A:128:ILE:CG1	1:A:129:THR:N	0.49	2.75	12	1
1:A:95:GLU:OE1	1:A:95:GLU:CA	0.49	2.60	20	1
1:A:104:PHE:CE1	1:A:120:MET:HG2	0.49	2.42	26	1
3:A:1:KDH:H41	3:A:1:KDH:C4	0.49	2.38	12	1
1:A:125:GLY:O	1:A:126:GLU:C	0.49	2.51	29	7
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:149:ASP:OD2	1:A:151:ASP:CB	0.48	2.61	11	1
1:A:104:PHE:CG	1:A:112:ILE:CD1	0.48	2.96	26	1
1:A:128:ILE:CG1	1:A:132:ASP:HB3	0.48	2.39	28	1
1:A:104:PHE:CD1	1:A:120:MET:SD	0.48	3.06	30	1
1:A:104:PHE:CZ	3:A:1:KDH:O03	0.48	2.67	19	3
1:A:114:LEU:CD1	1:A:137:MET:SD	0.48	2.99	7	1
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
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:N	1:A:154:LEU:CD2	0.48	2.76	27	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:ASP:N	1:A:109:ASP:OD1	0.48	2.46	28	4
1:A:149:ASP:N	1:A:149:ASP:OD1	0.47	2.45	2	3
1:A:153:PHE:CE2	1:A:157:MET:HG3	0.47	2.43	10	2
1:A:126:GLU:O	1:A:126:GLU:OE1	0.47	2.32	28	3
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: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:157:MET:C	1:A:158:LYS:CG	0.47	2.82	30	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: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:112:ILE:CG2	1:A:117:LEU:HG	0.47	2.39	16	5
1:A:101:PHE:C	1:A:101:PHE:CD1	0.47	2.88	3	2
1:A:104:PHE:CG	1:A:120:MET:HG3	0.47	2.45	7	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:104:PHE:O	1:A:105:ASP:C	0.47	2.53	23	2
1:A:105:ASP:OD2	1:A:108:ALA:CA	0.47	2.63	6	1
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:145:ASP:OD1	1:A:147:ARG:O	0.47	2.33	11	4
1:A:101:PHE:HB2	1:A:153:PHE:CE2	0.47	2.45	15	1
1:A:100:LEU:HB3	1:A:104:PHE:CE2	0.47	2.45	25	2
1:A:141:ASP:OD1	1:A:145:ASP:OD1	0.47	2.33	2	2
1:A:98:SER:CB	1:A:150:TYR:OH	0.47	2.63	6	1
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:141:ASP:OD2	1:A:147:ARG:O	0.47	2.33	2	7
1:A:149:ASP:OD1	1:A:152:GLU:CG	0.47	2.63	4	1
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:H41	3:A:1:KDH:C9	0.47	2.40	8	1
1:A:111:TYR:CE1	1:A:149:ASP:OD1	0.47	2.68	29	1
1:A:122:GLN:N	1:A:126:GLU:HG2	0.46	2.25	18	6
1:A:137:MET:CE	1:A:141:ASP:OD2	0.46	2.63	4	1
1:A:117:LEU:CD1	1:A:137:MET:CG	0.46	2.93	10	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:146:GLY:O	1:A:147:ARG:NH1	0.46	2.48	12	1
1:A:143:ASN:O	1:A:143:ASN:OD1	0.46	2.33	16	1
1:A:150:TYR:O	1:A:150:TYR:CD1	0.46	2.68	17	1
1:A:92:LYS:NZ	1:A:92:LYS:CB	0.46	2.78	23	1
1:A:107:ASN:O	1:A:108:ALA:O	0.46	2.33	10	3
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: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:N	1:A:145:ASP:OD1	0.46	2.49	4	3
1:A:137:MET:HE1	1:A:148:ILE:CD1	0.46	2.37	6	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:92:LYS:O	1:A:93:SER:O	0.46	2.34	15	1
1:A:154:LEU:N	1:A:154:LEU:HD22	0.46	2.26	27	1
1:A:104:PHE:CZ	1:A:120:MET:HE1	0.46	2.46	4	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:99:ASP:OD1	1:A:100:LEU:N	0.46	2.48	26	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:126:GLU:O	1:A:126:GLU:OE2	0.46	2.34	17	1
1:A:132:ASP:O	1:A:135:GLU:CB	0.46	2.64	1	1
1:A:141:ASP:OD2	1:A:144:ASN:O	0.46	2.34	12	3
1:A:107:ASN:ND2	1:A:109:ASP:OD1	0.46	2.49	7	1
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: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
1:A:149:ASP:OD2	1:A:152:GLU:OE1	0.45	2.34	30	1
1:A:101:PHE:CZ	1:A:112:ILE:HG13	0.45	2.46	3	1
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:145:ASP:O	1:A:145:ASP:CG	0.45	2.54	12	1
1:A:142:LYS:O	1:A:144:ASN:OD1	0.45	2.35	2	1
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: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:141:ASP:OD1	1:A:152:GLU:OE2	0.45	2.35	16	1
1:A:93:SER:O	1:A:94:GLU:C	0.45	2.55	13	5
1:A:107:ASN:HB2	1:A:116:GLU:OE2	0.45	2.11	12	2
1:A:113:ASP:CB	1:A:116:GLU:OE1	0.45	2.65	19	1
1:A:131:ASP:OD1	1:A:131:ASP:O	0.45	2.34	11	1
1:A:130:GLU:HG3	1:A:131:ASP:N	0.45	2.27	25	2
1:A:153:PHE:O	1:A:157:MET:SD	0.45	2.75	12	1
1:A:119:ILE:O	1:A:122:GLN:HG2	0.45	2.12	18	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:143:ASN:CG	0.44	2.56	14	2
1:A:143:ASN:O	1:A:144:ASN:CG	0.44	2.56	16	1
1:A:105:ASP:OD2	1:A:109:ASP:OD1	0.44	2.35	1	2
1:A:153:PHE:O	1:A:156:PHE:HB3	0.44	2.12	2	4
1:A:137:MET:O	1:A:138:LYS:C	0.44	2.56	21	4
1:A:105:ASP:OD1	1:A:109:ASP:OD1	0.44	2.35	14	1
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
1:A:109:ASP:OD1	1:A:109:ASP:N	0.44	2.50	24	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
3:A:1:KDH:H39	3:A:1:KDH:C9	0.44	2.43	17	2
1:A:120:MET:SD	1:A:120:MET:O	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	6	2
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
1:A:145:ASP:O	1:A:145:ASP:OD1	0.44	2.36	17	1
1:A:107:ASN:OD1	1:A:107:ASN:O	0.43	2.36	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:TYR:O	1:A:151:ASP:C	0.43	2.56	19	3
1:A:104:PHE:CE1	1:A:120:MET:HE1	0.43	2.49	4	1
1:A:136:LEU:O	1:A:137:MET:C	0.43	2.57	27	2
1:A:105:ASP:O	1:A:106:LYS:C	0.43	2.57	23	3
1:A:94:GLU:HG3	1:A:154:LEU:HD21	0.43	1.90	16	1
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:120:MET:HG3	1:A:121:LEU:N	0.43	2.29	2	3
1:A:121:LEU:HD21	3:A:1:KDH:O37	0.43	2.14	5	3
1:A:126:GLU:O	1:A:126:GLU:CD	0.43	2.57	5	10
1:A:107:ASN:C	1:A:109:ASP:OD1	0.43	2.57	7	1
1:A:122:GLN:O	1:A:123:ALA:C	0.43	2.57	14	4
1:A:114:LEU:HA	1:A:117:LEU:CD1	0.43	2.41	13	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:102:ARG:CG	1:A:103:MET:N	0.43	2.81	26	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:140:GLY:HA2	1:A:156:PHE:CA	0.43	2.43	6	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:137:MET:SD	1:A:148:ILE:CD1	0.43	2.99	1	1
1:A:122:GLN:O	1:A:124:THR:N	0.43	2.51	14	2
1:A:153:PHE:O	1:A:156:PHE:N	0.43	2.52	9	1
1:A:113:ASP:OD1	1:A:113:ASP:C	0.43	2.57	28	1
1:A:120:MET:SD	1:A:121:LEU:CD2	0.43	3.07	6	2
1:A:94:GLU:OE2	1:A:154:LEU:CD1	0.43	2.67	8	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: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: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:97:LEU:O	1:A:98:SER:C	0.43	2.57	3	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:128:ILE:CD1	1:A:133:ILE:HD13	0.43	2.44	21	1
1:A:105:ASP:OD2	1:A:109:ASP:CG	0.42	2.57	5	1
1:A:97:LEU:HA	1:A:100:LEU:HD21	0.42	1.91	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:ASP:O	1:A:102:ARG:HG3	0.42	2.14	7	2
1:A:98:SER:OG	1:A:99:ASP:N	0.42	2.52	8	2
1:A:133:ILE:O	1:A:134:GLU:C	0.42	2.57	8	1
1:A:129:THR:HG22	1:A:132:ASP:OD2	0.42	2.14	17	1
1:A:145:ASP:OD2	1:A:147:ARG:HG3	0.42	2.14	21	1
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:OD1	1:A:109:ASP:C	0.42	2.56	18	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:137:MET:HE2	1:A:148:ILE:HG13	0.42	1.90	17	2
1:A:137:MET:O	1:A:139:ASP:N	0.42	2.52	21	1
1:A:137:MET:CE	1:A:148:ILE:CG1	0.42	2.98	6	1
1:A:128:ILE:CG1	1:A:132:ASP:CB	0.42	2.97	7	1
1:A:144:ASN:ND2	1:A:144:ASN:O	0.42	2.52	10	1
1:A:122:GLN:N	1:A:126:GLU:HB3	0.42	2.29	14	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: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:104:PHE:CG	1:A:112:ILE:HD13	0.42	2.50	5	1
1:A:101:PHE:CD1	1:A:101:PHE:C	0.42	2.92	29	3
1:A:121:LEU:CB	1:A:126:GLU:HG2	0.42	2.44	12	1
1:A:143:ASN:O	1:A:144:ASN:HB3	0.42	2.15	20	3
1:A:107:ASN:O	1:A:108:ALA:C	0.42	2.58	19	1
1:A:94:GLU:O	1:A:95:GLU:C	0.42	2.57	20	2
1:A:101:PHE:O	1:A:102:ARG:C	0.42	2.57	28	1
1:A:157:MET:O	1:A:158:LYS:HG3	0.42	2.15	30	1
1:A:93:SER:O	1:A:97:LEU:HG	0.42	2.15	6	1
1:A:105:ASP:OD2	1:A:108:ALA:N	0.42	2.53	6	1
1:A:120:MET:CG	1:A:121:LEU:N	0.42	2.82	19	2
1:A:115:ASP:N	1:A:115:ASP:OD1	0.42	2.50	27	1
1:A:135:GLU:O	1:A:138:LYS:HD3	0.42	2.13	27	1
1:A:135:GLU:O	1:A:136:LEU:C	0.42	2.58	28	1
1:A:126:GLU:O	1:A:126:GLU:HG3	0.42	2.15	18	6
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:99:ASP:O	1:A:102:ARG:HG2	0.42	2.15	26	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:ASN:HB3	1:A:116:GLU:OE2	0.42	2.14	10	1
1:A:121:LEU:CD1	1:A:124:THR:HG21	0.42	2.45	12	1
1:A:138:LYS:CG	1:A:139:ASP:N	0.42	2.82	25	1
1:A:149:ASP:OD1	1:A:149:ASP:C	0.41	2.59	17	2
1:A:144:ASN:O	1:A:145:ASP:HB3	0.41	2.15	12	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:153:PHE:O	1:A:154:LEU:C	0.41	2.58	9	2
1:A:117:LEU:O	1:A:118:LYS:C	0.41	2.58	19	1
1:A:150:TYR:CD1	1:A:150:TYR:O	0.41	2.73	20	1
1:A:113:ASP:N	1:A:116:GLU:OE1	0.41	2.50	21	1
1:A:130:GLU:HG3	1:A:134:GLU:OE2	0.41	2.15	23	1
1:A:124:THR:O	1:A:124:THR:CG2	0.41	2.68	27	1
1:A:128:ILE:HG12	1:A:132:ASP:HB2	0.41	1.92	7	1
1:A:114:LEU:CG	1:A:137:MET:HG3	0.41	2.46	18	1
1:A:96:GLU:O	1:A:100:LEU:HB2	0.41	2.15	23	1
1:A:129:THR:O	1:A:130:GLU:C	0.41	2.59	26	1
1:A:112:ILE:CG2	1:A:117:LEU:CG	0.41	2.98	30	1
1:A:111:TYR:HB3	1:A:147:ARG:CG	0.41	2.46	3	1
1:A:97:LEU:HA	1:A:100:LEU:CD2	0.41	2.45	7	1
1:A:134:GLU:O	1:A:135:GLU:C	0.41	2.58	8	1
1:A:106:LYS:CG	1:A:119:ILE:HG21	0.41	2.46	16	1
1:A:112:ILE:HG22	1:A:148:ILE:HD12	0.41	1.91	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:97:LEU:O	1:A:100:LEU:N	0.41	2.52	27	1
1:A:107:ASN:HB3	1:A:116:GLU:OE1	0.41	2.16	28	2
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
1:A:143:ASN:HB2	1:A:145:ASP:OD2	0.41	2.14	9	1
3:A:1:KDH:H39	3:A:1:KDH:C6	0.41	2.46	17	1
1:A:147:ARG:NH1	1:A:147:ARG:HG2	0.41	2.31	23	1
1:A:99:ASP:O	1:A:102:ARG:HB3	0.41	2.16	2	1
1:A:157:MET:HG2	1:A:158:LYS:N	0.41	2.31	28	2
1:A:127:THR:O	1:A:127:THR:CG2	0.41	2.63	11	1
1:A:113:ASP:HB2	1:A:116:GLU:OE2	0.41	2.16	5	1
1:A:118:LYS:O	1:A:126:GLU:HG3	0.41	2.16	11	1
3:A:1:KDH:H39	3:A:1:KDH:C14	0.41	2.45	17	1
1:A:121:LEU:CD1	3:A:1:KDH:H39	0.41	2.45	21	1
1:A:141:ASP:CG	1:A:147:ARG:O	0.41	2.59	26	1
1:A:114:LEU:HG	1:A:137:MET:SD	0.41	2.56	30	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:125:GLY:O	1:A:126:GLU:HB2	0.41	2.15	16	1
1:A:149:ASP:OD1	1:A:152:GLU:OE1	0.41	2.39	21	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:108:ALA:O	1:A:109:ASP:HB3	0.41	2.16	8	2
1:A:104:PHE:CD1	1:A:112:ILE:CD1	0.41	3.04	13	1
1:A:98:SER:HB2	1:A:150:TYR:CE1	0.41	2.51	14	1
1:A:102:ARG:NH1	1:A:102:ARG:HG3	0.41	2.31	16	1
1:A:112:ILE:O	1:A:148:ILE:HG13	0.41	2.15	16	1
1:A:150:TYR:O	1:A:153:PHE:HB3	0.41	2.16	21	2
1:A:116:GLU:O	1:A:120:MET:N	0.41	2.53	23	1
1:A:113:ASP:O	1:A:117:LEU:HG	0.41	2.16	6	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:100:LEU:HD23	1:A:104:PHE:HD1	0.40	1.76	4	1
1:A:114:LEU:CA	1:A:117:LEU:HD12	0.40	2.41	13	1
1:A:126:GLU:CG	1:A:126:GLU:O	0.40	2.69	19	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: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
1:A:105:ASP:O	1:A:107:ASN:N	0.40	2.55	13	1
1:A:136:LEU:CD2	3:A:1:KDH:O37	0.40	2.69	6	1
1:A:101:PHE:CE2	1:A:112:ILE:HD11	0.40	2.51	12	1
1:A:149:ASP:OD1	1:A:149:ASP:N	0.40	2.55	27	1
1:A:113:ASP:OD1	1:A:116:GLU:HB2	0.40	2.16	28	1
1:A:107:ASN:O	1:A:107:ASN:OD1	0.40	2.38	5	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:99:ASP:O	1:A:102:ARG:HB2	0.40	2.16	12	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%)	6 36
All	All	2010/2160 (93%)	1657 (82%)	284 (14%)	69 (3%)	6 36

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	93	SER	5
1	A	158	LYS	5
1	A	92	LYS	5
1	A	141	ASP	2
1	A	129	THR	2
1	A	133	ILE	1
1	A	149	ASP	1
1	A	122	GLN	1

6.3.2 Protein sidechains (i)

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 22
All	All	1830/1920 (95%)	1346 (74%)	484 (26%)	2 22

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

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Mol	Chain	Res	Type	Models (Total)
1	A	103	MET	19
1	A	137	MET	18
1	A	106	LYS	17
1	A	122	GLN	16
1	A	132	ASP	16
1	A	92	LYS	15
1	A	97	LEU	15
1	A	118	LYS	14
1	A	138	LYS	14
1	A	121	LEU	14
1	A	96	GLU	13
1	A	129	THR	12
1	A	98	SER	12
1	A	135	GLU	10
1	A	141	ASP	10
1	A	147	ARG	10
1	A	120	MET	10
1	A	100	LEU	10
1	A	102	ARG	10
1	A	115	ASP	10
1	A	94	GLU	9
1	A	114	LEU	9
1	A	139	ASP	9
1	A	99	ASP	9
1	A	157	MET	9
1	A	104	PHE	9
1	A	151	ASP	8
1	A	113	ASP	8
1	A	131	ASP	7
1	A	93	SER	7
1	A	155	GLU	6
1	A	127	THR	6
1	A	145	ASP	6
1	A	154	LEU	6
1	A	95	GLU	6
1	A	144	ASN	5
1	A	150	TYR	5
1	A	136	LEU	4
1	A	128	ILE	4
1	A	130	GLU	4
1	A	143	ASN	4
1	A	124	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	134	GLU	3
1	A	105	ASP	2
1	A	149	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 monosaccharides 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	3.25±0.01	23±0 (63±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	1.07±0.01	4±0 (7±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. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	1	KDH	C14-C15	6.33	1.40	1.51	5	30
3	A	1	KDH	C01-C31	4.88	1.43	1.51	10	30
3	A	1	KDH	C20-C31	4.74	1.46	1.40	15	30
3	A	1	KDH	C49-C46	4.74	1.45	1.40	8	30
3	A	1	KDH	C4-C14	4.60	1.46	1.39	10	30
3	A	1	KDH	C26-C29	4.58	1.45	1.38	8	30
3	A	1	KDH	C9-C6	4.44	1.45	1.40	23	30
3	A	1	KDH	C38-C36	4.43	1.39	1.50	3	30
3	A	1	KDH	C39-C38	4.42	1.46	1.39	28	30
3	A	1	KDH	C12-C9	4.30	1.45	1.38	7	30
3	A	1	KDH	C4-C3	4.24	1.44	1.38	16	30
3	A	1	KDH	C43-C46	4.11	1.44	1.40	22	30
3	A	1	KDH	C12-C14	4.09	1.45	1.39	17	30
3	A	1	KDH	C39-C49	4.06	1.44	1.38	7	30
3	A	1	KDH	C41-C43	4.04	1.44	1.38	23	30
3	A	1	KDH	C41-C38	3.80	1.45	1.39	7	30
3	A	1	KDH	C3-C6	3.71	1.44	1.40	30	30
3	A	1	KDH	C26-C24	3.51	1.44	1.39	13	30
3	A	1	KDH	C21-C24	3.48	1.44	1.39	10	30
3	A	1	KDH	C21-C20	3.35	1.44	1.38	13	30
3	A	1	KDH	O01-C15	3.21	1.50	1.45	10	30
3	A	1	KDH	C01-C33	2.47	1.56	1.51	25	30
3	A	1	KDH	C29-C31	2.43	1.45	1.40	26	30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	1	KDH	O01-C15-C14	3.11	114.48	107.47	24	30
3	A	1	KDH	C20-O01-C15	2.58	121.99	116.38	10	30
3	A	1	KDH	C9-C6-C3	2.26	120.95	119.51	17	30
3	A	1	KDH	O35-C36-C38	2.23	115.52	111.92	28	8
3	A	1	KDH	O01-C20-C21	2.19	119.83	116.38	4	29

There are no chirality outliers.

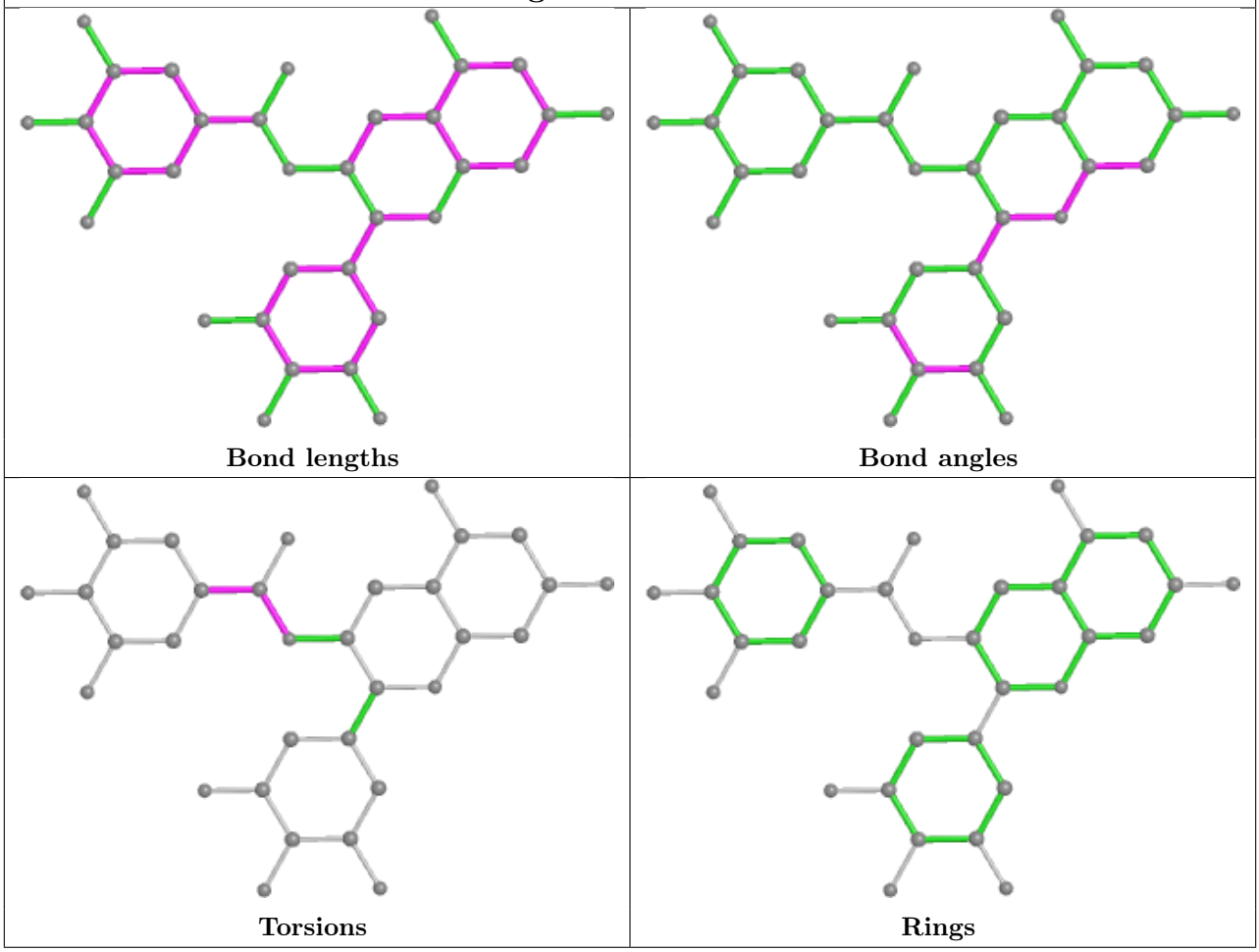
All unique torsion outliers are listed below.

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

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand KDH A 1



6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided