



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 06:33 AM UTC

PDB ID : 1IH0 / pdb_00001ih0
Title : Structure of the C-domain of Human Cardiac Troponin C in Complex with Ca²⁺ Sensitizer EMD 57033
Authors : Wang, X.; Li, M.X.; Spyropoulos, L.; Beier, N.; Chandra, M.; Solaro, R.J.; Sykes, B.D.
Deposited on : 2001-04-18

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

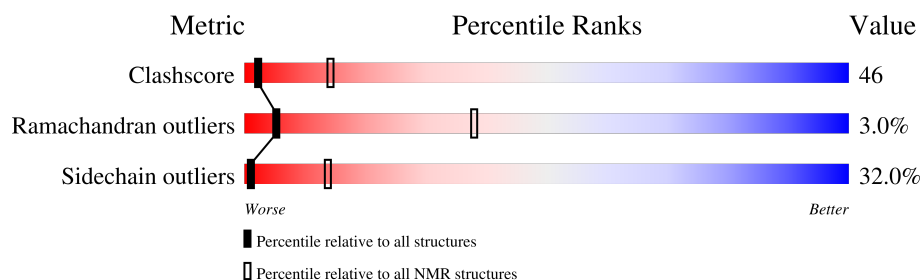
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

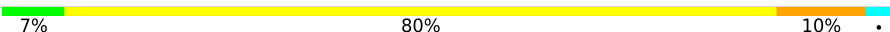
The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	71	

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:93-A:161 (69)	0.92	30

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 5 single-model clusters were found.

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

3 Entry composition [i](#)

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

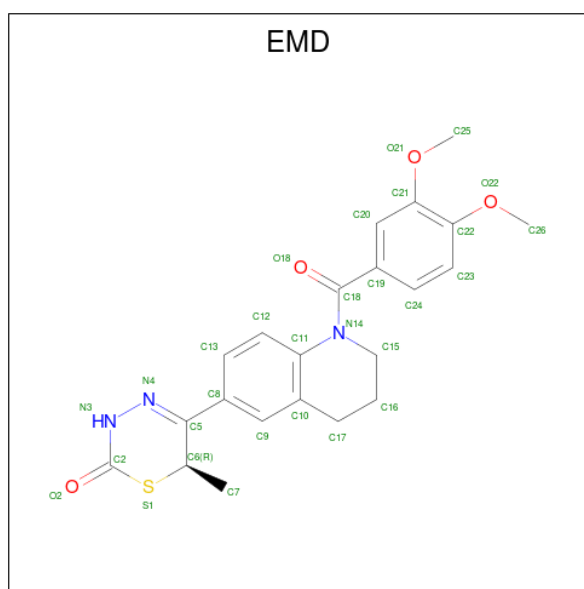
- Molecule 1 is a protein called TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES.

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

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

- Molecule 3 is 5-[1-(3,4-DIMETHOXY-BENZOYL)-1,2,3,4-TETRAHYDRO-QUINOLIN-6-YL]-6-METHYL-3,6-DIHYDRO-[1,3,4]THIADIAZIN-2-ONE (CCD ID: EMD) (formula: C₂₂H₂₃N₃O₄S).

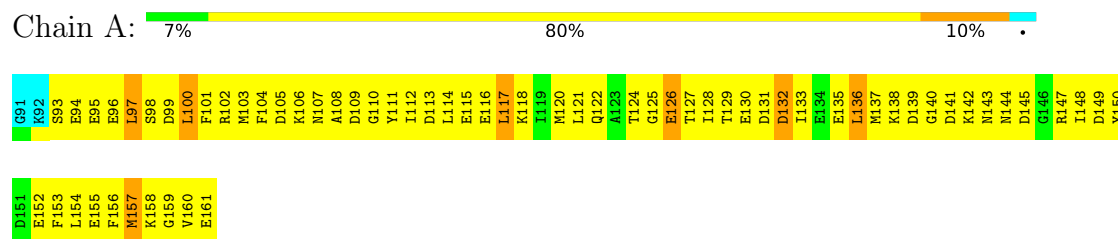


4 Residue-property plots

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

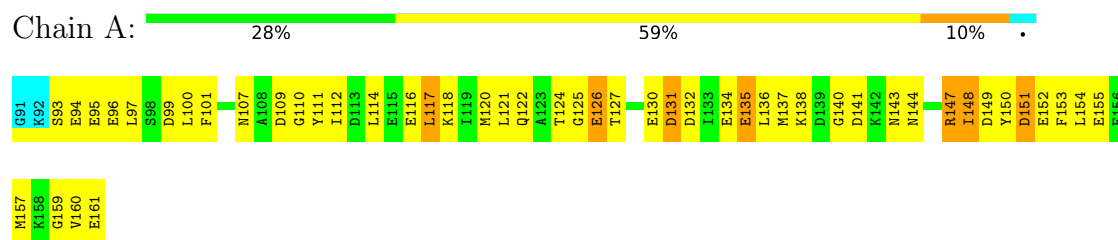


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

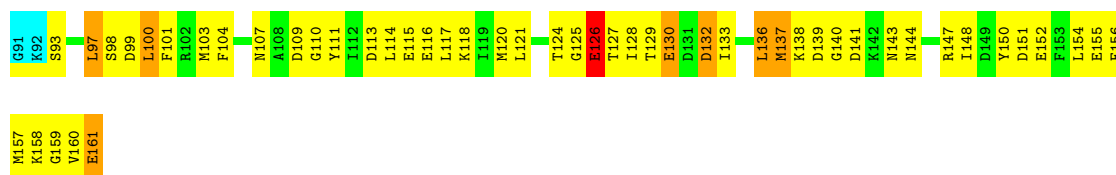
- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



4.2.2 Score per residue for model 2

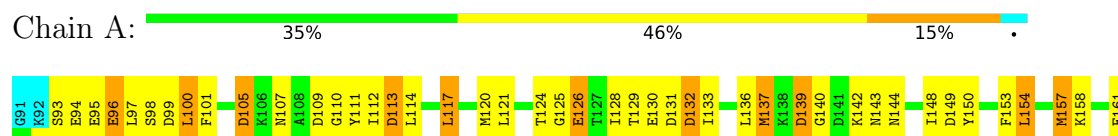
- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES





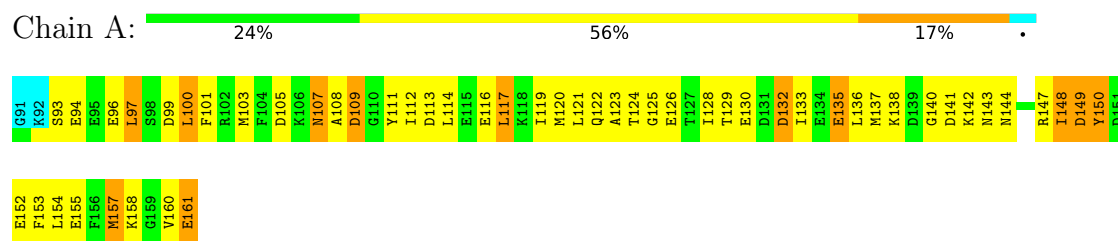
4.2.3 Score per residue for model 3

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



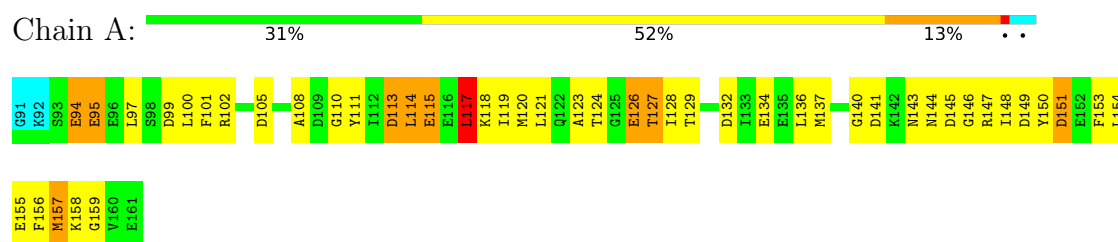
4.2.4 Score per residue for model 4

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



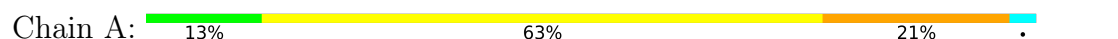
4.2.5 Score per residue for model 5

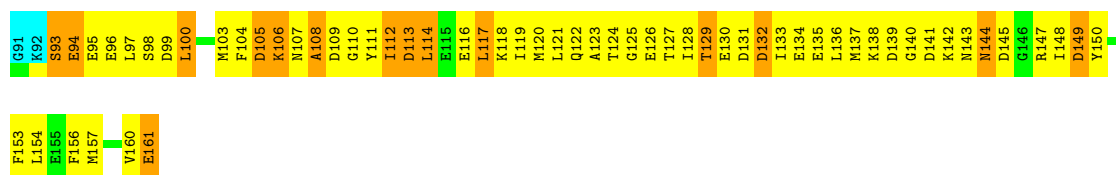
- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES



4.2.6 Score per residue for model 6

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

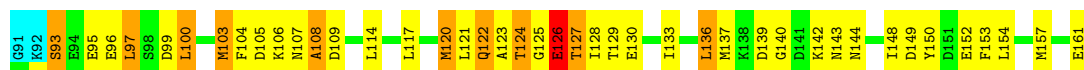




4.2.7 Score per residue for model 7

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

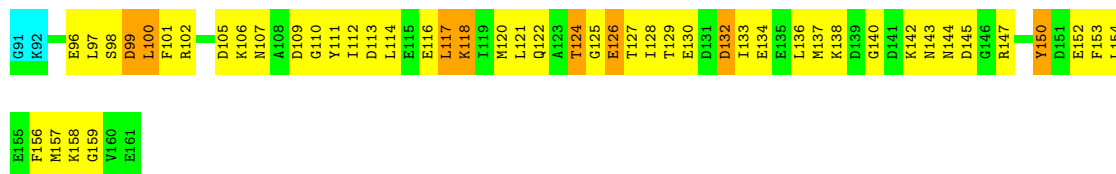
Chain A: 38% 44% 14% . .



4.2.8 Score per residue for model 8

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

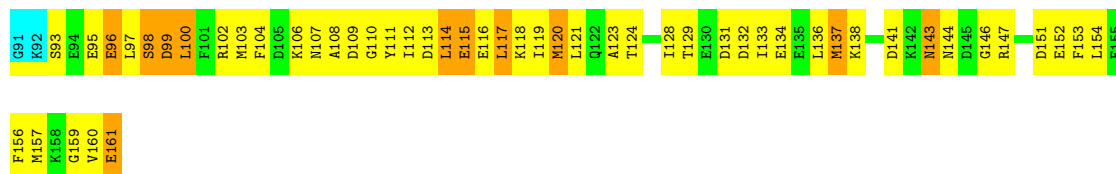
Chain A: 28% 58% 11% .



4.2.9 Score per residue for model 9

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

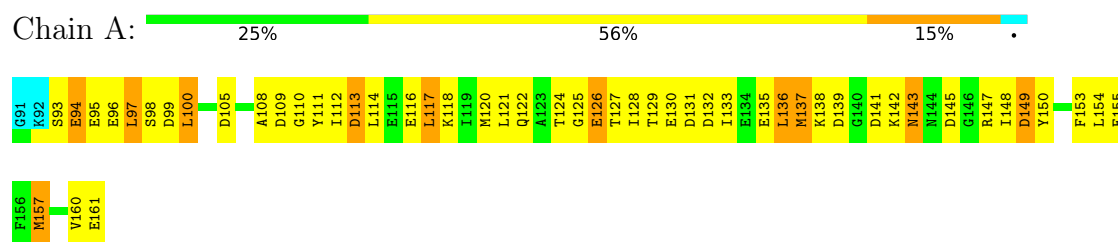
Chain A: 25% 56% 15% .



4.2.10 Score per residue for model 10

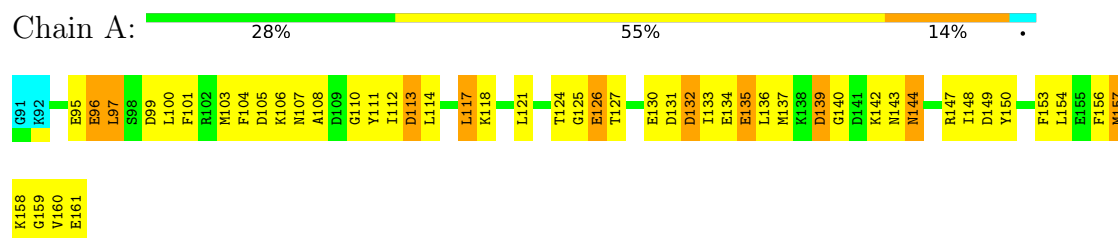
- Molecule 1: TROPONIN C, SLOW SKELETAL AND CARDIAC MUSCLES

Chain A: 35% 54% 8% .



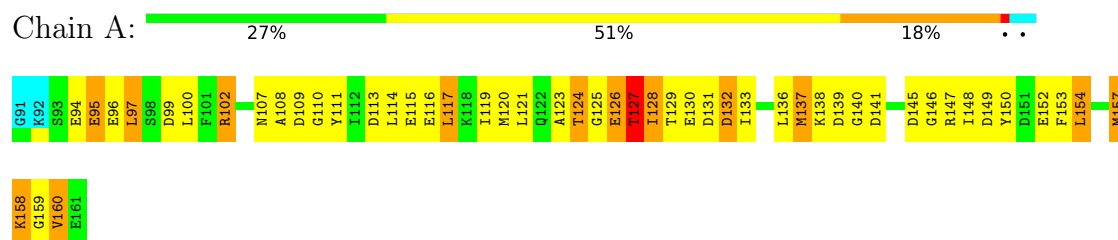
4.2.15 Score per residue for model 15

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



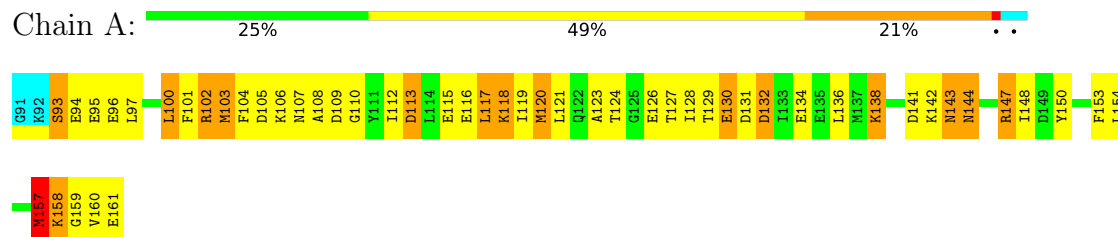
4.2.16 Score per residue for model 16

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



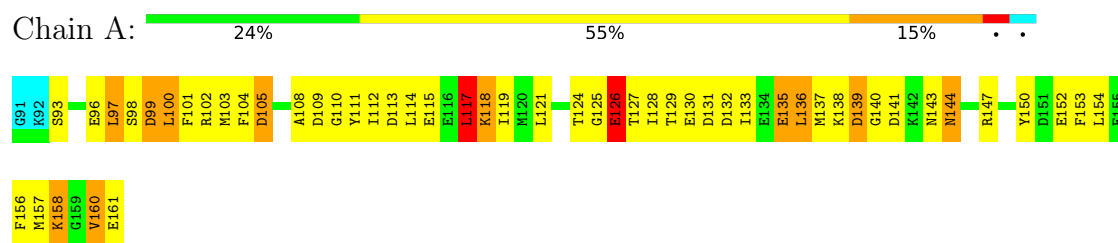
4.2.17 Score per residue for model 17

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



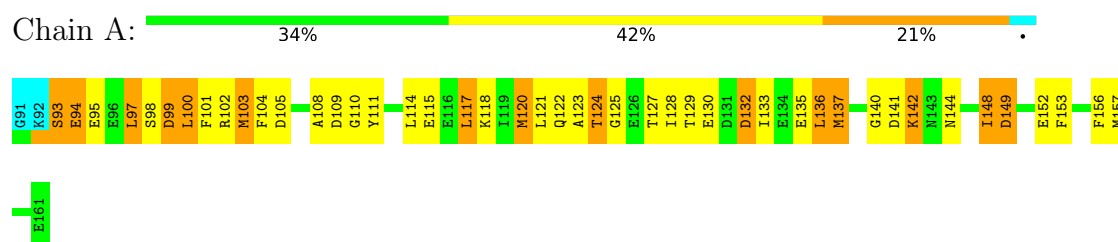
4.2.18 Score per residue for model 18

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



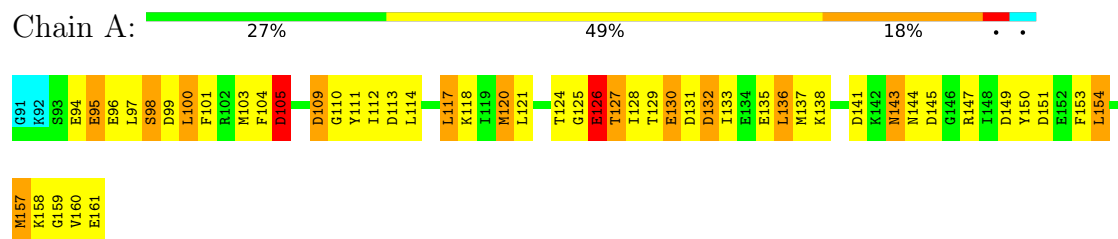
4.2.19 Score per residue for model 19

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



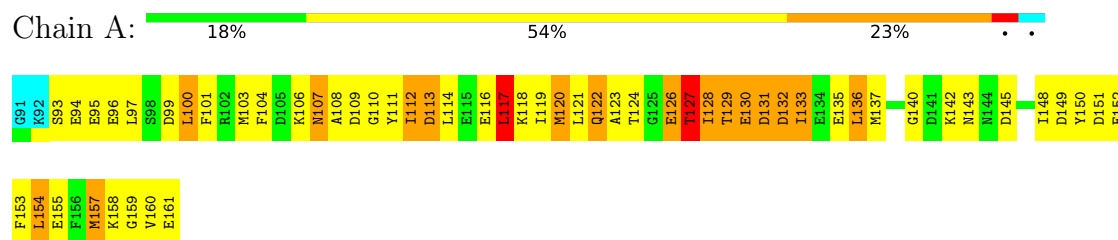
4.2.20 Score per residue for model 20

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



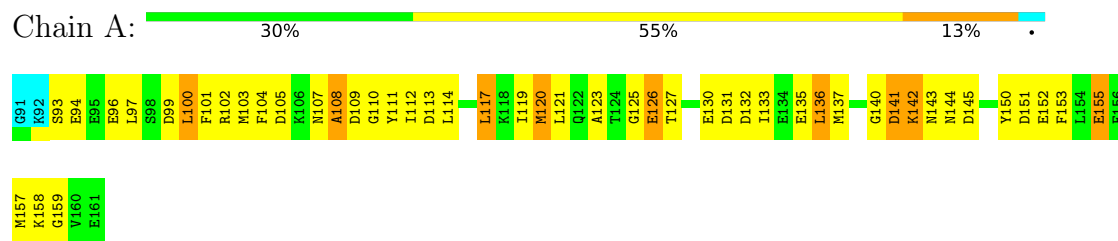
4.2.21 Score per residue for model 21

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



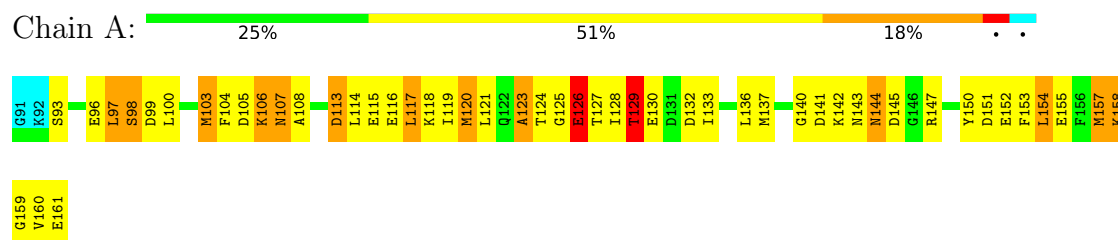
4.2.22 Score per residue for model 22

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



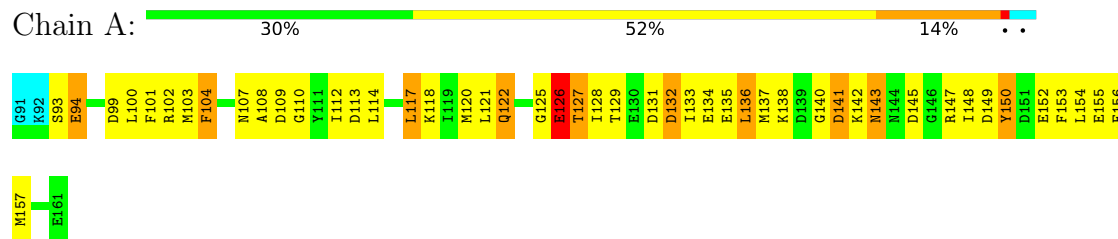
4.2.23 Score per residue for model 23

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



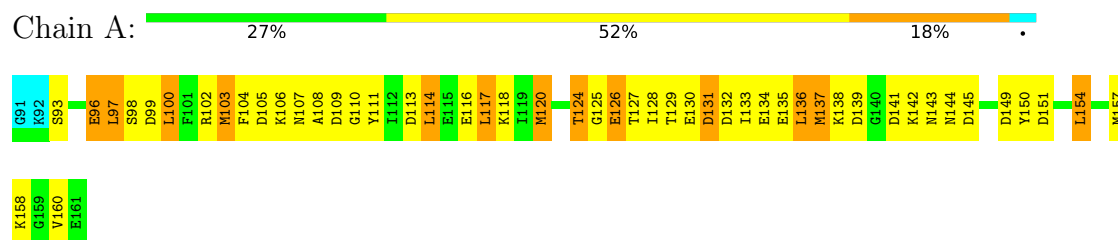
4.2.24 Score per residue for model 24

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



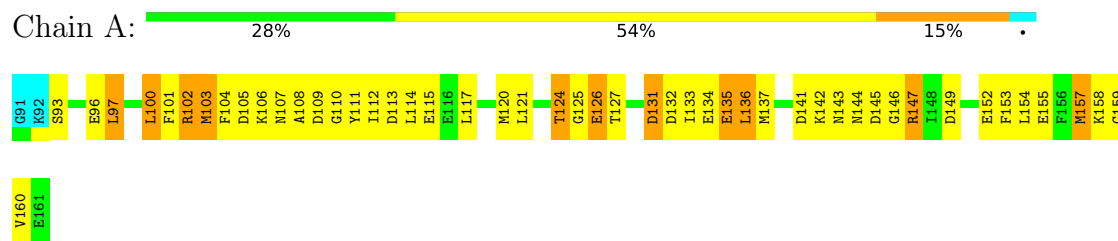
4.2.25 Score per residue for model 25

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



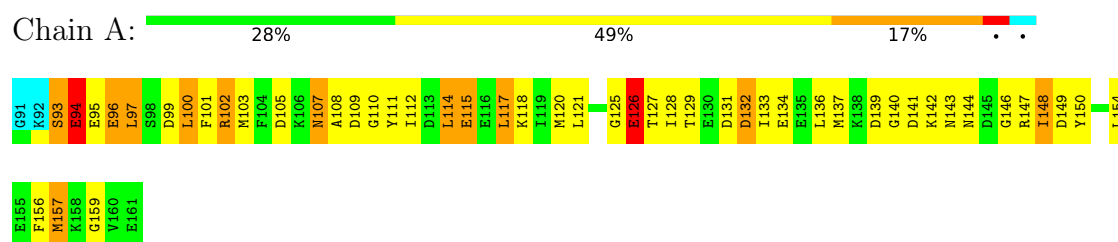
4.2.26 Score per residue for model 26

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



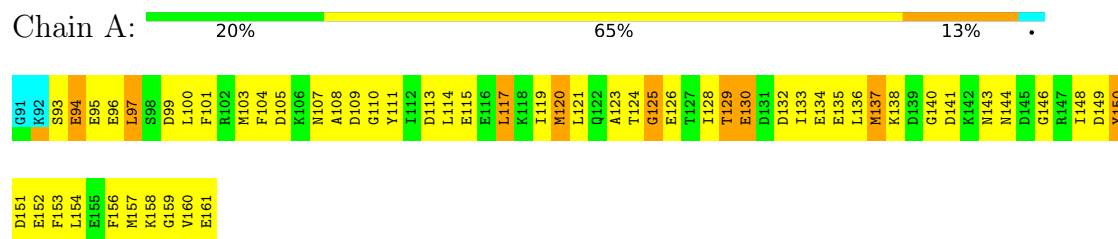
4.2.27 Score per residue for model 27

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



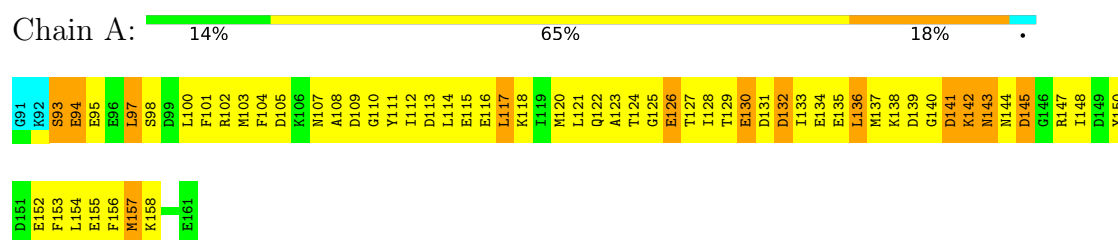
4.2.28 Score per residue for model 28

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



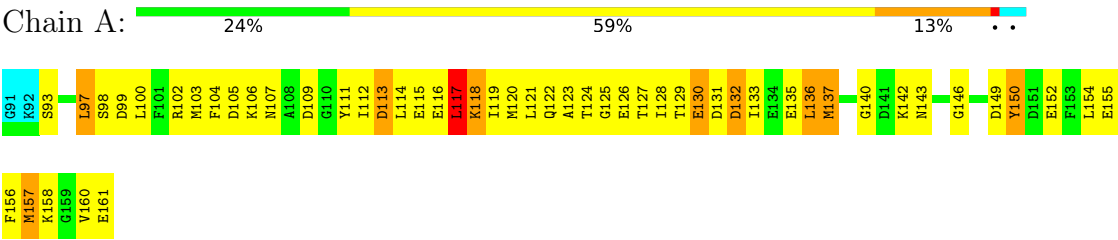
4.2.29 Score per residue for model 29

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



4.2.30 Score per residue for model 30 (medoid)

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



5 Refinement protocol and experimental data overview ⓘ

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

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

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

Software name	Classification	Version
X-PLOR	refinement	3.851

No chemical shift data was provided.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	563	520	520	50±10
3	A	30	23	23	8±4
All	All	17850	16290	16290	1561

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 46.

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

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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:LEU:HD13	1:A:157:MET:SD	0.88	2.09	17	2
1:A:117:LEU:CD2	1:A:136:LEU:HD22	0.86	2.00	6	3
1:A:136:LEU:HD21	3:A:1:EMD:C13	0.85	2.00	28	5
1:A:117:LEU:CD2	1:A:136:LEU:HD23	0.84	2.01	19	2
1:A:117:LEU:HD11	3:A:1:EMD:C7	0.83	2.02	6	6
1:A:127:THR:C	1:A:128:ILE:HD12	0.83	1.99	5	3
1:A:136:LEU:HD22	3:A:1:EMD:C13	0.83	2.04	26	11
1:A:136:LEU:HD11	3:A:1:EMD:C13	0.82	2.04	17	3
1:A:93:SER:C	1:A:97:LEU:HD23	0.82	2.00	28	2
1:A:114:LEU:CD1	1:A:133:ILE:HG22	0.82	2.04	20	1
1:A:97:LEU:CD1	1:A:154:LEU:HD23	0.81	2.06	6	1
1:A:104:PHE:CE2	3:A:1:EMD:H71	0.79	2.13	10	2
1:A:97:LEU:HD21	1:A:157:MET:O	0.78	1.78	7	15
1:A:121:LEU:HB3	1:A:128:ILE:HD13	0.77	1.55	24	2
1:A:136:LEU:HD21	3:A:1:EMD:C12	0.77	2.08	19	1
1:A:124:THR:HG21	3:A:1:EMD:C23	0.77	2.10	8	2
1:A:157:MET:HE1	3:A:1:EMD:H172	0.76	1.57	22	1
1:A:112:ILE:HD13	1:A:153:PHE:CE2	0.76	2.16	26	2
1:A:136:LEU:HD22	3:A:1:EMD:H13	0.75	1.56	26	6
1:A:117:LEU:HD21	1:A:136:LEU:HD22	0.75	1.59	23	2
1:A:128:ILE:HG22	1:A:129:THR:N	0.74	1.98	21	7
1:A:136:LEU:C	1:A:136:LEU:HD13	0.74	2.08	8	1
1:A:154:LEU:HD13	1:A:154:LEU:O	0.74	1.82	23	1
1:A:121:LEU:O	1:A:124:THR:HG22	0.73	1.83	5	8
1:A:136:LEU:HD23	1:A:136:LEU:O	0.73	1.82	16	7
1:A:137:MET:HG2	1:A:148:ILE:HD11	0.73	1.61	28	1
1:A:100:LEU:HD22	1:A:157:MET:CE	0.72	2.14	5	1
1:A:157:MET:HE1	3:A:1:EMD:C17	0.72	2.15	22	5
1:A:120:MET:O	1:A:124:THR:HG23	0.72	1.84	26	4
1:A:100:LEU:HD22	1:A:157:MET:HE3	0.72	1.62	7	3
1:A:160:VAL:HG12	1:A:160:VAL:O	0.71	1.86	6	2
1:A:121:LEU:HD13	1:A:128:ILE:CD1	0.71	2.15	12	1
1:A:121:LEU:HD22	1:A:128:ILE:HD13	0.71	1.61	18	2
1:A:150:TYR:CE1	1:A:154:LEU:HD23	0.70	2.21	23	1
1:A:136:LEU:HD21	1:A:156:PHE:CE1	0.70	2.21	12	1
1:A:112:ILE:HD13	1:A:153:PHE:CE1	0.70	2.21	17	1
1:A:114:LEU:HD11	1:A:133:ILE:CG2	0.70	2.16	18	7
1:A:136:LEU:HD22	3:A:1:EMD:N4	0.69	2.03	7	6
1:A:101:PHE:CD1	1:A:153:PHE:CG	0.69	2.81	22	1
1:A:128:ILE:HD13	1:A:132:ASP:OD2	0.68	1.88	17	1
1:A:136:LEU:HD11	3:A:1:EMD:H13	0.68	1.65	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:MET:HE1	3:A:1:EMD:H171	0.68	1.63	10	3
1:A:97:LEU:HD21	1:A:159:GLY:N	0.68	2.02	28	3
1:A:121:LEU:HD12	1:A:133:ILE:HG13	0.68	1.65	21	1
1:A:126:GLU:OE1	1:A:128:ILE:HD12	0.68	1.89	17	1
1:A:104:PHE:CZ	3:A:1:EMD:H71	0.68	2.22	7	2
1:A:136:LEU:HD21	3:A:1:EMD:H13	0.67	1.64	23	4
1:A:97:LEU:CD1	1:A:154:LEU:HD13	0.67	2.18	3	3
1:A:130:GLU:HA	1:A:133:ILE:HD12	0.67	1.67	20	5
1:A:100:LEU:CD1	1:A:157:MET:HE3	0.67	2.20	18	1
1:A:117:LEU:HD11	3:A:1:EMD:H73	0.66	1.66	13	9
1:A:100:LEU:HD11	1:A:157:MET:HE3	0.66	1.66	18	1
1:A:157:MET:HB2	1:A:160:VAL:HG22	0.65	1.68	20	1
1:A:124:THR:HG21	3:A:1:EMD:H24	0.65	1.66	26	1
1:A:101:PHE:CE1	1:A:112:ILE:HD12	0.65	2.26	22	1
1:A:97:LEU:HD13	1:A:154:LEU:HD22	0.65	1.69	13	1
1:A:97:LEU:HD22	1:A:154:LEU:HD22	0.65	1.67	30	3
1:A:121:LEU:HD12	1:A:133:ILE:HD11	0.64	1.67	10	1
1:A:114:LEU:HD13	1:A:137:MET:SD	0.64	2.32	22	2
1:A:150:TYR:O	1:A:154:LEU:HD12	0.64	1.92	4	4
1:A:124:THR:O	1:A:124:THR:HG23	0.64	1.93	13	3
1:A:137:MET:HE3	1:A:146:GLY:C	0.63	2.19	5	1
1:A:124:THR:HG21	3:A:1:EMD:C24	0.63	2.24	26	3
1:A:107:ASN:O	1:A:108:ALA:HB3	0.62	1.93	7	11
1:A:156:PHE:CE2	3:A:1:EMD:N4	0.62	2.66	6	1
1:A:104:PHE:CE1	1:A:112:ILE:HG21	0.62	2.30	22	3
1:A:114:LEU:HD11	1:A:133:ILE:HG23	0.62	1.71	18	1
1:A:120:MET:HE1	3:A:1:EMD:H172	0.62	1.69	29	1
1:A:160:VAL:HG12	1:A:161:GLU:OE1	0.62	1.93	4	1
1:A:150:TYR:O	1:A:154:LEU:HD23	0.62	1.94	16	4
1:A:97:LEU:HD22	1:A:154:LEU:HD23	0.62	1.71	13	2
1:A:118:LYS:CG	1:A:133:ILE:HD13	0.62	2.25	8	1
1:A:121:LEU:HD13	1:A:128:ILE:HD13	0.61	1.72	12	1
1:A:132:ASP:O	1:A:136:LEU:HD12	0.61	1.95	3	1
1:A:136:LEU:HD21	1:A:156:PHE:CZ	0.61	2.31	15	1
1:A:100:LEU:CD2	1:A:157:MET:HE3	0.61	2.26	7	1
1:A:120:MET:HE3	1:A:120:MET:HA	0.60	1.70	1	1
1:A:100:LEU:HD21	1:A:161:GLU:O	0.60	1.94	21	1
1:A:117:LEU:HD22	1:A:136:LEU:HD22	0.60	1.73	6	1
1:A:117:LEU:HD21	3:A:1:EMD:H71	0.60	1.72	28	1
1:A:121:LEU:HD12	1:A:133:ILE:HG12	0.60	1.73	27	3
1:A:103:MET:HE1	1:A:120:MET:HE1	0.60	1.72	30	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:MET:O	1:A:124:THR:HG22	0.59	1.97	13	4
1:A:153:PHE:CE1	1:A:157:MET:HE2	0.59	2.32	24	2
1:A:110:GLY:C	1:A:111:TYR:CD1	0.59	2.81	18	19
1:A:121:LEU:HD13	1:A:128:ILE:HG21	0.59	1.73	11	3
1:A:136:LEU:HD13	3:A:1:EMD:C12	0.59	2.28	12	2
1:A:128:ILE:HG21	1:A:132:ASP:HB2	0.59	1.73	17	1
1:A:97:LEU:CD2	1:A:159:GLY:CA	0.59	2.81	22	2
1:A:117:LEU:HD23	1:A:121:LEU:HD11	0.59	1.72	23	1
1:A:100:LEU:HD11	1:A:161:GLU:N	0.59	2.13	6	1
1:A:115:GLU:O	1:A:119:ILE:HD12	0.59	1.98	18	2
1:A:117:LEU:CD2	1:A:136:LEU:CD2	0.58	2.81	6	1
1:A:114:LEU:HD21	1:A:133:ILE:O	0.58	1.98	23	1
1:A:136:LEU:CD2	3:A:1:EMD:N4	0.58	2.66	7	9
1:A:148:ILE:HG21	3:A:1:EMD:S1	0.58	2.38	15	3
1:A:94:GLU:HG2	1:A:154:LEU:HD22	0.58	1.75	17	1
1:A:100:LEU:HD22	1:A:157:MET:HE2	0.58	1.76	5	2
1:A:156:PHE:CD1	3:A:1:EMD:N3	0.58	2.71	19	1
1:A:148:ILE:HD12	3:A:1:EMD:S1	0.57	2.39	15	4
1:A:97:LEU:HD21	1:A:159:GLY:H	0.57	1.57	28	1
1:A:127:THR:HG22	1:A:127:THR:O	0.57	1.97	19	5
1:A:97:LEU:HD21	1:A:159:GLY:CA	0.57	2.30	27	5
1:A:121:LEU:HD22	3:A:1:EMD:O18	0.57	1.99	30	2
1:A:153:PHE:CZ	1:A:157:MET:HE2	0.57	2.35	4	2
1:A:97:LEU:HD13	1:A:154:LEU:CD1	0.57	2.26	15	2
1:A:136:LEU:HD21	3:A:1:EMD:C5	0.57	2.29	6	1
1:A:143:ASN:O	1:A:144:ASN:CB	0.57	2.52	15	3
1:A:114:LEU:HD11	1:A:137:MET:SD	0.57	2.40	10	2
1:A:104:PHE:CE1	1:A:120:MET:SD	0.57	2.98	25	3
1:A:153:PHE:CD1	1:A:157:MET:SD	0.57	2.98	20	2
1:A:153:PHE:CZ	1:A:157:MET:SD	0.56	2.98	3	8
1:A:153:PHE:CE1	1:A:157:MET:SD	0.56	2.98	20	6
1:A:153:PHE:CE2	1:A:157:MET:SD	0.56	2.98	13	3
1:A:153:PHE:CZ	1:A:157:MET:CG	0.56	2.88	15	3
1:A:114:LEU:HD12	1:A:137:MET:HE2	0.56	1.77	6	1
1:A:150:TYR:CD2	1:A:154:LEU:HD11	0.56	2.35	27	2
1:A:128:ILE:CG2	1:A:132:ASP:CB	0.56	2.83	3	5
1:A:136:LEU:C	1:A:136:LEU:HD23	0.56	2.25	6	3
1:A:121:LEU:HD12	1:A:133:ILE:HD13	0.56	1.77	6	1
1:A:150:TYR:CD2	1:A:150:TYR:O	0.56	2.59	29	1
1:A:129:THR:O	1:A:129:THR:HG23	0.55	2.00	9	2
1:A:124:THR:HG21	3:A:1:EMD:H23	0.55	1.77	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:LEU:HD21	3:A:1:EMD:N4	0.55	2.17	6	2
1:A:114:LEU:N	1:A:137:MET:HE1	0.55	2.15	15	1
1:A:125:GLY:O	1:A:127:THR:HG23	0.55	2.01	22	1
1:A:153:PHE:CE1	1:A:157:MET:CG	0.55	2.90	5	2
1:A:119:ILE:O	1:A:123:ALA:HB2	0.54	2.02	6	2
1:A:120:MET:C	1:A:124:THR:HG22	0.54	2.27	23	1
1:A:97:LEU:HD23	1:A:153:PHE:CE2	0.54	2.37	19	1
1:A:111:TYR:CZ	1:A:149:ASP:OD1	0.54	2.61	21	1
1:A:118:LYS:HE2	1:A:133:ILE:HG21	0.54	1.79	18	1
1:A:150:TYR:CE1	1:A:154:LEU:CD2	0.54	2.91	21	1
1:A:104:PHE:CZ	1:A:120:MET:SD	0.54	3.01	9	2
1:A:110:GLY:O	1:A:111:TYR:CD1	0.54	2.61	28	9
1:A:150:TYR:O	1:A:150:TYR:CG	0.54	2.60	29	1
1:A:126:GLU:O	1:A:128:ILE:CD1	0.54	2.56	16	1
1:A:104:PHE:CD1	1:A:120:MET:SD	0.54	3.00	23	3
1:A:101:PHE:CZ	1:A:110:GLY:O	0.54	2.61	24	5
1:A:119:ILE:O	1:A:123:ALA:CB	0.54	2.56	6	4
1:A:129:THR:OG1	1:A:130:GLU:N	0.54	2.41	21	5
1:A:143:ASN:OD1	1:A:145:ASP:CB	0.53	2.56	24	2
1:A:136:LEU:C	1:A:136:LEU:CD1	0.53	2.80	8	1
1:A:122:GLN:N	1:A:126:GLU:OE2	0.53	2.40	21	1
1:A:128:ILE:C	1:A:129:THR:HG22	0.53	2.29	23	1
1:A:125:GLY:C	1:A:126:GLU:CG	0.53	2.81	6	10
1:A:128:ILE:CG2	1:A:129:THR:N	0.53	2.71	9	8
1:A:104:PHE:CZ	1:A:120:MET:CB	0.53	2.92	17	2
1:A:112:ILE:CG2	1:A:113:ASP:N	0.53	2.71	21	1
1:A:131:ASP:O	1:A:135:GLU:CB	0.53	2.56	18	8
1:A:126:GLU:O	1:A:127:THR:CG2	0.53	2.56	1	1
1:A:99:ASP:O	1:A:103:MET:N	0.53	2.41	23	5
1:A:150:TYR:O	1:A:154:LEU:CD1	0.53	2.57	13	2
1:A:137:MET:CE	1:A:146:GLY:O	0.53	2.57	9	2
1:A:132:ASP:O	1:A:136:LEU:CB	0.53	2.57	25	9
1:A:153:PHE:O	1:A:157:MET:CB	0.53	2.57	12	6
1:A:104:PHE:CZ	1:A:120:MET:HB2	0.53	2.39	28	2
1:A:121:LEU:CD2	3:A:1:EMD:O18	0.53	2.57	14	14
1:A:140:GLY:CA	3:A:1:EMD:O2	0.53	2.56	13	10
1:A:125:GLY:O	1:A:127:THR:N	0.53	2.42	20	7
1:A:128:ILE:CG2	1:A:132:ASP:CG	0.53	2.81	23	1
1:A:107:ASN:O	1:A:108:ALA:CB	0.53	2.56	7	5
1:A:136:LEU:HD13	1:A:136:LEU:O	0.53	2.04	8	1
1:A:101:PHE:CA	1:A:153:PHE:CE2	0.53	2.92	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:LEU:O	1:A:120:MET:N	0.52	2.42	6	8
1:A:121:LEU:O	1:A:125:GLY:N	0.52	2.42	19	4
1:A:137:MET:O	1:A:141:ASP:CB	0.52	2.57	10	2
1:A:109:ASP:OD1	1:A:110:GLY:N	0.52	2.43	18	7
1:A:100:LEU:HD22	1:A:157:MET:CG	0.52	2.35	2	1
1:A:150:TYR:O	1:A:154:LEU:N	0.52	2.42	20	7
1:A:107:ASN:ND2	1:A:116:GLU:OE2	0.52	2.42	4	3
1:A:158:LYS:O	1:A:158:LYS:CG	0.52	2.57	12	3
1:A:107:ASN:OD1	1:A:108:ALA:N	0.52	2.43	7	2
1:A:107:ASN:CB	1:A:116:GLU:OE2	0.52	2.57	11	2
1:A:136:LEU:HD23	1:A:136:LEU:C	0.52	2.30	16	1
1:A:128:ILE:CG2	1:A:132:ASP:HB2	0.52	2.34	19	9
1:A:147:ARG:C	1:A:148:ILE:HD13	0.52	2.30	4	1
1:A:117:LEU:HD13	1:A:137:MET:HG3	0.52	1.82	25	1
1:A:143:ASN:ND2	1:A:152:GLU:OE2	0.52	2.43	26	8
1:A:101:PHE:HA	1:A:153:PHE:CE2	0.52	2.40	13	3
1:A:113:ASP:OD1	1:A:115:GLU:N	0.52	2.43	9	1
1:A:101:PHE:N	1:A:153:PHE:CE2	0.52	2.78	19	1
1:A:101:PHE:HE1	1:A:112:ILE:HD12	0.52	1.63	22	1
1:A:154:LEU:O	1:A:154:LEU:CD1	0.52	2.57	23	1
1:A:101:PHE:C	1:A:101:PHE:CD1	0.52	2.87	11	10
1:A:160:VAL:HG12	1:A:161:GLU:N	0.52	2.19	9	2
1:A:137:MET:O	1:A:140:GLY:N	0.52	2.43	8	1
1:A:143:ASN:ND2	1:A:152:GLU:CD	0.52	2.68	12	4
1:A:126:GLU:O	1:A:128:ILE:HD12	0.52	2.03	16	2
1:A:137:MET:O	1:A:141:ASP:N	0.52	2.43	28	5
1:A:143:ASN:OD1	1:A:144:ASN:N	0.52	2.43	2	3
1:A:112:ILE:O	1:A:147:ARG:CG	0.52	2.58	6	2
1:A:97:LEU:HD11	1:A:158:LYS:HA	0.52	1.80	16	2
1:A:120:MET:O	1:A:124:THR:CG2	0.52	2.58	23	2
1:A:101:PHE:HA	1:A:153:PHE:CZ	0.52	2.40	19	6
1:A:133:ILE:O	1:A:137:MET:CB	0.52	2.57	4	3
1:A:148:ILE:HD12	3:A:1:EMD:O2	0.52	2.05	15	2
1:A:96:GLU:O	1:A:99:ASP:N	0.52	2.43	28	6
1:A:104:PHE:CD2	1:A:157:MET:HE1	0.52	2.40	12	2
1:A:114:LEU:CD1	1:A:133:ILE:O	0.52	2.58	20	1
1:A:145:ASP:OD2	1:A:147:ARG:NH1	0.52	2.43	29	1
1:A:114:LEU:O	1:A:117:LEU:N	0.52	2.43	5	1
1:A:119:ILE:HD13	1:A:119:ILE:N	0.52	2.19	22	1
1:A:99:ASP:O	1:A:102:ARG:CG	0.52	2.58	25	1
1:A:101:PHE:CD2	1:A:153:PHE:CG	0.51	2.99	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:PHE:O	1:A:157:MET:N	0.51	2.43	7	4
1:A:135:GLU:O	1:A:138:LYS:N	0.51	2.43	11	1
1:A:114:LEU:HD22	1:A:133:ILE:HG22	0.51	1.79	23	1
1:A:141:ASP:O	1:A:144:ASN:N	0.51	2.44	22	13
1:A:128:ILE:CG2	1:A:132:ASP:HB3	0.51	2.35	3	1
1:A:153:PHE:CZ	1:A:157:MET:CE	0.51	2.94	4	2
1:A:153:PHE:CE1	1:A:157:MET:HG2	0.51	2.40	5	2
1:A:109:ASP:OD1	1:A:109:ASP:N	0.51	2.44	24	5
1:A:114:LEU:CG	1:A:133:ILE:HG22	0.51	2.35	20	1
1:A:105:ASP:OD2	1:A:111:TYR:N	0.51	2.44	28	2
1:A:129:THR:HG23	1:A:130:GLU:N	0.51	2.21	2	2
1:A:153:PHE:CE1	1:A:157:MET:HB3	0.51	2.41	12	2
1:A:101:PHE:CE1	1:A:110:GLY:C	0.51	2.88	17	1
1:A:124:THR:OG1	1:A:125:GLY:N	0.51	2.42	29	1
1:A:156:PHE:CD2	3:A:1:EMD:N4	0.51	2.78	6	1
1:A:112:ILE:HG22	1:A:117:LEU:HD12	0.51	1.80	8	2
1:A:121:LEU:CD1	1:A:133:ILE:CD1	0.51	2.88	13	1
1:A:143:ASN:ND2	1:A:145:ASP:OD2	0.51	2.44	13	1
1:A:129:THR:O	1:A:133:ILE:HD12	0.51	2.04	2	1
1:A:160:VAL:O	1:A:160:VAL:CG1	0.51	2.58	6	1
1:A:121:LEU:O	1:A:124:THR:N	0.51	2.44	29	6
1:A:125:GLY:O	1:A:126:GLU:C	0.51	2.54	2	20
1:A:135:GLU:O	1:A:139:ASP:N	0.51	2.44	15	2
1:A:147:ARG:CG	1:A:148:ILE:N	0.51	2.74	2	3
1:A:130:GLU:O	1:A:133:ILE:N	0.51	2.44	12	2
1:A:109:ASP:N	1:A:109:ASP:OD1	0.51	2.43	27	5
1:A:128:ILE:HG22	1:A:129:THR:H	0.51	1.66	17	1
1:A:126:GLU:N	1:A:126:GLU:OE1	0.51	2.42	21	1
1:A:126:GLU:C	1:A:127:THR:HG22	0.51	2.31	1	3
1:A:93:SER:O	1:A:95:GLU:N	0.51	2.44	27	3
1:A:149:ASP:N	1:A:149:ASP:OD1	0.51	2.44	13	2
1:A:99:ASP:O	1:A:103:MET:CG	0.51	2.59	15	3
1:A:157:MET:CE	1:A:160:VAL:O	0.51	2.59	16	1
1:A:97:LEU:O	1:A:100:LEU:N	0.50	2.43	21	4
1:A:150:TYR:CD2	1:A:154:LEU:CD2	0.50	2.94	15	1
1:A:102:ARG:O	1:A:105:ASP:N	0.50	2.43	27	4
1:A:114:LEU:HD11	1:A:133:ILE:O	0.50	2.06	20	1
1:A:140:GLY:O	1:A:141:ASP:C	0.50	2.54	22	1
1:A:143:ASN:N	1:A:152:GLU:OE2	0.50	2.44	1	6
1:A:156:PHE:CD2	3:A:1:EMD:N3	0.50	2.79	28	2
1:A:126:GLU:OE1	1:A:127:THR:N	0.50	2.45	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:SER:O	1:A:97:LEU:HD23	0.50	2.06	28	1
1:A:137:MET:CE	1:A:146:GLY:C	0.50	2.84	5	1
1:A:153:PHE:CD1	1:A:157:MET:HB2	0.50	2.42	6	1
1:A:121:LEU:O	1:A:124:THR:CG2	0.50	2.59	2	2
1:A:118:LYS:HG3	1:A:133:ILE:HD13	0.50	1.82	8	1
1:A:136:LEU:HD13	3:A:1:EMD:H12	0.50	1.82	22	1
1:A:114:LEU:HD13	1:A:137:MET:HG3	0.50	1.83	2	2
1:A:136:LEU:HD23	1:A:139:ASP:HB2	0.50	1.83	2	1
1:A:148:ILE:CG2	3:A:1:EMD:S1	0.50	2.99	15	1
1:A:120:MET:O	1:A:123:ALA:HB3	0.50	2.07	16	1
1:A:107:ASN:ND2	1:A:109:ASP:OD1	0.50	2.45	16	2
1:A:114:LEU:N	1:A:137:MET:HE3	0.50	2.22	19	2
1:A:114:LEU:H	1:A:114:LEU:HD12	0.50	1.67	21	1
1:A:106:LYS:HE2	1:A:119:ILE:HD13	0.50	1.81	23	1
1:A:151:ASP:OD1	1:A:151:ASP:N	0.50	2.44	5	1
1:A:136:LEU:O	1:A:136:LEU:HD22	0.50	2.06	8	1
1:A:153:PHE:CD1	1:A:153:PHE:O	0.50	2.64	11	1
1:A:129:THR:O	1:A:130:GLU:CB	0.50	2.59	12	2
1:A:151:ASP:CG	1:A:152:GLU:N	0.49	2.70	2	1
1:A:143:ASN:O	1:A:144:ASN:CG	0.49	2.55	15	3
1:A:128:ILE:HD12	1:A:128:ILE:N	0.49	2.22	5	1
1:A:148:ILE:HD12	3:A:1:EMD:C2	0.49	2.37	15	2
1:A:94:GLU:O	1:A:97:LEU:N	0.49	2.45	14	1
1:A:126:GLU:O	1:A:127:THR:C	0.49	2.55	18	4
1:A:117:LEU:HD11	3:A:1:EMD:H71	0.49	1.83	15	1
1:A:139:ASP:OD1	1:A:139:ASP:C	0.49	2.55	18	1
1:A:107:ASN:ND2	1:A:109:ASP:OD2	0.49	2.44	27	1
1:A:126:GLU:C	1:A:127:THR:CG2	0.49	2.85	16	3
1:A:105:ASP:CG	1:A:108:ALA:C	0.49	2.80	17	1
1:A:153:PHE:CZ	1:A:157:MET:CB	0.49	2.95	16	1
1:A:100:LEU:HD13	1:A:157:MET:CG	0.49	2.38	22	2
1:A:103:MET:HE2	1:A:103:MET:O	0.49	2.06	19	2
1:A:113:ASP:N	1:A:113:ASP:OD1	0.49	2.45	5	2
3:A:1:EMD:C15	3:A:1:EMD:C24	0.49	2.91	5	5
1:A:96:GLU:O	1:A:97:LEU:C	0.49	2.56	23	13
1:A:100:LEU:O	1:A:103:MET:N	0.49	2.46	23	2
1:A:107:ASN:CG	1:A:108:ALA:N	0.49	2.70	17	2
1:A:93:SER:O	1:A:94:GLU:C	0.49	2.55	27	7
1:A:153:PHE:CE1	1:A:157:MET:HB2	0.49	2.43	29	3
1:A:120:MET:HE2	3:A:1:EMD:H24	0.49	1.85	22	1
1:A:121:LEU:CD1	1:A:133:ILE:HG12	0.49	2.38	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:LEU:CD2	3:A:1:EMD:C13	0.49	2.90	19	2
1:A:153:PHE:CZ	1:A:157:MET:HG2	0.49	2.43	5	5
1:A:143:ASN:OD1	1:A:143:ASN:C	0.49	2.56	2	3
1:A:113:ASP:OD1	1:A:113:ASP:N	0.49	2.45	6	4
1:A:150:TYR:O	1:A:154:LEU:CG	0.49	2.61	27	4
1:A:124:THR:CG2	3:A:1:EMD:C23	0.49	2.88	8	1
1:A:121:LEU:C	1:A:126:GLU:CD	0.49	2.81	21	1
1:A:112:ILE:O	1:A:147:ARG:CB	0.48	2.61	1	1
1:A:135:GLU:CD	1:A:135:GLU:C	0.48	2.81	12	1
1:A:107:ASN:OD1	1:A:109:ASP:CG	0.48	2.56	6	3
1:A:127:THR:O	1:A:127:THR:OG1	0.48	2.31	16	1
1:A:100:LEU:HD23	1:A:103:MET:SD	0.48	2.48	29	2
1:A:121:LEU:O	1:A:122:GLN:C	0.48	2.56	7	4
1:A:157:MET:HE2	1:A:160:VAL:HB	0.48	1.86	30	1
1:A:143:ASN:C	1:A:144:ASN:CG	0.48	2.82	25	3
3:A:1:EMD:C24	3:A:1:EMD:H151	0.48	2.38	5	9
1:A:118:LYS:CG	1:A:133:ILE:CD1	0.48	2.92	24	1
1:A:121:LEU:HD21	3:A:1:EMD:O18	0.48	2.08	15	4
1:A:114:LEU:O	1:A:115:GLU:C	0.48	2.57	5	4
1:A:113:ASP:C	1:A:137:MET:CE	0.48	2.86	6	1
1:A:111:TYR:CD1	1:A:147:ARG:HD2	0.48	2.43	8	2
1:A:128:ILE:HG21	1:A:133:ILE:CD1	0.48	2.38	16	1
1:A:157:MET:HE2	1:A:160:VAL:O	0.48	2.08	16	1
1:A:102:ARG:HG3	1:A:103:MET:N	0.48	2.22	30	3
1:A:157:MET:SD	1:A:160:VAL:CG2	0.48	3.02	28	1
1:A:160:VAL:CG1	1:A:161:GLU:N	0.48	2.75	9	1
1:A:117:LEU:HD21	3:A:1:EMD:N4	0.48	2.23	21	4
1:A:124:THR:O	3:A:1:EMD:C24	0.48	2.62	12	1
1:A:112:ILE:HG22	1:A:113:ASP:N	0.48	2.23	21	1
1:A:136:LEU:O	1:A:139:ASP:OD2	0.48	2.31	18	1
1:A:156:PHE:CE1	3:A:1:EMD:N4	0.48	2.81	19	1
1:A:121:LEU:O	1:A:126:GLU:CB	0.48	2.62	28	1
1:A:112:ILE:N	1:A:112:ILE:HD13	0.48	2.23	20	2
1:A:131:ASP:N	1:A:131:ASP:OD1	0.48	2.46	10	1
1:A:112:ILE:O	1:A:148:ILE:N	0.48	2.44	29	2
1:A:125:GLY:O	1:A:126:GLU:CD	0.48	2.56	27	1
1:A:97:LEU:O	1:A:98:SER:C	0.48	2.57	29	15
1:A:140:GLY:C	3:A:1:EMD:O2	0.48	2.57	3	6
1:A:117:LEU:O	1:A:118:LYS:C	0.48	2.57	21	12
1:A:100:LEU:HD22	1:A:157:MET:HE1	0.48	1.86	13	1
1:A:100:LEU:O	1:A:103:MET:CG	0.48	2.61	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:MET:HE1	1:A:146:GLY:HA2	0.48	1.85	30	1
1:A:143:ASN:CG	1:A:152:GLU:OE2	0.47	2.57	18	4
1:A:100:LEU:O	1:A:101:PHE:C	0.47	2.57	18	5
1:A:153:PHE:CE1	1:A:157:MET:CB	0.47	2.97	6	4
1:A:148:ILE:C	1:A:149:ASP:OD1	0.47	2.57	14	2
1:A:153:PHE:CE1	1:A:157:MET:HE3	0.47	2.44	9	1
1:A:132:ASP:O	1:A:136:LEU:N	0.47	2.45	23	3
1:A:105:ASP:OD1	1:A:108:ALA:HB3	0.47	2.09	19	1
1:A:136:LEU:O	1:A:139:ASP:N	0.47	2.47	3	3
1:A:143:ASN:O	1:A:144:ASN:C	0.47	2.57	3	1
1:A:100:LEU:HD12	1:A:159:GLY:HA2	0.47	1.84	8	1
1:A:149:ASP:N	1:A:152:GLU:OE1	0.47	2.47	26	2
1:A:148:ILE:HG21	1:A:153:PHE:HD1	0.47	1.69	17	1
1:A:110:GLY:C	1:A:111:TYR:CG	0.47	2.92	14	3
1:A:97:LEU:CD2	1:A:159:GLY:N	0.47	2.77	5	2
1:A:111:TYR:CD2	1:A:147:ARG:HD3	0.47	2.44	5	2
1:A:150:TYR:CE2	1:A:154:LEU:HD11	0.47	2.44	27	1
3:A:1:EMD:C24	3:A:1:EMD:C15	0.47	2.92	12	4
1:A:143:ASN:OD1	1:A:145:ASP:CG	0.47	2.58	14	2
1:A:132:ASP:O	1:A:136:LEU:HB2	0.47	2.10	25	13
1:A:145:ASP:OD1	1:A:146:GLY:N	0.47	2.47	26	2
1:A:121:LEU:O	1:A:126:GLU:N	0.47	2.46	23	1
1:A:136:LEU:CD1	3:A:1:EMD:H13	0.47	2.38	23	1
1:A:153:PHE:O	1:A:157:MET:CG	0.47	2.63	24	1
1:A:126:GLU:HG3	1:A:127:THR:N	0.47	2.25	1	2
1:A:110:GLY:O	1:A:111:TYR:CG	0.47	2.67	8	5
1:A:121:LEU:HD23	1:A:121:LEU:N	0.47	2.24	5	1
1:A:93:SER:C	1:A:95:GLU:N	0.47	2.71	28	4
1:A:109:ASP:OD2	1:A:111:TYR:O	0.47	2.33	14	6
1:A:107:ASN:OD1	1:A:107:ASN:C	0.47	2.57	2	4
1:A:149:ASP:O	1:A:150:TYR:C	0.47	2.57	28	5
1:A:121:LEU:O	1:A:123:ALA:N	0.47	2.48	7	1
1:A:107:ASN:O	1:A:107:ASN:CG	0.47	2.57	8	3
1:A:144:ASN:ND2	1:A:144:ASN:O	0.47	2.47	8	1
1:A:128:ILE:HG23	1:A:132:ASP:HB2	0.47	1.86	12	1
1:A:143:ASN:CB	1:A:152:GLU:OE2	0.47	2.63	13	2
1:A:150:TYR:CE1	1:A:154:LEU:HD21	0.47	2.45	21	1
1:A:149:ASP:O	1:A:153:PHE:CB	0.47	2.63	1	3
1:A:143:ASN:O	1:A:144:ASN:ND2	0.47	2.48	3	1
1:A:97:LEU:CD1	1:A:154:LEU:CD2	0.47	2.92	9	1
1:A:121:LEU:HD13	1:A:128:ILE:HD12	0.47	1.84	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:LEU:HD12	1:A:133:ILE:CD1	0.47	2.40	13	2
1:A:111:TYR:CD1	1:A:147:ARG:HD3	0.47	2.45	14	1
1:A:143:ASN:O	1:A:144:ASN:OD1	0.47	2.33	15	1
1:A:97:LEU:CD2	1:A:159:GLY:HA2	0.47	2.39	21	1
1:A:154:LEU:O	1:A:157:MET:N	0.47	2.47	13	1
1:A:105:ASP:OD1	1:A:108:ALA:C	0.47	2.57	17	1
1:A:99:ASP:N	1:A:99:ASP:OD1	0.47	2.45	19	1
1:A:104:PHE:CD1	1:A:112:ILE:HG12	0.47	2.45	22	1
1:A:118:LYS:HG2	1:A:133:ILE:CD1	0.47	2.40	24	1
1:A:144:ASN:O	1:A:144:ASN:OD1	0.47	2.33	20	2
1:A:118:LYS:HE3	1:A:133:ILE:HG21	0.47	1.87	6	1
1:A:118:LYS:O	1:A:121:LEU:N	0.47	2.44	27	2
1:A:136:LEU:HD11	3:A:1:EMD:H12	0.47	1.79	17	1
1:A:104:PHE:CG	1:A:120:MET:SD	0.47	3.08	19	2
1:A:118:LYS:HE2	1:A:133:ILE:HD13	0.47	1.86	20	1
1:A:114:LEU:HD22	1:A:133:ILE:CG2	0.47	2.40	23	1
1:A:105:ASP:OD2	1:A:109:ASP:OD1	0.46	2.33	26	6
1:A:158:LYS:O	1:A:159:GLY:C	0.46	2.57	17	1
1:A:148:ILE:CG2	1:A:149:ASP:N	0.46	2.78	19	1
1:A:149:ASP:OD1	1:A:150:TYR:N	0.46	2.46	5	2
1:A:113:ASP:OD1	1:A:116:GLU:OE2	0.46	2.34	6	3
1:A:105:ASP:OD1	1:A:109:ASP:OD1	0.46	2.32	8	2
1:A:100:LEU:HD22	1:A:157:MET:HG2	0.46	1.88	2	2
1:A:157:MET:CE	3:A:1:EMD:H171	0.46	2.40	8	1
1:A:144:ASN:CG	1:A:144:ASN:O	0.46	2.57	15	1
1:A:128:ILE:CG2	1:A:133:ILE:CD1	0.46	2.93	16	1
1:A:97:LEU:HD11	1:A:159:GLY:N	0.46	2.25	23	1
1:A:141:ASP:OD1	1:A:143:ASN:OD1	0.46	2.33	2	2
1:A:147:ARG:HG2	1:A:148:ILE:N	0.46	2.25	2	1
1:A:97:LEU:HD12	1:A:154:LEU:CD2	0.46	2.41	9	2
1:A:113:ASP:HA	1:A:137:MET:HE1	0.46	1.88	23	1
1:A:141:ASP:OD1	1:A:147:ARG:O	0.46	2.33	29	5
1:A:121:LEU:C	1:A:123:ALA:N	0.46	2.72	7	3
1:A:137:MET:O	1:A:138:LYS:C	0.46	2.59	12	1
1:A:150:TYR:CD2	1:A:154:LEU:HD21	0.46	2.45	15	1
1:A:141:ASP:O	1:A:142:LYS:C	0.46	2.59	27	5
1:A:122:GLN:O	1:A:126:GLU:CG	0.46	2.63	24	1
1:A:126:GLU:OE1	3:A:1:EMD:C26	0.46	2.64	28	1
1:A:111:TYR:CE2	1:A:149:ASP:OD2	0.46	2.69	30	1
1:A:114:LEU:HD11	1:A:133:ILE:C	0.46	2.35	20	1
1:A:150:TYR:O	1:A:151:ASP:C	0.46	2.58	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:LEU:CD2	3:A:1:EMD:H13	0.46	2.41	6	2
1:A:136:LEU:HD13	3:A:1:EMD:C13	0.46	2.41	12	1
1:A:113:ASP:O	1:A:117:LEU:HD12	0.46	2.10	22	2
1:A:116:GLU:O	1:A:119:ILE:N	0.46	2.49	16	1
1:A:149:ASP:OD1	1:A:149:ASP:C	0.46	2.58	24	1
1:A:121:LEU:HD11	1:A:136:LEU:HD22	0.46	1.87	28	1
1:A:107:ASN:OD1	1:A:109:ASP:OD1	0.46	2.34	1	2
1:A:140:GLY:O	3:A:1:EMD:O2	0.46	2.33	5	2
1:A:136:LEU:CG	3:A:1:EMD:H13	0.46	2.40	6	1
1:A:121:LEU:CD1	1:A:133:ILE:HG13	0.46	2.41	16	2
1:A:104:PHE:O	1:A:106:LYS:N	0.46	2.49	11	1
1:A:131:ASP:O	1:A:132:ASP:C	0.46	2.59	21	1
1:A:130:GLU:O	1:A:131:ASP:C	0.46	2.59	12	4
1:A:125:GLY:C	1:A:126:GLU:HG2	0.46	2.36	10	3
1:A:125:GLY:O	1:A:126:GLU:O	0.46	2.34	26	2
3:A:1:EMD:O18	3:A:1:EMD:H12	0.46	2.11	13	12
3:A:1:EMD:H12	3:A:1:EMD:O18	0.46	2.11	6	18
1:A:121:LEU:CD1	1:A:133:ILE:HD11	0.46	2.41	10	1
1:A:153:PHE:O	1:A:157:MET:HB3	0.45	2.11	21	2
1:A:103:MET:HG3	1:A:104:PHE:N	0.45	2.26	29	4
1:A:157:MET:SD	1:A:160:VAL:HG21	0.45	2.51	9	1
1:A:129:THR:O	1:A:131:ASP:N	0.45	2.47	25	3
1:A:111:TYR:CD2	1:A:148:ILE:O	0.45	2.68	21	1
1:A:156:PHE:CD1	1:A:156:PHE:O	0.45	2.70	29	1
1:A:103:MET:SD	1:A:104:PHE:N	0.45	2.89	30	1
1:A:107:ASN:OD1	1:A:109:ASP:CB	0.45	2.64	6	1
1:A:126:GLU:O	1:A:128:ILE:N	0.45	2.50	20	4
1:A:157:MET:O	1:A:157:MET:CG	0.45	2.62	4	2
1:A:109:ASP:OD1	1:A:109:ASP:C	0.45	2.58	21	1
1:A:137:MET:O	1:A:141:ASP:HB2	0.45	2.11	10	7
1:A:128:ILE:HG23	1:A:132:ASP:CG	0.45	2.37	13	1
1:A:136:LEU:CD1	3:A:1:EMD:C12	0.45	2.94	22	1
1:A:140:GLY:HA2	1:A:156:PHE:CE2	0.45	2.46	11	1
1:A:148:ILE:HG21	1:A:153:PHE:CD1	0.45	2.47	16	1
1:A:128:ILE:O	1:A:129:THR:CB	0.45	2.64	23	1
1:A:128:ILE:CG1	1:A:132:ASP:HB2	0.45	2.42	24	1
1:A:114:LEU:HG	1:A:137:MET:HE2	0.45	1.87	29	1
1:A:144:ASN:O	1:A:144:ASN:CG	0.45	2.59	8	2
1:A:120:MET:O	1:A:124:THR:HG21	0.45	2.12	21	1
1:A:152:GLU:O	1:A:155:GLU:N	0.45	2.50	22	1
1:A:128:ILE:HG12	1:A:132:ASP:CB	0.45	2.42	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:THR:HG23	1:A:127:THR:O	0.45	2.11	25	1
1:A:125:GLY:C	1:A:127:THR:N	0.45	2.75	7	5
1:A:131:ASP:O	1:A:135:GLU:HB3	0.45	2.12	18	5
1:A:160:VAL:O	1:A:161:GLU:O	0.45	2.35	18	1
1:A:101:PHE:CD1	1:A:101:PHE:O	0.45	2.70	27	1
1:A:153:PHE:CD2	1:A:157:MET:SD	0.45	3.10	4	1
1:A:143:ASN:O	1:A:143:ASN:OD1	0.45	2.35	5	1
1:A:117:LEU:HD21	1:A:136:LEU:CD2	0.45	2.37	23	2
1:A:157:MET:HE3	3:A:1:EMD:H9	0.45	1.88	8	1
1:A:153:PHE:CE1	1:A:157:MET:CE	0.45	2.99	19	3
1:A:149:ASP:OD1	1:A:149:ASP:N	0.45	2.47	14	1
1:A:157:MET:CE	3:A:1:EMD:C17	0.45	2.95	8	1
1:A:120:MET:C	1:A:121:LEU:HD23	0.45	2.36	11	2
1:A:101:PHE:O	1:A:105:ASP:N	0.45	2.45	13	1
1:A:128:ILE:HG23	1:A:132:ASP:OD2	0.45	2.11	13	1
1:A:97:LEU:C	1:A:99:ASP:N	0.44	2.75	11	3
1:A:121:LEU:O	1:A:126:GLU:HA	0.44	2.12	23	1
1:A:105:ASP:CG	1:A:109:ASP:OD1	0.44	2.60	8	1
1:A:153:PHE:CZ	1:A:157:MET:HE3	0.44	2.48	9	1
1:A:157:MET:SD	1:A:160:VAL:HG23	0.44	2.53	11	1
1:A:121:LEU:CD1	1:A:133:ILE:HD13	0.44	2.42	22	2
1:A:125:GLY:O	1:A:126:GLU:HG3	0.44	2.12	11	8
1:A:156:PHE:CB	3:A:1:EMD:O2	0.44	2.65	5	1
1:A:113:ASP:O	1:A:114:LEU:C	0.44	2.60	8	3
1:A:114:LEU:HG	1:A:133:ILE:CG2	0.44	2.43	11	2
1:A:153:PHE:O	1:A:157:MET:HB2	0.44	2.12	17	3
1:A:114:LEU:HD23	1:A:133:ILE:CG2	0.44	2.41	10	1
1:A:127:THR:C	1:A:128:ILE:CG1	0.44	2.90	17	1
1:A:141:ASP:OD2	1:A:146:GLY:N	0.44	2.50	27	1
1:A:107:ASN:OD1	1:A:109:ASP:N	0.44	2.51	2	1
1:A:118:LYS:HG2	1:A:133:ILE:HD13	0.44	1.89	8	2
1:A:114:LEU:HD23	1:A:133:ILE:HG22	0.44	1.88	10	1
1:A:157:MET:HE1	3:A:1:EMD:H9	0.44	1.88	10	1
1:A:94:GLU:HG3	1:A:154:LEU:HD22	0.44	1.89	24	1
1:A:153:PHE:CE2	1:A:157:MET:CE	0.44	3.00	4	1
1:A:125:GLY:O	1:A:126:GLU:HG2	0.44	2.13	8	1
1:A:129:THR:O	1:A:130:GLU:HB2	0.44	2.12	12	1
1:A:153:PHE:CD1	1:A:157:MET:HB3	0.44	2.47	12	2
1:A:144:ASN:OD1	1:A:144:ASN:C	0.44	2.60	15	1
1:A:114:LEU:CD1	1:A:137:MET:HB2	0.44	2.43	6	1
1:A:102:ARG:CG	1:A:103:MET:N	0.44	2.81	30	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:ILE:CD1	3:A:1:EMD:S1	0.44	3.06	4	2
1:A:107:ASN:HB2	1:A:116:GLU:OE2	0.44	2.13	8	2
1:A:137:MET:SD	1:A:137:MET:C	0.44	3.00	8	1
1:A:107:ASN:OD1	1:A:107:ASN:O	0.44	2.36	9	1
1:A:101:PHE:CD2	1:A:153:PHE:CD2	0.44	3.06	13	1
1:A:113:ASP:O	1:A:116:GLU:N	0.44	2.50	25	2
1:A:124:THR:CG2	1:A:125:GLY:N	0.44	2.80	28	1
1:A:125:GLY:C	1:A:126:GLU:HG3	0.44	2.38	2	1
1:A:157:MET:O	1:A:157:MET:HG2	0.44	2.13	4	2
1:A:133:ILE:O	1:A:137:MET:HB2	0.44	2.13	25	4
1:A:157:MET:HE2	3:A:1:EMD:H171	0.44	1.88	18	1
1:A:94:GLU:OE1	1:A:94:GLU:CA	0.44	2.63	27	1
1:A:114:LEU:O	1:A:114:LEU:HD12	0.43	2.12	3	1
1:A:143:ASN:OD1	1:A:145:ASP:N	0.43	2.51	26	2
1:A:160:VAL:O	1:A:161:GLU:C	0.43	2.61	12	1
1:A:153:PHE:O	1:A:154:LEU:C	0.43	2.61	16	1
1:A:150:TYR:O	1:A:154:LEU:CB	0.43	2.66	27	2
1:A:153:PHE:CD1	1:A:153:PHE:C	0.43	2.96	4	2
1:A:126:GLU:O	1:A:127:THR:HB	0.43	2.13	14	3
1:A:105:ASP:OD1	1:A:116:GLU:OE2	0.43	2.36	12	1
1:A:109:ASP:CG	1:A:109:ASP:O	0.43	2.61	17	1
1:A:112:ILE:O	1:A:147:ARG:HG2	0.43	2.11	6	1
1:A:149:ASP:CG	1:A:150:TYR:N	0.43	2.76	10	3
1:A:132:ASP:OD1	1:A:136:LEU:HD12	0.43	2.13	15	1
1:A:130:GLU:N	1:A:130:GLU:CD	0.43	2.76	25	1
1:A:94:GLU:CA	1:A:97:LEU:HB2	0.43	2.42	12	1
1:A:122:GLN:HA	1:A:126:GLU:CB	0.43	2.43	13	1
1:A:128:ILE:O	1:A:129:THR:HB	0.43	2.13	21	1
1:A:101:PHE:CE1	1:A:112:ILE:CD1	0.43	3.00	22	1
1:A:140:GLY:HA3	3:A:1:EMD:O2	0.43	2.13	28	6
1:A:100:LEU:O	1:A:103:MET:HG2	0.43	2.13	22	1
1:A:153:PHE:C	1:A:153:PHE:CD1	0.43	2.96	23	1
1:A:153:PHE:O	1:A:157:MET:HG2	0.43	2.13	24	1
1:A:149:ASP:OD1	1:A:152:GLU:CG	0.43	2.67	1	1
1:A:111:TYR:CD2	1:A:147:ARG:HD2	0.43	2.49	2	1
1:A:143:ASN:ND2	1:A:143:ASN:C	0.43	2.76	17	1
1:A:105:ASP:OD2	1:A:109:ASP:CG	0.43	2.62	20	1
1:A:112:ILE:O	1:A:147:ARG:CA	0.43	2.67	1	1
1:A:131:ASP:O	1:A:135:GLU:HB2	0.43	2.13	12	3
1:A:97:LEU:CD2	1:A:157:MET:O	0.43	2.62	3	1
1:A:121:LEU:O	1:A:124:THR:OG1	0.43	2.33	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:ASP:OD2	1:A:152:GLU:OE2	0.43	2.37	4	1
1:A:106:LYS:HE2	1:A:119:ILE:CD1	0.43	2.44	6	1
1:A:114:LEU:O	1:A:116:GLU:N	0.43	2.52	9	1
1:A:157:MET:SD	1:A:160:VAL:O	0.43	2.76	11	1
1:A:140:GLY:O	1:A:148:ILE:CD1	0.43	2.66	13	1
1:A:107:ASN:OD1	1:A:107:ASN:N	0.43	2.51	16	1
1:A:115:GLU:O	1:A:119:ILE:CD1	0.43	2.66	17	1
1:A:113:ASP:OD1	1:A:113:ASP:C	0.43	2.61	18	2
1:A:121:LEU:HD22	1:A:128:ILE:CD1	0.43	2.43	23	1
1:A:106:LYS:N	1:A:116:GLU:OE2	0.43	2.47	30	1
1:A:153:PHE:CG	1:A:157:MET:SD	0.43	3.12	4	1
1:A:160:VAL:O	1:A:161:GLU:OXT	0.43	2.36	6	1
1:A:114:LEU:CD1	1:A:137:MET:HG3	0.43	2.44	16	1
1:A:141:ASP:OD1	1:A:144:ASN:N	0.43	2.50	19	1
1:A:97:LEU:HD11	1:A:158:LYS:C	0.43	2.38	26	1
1:A:127:THR:O	1:A:127:THR:CG2	0.43	2.67	19	1
1:A:114:LEU:C	1:A:116:GLU:N	0.42	2.75	9	1
1:A:114:LEU:H	1:A:137:MET:HE1	0.42	1.74	15	1
1:A:141:ASP:C	1:A:143:ASN:N	0.42	2.77	22	2
1:A:134:GLU:O	1:A:138:LYS:N	0.42	2.50	25	1
1:A:156:PHE:CG	3:A:1:EMD:C2	0.42	3.02	8	1
1:A:157:MET:HE3	1:A:160:VAL:HB	0.42	1.91	15	1
1:A:126:GLU:C	1:A:128:ILE:N	0.42	2.77	20	2
1:A:145:ASP:OD2	1:A:147:ARG:NE	0.42	2.51	20	2
1:A:107:ASN:O	1:A:108:ALA:C	0.42	2.62	22	1
1:A:132:ASP:O	1:A:136:LEU:HD13	0.42	2.13	28	1
1:A:94:GLU:HA	1:A:97:LEU:HB2	0.42	1.91	12	1
1:A:149:ASP:CG	1:A:152:GLU:OE1	0.42	2.62	19	1
1:A:149:ASP:OD2	1:A:152:GLU:OE1	0.42	2.37	19	1
1:A:102:ARG:HB2	1:A:102:ARG:NH1	0.42	2.29	16	1
1:A:129:THR:O	1:A:130:GLU:C	0.42	2.63	30	1
1:A:94:GLU:O	1:A:95:GLU:C	0.42	2.62	20	4
1:A:100:LEU:O	1:A:103:MET:HG3	0.42	2.13	21	3
1:A:109:ASP:OD1	1:A:111:TYR:N	0.42	2.47	21	1
1:A:143:ASN:ND2	1:A:152:GLU:OE1	0.42	2.51	21	1
1:A:99:ASP:O	1:A:102:ARG:HG2	0.42	2.12	25	1
1:A:117:LEU:HD21	3:A:1:EMD:C7	0.42	2.42	28	1
1:A:156:PHE:CD2	3:A:1:EMD:C2	0.42	3.03	28	1
1:A:131:ASP:O	1:A:132:ASP:CB	0.42	2.67	30	1
1:A:93:SER:O	1:A:96:GLU:N	0.42	2.49	22	1
1:A:99:ASP:O	1:A:100:LEU:C	0.42	2.63	13	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:GLU:O	1:A:117:LEU:C	0.42	2.62	16	2
1:A:128:ILE:HG23	1:A:132:ASP:CB	0.42	2.45	3	1
1:A:125:GLY:O	1:A:126:GLU:CG	0.42	2.68	26	2
1:A:140:GLY:O	1:A:148:ILE:HG12	0.42	2.14	19	1
1:A:157:MET:HE1	3:A:1:EMD:C9	0.42	2.44	26	1
1:A:143:ASN:O	1:A:144:ASN:HB3	0.42	2.15	27	1
1:A:105:ASP:OD2	1:A:109:ASP:N	0.42	2.44	29	1
1:A:115:GLU:O	1:A:118:LYS:HG2	0.42	2.15	30	1
1:A:140:GLY:HA2	1:A:156:PHE:CD1	0.42	2.50	30	1
1:A:122:GLN:HA	1:A:126:GLU:CA	0.42	2.44	1	1
1:A:143:ASN:OD1	1:A:145:ASP:HB2	0.42	2.13	24	2
1:A:113:ASP:CG	1:A:116:GLU:OE2	0.42	2.63	23	1
1:A:134:GLU:O	1:A:138:LYS:CB	0.42	2.68	25	1
1:A:97:LEU:HG	1:A:154:LEU:HD23	0.42	1.91	28	1
1:A:105:ASP:OD2	1:A:110:GLY:N	0.42	2.51	6	1
1:A:114:LEU:HG	1:A:133:ILE:HG21	0.42	1.91	9	1
1:A:157:MET:CE	1:A:160:VAL:HB	0.42	2.45	15	1
1:A:134:GLU:O	1:A:138:LYS:HB2	0.42	2.14	17	1
1:A:117:LEU:HD21	3:A:1:EMD:H13	0.42	1.91	18	1
1:A:136:LEU:O	1:A:140:GLY:N	0.42	2.52	21	1
1:A:136:LEU:O	1:A:137:MET:C	0.42	2.63	3	1
1:A:141:ASP:CG	1:A:141:ASP:O	0.42	2.60	6	1
1:A:105:ASP:HB2	1:A:112:ILE:CD1	0.42	2.45	8	1
1:A:124:THR:O	1:A:124:THR:CG2	0.42	2.64	13	1
1:A:102:ARG:O	1:A:103:MET:C	0.42	2.63	26	4
1:A:126:GLU:O	1:A:128:ILE:HG12	0.42	2.15	20	1
1:A:102:ARG:C	1:A:104:PHE:N	0.42	2.76	26	1
1:A:126:GLU:CD	3:A:1:EMD:O21	0.41	2.63	5	1
1:A:107:ASN:OD1	1:A:109:ASP:HB3	0.41	2.15	6	1
1:A:136:LEU:C	1:A:136:LEU:CD2	0.41	2.93	16	1
1:A:129:THR:CG2	1:A:132:ASP:OD1	0.41	2.68	23	1
1:A:107:ASN:O	1:A:107:ASN:OD1	0.41	2.37	24	2
1:A:112:ILE:O	1:A:147:ARG:HA	0.41	2.15	1	1
1:A:153:PHE:CD1	3:A:1:EMD:S1	0.41	3.13	17	1
1:A:154:LEU:HD22	1:A:154:LEU:HA	0.41	1.75	25	2
1:A:111:TYR:HB3	1:A:147:ARG:CD	0.41	2.45	6	1
1:A:95:GLU:HG3	1:A:96:GLU:N	0.41	2.30	9	1
1:A:99:ASP:OD1	1:A:99:ASP:N	0.41	2.51	14	1
1:A:153:PHE:CZ	1:A:157:MET:HG3	0.41	2.50	17	1
1:A:152:GLU:O	1:A:156:PHE:HB2	0.41	2.15	24	1
1:A:139:ASP:OD1	1:A:156:PHE:CE1	0.41	2.73	27	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:GLY:HA2	3:A:1:EMD:O2	0.41	2.15	29	1
1:A:126:GLU:O	1:A:127:THR:HG22	0.41	2.15	1	1
1:A:121:LEU:HD13	1:A:128:ILE:CG2	0.41	2.45	10	1
1:A:128:ILE:HD13	1:A:132:ASP:HB3	0.41	1.93	12	1
1:A:117:LEU:CD1	1:A:137:MET:HE3	0.41	2.45	24	1
1:A:113:ASP:C	1:A:115:GLU:N	0.41	2.77	28	1
1:A:121:LEU:O	1:A:126:GLU:HB2	0.41	2.15	28	1
1:A:131:ASP:OD1	1:A:135:GLU:OE2	0.41	2.37	30	1
1:A:126:GLU:O	1:A:127:THR:CB	0.41	2.68	8	1
1:A:143:ASN:HB3	1:A:152:GLU:OE2	0.41	2.16	13	1
1:A:152:GLU:O	1:A:153:PHE:C	0.41	2.63	16	1
1:A:149:ASP:OD1	1:A:152:GLU:HG3	0.41	2.16	1	1
1:A:133:ILE:O	1:A:137:MET:HB3	0.41	2.14	4	1
1:A:118:LYS:HE3	1:A:133:ILE:CG2	0.41	2.45	6	1
1:A:113:ASP:HA	1:A:137:MET:CE	0.41	2.45	23	1
1:A:145:ASP:OD1	1:A:145:ASP:N	0.41	2.49	23	1
1:A:140:GLY:HA3	3:A:1:EMD:C2	0.41	2.45	3	1
1:A:149:ASP:O	1:A:153:PHE:HB2	0.41	2.15	11	2
1:A:99:ASP:O	1:A:102:ARG:N	0.41	2.54	9	1
1:A:104:PHE:CE1	1:A:120:MET:HB2	0.41	2.50	11	1
1:A:121:LEU:HA	1:A:124:THR:OG1	0.41	2.16	11	1
1:A:113:ASP:CG	1:A:116:GLU:HG3	0.41	2.41	2	1
1:A:97:LEU:CD2	1:A:153:PHE:CD2	0.41	3.04	19	1
1:A:100:LEU:HB3	1:A:153:PHE:CE2	0.41	2.51	15	1
1:A:138:LYS:O	1:A:138:LYS:CG	0.41	2.68	16	1
1:A:153:PHE:CE2	1:A:157:MET:HG2	0.41	2.50	16	1
1:A:104:PHE:CD1	1:A:112:ILE:HG21	0.41	2.51	17	1
1:A:151:ASP:O	1:A:154:LEU:HB2	0.41	2.16	21	1
1:A:113:ASP:OD2	1:A:116:GLU:OE2	0.41	2.39	23	1
1:A:114:LEU:C	1:A:118:LYS:HD3	0.41	2.41	30	1
1:A:136:LEU:O	1:A:139:ASP:HB2	0.41	2.15	6	1
1:A:100:LEU:HA	1:A:103:MET:CG	0.41	2.46	9	1
1:A:113:ASP:C	1:A:113:ASP:OD1	0.41	2.62	12	1
1:A:97:LEU:CD2	1:A:154:LEU:HD23	0.41	2.42	13	1
1:A:121:LEU:HD12	1:A:133:ILE:CG1	0.41	2.46	16	1
1:A:104:PHE:CD2	1:A:120:MET:SD	0.41	3.14	19	1
1:A:99:ASP:O	1:A:103:MET:HG3	0.41	2.16	27	1
1:A:114:LEU:O	1:A:118:LYS:CD	0.41	2.69	30	1
1:A:157:MET:O	1:A:159:GLY:N	0.40	2.53	13	2
1:A:97:LEU:O	1:A:99:ASP:N	0.40	2.54	11	1
1:A:144:ASN:OD1	1:A:144:ASN:N	0.40	2.52	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:ASP:OD1	1:A:108:ALA:N	0.40	2.54	17	1
1:A:114:LEU:CD1	1:A:133:ILE:CG2	0.40	2.91	20	1
1:A:122:GLN:O	1:A:126:GLU:HG3	0.40	2.14	24	1
1:A:137:MET:SD	1:A:148:ILE:HD11	0.40	2.55	1	1
1:A:139:ASP:O	1:A:156:PHE:CD1	0.40	2.73	2	1
1:A:161:GLU:OE1	1:A:161:GLU:O	0.40	2.40	2	1
1:A:119:ILE:O	1:A:123:ALA:N	0.40	2.49	5	1
1:A:157:MET:O	1:A:157:MET:HG3	0.40	2.16	10	2
1:A:127:THR:C	1:A:128:ILE:HG12	0.40	2.42	25	1
1:A:143:ASN:C	1:A:144:ASN:ND2	0.40	2.79	6	1
1:A:113:ASP:OD1	1:A:115:GLU:HB2	0.40	2.17	9	1
1:A:107:ASN:ND2	1:A:109:ASP:HB3	0.40	2.30	13	1
1:A:97:LEU:HD23	1:A:153:PHE:CD2	0.40	2.51	19	1
1:A:107:ASN:OD1	1:A:116:GLU:OE2	0.40	2.39	21	1
1:A:127:THR:O	1:A:127:THR:HG22	0.40	2.16	26	1
1:A:149:ASP:OD2	1:A:151:ASP:HB2	0.40	2.16	1	1
1:A:145:ASP:O	1:A:145:ASP:OD1	0.40	2.40	10	1
1:A:140:GLY:O	1:A:148:ILE:HD13	0.40	2.16	13	1
1:A:128:ILE:HG12	1:A:132:ASP:HB3	0.40	1.93	16	1
1:A:126:GLU:CD	1:A:128:ILE:HB	0.40	2.41	17	1
1:A:101:PHE:CD1	1:A:153:PHE:CD2	0.40	3.09	22	1
1:A:146:GLY:O	1:A:147:ARG:HB3	0.40	2.17	26	1
1:A:137:MET:HE1	1:A:146:GLY:C	0.40	2.42	28	1
1:A:110:GLY:C	1:A:111:TYR:CD2	0.40	3.00	9	1
1:A:150:TYR:CE2	1:A:154:LEU:HD21	0.40	2.52	15	1
1:A:130:GLU:O	1:A:133:ILE:HB	0.40	2.17	16	1
1:A:99:ASP:O	1:A:103:MET:HB2	0.40	2.17	18	1
1:A:135:GLU:O	1:A:136:LEU:C	0.40	2.64	25	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	68/71 (96%)	51±4 (75±5%)	15±4 (22±6%)	2±1 (3±2%)	5	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2040/2130 (96%)	1527 (75%)	452 (22%)	61 (3%)	5	38

All 24 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	126	GLU	14
1	A	108	ALA	8
1	A	105	ASP	5
1	A	117	LEU	4
1	A	129	THR	3
1	A	127	THR	3
1	A	124	THR	2
1	A	133	ILE	2
1	A	144	ASN	2
1	A	147	ARG	2
1	A	159	GLY	2
1	A	94	GLU	2
1	A	135	GLU	1
1	A	122	GLN	1
1	A	115	GLU	1
1	A	95	GLU	1
1	A	155	GLU	1
1	A	157	MET	1
1	A	158	LYS	1
1	A	156	PHE	1
1	A	128	ILE	1
1	A	123	ALA	1
1	A	125	GLY	1
1	A	132	ASP	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	62/63 (98%)	42±3 (68±5%)	20±3 (32±5%)	1	14
All	All	1860/1890 (98%)	1265 (68%)	595 (32%)	1	14

All 55 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	117	LEU	30
1	A	132	ASP	22
1	A	100	LEU	20
1	A	136	LEU	19
1	A	97	LEU	19
1	A	130	GLU	18
1	A	93	SER	18
1	A	120	MET	18
1	A	158	LYS	18
1	A	142	LYS	17
1	A	138	LYS	15
1	A	161	GLU	15
1	A	157	MET	15
1	A	155	GLU	14
1	A	126	GLU	14
1	A	137	MET	14
1	A	95	GLU	13
1	A	96	GLU	13
1	A	134	GLU	13
1	A	113	ASP	13
1	A	106	LYS	13
1	A	94	GLU	12
1	A	112	ILE	12
1	A	129	THR	12
1	A	103	MET	11
1	A	99	ASP	11
1	A	114	LEU	10
1	A	118	LYS	10
1	A	135	GLU	10
1	A	150	TYR	10
1	A	127	THR	10
1	A	105	ASP	9
1	A	139	ASP	9
1	A	122	GLN	9
1	A	131	ASP	8
1	A	102	ARG	8
1	A	145	ASP	8
1	A	151	ASP	7
1	A	115	GLU	7
1	A	160	VAL	7
1	A	143	ASN	7

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Mol	Chain	Res	Type	Models (Total)
1	A	147	ARG	6
1	A	154	LEU	6
1	A	98	SER	6
1	A	148	ILE	5
1	A	149	ASP	5
1	A	144	ASN	5
1	A	124	THR	5
1	A	107	ASN	4
1	A	104	PHE	4
1	A	141	ASP	4
1	A	109	ASP	2
1	A	156	PHE	2
1	A	128	ILE	2
1	A	152	GLU	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 oligosaccharides 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	Counts	Bond lengths	
						RMSZ	#Z>2
3	EMD	A	1	-	31,33,33	2.10±0.01	7±1 (21±3%)

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	Counts	Bond angles	
						RMSZ	#Z>2
3	EMD	A	1	-	38,47,47	3.07±0.01	10±0 (26±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	EMD	A	1	-	-	0±0,16,39,39	0±0,3,4,4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	1	EMD	C11-N14	6.79	1.52	1.41	30	30
3	A	1	EMD	C8-C5	6.39	1.57	1.48	10	30
3	A	1	EMD	C15-N14	3.09	1.52	1.47	11	30
3	A	1	EMD	C2-N3	2.73	1.33	1.36	20	30
3	A	1	EMD	C6-S1	2.17	1.81	1.82	21	5
3	A	1	EMD	C19-C18	2.14	1.53	1.50	24	28
3	A	1	EMD	C18-N14	2.12	1.39	1.36	13	22
3	A	1	EMD	O21-C21	2.07	1.40	1.37	7	22
3	A	1	EMD	O22-C22	2.05	1.40	1.37	5	7

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

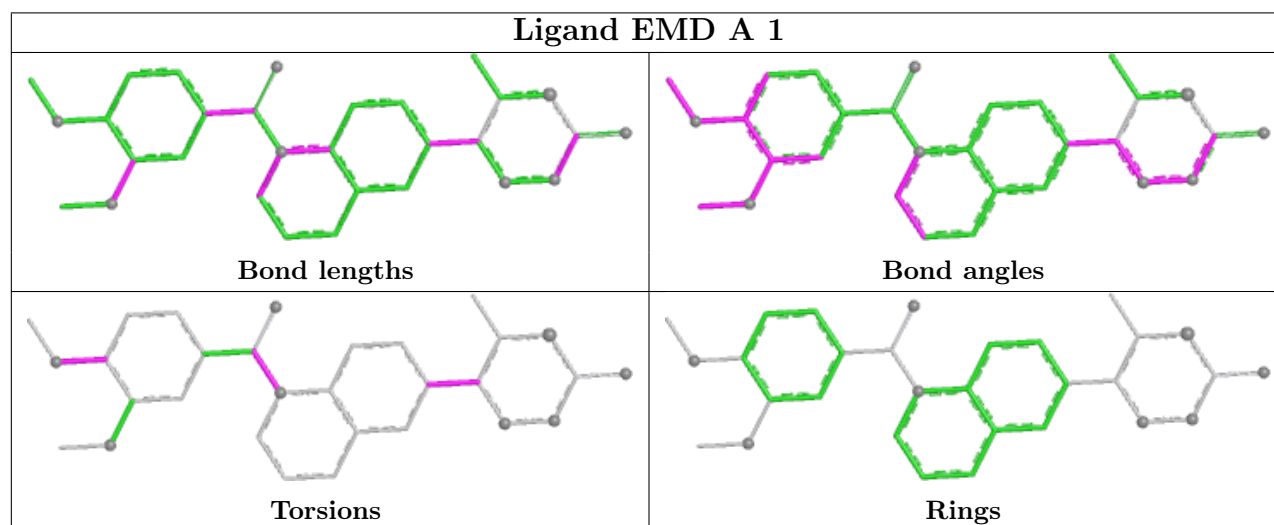
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
3	A	1	EMD	C5-N4-N3	14.07	133.33	117.20	7	30
3	A	1	EMD	O22-C22-C21	5.25	122.52	115.40	13	30
3	A	1	EMD	O21-C21-C22	5.03	122.23	115.40	23	30
3	A	1	EMD	C25-O21-C21	4.86	124.65	117.51	17	30
3	A	1	EMD	C26-O22-C22	4.82	124.58	117.51	12	30
3	A	1	EMD	O22-C22-C23	4.18	117.26	124.30	13	30
3	A	1	EMD	C16-C15-N14	3.75	116.85	109.95	20	30
3	A	1	EMD	O21-C21-C20	3.75	117.62	124.08	23	30
3	A	1	EMD	C8-C5-N4	3.41	119.94	117.03	13	30
3	A	1	EMD	C2-N3-N4	2.21	124.57	126.87	8	30
3	A	1	EMD	C19-C18-N14	2.14	121.74	118.29	13	4

There are no chirality outliers.

There are no torsion outliers.

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 than 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.



6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided