Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1LXF
Title	:	Structure of the Regulatory N-domain of Human Cardiac Troponin C in Complex with Human Cardiac Troponin-I(147-163) and Bepridil
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Deposited on	:	2002-06-05

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

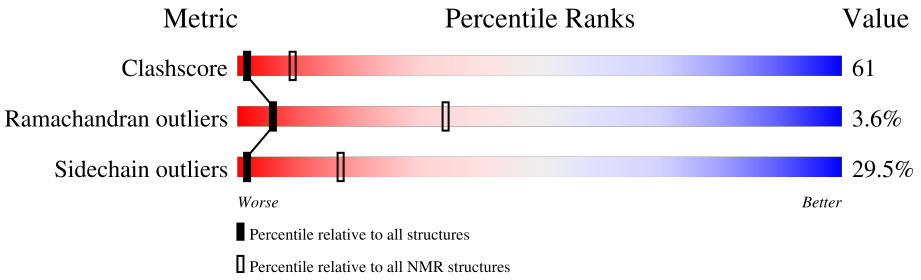
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	C	89	19% 64% 9% 8%
2	I	17	12% 35% 12% 41%

2 Ensemble composition and analysis (i)

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

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

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

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

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

The models can be grouped into 4 clusters and 7 single-model clusters were found.

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

3 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1687 atoms, of which 837 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	C	89	1364	432	666	107	150	9	0

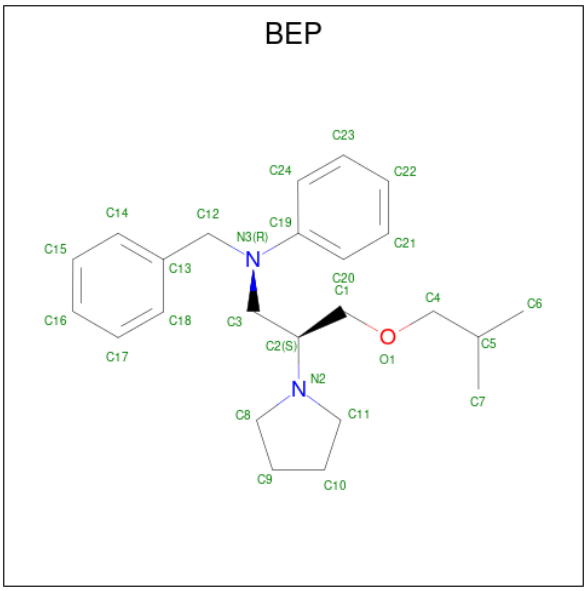
- Molecule 2 is a protein called Troponin I, cardiac muscle.

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

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

Mol	Chain	Residues	Atoms	
			Total	Ca
3	C	1	1	1

- Molecule 4 is 1-ISOBUTOXY-2-PYRROLIDINO-3[N-BENZYLANILINO] PROPANE (three-letter code: BEP) (formula: $C_{24}H_{34}N_2O$).



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

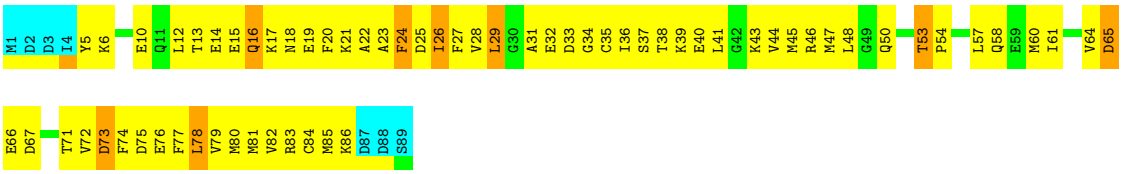
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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 C: 19% 64% 9% 8%



• Molecule 2: Troponin I, cardiac muscle

Chain I: 12% 35% 12% 41%

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 C: 35% 42% 16% 8%

• Molecule 2: Troponin I, cardiac muscle

Chain I: 6% 35% 18% 41%

R147 I148 S149 A150 D151 A152 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.2 Score per residue for model 2

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

Chain C: 28% 47% 16% • 8%

M1 D2 D3 I4 Y5 K6 V9 E10 Q11 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M47 L48 N51 P52 T53 P54 L57 Q58 E59 M60 E63 V64 S69

G70 T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 K86 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 29% 24% 6% 41%

R147 I148 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.3 Score per residue for model 3

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

Chain C: 36% 42% 15% 8%

M1 D2 D3 I4 Y5 K6 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 S37 T38 K39 E40 K43 V44 M45 R46 M47 L48 G49 Q50 N51 P52 T53 P54 L57 Q58 E59 M60 I61 V64 D65 E66

T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 24% 24% 12% 41%

R147 I148 S149 A150 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.4 Score per residue for model 4

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

Chain C: 27% 51% 15% 8%

M1 D2 D3 I4 Y5 K6 A7 A8 V9 E10 Q11 L12 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 M47 L48 G49 Q50 T53 P54 E55 E56 L57 Q58 E59 M60 I61 V64

D65 E66 D67 G68 S69 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 C84 M85 K86 D87 D88 S89

• Molecule 2: Troponin I, cardiac muscle

Chain I: 12% 35% 12% 41%

R147 I148 S149 A150 D151 A152 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.5 Score per residue for model 5

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

Chain C: 21% 53% 18% 8%

M1 D2 D3 I4 Y5 K6 A7 E10 Q11 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 M47 L48 N51 P52 T53 P54 L57 Q58 E59 M60 I61 V64 D65

E66 D67 G68 S69 G70 T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 C84 M85 K86 D87 D88 S89

• Molecule 2: Troponin I, cardiac muscle

Chain I: 12% 35% 12% 41%

R147 I148 S149 A150 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.6 Score per residue for model 6

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

Chain C: 33% 47% 12% 8%

M1 D2 D3 I4 Y5 V9 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 M47 L48 T53 L57 Q58 E59 M60 I61 D62 E63 V64 D65 E66 D67

G70 T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 D87 D88 S89

• Molecule 2: Troponin I, cardiac muscle

Chain I: 18% 35% 6% 41%

R147 I148 S149 A150 D151 A152 M153 M154 L157 L158 G159 A160 R161 A162 K163

4.2.7 Score per residue for model 7

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

Chain C: 27% 49% 15% • 8%

M1 D2 D3 I4 Y5 K6 E10 Q11 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 D33 G34 C35 I36 S37 T38 L41 G42 K43 V44 M45 R46 M47 L48 G49 Q50 N51 P52 T53 P54 L57 M60 I61 D62 E63 V64 D65 E66 D67

V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 C84 M85 K86 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 12% 24% 18% 6% 41%

R147 I148 S149 A150 D151 A152 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.8 Score per residue for model 8

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

Chain C: 31% 44% 17% 8%

M1 D2 D3 I4 Y5 K6 A7 E10 Q11 L12 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 D33 G34 C35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 M47 L48 N51 P52 T53 P54 L57 M60 I61 D62 E63 V64 D65 V72 D73

F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 C84 M85 K86 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 6% 35% 18% 41%

R147 I148 S149 A150 D151 A152 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.9 Score per residue for model 9

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

Chain C: 27% 51% 12% • 8%

M1 D2 D3 I4 Y5 K6 E10 Q11 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 M47 L48 G49 T53 P54 E55 E56 L57 M60 I61 V64 D65 E66

D67 V72 D73 F74 D75 E76 F77 L78 V79 M80 R83 K86 D87 D88 S89

• Molecule 2: Troponin I, cardiac muscle

Chain I: 18% 12% 29% 41%

R147 I148 S149 A150 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.10 Score per residue for model 10

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

Chain C: 30% 48% 13% 8%

M1 D2 D3 I4 Y5 K6 A7 A8 V9 E10 Q11 L12 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 D33 G34 C35 I36 S37 T38 K39 E40 L41 V44 M45 R46 M47 L48 G49 T53 P54 L57 Q58 E59 M60 I61 D62 E63 V64 D65 V72 D73

F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 C84 M85 K86 D87 D88 S89

• Molecule 2: Troponin I, cardiac muscle

Chain I: 12% 35% 12% 41%

R147 I148 S149 A150 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.11 Score per residue for model 11

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

Chain C: 28% 43% 21% 8%

M1 D2 D3 I4 Y5 K6 A7 A8 V9 E10 Q11 L12 T13 E14 E15 Q16 K17 N18 E19 F20 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 E40 L41 G42 K43 V44 M45 R46 M47 L48 G49 Q50 N51 P52 T53 P54 L57 Q58 E59 M60 I61 D62 E63 V64

D65 E66 D67 T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 C84 M85 K86 D87 D88 S89

• Molecule 2: Troponin I, cardiac muscle

Chain I: 6% 29% 24% 41%

R147 I148 S149 A150 D151 A152 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.12 Score per residue for model 12

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

Chain C: 26% 48% 18% 8%

M1 D2 D3 I4 Y5 K6 V9 E10 Q11 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 V44 M47 L48 T53 P54 L57 Q58 E59 M60 I61 D62 E63 V64 D65 E66 D67

G68 S69 G70 T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 C84 M85 K86 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 18% 35% 6% 41%

R147 I148 D151 A152 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.13 Score per residue for model 13

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

Chain C: 31% 44% 16% • 8%

M1 D2 D3 I4 Y5 K6 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 E40 L41 V44 M45 R46 M47 L48 N51 P52 T53 P54 E55 E56 L57 Q58 E59 M60 I61 D62 E63 V64 D65 E66 D67 G68 S69

V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 M85 K86 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 18% 29% 12% 41%

R147 I148 S149 A150 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.14 Score per residue for model 14

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

Chain C: 33% 44% 16% 8%

M1 D2 D3 I4 Y5 K6 V9 E10 Q11 L12 T13 E14 E15 Q16 K17 N18 E19 F20 A23 F24 D25 I26 F27 V28 L29 D33 G34 C35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 M47 L48 G49 Q50 T53 P54 L57 M60 I61 D62 E63 V64 D65 E66 D67

G68 S69 G70 T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 K86 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 24% 24% 12% 41%

R147 I148 S149 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.15 Score per residue for model 15

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

Chain C: 35% 43% 15% 8%

M1 D2 D3 I4 Y5 K6 V9 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 D33 G34 C35 I36 S37 L41 G42 K43 V44 M45 R46 M47 L48 G49 Q50 T53 P54 L57 M60 I61 D62 E63 V64 D65 T71 V72 D73

F74 D75 E76 F77 L78 V79 M80 M81 C84 M85 K86 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 12% 35% 12% 41%

R147 I148 S149 A150 D151 A152 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.16 Score per residue for model 16

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

Chain C: 28% 53% 11% 8%

M1 D2 D3 I4 Y5 K6 V9 E10 Q11 L12 T13 E14 E15 Q16 K17 N18 E19 A22 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 M47 L48 T53 P54 L57 Q58 E59 M60 I61 D62 E63 V64 D65 E66

D67 G70 T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 C84 M85 K86 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 12% 24% 24% 41%

R147 I148 S149 A150 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.17 Score per residue for model 17

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

Chain C: 28% 47% 17% 8%

M1 D2 D3 I4 Y5 K6 E10 Q11 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 M47 L48 G49 Q50 N51 P52 T53 P54 Q58 E59 M60 I61 D62 E63 V64

D65 E66 D67 G68 S69 G70 T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 12% 24% 24% 41%

R147 I148 S149 A150 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.18 Score per residue for model 18

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

Chain C: 26% 45% 21% 8%

M1 D2 D3 I4 Y5 K6 A7 E10 Q11 L12 T13 E14 E15 Q16 K17 N18 E19 F20 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 M47 L48 G49 Q50 N51 P52 T53 P54 E55 E56 L57 Q58 E59 M60 I61 D62

E63 V64 D65 E66 D67 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 C84 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 18% 41% 41%

R147 I148 S149 A150 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.19 Score per residue for model 19

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

Chain C: 24% 51% 18% 8%

M1 D2 D3 I4 Y5 K6 A7 Q11 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 M47 L48 G49 T53 P54 E55 E56 L57 Q58 E59 M60 I61 D62 E63 V64

D65 E66 D67 G68 S69 G70 T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 C84 M85 K86 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 6% 35% 12% 6% 41%

R147 I148 S149 A150 D151 A152 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.20 Score per residue for model 20

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

Chain C: 25% 52% 15% • 8%

M1 D2 D3 I4 Y5 K6 A7 E10 Q11 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 M47 L48 G49 Q50 T53 P54 E55 E56 L57 Q58 I61 D62 E63

V64 D65 E66 D67 G68 S69 G70 T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 C84 M85 K86 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 24% 18% 18% 41%

R147 I148 S149 A150 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.21 Score per residue for model 21

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

Chain C: 31% 40% 20% 8%

M1 D2 D3 I4 Y5 K6 A7 E10 Q11 L12 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 M47 L48 T53 L57 Q58 E59 M60 I61 D62 E63 V64 D65 E66 D67 G68 S69

V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 18% 29% 12% 41%

R147 I148 S149 A150 D151 A152 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.22 Score per residue for model 22

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

Chain C: 29% 46% 16% • 8%

M1 D2 D3 I4 Y5 K6 E10 Q11 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 M47 L48 G49 T53 P54 L57 M60 I61 D62 E63 V64 D65 E66

V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 C84 M85 K86 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 18% 29% 12% 41%

R147 I148 A152 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.23 Score per residue for model 23

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

Chain C: 24% 49% 19% 8%

M1 D2 D3 I4 Y5 K6 L12 T13 E14 E15 Q16 K17 N18 K21 A22 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 M47 L48 G49 Q50 N51 P52 T53 P54 L57 Q58 E59 M60 I61 V64 D65 G70

T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 C84 M85 K86 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 35% 24% 41%

R147 I148 S149 A150 D151 A152 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.24 Score per residue for model 24

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

Chain C: 28% 47% 17% 8%

M1 D2 D3 I4 Y5 K6 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 D33 G34 C35 I36 S37 T38 L41 G42 K43 V44 M45 R46 M47 L48 G49 Q50 T53 P54 E55 E56 L57 Q58 E59 M60 I61 D65 E66 D67 G70 T71

V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 C84 M85 K86 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 24% 29% 6% 41%

R147 I148 S149 A150 M153 A156 L157 L158 G159 A160 R161 A162 K163

4.2.25 Score per residue for model 25

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

Chain C: 24% 52% 16% • 8%

M1 D2 D3 I4 Y5 K6 A7 A8 V9 E10 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 V44 M45 R46 M47 L48 G49 Q50 T53 P54 E55 E56 L57 Q58 E59 M60 I61 V64

D65 E66 T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 29% 18% 12% 41%

R147 I148 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.26 Score per residue for model 26

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

Chain C: 25% 47% 19% • 8%

M1 D2 D3 I4 Y5 K6 V9 E10 Q11 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 G42 K43 V44 M45 R46 M47 L48 G49 Q50 N51 P52 T53 P54 E55 E56 L57 M60 I61 D62 E63

V64 D65 E66 T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 C84 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 24% 35% 41%

R147 I148 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.27 Score per residue for model 27

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

Chain C: 30% 52% 9% • 8%

M1 D2 D3 I4 Y5 K6 A7 E10 Q11 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 D33 G34 C35 I36 K39 E40 L41 V44 M45 R46 M47 L48 G49 Q50 T53 P54 L57 Q58 E59 M60 I61 D62 E63 V64 D65 G70 T71 V72 D73

F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 C84 M85 K86 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 12% 35% 12% 41%

R147 I148 S149 A150 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.28 Score per residue for model 28

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

Chain C: 28% 49% 15% 8%

M1 D2 D3 I4 Y5 K6 A7 E10 Q11 L12 T13 Q16 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 V44 M45 R46 M47 L48 G49 Q50 N51 P52 T53 P54 L57 Q58 E59 M60 I61 D62 E63 V64 D65 E66

D67 T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 K86 D87 D88 S89

- Molecule 2: Troponin I, cardiac muscle

Chain I: 6% 29% 18% 6% 41%

R147 I148 S149 A150 D151 A152 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.29 Score per residue for model 29 (medoid)

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

Chain C: 26% 54% 11% • 8%

M1 D2 D3 I4 Y5 K6 A7 A8 V9 E10 Q11 L12 Q16 K17 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 V44 M45 R46 M47 L48 G49 Q50 T53 P54 L57 Q58 E59 M60 E63 V64 D65 E66 D67

T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 K86 D87 D88 S89

• Molecule 2: Troponin I, cardiac muscle

Chain I: 6% 29% 24% 41%

R147 I148 S149 A150 D151 A152 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

4.2.30 Score per residue for model 30

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

Chain C: 26% 47% 18% • 8%

M1 D2 D3 I4 Y5 L12 T13 E14 E15 Q16 K17 N18 E19 F20 K21 A22 A23 F24 D25 I26 F27 V28 L29 G30 A31 E32 D33 G34 C35 I36 S37 T38 K39 E40 L41 V44 M45 R46 M47 Q50 N51 P52 T53 P54 E55 E56 L57 M60 I61 D62 E63 V64 D65 E66 D67

G70 T71 V72 D73 F74 D75 E76 F77 L78 V79 M80 M81 V82 R83 C84 M85 K86 D87 D88 S89

• Molecule 2: Troponin I, cardiac muscle

Chain I: 18% 29% 12% 41%

R147 I148 S149 A150 M153 M154 Q155 A156 L157 L158 G159 A160 R161 A162 K163

5 Refinement protocol and experimental data overview (i)

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

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

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

Software name	Classification	Version
X-PLOR	refinement	3.85

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, BEP

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (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	C	643	623	622	78±10
2	I	70	72	72	18±5
4	C	27	34	34	12±4
All	All	22230	21870	21847	2678

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 61.

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

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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:36:ILE:HD11	1:C:77:PHE:CE2	0.89	2.02	5	2
4:C:92:BEP:N2	2:I:148:ILE:HD11	0.88	1.83	5	5
1:C:29:LEU:O	1:C:29:LEU:HD12	0.88	1.69	11	11
1:C:36:ILE:HD11	1:C:77:PHE:CG	0.87	2.05	23	3
1:C:36:ILE:O	1:C:71:THR:HG22	0.86	1.70	12	3
1:C:41:LEU:HD23	1:C:57:LEU:CD2	0.86	2.00	26	9
1:C:26:ILE:HD13	2:I:157:LEU:HD21	0.86	1.45	27	1
1:C:57:LEU:HD23	1:C:60:MET:SD	0.86	2.10	11	6
1:C:36:ILE:HG21	1:C:41:LEU:HD21	0.86	1.46	16	1
1:C:26:ILE:CG2	1:C:44:VAL:HG22	0.86	2.01	27	4
1:C:64:VAL:HG13	1:C:80:MET:SD	0.86	2.10	18	8
1:C:28:VAL:HG11	1:C:34:GLY:C	0.85	1.92	28	16
1:C:5:TYR:O	1:C:9:VAL:HG22	0.85	1.71	25	3
1:C:48:LEU:HD23	2:I:152:ALA:O	0.85	1.71	4	1
4:C:92:BEP:H181	2:I:148:ILE:HD13	0.85	1.48	5	2
1:C:38:THR:HG22	1:C:61:ILE:HG13	0.85	1.47	4	8
2:I:156:ALA:C	2:I:157:LEU:HD13	0.84	1.92	30	6
2:I:156:ALA:C	2:I:157:LEU:HD22	0.84	1.93	27	5
1:C:48:LEU:CD2	2:I:156:ALA:HB2	0.84	2.03	17	8
1:C:23:ALA:CB	2:I:157:LEU:HD21	0.83	2.02	6	5
1:C:12:LEU:HD13	1:C:16:GLN:CD	0.83	1.92	28	12
2:I:156:ALA:O	2:I:157:LEU:HD13	0.83	1.74	8	6
1:C:27:PHE:CE2	1:C:28:VAL:HG13	0.82	2.09	18	1
2:I:157:LEU:N	2:I:157:LEU:HD13	0.82	1.89	15	2
1:C:12:LEU:HD13	1:C:16:GLN:NE2	0.82	1.89	21	15
1:C:72:VAL:HG21	4:C:92:BEP:H221	0.81	1.50	10	10
2:I:157:LEU:HD13	2:I:157:LEU:N	0.81	1.89	20	4
1:C:24:PHE:O	1:C:28:VAL:HG22	0.80	1.76	5	17
1:C:26:ILE:HD11	2:I:157:LEU:HD11	0.80	1.52	3	4
1:C:36:ILE:HD12	1:C:72:VAL:HB	0.80	1.52	30	3
1:C:26:ILE:HG13	2:I:157:LEU:HD12	0.80	1.49	30	5
1:C:41:LEU:HD11	4:C:92:BEP:C23	0.80	2.07	16	1
1:C:74:PHE:CE1	1:C:78:LEU:HD11	0.79	2.11	20	2
1:C:12:LEU:HD22	1:C:16:GLN:OE1	0.79	1.76	30	6
2:I:157:LEU:HD22	2:I:157:LEU:N	0.79	1.93	29	6
1:C:19:GLU:O	2:I:157:LEU:HD23	0.79	1.78	22	2
1:C:27:PHE:CD1	1:C:28:VAL:HG13	0.78	2.13	30	4
2:I:153:MET:O	2:I:157:LEU:HD21	0.78	1.79	30	3
1:C:74:PHE:CZ	1:C:78:LEU:HD11	0.78	2.13	20	5
1:C:48:LEU:HD11	2:I:156:ALA:HB2	0.77	1.53	15	5
1:C:36:ILE:HD11	1:C:77:PHE:CD2	0.77	2.15	27	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:92:BEP:H81	4:C:92:BEP:H63	0.77	1.56	5	1
1:C:47:MET:HE2	2:I:156:ALA:HB1	0.77	1.55	18	9
1:C:28:VAL:HB	1:C:31:ALA:HB3	0.76	1.55	16	10
1:C:48:LEU:HB3	2:I:152:ALA:HB1	0.76	1.56	11	1
2:I:153:MET:O	2:I:157:LEU:HD23	0.76	1.80	3	1
1:C:23:ALA:HA	2:I:157:LEU:HD11	0.74	1.57	8	6
4:C:92:BEP:H73	4:C:92:BEP:H111	0.74	1.57	23	1
4:C:92:BEP:C17	2:I:148:ILE:HD11	0.74	2.13	7	1
1:C:64:VAL:HG21	1:C:72:VAL:HG22	0.74	1.59	13	10
1:C:41:LEU:HD21	4:C:92:BEP:C21	0.74	2.10	1	2
1:C:26:ILE:O	1:C:29:LEU:HD22	0.74	1.81	18	3
1:C:77:PHE:CE1	1:C:81:MET:HE1	0.74	2.18	20	2
1:C:48:LEU:CD1	2:I:156:ALA:HB2	0.73	2.13	12	8
2:I:148:ILE:HG23	2:I:148:ILE:O	0.73	1.83	22	4
1:C:29:LEU:HD23	1:C:29:LEU:O	0.73	1.84	10	3
1:C:48:LEU:N	1:C:48:LEU:HD23	0.73	1.98	27	9
1:C:26:ILE:HG22	1:C:44:VAL:HG23	0.73	1.60	22	1
2:I:156:ALA:C	2:I:157:LEU:HD23	0.72	2.05	13	5
1:C:53:THR:HG22	1:C:54:PRO:CD	0.72	2.14	19	13
1:C:41:LEU:HD22	4:C:92:BEP:C21	0.72	2.15	11	3
1:C:5:TYR:CD2	1:C:79:VAL:HG13	0.72	2.20	5	6
1:C:12:LEU:HD13	1:C:16:GLN:OE1	0.72	1.85	9	4
1:C:22:ALA:HB3	2:I:157:LEU:HD13	0.72	1.60	21	3
4:C:92:BEP:H21	2:I:148:ILE:HD11	0.71	1.61	29	6
1:C:47:MET:O	1:C:48:LEU:HD12	0.71	1.85	21	3
1:C:47:MET:C	1:C:48:LEU:HD23	0.71	2.05	14	5
2:I:157:LEU:N	2:I:157:LEU:HD23	0.71	2.00	5	3
1:C:22:ALA:HB1	2:I:157:LEU:CB	0.71	2.16	27	1
1:C:78:LEU:O	1:C:82:VAL:HG23	0.71	1.86	27	8
1:C:27:PHE:CE1	1:C:28:VAL:HG13	0.71	2.20	30	4
1:C:24:PHE:CE2	1:C:77:PHE:CD2	0.71	2.79	14	11
1:C:41:LEU:HB3	1:C:57:LEU:HD22	0.71	1.62	2	1
1:C:41:LEU:HD12	1:C:57:LEU:CD2	0.70	2.15	16	1
4:C:92:BEP:H62	4:C:92:BEP:H11	0.70	1.61	18	1
1:C:26:ILE:CD1	2:I:157:LEU:HD21	0.70	2.15	27	1
1:C:28:VAL:HG12	1:C:35:CYS:O	0.70	1.86	19	19
1:C:26:ILE:HD11	2:I:157:LEU:CD1	0.70	2.16	14	5
4:C:92:BEP:H141	2:I:148:ILE:HD13	0.70	1.64	8	1
1:C:29:LEU:HD22	1:C:29:LEU:C	0.70	2.06	29	3
1:C:48:LEU:HD23	1:C:48:LEU:N	0.70	2.00	14	1
1:C:48:LEU:HD21	2:I:156:ALA:HB2	0.70	1.64	20	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:I:157:LEU:HD23	2:I:157:LEU:N	0.70	2.02	13	3
1:C:24:PHE:CD1	1:C:27:PHE:CZ	0.69	2.80	29	2
1:C:24:PHE:CZ	1:C:77:PHE:CD2	0.69	2.80	6	15
1:C:26:ILE:HG13	2:I:157:LEU:HD22	0.69	1.63	16	2
1:C:27:PHE:CE1	1:C:28:VAL:HG22	0.69	2.22	30	5
1:C:22:ALA:HB3	2:I:157:LEU:HD23	0.69	1.64	12	4
1:C:44:VAL:O	1:C:48:LEU:HD12	0.69	1.88	4	1
1:C:27:PHE:CD2	1:C:28:VAL:HG13	0.69	2.23	18	1
1:C:36:ILE:HD12	4:C:92:BEP:H231	0.69	1.64	4	1
1:C:29:LEU:HD13	1:C:29:LEU:C	0.69	2.09	6	3
1:C:27:PHE:CE1	1:C:44:VAL:HG21	0.69	2.22	24	4
1:C:28:VAL:HG11	1:C:34:GLY:CA	0.69	2.18	28	6
1:C:64:VAL:HG13	1:C:80:MET:HG3	0.68	1.65	2	4
4:C:92:BEP:C18	2:I:148:ILE:HD13	0.68	2.17	5	1
1:C:26:ILE:HG22	1:C:44:VAL:CG2	0.68	2.05	10	2
1:C:24:PHE:CE2	1:C:74:PHE:CE1	0.68	2.81	10	9
1:C:29:LEU:HD23	1:C:30:GLY:N	0.68	2.03	21	3
1:C:24:PHE:CE2	1:C:74:PHE:CD2	0.68	2.81	27	2
1:C:27:PHE:CZ	1:C:44:VAL:HG11	0.68	2.23	1	1
4:C:92:BEP:C14	2:I:148:ILE:HD11	0.68	2.17	15	1
1:C:53:THR:O	1:C:57:LEU:HD12	0.68	1.87	26	1
1:C:22:ALA:O	1:C:26:ILE:HD11	0.68	1.89	16	1
1:C:41:LEU:HD11	4:C:92:BEP:C15	0.68	2.19	23	2
1:C:48:LEU:HD22	2:I:156:ALA:HA	0.68	1.64	27	1
1:C:27:PHE:CD2	1:C:77:PHE:CZ	0.68	2.81	23	3
1:C:27:PHE:CE2	1:C:77:PHE:CZ	0.67	2.81	3	7
1:C:23:ALA:HB1	1:C:27:PHE:CZ	0.67	2.24	22	5
4:C:92:BEP:H31	2:I:148:ILE:HD11	0.67	1.65	26	3
1:C:47:MET:CE	2:I:156:ALA:HB1	0.67	2.20	22	9
1:C:60:MET:HE2	4:C:92:BEP:N3	0.67	2.04	16	2
1:C:44:VAL:HG12	1:C:48:LEU:HD13	0.67	1.64	1	2
1:C:48:LEU:HD13	2:I:153:MET:CB	0.67	2.19	14	1
1:C:48:LEU:HD13	2:I:153:MET:HA	0.67	1.67	18	2
1:C:63:GLU:OE2	4:C:92:BEP:H62	0.66	1.89	2	1
1:C:24:PHE:CD1	1:C:77:PHE:CE2	0.66	2.83	5	1
2:I:153:MET:O	2:I:157:LEU:HD11	0.66	1.90	30	2
1:C:26:ILE:HD11	2:I:157:LEU:HD12	0.66	1.67	8	1
1:C:12:LEU:HD13	1:C:16:GLN:CG	0.66	2.20	24	3
1:C:26:ILE:O	1:C:29:LEU:HD23	0.66	1.90	1	5
1:C:12:LEU:HD13	1:C:16:GLN:HG2	0.66	1.66	24	3
1:C:24:PHE:CZ	1:C:74:PHE:CD1	0.66	2.84	22	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:22:ALA:HB1	2:I:157:LEU:HB2	0.66	1.67	27	2
1:C:41:LEU:HD11	4:C:92:BEP:C17	0.66	2.21	22	1
1:C:27:PHE:HE1	1:C:44:VAL:HG11	0.66	1.44	13	3
4:C:92:BEP:H72	4:C:92:BEP:H111	0.66	1.65	29	1
4:C:92:BEP:H141	2:I:148:ILE:HD11	0.65	1.67	15	1
1:C:45:MET:HE3	4:C:92:BEP:H82	0.65	1.68	19	1
1:C:24:PHE:CD2	1:C:74:PHE:CE1	0.65	2.84	3	2
2:I:149:SER:O	2:I:150:ALA:HB3	0.65	1.92	17	14
1:C:26:ILE:HD12	1:C:26:ILE:N	0.65	2.06	27	4
1:C:45:MET:HE1	4:C:92:BEP:C15	0.65	2.21	5	1
1:C:23:ALA:HB1	2:I:153:MET:HE3	0.64	1.67	17	1
1:C:27:PHE:CE2	1:C:28:VAL:CG1	0.64	2.80	18	1
2:I:149:SER:O	2:I:150:ALA:HB2	0.64	1.92	4	6
1:C:27:PHE:HD1	1:C:44:VAL:HG21	0.64	1.50	20	3
1:C:12:LEU:HD22	1:C:16:GLN:NE2	0.64	2.07	12	1
4:C:92:BEP:C2	2:I:148:ILE:HD11	0.64	2.22	19	4
1:C:36:ILE:HD12	1:C:72:VAL:CB	0.64	2.22	30	2
4:C:92:BEP:C4	2:I:148:ILE:HD11	0.64	2.23	6	1
1:C:47:MET:C	1:C:48:LEU:HD12	0.64	2.13	21	3
1:C:36:ILE:HG21	1:C:41:LEU:CD2	0.64	2.23	16	2
4:C:92:BEP:H21	2:I:148:ILE:HD13	0.63	1.69	2	3
1:C:74:PHE:O	1:C:78:LEU:HD23	0.63	1.92	5	1
1:C:77:PHE:CE1	1:C:81:MET:CE	0.63	2.81	20	3
1:C:74:PHE:CE2	1:C:78:LEU:CD1	0.63	2.81	25	2
4:C:92:BEP:C2	2:I:148:ILE:HD13	0.63	2.23	2	2
1:C:24:PHE:CZ	1:C:74:PHE:CD2	0.63	2.87	2	1
1:C:64:VAL:HG21	1:C:72:VAL:CG1	0.63	2.23	20	3
1:C:24:PHE:CD2	1:C:74:PHE:CE2	0.63	2.87	1	4
1:C:27:PHE:CZ	1:C:28:VAL:CG2	0.63	2.82	26	3
1:C:24:PHE:CE1	1:C:74:PHE:CD1	0.63	2.86	29	1
1:C:48:LEU:HD12	2:I:156:ALA:HB2	0.62	1.69	12	2
1:C:27:PHE:HA	1:C:44:VAL:HG21	0.62	1.70	28	5
1:C:38:THR:O	1:C:57:LEU:HD12	0.62	1.94	29	1
1:C:23:ALA:N	2:I:157:LEU:HD13	0.62	2.09	2	2
1:C:38:THR:HG22	1:C:58:GLN:HA	0.62	1.70	10	6
1:C:63:GLU:OE1	4:C:92:BEP:H62	0.62	1.94	21	1
1:C:41:LEU:HD22	4:C:92:BEP:C20	0.62	2.24	7	9
1:C:29:LEU:HD12	1:C:29:LEU:C	0.62	2.14	11	5
2:I:157:LEU:N	2:I:157:LEU:CD1	0.62	2.62	15	5
1:C:24:PHE:CE1	1:C:27:PHE:CZ	0.62	2.88	29	1
1:C:44:VAL:HG12	1:C:48:LEU:CD1	0.61	2.24	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:24:PHE:CE1	1:C:74:PHE:CD2	0.61	2.89	2	2
1:C:53:THR:HG22	1:C:54:PRO:HD3	0.61	1.71	19	1
1:C:24:PHE:CE2	1:C:74:PHE:CD1	0.61	2.88	24	10
1:C:27:PHE:CE1	1:C:28:VAL:CG1	0.61	2.83	14	4
1:C:48:LEU:HD21	2:I:153:MET:HA	0.61	1.71	2	5
1:C:24:PHE:CZ	1:C:77:PHE:CE2	0.61	2.88	14	1
1:C:74:PHE:CG	1:C:74:PHE:O	0.61	2.53	4	6
1:C:45:MET:HE2	4:C:92:BEP:C16	0.61	2.25	28	2
1:C:41:LEU:HD21	1:C:57:LEU:HD22	0.61	1.72	14	1
1:C:23:ALA:HB1	1:C:27:PHE:CE1	0.61	2.30	27	1
2:I:156:ALA:CB	2:I:157:LEU:HD22	0.61	2.26	27	1
2:I:156:ALA:C	2:I:157:LEU:HD12	0.61	2.16	26	3
2:I:153:MET:O	2:I:157:LEU:HD13	0.61	1.96	22	6
1:C:64:VAL:HG21	1:C:72:VAL:HG13	0.61	1.73	15	10
1:C:60:MET:HE1	4:C:92:BEP:H32	0.61	1.73	27	1
2:I:157:LEU:CD1	2:I:157:LEU:N	0.60	2.64	26	11
1:C:24:PHE:CE2	1:C:78:LEU:HD12	0.60	2.31	18	2
1:C:74:PHE:CZ	1:C:78:LEU:HD13	0.60	2.31	25	1
1:C:64:VAL:CG2	1:C:72:VAL:HG22	0.60	2.27	4	9
1:C:36:ILE:CD1	1:C:77:PHE:CD2	0.60	2.85	7	3
1:C:24:PHE:O	1:C:27:PHE:CE1	0.60	2.55	18	3
1:C:74:PHE:CD2	1:C:74:PHE:O	0.60	2.55	29	11
1:C:48:LEU:HD22	2:I:153:MET:HA	0.60	1.74	14	2
1:C:53:THR:CB	1:C:54:PRO:CD	0.60	2.80	24	27
1:C:75:ASP:O	1:C:79:VAL:HG23	0.60	1.96	27	2
1:C:84:CYS:SG	4:C:92:BEP:H72	0.60	2.37	19	1
1:C:27:PHE:CE1	1:C:28:VAL:CG2	0.60	2.85	29	4
1:C:41:LEU:HD21	4:C:92:BEP:H122	0.60	1.74	27	1
1:C:80:MET:HE2	4:C:92:BEP:H32	0.60	1.71	1	2
1:C:23:ALA:HB1	2:I:153:MET:CE	0.60	2.26	17	1
1:C:77:PHE:CD1	1:C:81:MET:CE	0.60	2.85	23	1
1:C:61:ILE:CD1	1:C:61:ILE:N	0.59	2.65	1	14
2:I:157:LEU:N	2:I:157:LEU:HD12	0.59	2.13	17	7
1:C:5:TYR:CE1	1:C:79:VAL:HG13	0.59	2.31	17	1
1:C:74:PHE:O	1:C:78:LEU:HD12	0.59	1.97	28	1
1:C:27:PHE:CD1	1:C:44:VAL:CG2	0.59	2.84	9	5
1:C:26:ILE:HG21	1:C:44:VAL:HG23	0.59	1.73	22	2
1:C:44:VAL:CG1	1:C:45:MET:N	0.59	2.66	22	4
1:C:24:PHE:O	1:C:27:PHE:CE2	0.59	2.56	26	2
1:C:27:PHE:CZ	1:C:28:VAL:HG22	0.59	2.32	14	3
1:C:80:MET:CE	4:C:92:BEP:C23	0.59	2.81	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:41:LEU:CD2	4:C:92:BEP:C21	0.59	2.80	11	2
1:C:74:PHE:O	1:C:74:PHE:CD1	0.59	2.56	1	8
1:C:48:LEU:HD13	2:I:153:MET:CA	0.59	2.27	14	1
1:C:45:MET:CE	4:C:92:BEP:C16	0.59	2.81	4	3
1:C:61:ILE:N	1:C:61:ILE:HD13	0.59	2.13	27	3
1:C:41:LEU:CD2	4:C:92:BEP:C20	0.59	2.81	12	7
1:C:41:LEU:CD1	4:C:92:BEP:C16	0.59	2.81	18	1
1:C:22:ALA:CB	2:I:157:LEU:HD13	0.59	2.27	21	1
1:C:24:PHE:O	1:C:27:PHE:CD1	0.58	2.56	30	2
1:C:28:VAL:HG11	1:C:34:GLY:HA2	0.58	1.74	28	5
1:C:27:PHE:CD1	1:C:27:PHE:N	0.58	2.64	20	1
1:C:24:PHE:CE2	1:C:74:PHE:CE2	0.58	2.91	30	5
4:C:92:BEP:C3	2:I:148:ILE:HD12	0.58	2.28	12	1
1:C:80:MET:CE	4:C:92:BEP:C21	0.58	2.81	14	1
1:C:41:LEU:CD1	4:C:92:BEP:C23	0.58	2.80	16	1
1:C:23:ALA:HB1	2:I:153:MET:SD	0.58	2.39	8	1
1:C:23:ALA:N	2:I:157:LEU:HD21	0.58	2.13	12	2
1:C:41:LEU:CD2	4:C:92:BEP:C24	0.58	2.81	20	1
1:C:24:PHE:CD2	1:C:74:PHE:CD2	0.58	2.90	26	1
2:I:157:LEU:N	2:I:157:LEU:CD2	0.58	2.65	29	10
4:C:92:BEP:C15	2:I:153:MET:HE3	0.58	2.28	15	1
4:C:92:BEP:C3	2:I:148:ILE:HD11	0.58	2.28	17	2
1:C:24:PHE:CZ	1:C:78:LEU:HD12	0.58	2.33	26	2
1:C:24:PHE:CE2	1:C:78:LEU:HD11	0.58	2.34	25	3
1:C:41:LEU:HD21	4:C:92:BEP:C12	0.58	2.29	17	2
1:C:48:LEU:HD13	2:I:152:ALA:O	0.58	1.97	23	1
1:C:41:LEU:CD2	1:C:57:LEU:CD2	0.58	2.81	26	1
1:C:64:VAL:CG1	1:C:80:MET:CG	0.58	2.82	4	2
1:C:23:ALA:HB2	2:I:153:MET:SD	0.58	2.39	10	4
1:C:26:ILE:HG13	2:I:157:LEU:HD11	0.58	1.74	6	2
1:C:60:MET:CE	4:C:92:BEP:N2	0.58	2.67	29	3
1:C:19:GLU:CG	1:C:20:PHE:N	0.58	2.66	19	2
1:C:36:ILE:CD1	1:C:77:PHE:CD1	0.58	2.87	23	3
1:C:48:LEU:HD21	2:I:153:MET:HE1	0.58	1.76	3	1
1:C:24:PHE:CD1	1:C:24:PHE:O	0.58	2.57	8	2
4:C:92:BEP:C1	2:I:148:ILE:HD11	0.57	2.28	6	2
1:C:5:TYR:CE2	1:C:79:VAL:HG13	0.57	2.33	5	4
1:C:48:LEU:HD21	2:I:153:MET:SD	0.57	2.38	5	1
1:C:12:LEU:CD1	1:C:16:GLN:CG	0.57	2.81	24	1
1:C:74:PHE:CE1	1:C:78:LEU:CD1	0.57	2.86	20	5
1:C:80:MET:CE	4:C:92:BEP:C22	0.57	2.82	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:24:PHE:CZ	1:C:78:LEU:CD1	0.57	2.87	26	2
1:C:74:PHE:O	1:C:74:PHE:CG	0.57	2.58	13	12
4:C:92:BEP:C1	2:I:148:ILE:CD1	0.57	2.82	4	1
1:C:27:PHE:CE1	1:C:44:VAL:CG1	0.57	2.87	5	3
1:C:36:ILE:CD1	1:C:77:PHE:CG	0.57	2.86	23	2
1:C:36:ILE:HD11	1:C:77:PHE:CD1	0.57	2.35	23	3
1:C:29:LEU:C	1:C:29:LEU:HD12	0.57	2.20	15	4
4:C:92:BEP:H63	2:I:148:ILE:HB	0.57	1.77	4	1
1:C:60:MET:HE1	4:C:92:BEP:C3	0.57	2.29	27	1
1:C:36:ILE:HG22	1:C:41:LEU:HB2	0.57	1.76	30	1
1:C:74:PHE:O	1:C:74:PHE:CD2	0.57	2.58	4	4
1:C:53:THR:HG22	1:C:54:PRO:HD2	0.57	1.76	3	13
4:C:92:BEP:C15	2:I:153:MET:CE	0.57	2.82	15	1
1:C:48:LEU:HD22	4:C:92:BEP:H161	0.56	1.76	10	1
1:C:72:VAL:HG12	1:C:76:GLU:HG3	0.56	1.76	14	10
1:C:64:VAL:HG12	1:C:80:MET:SD	0.56	2.40	5	1
4:C:92:BEP:H72	4:C:92:BEP:H91	0.56	1.78	20	1
1:C:52:PRO:CG	1:C:57:LEU:HD21	0.56	2.31	28	1
1:C:60:MET:CE	4:C:92:BEP:C12	0.56	2.83	16	2
1:C:27:PHE:CD1	1:C:41:LEU:HD12	0.56	2.35	5	1
1:C:45:MET:HE2	4:C:92:BEP:H91	0.56	1.76	14	1
1:C:5:TYR:O	1:C:9:VAL:HG23	0.56	2.01	16	1
4:C:92:BEP:C11	2:I:148:ILE:HD11	0.56	2.31	10	1
1:C:77:PHE:CE1	1:C:81:MET:SD	0.56	2.99	4	1
1:C:12:LEU:CD2	1:C:12:LEU:N	0.56	2.68	9	3
1:C:36:ILE:HD12	1:C:77:PHE:CD2	0.56	2.36	9	1
1:C:53:THR:CG2	1:C:54:PRO:CD	0.56	2.84	19	5
1:C:64:VAL:HG21	1:C:72:VAL:CG2	0.56	2.31	20	10
1:C:23:ALA:O	1:C:27:PHE:CD2	0.56	2.59	9	2
4:C:92:BEP:C11	4:C:92:BEP:O1	0.55	2.54	15	2
1:C:44:VAL:HG11	2:I:153:MET:HE2	0.55	1.76	17	1
2:I:153:MET:O	2:I:157:LEU:HD22	0.55	2.01	6	2
2:I:149:SER:O	2:I:150:ALA:CB	0.55	2.55	13	19
1:C:74:PHE:CZ	1:C:78:LEU:CD1	0.55	2.89	25	4
1:C:64:VAL:CG2	1:C:72:VAL:HG21	0.55	2.30	18	1
1:C:16:GLN:O	1:C:19:GLU:N	0.55	2.40	19	2
1:C:27:PHE:CD1	1:C:36:ILE:HD13	0.55	2.37	10	1
1:C:41:LEU:HD12	1:C:57:LEU:HD22	0.55	1.78	16	1
1:C:64:VAL:HG12	1:C:80:MET:HG3	0.55	1.78	20	2
1:C:27:PHE:CD2	1:C:36:ILE:HG12	0.55	2.37	29	3
1:C:12:LEU:HD13	1:C:16:GLN:HE21	0.55	1.61	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:80:MET:HE3	4:C:92:BEP:C21	0.55	2.32	14	1
1:C:48:LEU:CD1	2:I:156:ALA:CB	0.55	2.84	12	2
1:C:22:ALA:O	1:C:26:ILE:CD1	0.55	2.55	22	2
1:C:61:ILE:HD13	4:C:92:BEP:H211	0.55	1.77	27	1
1:C:23:ALA:HA	2:I:157:LEU:HD22	0.54	1.78	2	5
1:C:48:LEU:N	1:C:48:LEU:CD2	0.54	2.68	18	2
1:C:64:VAL:HG12	1:C:80:MET:HB2	0.54	1.79	30	1
1:C:29:LEU:O	1:C:29:LEU:CD2	0.54	2.56	22	3
1:C:6:LYS:HA	1:C:9:VAL:CG2	0.54	2.31	12	5
1:C:61:ILE:O	1:C:65:ASP:N	0.54	2.40	19	16
2:I:148:ILE:O	2:I:149:SER:CB	0.54	2.55	10	1
1:C:19:GLU:OE2	2:I:150:ALA:HB1	0.54	2.02	16	1
1:C:26:ILE:N	1:C:26:ILE:HD13	0.54	2.18	3	2
1:C:19:GLU:O	2:I:157:LEU:CD1	0.54	2.56	2	1
1:C:27:PHE:HD2	1:C:36:ILE:HD13	0.54	1.63	11	3
1:C:53:THR:CG2	1:C:54:PRO:HD2	0.54	2.32	19	10
1:C:23:ALA:O	1:C:27:PHE:CE1	0.54	2.60	20	1
1:C:74:PHE:C	1:C:74:PHE:CD1	0.54	2.81	26	1
1:C:77:PHE:CZ	1:C:81:MET:HG3	0.54	2.38	4	1
1:C:78:LEU:HD23	1:C:81:MET:SD	0.54	2.43	7	1
4:C:92:BEP:C17	2:I:153:MET:CE	0.54	2.85	24	1
1:C:6:LYS:O	1:C:10:GLU:CG	0.54	2.56	11	10
1:C:45:MET:HE2	4:C:92:BEP:H102	0.54	1.80	6	1
4:C:92:BEP:H31	2:I:148:ILE:HD12	0.54	1.80	12	1
4:C:92:BEP:C3	4:C:92:BEP:C18	0.54	2.85	17	1
1:C:17:LYS:CD	1:C:18:ASN:N	0.54	2.71	24	1
2:I:148:ILE:O	2:I:148:ILE:CG2	0.54	2.56	18	4
1:C:16:GLN:O	1:C:19:GLU:CG	0.53	2.56	27	7
1:C:27:PHE:CE2	1:C:41:LEU:HD13	0.53	2.38	13	2
1:C:64:VAL:HG13	1:C:80:MET:CG	0.53	2.32	2	1
4:C:92:BEP:O1	4:C:92:BEP:C8	0.53	2.56	21	2
1:C:80:MET:CE	4:C:92:BEP:C24	0.53	2.87	24	2
2:I:153:MET:O	2:I:156:ALA:N	0.53	2.42	25	5
1:C:21:LYS:O	1:C:25:ASP:N	0.53	2.42	24	3
1:C:23:ALA:HB1	1:C:27:PHE:CE2	0.53	2.39	9	3
1:C:48:LEU:HD21	2:I:153:MET:HB3	0.53	1.80	6	1
2:I:148:ILE:O	2:I:148:ILE:HG22	0.53	2.02	24	4
1:C:81:MET:O	1:C:85:MET:CE	0.53	2.57	12	1
1:C:77:PHE:CD1	1:C:81:MET:HE2	0.53	2.39	23	1
1:C:24:PHE:O	1:C:28:VAL:CG2	0.53	2.57	27	7
4:C:92:BEP:H12	2:I:148:ILE:HD13	0.53	1.80	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:I:153:MET:O	2:I:157:LEU:CD2	0.53	2.56	30	5
2:I:153:MET:HE3	2:I:157:LEU:HD21	0.53	1.80	5	1
1:C:27:PHE:CD1	1:C:36:ILE:HG12	0.53	2.39	26	2
1:C:74:PHE:CE2	1:C:78:LEU:HD11	0.53	2.38	23	2
1:C:15:GLU:O	1:C:19:GLU:CG	0.53	2.57	24	1
1:C:28:VAL:HG21	1:C:34:GLY:HA2	0.53	1.79	5	3
2:I:157:LEU:CD2	2:I:157:LEU:O	0.53	2.57	23	2
1:C:42:GLY:CA	1:C:57:LEU:HD11	0.53	2.33	23	1
1:C:77:PHE:CZ	1:C:81:MET:CG	0.53	2.92	4	1
1:C:45:MET:SD	4:C:92:BEP:C16	0.53	2.97	22	2
1:C:28:VAL:CG1	1:C:35:CYS:O	0.53	2.57	26	5
2:I:154:MET:HA	2:I:157:LEU:HD21	0.53	1.81	20	2
1:C:21:LYS:O	1:C:24:PHE:CB	0.53	2.57	3	3
1:C:45:MET:CE	4:C:92:BEP:C15	0.53	2.87	25	3
2:I:157:LEU:O	2:I:157:LEU:HD23	0.53	2.03	23	2
1:C:19:GLU:O	1:C:22:ALA:HB3	0.53	2.03	10	3
1:C:27:PHE:CE2	1:C:28:VAL:HG22	0.53	2.39	26	2
1:C:41:LEU:HB2	1:C:57:LEU:HD22	0.53	1.80	16	1
1:C:26:ILE:CD1	2:I:157:LEU:HD11	0.52	2.30	3	4
1:C:77:PHE:C	1:C:77:PHE:CD1	0.52	2.80	7	6
4:C:92:BEP:H112	4:C:92:BEP:H72	0.52	1.81	7	1
4:C:92:BEP:C14	2:I:153:MET:CE	0.52	2.87	21	1
1:C:22:ALA:HB1	2:I:157:LEU:HG	0.52	1.81	3	2
1:C:72:VAL:HG13	1:C:76:GLU:HG3	0.52	1.81	29	4
1:C:85:MET:HE2	2:I:148:ILE:HG22	0.52	1.80	12	1
1:C:64:VAL:HG21	1:C:72:VAL:HG21	0.52	1.80	18	3
1:C:5:TYR:CD1	1:C:79:VAL:CG1	0.52	2.92	7	1
1:C:81:MET:HG2	1:C:82:VAL:N	0.52	2.19	7	1
2:I:156:ALA:HB3	2:I:157:LEU:CD1	0.52	2.33	7	5
1:C:41:LEU:O	1:C:44:VAL:N	0.52	2.43	11	3
1:C:19:GLU:O	2:I:157:LEU:CD2	0.52	2.55	22	2
1:C:73:ASP:OD1	1:C:75:ASP:N	0.52	2.41	7	17
1:C:43:LYS:O	1:C:46:ARG:CG	0.52	2.58	22	4
1:C:72:VAL:HG13	1:C:76:GLU:CD	0.52	2.25	18	1
1:C:21:LYS:O	1:C:24:PHE:N	0.52	2.43	23	7
1:C:12:LEU:CD1	1:C:16:GLN:OE1	0.52	2.57	9	2
1:C:45:MET:SD	4:C:92:BEP:C18	0.52	2.98	9	1
1:C:48:LEU:HD11	4:C:92:BEP:H171	0.52	1.80	23	2
1:C:57:LEU:O	1:C:60:MET:N	0.52	2.43	28	15
4:C:92:BEP:C1	2:I:148:ILE:HD13	0.52	2.35	2	1
1:C:53:THR:CB	1:C:54:PRO:HD2	0.52	2.35	25	26

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:64:VAL:CG1	1:C:80:MET:SD	0.52	2.98	8	4
1:C:29:LEU:O	1:C:29:LEU:CG	0.52	2.57	18	2
1:C:26:ILE:HB	1:C:44:VAL:HG22	0.52	1.82	11	3
1:C:73:ASP:OD1	1:C:76:GLU:CG	0.52	2.58	13	4
1:C:82:VAL:O	1:C:85:MET:N	0.52	2.43	27	1
1:C:60:MET:SD	4:C:92:BEP:C10	0.52	2.98	30	1
1:C:81:MET:O	1:C:84:CYS:N	0.52	2.43	18	2
1:C:5:TYR:CZ	1:C:83:ARG:HB3	0.52	2.40	27	1
1:C:44:VAL:O	1:C:47:MET:N	0.52	2.43	12	14
1:C:23:ALA:CA	2:I:157:LEU:HD21	0.52	2.35	12	2
1:C:63:GLU:N	1:C:63:GLU:OE1	0.52	2.42	30	2
1:C:37:SER:O	1:C:40:GLU:N	0.52	2.43	18	3
1:C:34:GLY:O	1:C:74:PHE:N	0.51	2.44	18	1
1:C:41:LEU:HD11	4:C:92:BEP:H181	0.51	1.82	28	1
1:C:36:ILE:CG2	1:C:41:LEU:HD23	0.51	2.36	2	1
2:I:154:MET:HA	2:I:157:LEU:HD23	0.51	1.82	8	1
2:I:148:ILE:O	2:I:150:ALA:N	0.51	2.42	9	1
1:C:24:PHE:CZ	1:C:78:LEU:HG	0.51	2.40	18	4
1:C:17:LYS:HD2	1:C:18:ASN:N	0.51	2.21	24	1
2:I:157:LEU:N	2:I:157:LEU:HD22	0.51	2.19	30	3
4:C:92:BEP:C19	4:C:92:BEP:C18	0.51	2.88	18	1
1:C:80:MET:SD	4:C:92:BEP:C20	0.51	2.98	23	1
1:C:48:LEU:HD22	2:I:156:ALA:CA	0.51	2.34	27	1
1:C:74:PHE:CD1	1:C:74:PHE:C	0.51	2.83	30	4
1:C:48:LEU:HD11	2:I:156:ALA:CB	0.51	2.35	12	2
1:C:26:ILE:CD1	2:I:157:LEU:CD1	0.51	2.88	14	3
1:C:27:PHE:CE1	4:C:92:BEP:H171	0.51	2.40	20	2
1:C:26:ILE:HD13	2:I:157:LEU:CD2	0.51	2.28	27	1
4:C:92:BEP:H41	2:I:148:ILE:HD11	0.51	1.81	6	1
1:C:26:ILE:HB	1:C:44:VAL:HG23	0.51	1.82	7	1
2:I:150:ALA:O	2:I:153:MET:N	0.51	2.44	17	4
1:C:17:LYS:O	1:C:20:PHE:N	0.51	2.44	22	1
1:C:84:CYS:SG	4:C:92:BEP:H62	0.51	2.46	27	1
1:C:63:GLU:OE1	1:C:63:GLU:CA	0.51	2.58	30	2
1:C:6:LYS:O	1:C:10:GLU:N	0.51	2.43	2	8
1:C:7:ALA:O	1:C:10:GLU:N	0.51	2.44	20	7
1:C:77:PHE:O	1:C:80:MET:N	0.51	2.44	4	2
1:C:41:LEU:HD22	4:C:92:BEP:C23	0.51	2.35	23	2
1:C:63:GLU:OE1	4:C:92:BEP:C6	0.51	2.58	21	1
1:C:16:GLN:NE2	1:C:20:PHE:CD2	0.51	2.78	25	1
1:C:24:PHE:HE2	1:C:78:LEU:HD11	0.51	1.66	30	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:14:GLU:O	1:C:18:ASN:ND2	0.51	2.44	13	5
1:C:9:VAL:O	1:C:17:LYS:NZ	0.51	2.44	4	1
1:C:60:MET:HB3	4:C:92:BEP:C24	0.51	2.36	16	1
1:C:40:GLU:O	1:C:43:LYS:N	0.51	2.43	17	1
1:C:45:MET:CE	4:C:92:BEP:C17	0.51	2.89	26	1
1:C:45:MET:HE3	4:C:92:BEP:C17	0.51	2.36	26	2
1:C:36:ILE:HD12	1:C:72:VAL:CG1	0.51	2.36	30	2
1:C:5:TYR:O	1:C:9:VAL:N	0.51	2.43	2	2
1:C:45:MET:O	1:C:48:LEU:N	0.51	2.43	29	4
2:I:153:MET:CE	2:I:157:LEU:HD21	0.51	2.36	5	1
1:C:64:VAL:CG2	1:C:72:VAL:HG13	0.51	2.35	20	2
1:C:36:ILE:O	1:C:72:VAL:HG23	0.51	2.06	19	2
1:C:44:VAL:CG1	2:I:153:MET:SD	0.50	2.99	17	2
1:C:23:ALA:HB2	2:I:153:MET:HG2	0.50	1.83	7	2
1:C:80:MET:O	1:C:83:ARG:CB	0.50	2.59	10	1
1:C:46:ARG:CD	1:C:51:ASN:OD1	0.50	2.59	13	1
1:C:27:PHE:CZ	4:C:92:BEP:H161	0.50	2.42	3	2
1:C:29:LEU:C	1:C:29:LEU:CD2	0.50	2.76	29	3
2:I:157:LEU:HD22	2:I:157:LEU:H	0.50	1.65	30	4
1:C:35:CYS:CB	1:C:72:VAL:O	0.50	2.59	15	1
1:C:84:CYS:SG	4:C:92:BEP:C8	0.50	2.99	26	1
1:C:80:MET:CE	4:C:92:BEP:C3	0.50	2.88	4	1
1:C:80:MET:HE2	4:C:92:BEP:C23	0.50	2.37	9	1
1:C:19:GLU:HG3	1:C:20:PHE:N	0.50	2.20	19	2
1:C:41:LEU:HD12	1:C:41:LEU:O	0.50	2.06	15	2
1:C:63:GLU:OE2	4:C:92:BEP:H61	0.50	2.05	19	1
1:C:12:LEU:CD2	1:C:16:GLN:OE1	0.50	2.58	28	1
1:C:27:PHE:HB3	1:C:36:ILE:HG23	0.50	1.82	4	3
1:C:5:TYR:CE2	1:C:79:VAL:CG1	0.50	2.95	5	3
1:C:21:LYS:HA	1:C:24:PHE:CD2	0.50	2.41	25	3
1:C:24:PHE:CE1	1:C:77:PHE:CE2	0.50	3.00	27	4
1:C:60:MET:HE3	4:C:92:BEP:H112	0.50	1.83	5	1
1:C:8:ALA:CB	1:C:82:VAL:HG13	0.50	2.36	11	1
1:C:44:VAL:O	1:C:48:LEU:HD13	0.50	2.06	1	1
2:I:151:ASP:OD1	2:I:152:ALA:N	0.50	2.45	29	2
4:C:92:BEP:C18	2:I:148:ILE:HD11	0.50	2.36	7	1
1:C:36:ILE:HG22	1:C:37:SER:N	0.50	2.21	9	4
1:C:67:ASP:OD1	1:C:69:SER:N	0.50	2.45	12	1
1:C:77:PHE:CD2	1:C:78:LEU:N	0.50	2.80	12	10
1:C:23:ALA:CB	2:I:153:MET:SD	0.50	2.99	8	6
4:C:92:BEP:H12	2:I:148:ILE:CD1	0.50	2.35	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:51:ASN:O	1:C:51:ASN:ND2	0.50	2.44	5	2
1:C:33:ASP:N	1:C:33:ASP:OD1	0.50	2.44	12	4
1:C:65:ASP:OD2	1:C:70:GLY:CA	0.50	2.60	24	4
1:C:80:MET:HE2	4:C:92:BEP:C24	0.50	2.36	21	1
1:C:45:MET:HE3	4:C:92:BEP:C16	0.50	2.36	4	1
1:C:27:PHE:CD2	1:C:41:LEU:HD13	0.50	2.42	11	1
1:C:27:PHE:CE2	1:C:36:ILE:HG12	0.50	2.41	18	1
1:C:36:ILE:CG2	1:C:41:LEU:CD2	0.49	2.89	16	2
2:I:154:MET:O	2:I:157:LEU:N	0.49	2.45	17	3
1:C:23:ALA:CA	2:I:157:LEU:HD11	0.49	2.36	22	1
1:C:20:PHE:O	1:C:24:PHE:N	0.49	2.44	2	1
1:C:27:PHE:CE1	4:C:92:BEP:C16	0.49	2.95	3	1
1:C:67:ASP:N	1:C:67:ASP:OD1	0.49	2.43	17	7
1:C:78:LEU:C	1:C:81:MET:CE	0.49	2.80	7	1
1:C:84:CYS:HB2	4:C:92:BEP:H72	0.49	1.84	15	1
4:C:92:BEP:C16	2:I:153:MET:SD	0.49	3.01	24	2
1:C:20:PHE:CZ	1:C:81:MET:HB3	0.49	2.42	4	1
1:C:80:MET:O	1:C:83:ARG:N	0.49	2.45	25	2
1:C:77:PHE:CD1	1:C:77:PHE:O	0.49	2.65	26	2
1:C:16:GLN:OE1	1:C:20:PHE:CD2	0.49	2.65	10	1
1:C:60:MET:HB3	4:C:92:BEP:C20	0.49	2.38	12	3
1:C:41:LEU:HD21	4:C:92:BEP:H141	0.49	1.83	23	1
1:C:48:LEU:HD21	2:I:153:MET:CB	0.49	2.37	6	1
1:C:27:PHE:CD1	1:C:44:VAL:HG11	0.49	2.42	24	2
4:C:92:BEP:H63	4:C:92:BEP:H91	0.49	1.84	7	2
1:C:41:LEU:CD2	4:C:92:BEP:H201	0.49	2.38	25	3
1:C:85:MET:CE	2:I:148:ILE:HG22	0.49	2.38	12	1
1:C:60:MET:HE3	4:C:92:BEP:H91	0.49	1.84	21	1
1:C:29:LEU:CG	1:C:29:LEU:O	0.49	2.61	15	2
2:I:153:MET:O	2:I:157:LEU:CG	0.49	2.60	21	1
1:C:60:MET:HE3	4:C:92:BEP:H11	0.49	1.83	6	1
1:C:24:PHE:HA	1:C:27:PHE:CE2	0.49	2.42	20	3
1:C:50:GLN:OE1	4:C:92:BEP:C9	0.49	2.61	14	1
1:C:29:LEU:HD12	1:C:29:LEU:O	0.49	2.08	15	4
1:C:61:ILE:CG2	1:C:65:ASP:CG	0.49	2.81	21	2
1:C:12:LEU:CD1	1:C:16:GLN:CD	0.49	2.80	24	1
4:C:92:BEP:H11	2:I:148:ILE:HD11	0.49	1.85	1	1
2:I:156:ALA:HB3	2:I:157:LEU:HD13	0.49	1.84	15	3
1:C:59:GLU:O	1:C:63:GLU:CG	0.49	2.61	27	3
1:C:27:PHE:CA	1:C:44:VAL:HG21	0.49	2.38	17	1
1:C:23:ALA:CB	1:C:27:PHE:CZ	0.49	2.96	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:27:PHE:CD1	1:C:28:VAL:N	0.49	2.81	30	2
1:C:15:GLU:O	1:C:18:ASN:N	0.49	2.46	23	4
1:C:45:MET:HE3	1:C:45:MET:HA	0.49	1.84	8	1
1:C:27:PHE:CD1	1:C:28:VAL:HG22	0.49	2.43	29	3
1:C:28:VAL:O	1:C:31:ALA:N	0.49	2.46	22	1
1:C:22:ALA:HB3	2:I:157:LEU:CD2	0.49	2.37	26	1
1:C:64:VAL:O	1:C:66:GLU:N	0.48	2.45	30	4
1:C:27:PHE:CE2	1:C:41:LEU:CD1	0.48	2.96	11	2
1:C:80:MET:HE1	4:C:92:BEP:C24	0.48	2.37	24	2
1:C:41:LEU:CB	1:C:57:LEU:HD22	0.48	2.38	16	1
1:C:28:VAL:HG11	1:C:35:CYS:N	0.48	2.23	26	1
1:C:5:TYR:OH	1:C:83:ARG:NH1	0.48	2.45	2	3
1:C:41:LEU:HD11	1:C:45:MET:SD	0.48	2.48	9	1
1:C:29:LEU:HD21	1:C:43:LYS:HD3	0.48	1.85	16	1
4:C:92:BEP:C19	4:C:92:BEP:H181	0.48	2.39	18	1
1:C:61:ILE:HG22	1:C:65:ASP:CG	0.48	2.29	17	2
1:C:7:ALA:O	1:C:11:GLN:CG	0.48	2.62	27	3
4:C:92:BEP:H31	4:C:92:BEP:C18	0.48	2.36	17	1
1:C:46:ARG:N	1:C:50:GLN:O	0.48	2.46	24	3
1:C:24:PHE:CD1	1:C:27:PHE:CE1	0.48	3.01	29	1
1:C:26:ILE:CG2	1:C:47:MET:CE	0.48	2.92	19	3
1:C:24:PHE:CE2	1:C:78:LEU:HD21	0.48	2.44	5	1
1:C:78:LEU:O	1:C:81:MET:N	0.48	2.43	19	5
1:C:81:MET:O	1:C:85:MET:CG	0.48	2.62	15	2
1:C:27:PHE:HA	1:C:44:VAL:CG2	0.48	2.38	18	5
1:C:80:MET:CE	4:C:92:BEP:H31	0.48	2.39	4	3
1:C:29:LEU:C	1:C:29:LEU:CD1	0.48	2.77	29	5
1:C:12:LEU:N	1:C:12:LEU:HD23	0.48	2.24	16	3
1:C:48:LEU:HD23	2:I:156:ALA:HB2	0.48	1.82	17	1
1:C:27:PHE:CD2	1:C:36:ILE:CG1	0.48	2.97	30	2
1:C:72:VAL:O	1:C:73:ASP:O	0.48	2.32	10	4
1:C:7:ALA:O	1:C:11:GLN:N	0.48	2.43	20	2
1:C:64:VAL:CG1	1:C:80:MET:HG3	0.48	2.39	13	7
4:C:92:BEP:H21	2:I:148:ILE:CD1	0.48	2.38	2	7
1:C:27:PHE:CE2	1:C:77:PHE:CE2	0.48	3.01	3	1
4:C:92:BEP:C16	2:I:153:MET:CE	0.48	2.92	3	1
1:C:38:THR:CG2	1:C:58:GLN:HA	0.48	2.38	17	4
1:C:48:LEU:HD22	2:I:152:ALA:O	0.48	2.09	11	2
1:C:67:ASP:OD1	1:C:67:ASP:N	0.48	2.44	18	4
1:C:27:PHE:CZ	4:C:92:BEP:H171	0.48	2.44	16	1
1:C:41:LEU:CD1	4:C:92:BEP:C15	0.48	2.91	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:23:ALA:HA	1:C:26:ILE:CG1	0.48	2.39	15	16
1:C:36:ILE:O	1:C:72:VAL:N	0.47	2.47	2	3
4:C:92:BEP:C16	2:I:148:ILE:HD11	0.47	2.39	7	1
1:C:24:PHE:HA	1:C:27:PHE:CD2	0.47	2.44	20	5
1:C:64:VAL:O	1:C:76:GLU:OE1	0.47	2.32	12	3
1:C:16:GLN:O	1:C:19:GLU:HG2	0.47	2.09	11	5
1:C:35:CYS:CB	1:C:71:THR:HB	0.47	2.39	20	2
1:C:23:ALA:HB2	2:I:153:MET:CG	0.47	2.39	13	1
1:C:14:GLU:O	1:C:18:ASN:N	0.47	2.46	26	1
1:C:41:LEU:HD21	4:C:92:BEP:H241	0.47	1.87	14	1
1:C:38:THR:O	1:C:57:LEU:CD1	0.47	2.60	30	4
1:C:60:MET:HE2	4:C:92:BEP:H31	0.47	1.86	28	1
4:C:92:BEP:H81	2:I:148:ILE:CG1	0.47	2.39	30	1
1:C:16:GLN:OE1	1:C:16:GLN:O	0.47	2.32	10	2
1:C:61:ILE:O	1:C:64:VAL:N	0.47	2.43	11	3
1:C:41:LEU:HD21	4:C:92:BEP:H121	0.47	1.85	17	2
1:C:27:PHE:CD1	1:C:27:PHE:C	0.47	2.88	29	2
1:C:25:ASP:C	1:C:26:ILE:HD13	0.47	2.30	30	1
1:C:16:GLN:O	1:C:19:GLU:HG3	0.47	2.10	27	11
2:I:148:ILE:CG1	2:I:148:ILE:O	0.47	2.62	28	1
1:C:53:THR:HB	1:C:54:PRO:HD2	0.47	1.86	5	11
1:C:16:GLN:HG3	1:C:17:LYS:N	0.47	2.25	6	10
1:C:19:GLU:OE1	1:C:20:PHE:N	0.47	2.46	4	1
1:C:77:PHE:CE2	1:C:81:MET:HG3	0.47	2.44	4	1
2:I:156:ALA:C	2:I:157:LEU:CD1	0.47	2.79	23	2
1:C:80:MET:CE	4:C:92:BEP:H12	0.47	2.40	21	3
1:C:73:ASP:OD1	1:C:76:GLU:OE2	0.47	2.33	9	2
1:C:73:ASP:OD1	1:C:76:GLU:HG3	0.47	2.10	15	2
1:C:33:ASP:OD1	1:C:33:ASP:N	0.47	2.46	13	2
1:C:25:ASP:O	1:C:29:LEU:CB	0.47	2.63	22	2
1:C:47:MET:CE	2:I:156:ALA:CB	0.47	2.92	22	1
1:C:58:GLN:O	1:C:58:GLN:NE2	0.47	2.47	29	1
1:C:80:MET:HE1	4:C:92:BEP:C20	0.47	2.39	30	1
1:C:79:VAL:O	1:C:83:ARG:N	0.47	2.46	9	4
1:C:42:GLY:HA2	1:C:57:LEU:HD11	0.47	1.86	23	1
1:C:60:MET:CE	4:C:92:BEP:C3	0.47	2.93	27	2
1:C:65:ASP:OD1	1:C:71:THR:O	0.47	2.33	29	7
1:C:38:THR:HG21	1:C:58:GLN:OE1	0.47	2.10	6	1
1:C:33:ASP:OD1	1:C:35:CYS:SG	0.47	2.73	11	3
1:C:73:ASP:OD1	1:C:73:ASP:C	0.47	2.53	7	4
4:C:92:BEP:H111	2:I:148:ILE:HD13	0.47	1.85	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:36:ILE:CG2	1:C:41:LEU:HD21	0.47	2.31	16	1
1:C:36:ILE:HG22	1:C:37:SER:H	0.47	1.69	16	1
1:C:30:GLY:O	1:C:31:ALA:O	0.47	2.33	25	2
1:C:26:ILE:CD1	1:C:26:ILE:N	0.47	2.77	27	1
1:C:73:ASP:OD2	1:C:76:GLU:OE2	0.46	2.33	22	5
1:C:24:PHE:HE2	1:C:78:LEU:HD12	0.46	1.71	3	1
1:C:48:LEU:CD1	1:C:48:LEU:N	0.46	2.77	5	1
1:C:73:ASP:OD1	1:C:76:GLU:HG2	0.46	2.10	13	5
2:I:149:SER:OG	2:I:150:ALA:N	0.46	2.47	9	1
1:C:8:ALA:HB3	1:C:82:VAL:CG1	0.46	2.40	11	1
4:C:92:BEP:H31	2:I:148:ILE:CD1	0.46	2.40	12	3
1:C:26:ILE:CG1	2:I:157:LEU:HD11	0.46	2.40	24	3
1:C:84:CYS:O	1:C:86:LYS:N	0.46	2.48	16	1
1:C:53:THR:O	1:C:57:LEU:CG	0.46	2.63	21	1
1:C:14:GLU:O	1:C:18:ASN:CB	0.46	2.64	24	1
1:C:22:ALA:CB	2:I:157:LEU:HB2	0.46	2.38	27	1
1:C:80:MET:HE1	4:C:92:BEP:C21	0.46	2.40	27	1
1:C:20:PHE:O	1:C:24:PHE:CD2	0.46	2.68	28	1
4:C:92:BEP:C15	2:I:153:MET:SD	0.46	3.04	1	1
1:C:80:MET:HE1	4:C:92:BEP:H31	0.46	1.87	4	1
1:C:36:ILE:O	1:C:71:THR:CG2	0.46	2.59	11	1
1:C:73:ASP:CG	1:C:76:GLU:CG	0.46	2.84	11	1
1:C:36:ILE:HG13	1:C:72:VAL:O	0.46	2.10	18	1
1:C:77:PHE:O	1:C:81:MET:CE	0.46	2.64	23	1
1:C:52:PRO:HG2	1:C:57:LEU:HD21	0.46	1.87	28	1
1:C:61:ILE:N	1:C:61:ILE:HD12	0.46	2.24	9	5
1:C:77:PHE:CE1	4:C:92:BEP:H211	0.46	2.46	3	1
4:C:92:BEP:H11	2:I:148:ILE:CD1	0.46	2.40	4	1
1:C:82:VAL:O	1:C:86:LYS:N	0.46	2.44	7	1
1:C:27:PHE:CZ	1:C:28:VAL:HG21	0.46	2.45	26	2
1:C:41:LEU:CD1	4:C:92:BEP:C24	0.46	2.94	16	1
1:C:73:ASP:OD1	1:C:73:ASP:N	0.46	2.47	9	1
2:I:154:MET:HA	2:I:157:LEU:CD2	0.46	2.41	15	2
4:C:92:BEP:H81	2:I:148:ILE:HD11	0.46	1.87	17	1
1:C:21:LYS:O	1:C:24:PHE:HB2	0.46	2.11	7	11
1:C:80:MET:CE	4:C:92:BEP:C19	0.46	2.93	1	2
4:C:92:BEP:H121	2:I:148:ILE:CD1	0.46	2.40	22	2
1:C:48:LEU:HD13	2:I:153:MET:HB3	0.46	1.85	14	1
4:C:92:BEP:C20	4:C:92:BEP:H11	0.46	2.40	17	2
1:C:28:VAL:HG12	1:C:31:ALA:CB	0.46	2.41	19	1
1:C:48:LEU:N	1:C:48:LEU:CD1	0.46	2.78	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:24:PHE:CD1	1:C:74:PHE:CD1	0.46	3.04	29	1
1:C:27:PHE:CG	1:C:44:VAL:HG21	0.46	2.45	1	1
1:C:48:LEU:HD21	2:I:153:MET:CA	0.46	2.41	6	3
1:C:53:THR:HB	1:C:54:PRO:CD	0.46	2.40	5	3
1:C:80:MET:HE1	4:C:92:BEP:H42	0.46	1.88	5	1
1:C:8:ALA:CB	1:C:82:VAL:CG1	0.46	2.94	11	1
1:C:13:THR:O	1:C:15:GLU:N	0.46	2.48	12	2
1:C:26:ILE:CG2	1:C:47:MET:HE1	0.46	2.41	19	2
1:C:5:TYR:CD1	1:C:5:TYR:N	0.46	2.83	27	2
1:C:63:GLU:HA	1:C:63:GLU:OE1	0.46	2.11	29	1
1:C:48:LEU:O	2:I:155:GLN:NE2	0.46	2.49	5	1
1:C:78:LEU:O	1:C:81:MET:SD	0.46	2.74	7	1
1:C:60:MET:HB3	4:C:92:BEP:C21	0.46	2.41	15	4
1:C:26:ILE:C	1:C:44:VAL:CG2	0.46	2.84	30	1
1:C:40:GLU:O	1:C:43:LYS:CB	0.46	2.63	1	1
4:C:92:BEP:C14	2:I:148:ILE:HD12	0.46	2.40	1	1
1:C:27:PHE:CE2	1:C:77:PHE:CE1	0.46	3.04	2	2
1:C:64:VAL:CG1	1:C:80:MET:HB2	0.46	2.41	12	6
1:C:29:LEU:O	1:C:29:LEU:HG	0.46	2.11	23	3
1:C:60:MET:CE	4:C:92:BEP:H31	0.46	2.40	15	3
1:C:77:PHE:CE1	1:C:81:MET:HE2	0.46	2.45	23	1
1:C:58:GLN:O	1:C:58:GLN:OE1	0.46	2.33	27	1
1:C:24:PHE:CD2	1:C:74:PHE:CZ	0.46	3.04	3	1
1:C:27:PHE:O	1:C:36:ILE:HG23	0.46	2.11	11	1
1:C:27:PHE:CZ	2:I:153:MET:CE	0.46	2.99	17	1
1:C:33:ASP:OD2	1:C:35:CYS:SG	0.46	2.74	17	2
1:C:80:MET:SD	4:C:92:BEP:C23	0.46	3.04	21	1
1:C:64:VAL:HG12	1:C:80:MET:CB	0.46	2.41	23	1
1:C:15:GLU:O	1:C:19:GLU:OE2	0.46	2.34	25	1
1:C:60:MET:CE	4:C:92:BEP:H12	0.46	2.41	26	1
2:I:157:LEU:HD12	2:I:157:LEU:N	0.46	2.24	26	1
1:C:16:GLN:O	1:C:16:GLN:OE1	0.46	2.34	27	1
1:C:61:ILE:O	1:C:64:VAL:CG2	0.46	2.64	26	2
1:C:60:MET:CE	4:C:92:BEP:H82	0.46	2.41	29	1
1:C:80:MET:SD	1:C:80:MET:O	0.45	2.74	4	1
1:C:45:MET:SD	4:C:92:BEP:C15	0.45	3.04	5	1
1:C:61:ILE:HG13	1:C:72:VAL:HG23	0.45	1.87	11	1
4:C:92:BEP:H181	4:C:92:BEP:C24	0.45	2.41	22	2
1:C:79:VAL:O	1:C:82:VAL:N	0.45	2.49	27	5
1:C:41:LEU:CD1	4:C:92:BEP:H171	0.45	2.41	22	1
1:C:27:PHE:CE1	1:C:36:ILE:HG12	0.45	2.46	26	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:61:ILE:O	1:C:64:VAL:HG22	0.45	2.10	15	1
4:C:92:BEP:C3	4:C:92:BEP:H181	0.45	2.40	17	1
1:C:64:VAL:O	1:C:64:VAL:CG2	0.45	2.64	21	1
1:C:15:GLU:O	1:C:19:GLU:HG3	0.45	2.10	24	1
1:C:58:GLN:O	1:C:61:ILE:N	0.45	2.44	4	4
1:C:84:CYS:SG	1:C:85:MET:N	0.45	2.90	20	4
2:I:156:ALA:CB	2:I:157:LEU:HD13	0.45	2.42	15	2
1:C:22:ALA:CB	2:I:157:LEU:HG	0.45	2.41	28	2
4:C:92:BEP:H81	4:C:92:BEP:H72	0.45	1.86	13	1
1:C:16:GLN:O	1:C:16:GLN:NE2	0.45	2.49	14	1
1:C:60:MET:SD	4:C:92:BEP:O1	0.45	2.74	17	2
1:C:45:MET:CE	4:C:92:BEP:H141	0.45	2.40	17	1
1:C:56:GLU:OE1	1:C:56:GLU:N	0.45	2.49	24	1
1:C:60:MET:HE2	4:C:92:BEP:H12	0.45	1.88	10	1
1:C:46:ARG:HG3	1:C:47:MET:N	0.45	2.26	26	5
1:C:60:MET:CB	4:C:92:BEP:C24	0.45	2.95	16	1
1:C:64:VAL:HB	1:C:76:GLU:CB	0.45	2.41	13	3
1:C:81:MET:O	1:C:85:MET:HE2	0.45	2.11	12	1
1:C:29:LEU:O	1:C:29:LEU:CD1	0.45	2.59	28	4
1:C:81:MET:HA	1:C:81:MET:CE	0.45	2.42	28	1
1:C:44:VAL:O	1:C:48:LEU:CD1	0.45	2.65	1	2
1:C:18:ASN:O	1:C:20:PHE:N	0.45	2.50	5	5
1:C:77:PHE:CD1	1:C:77:PHE:C	0.45	2.89	26	2
1:C:77:PHE:CD1	1:C:81:MET:HE1	0.45	2.46	23	2
1:C:48:LEU:CD2	2:I:156:ALA:HA	0.45	2.39	27	1
1:C:26:ILE:HB	1:C:44:VAL:CG2	0.45	2.42	3	2
1:C:28:VAL:HG13	1:C:36:ILE:HG12	0.45	1.89	11	1
2:I:153:MET:O	2:I:155:GLN:N	0.45	2.50	19	2
1:C:25:ASP:O	1:C:29:LEU:CA	0.45	2.64	22	1
2:I:153:MET:O	2:I:157:LEU:CD1	0.45	2.64	30	1
1:C:72:VAL:CG1	1:C:76:GLU:HG3	0.45	2.42	25	14
1:C:28:VAL:HG23	1:C:28:VAL:O	0.45	2.11	4	1
4:C:92:BEP:H12	2:I:148:ILE:HD11	0.45	1.88	6	2
1:C:57:LEU:CD2	1:C:60:MET:SD	0.45	3.01	22	1
1:C:47:MET:HE1	2:I:156:ALA:HB1	0.45	1.87	25	1
1:C:36:ILE:HD12	4:C:92:BEP:C23	0.45	2.40	4	1
1:C:28:VAL:O	1:C:28:VAL:HG23	0.45	2.11	5	1
1:C:43:LYS:O	1:C:47:MET:CG	0.45	2.65	6	1
1:C:81:MET:HB3	1:C:85:MET:CE	0.45	2.41	11	2
1:C:61:ILE:HA	1:C:64:VAL:CG2	0.45	2.42	14	1
1:C:41:LEU:HD11	4:C:92:BEP:C16	0.45	2.42	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:43:LYS:O	1:C:46:ARG:HG3	0.45	2.12	18	2
1:C:80:MET:SD	1:C:81:MET:SD	0.45	3.14	20	2
1:C:5:TYR:OH	1:C:83:ARG:CG	0.45	2.65	1	1
1:C:43:LYS:O	1:C:46:ARG:HG2	0.45	2.12	22	3
1:C:48:LEU:N	1:C:48:LEU:HD12	0.45	2.27	5	1
4:C:92:BEP:C16	2:I:153:MET:HG2	0.45	2.42	5	1
1:C:13:THR:OG1	1:C:16:GLN:CG	0.45	2.64	9	1
1:C:86:LYS:CD	1:C:86:LYS:N	0.45	2.80	23	1
1:C:80:MET:CE	4:C:92:BEP:H32	0.44	2.42	1	1
1:C:79:VAL:O	1:C:82:VAL:HG12	0.44	2.11	4	2
1:C:37:SER:O	1:C:39:LYS:N	0.44	2.51	5	1
1:C:45:MET:CB	1:C:52:PRO:HG3	0.44	2.42	7	1
1:C:60:MET:CE	4:C:92:BEP:H122	0.44	2.42	12	3
1:C:24:PHE:HA	1:C:27:PHE:CD1	0.44	2.47	18	1
1:C:64:VAL:CG2	1:C:72:VAL:CG2	0.44	2.95	26	2
1:C:84:CYS:SG	4:C:92:BEP:C9	0.44	3.05	12	2
4:C:92:BEP:C2	2:I:148:ILE:CD1	0.44	2.95	13	1
1:C:41:LEU:HD21	4:C:92:BEP:C24	0.44	2.41	20	1
1:C:60:MET:CE	4:C:92:BEP:C8	0.44	2.95	22	2
1:C:77:PHE:O	1:C:78:LEU:C	0.44	2.56	12	10
1:C:70:GLY:O	1:C:71:THR:HG23	0.44	2.13	23	1
1:C:45:MET:HE2	4:C:92:BEP:C15	0.44	2.43	25	1
1:C:16:GLN:O	1:C:20:PHE:CD2	0.44	2.70	26	1
1:C:27:PHE:CZ	4:C:92:BEP:C16	0.44	3.01	3	1
1:C:79:VAL:O	1:C:80:MET:C	0.44	2.56	22	12
1:C:23:ALA:N	2:I:157:LEU:CD2	0.44	2.79	12	1
1:C:35:CYS:HA	1:C:72:VAL:O	0.44	2.12	15	2
1:C:72:VAL:HG13	1:C:76:GLU:CG	0.44	2.43	18	1
1:C:26:ILE:HD11	2:I:157:LEU:HB3	0.44	1.88	20	2
1:C:48:LEU:CD2	1:C:48:LEU:N	0.44	2.70	23	1
1:C:72:VAL:HG13	1:C:76:GLU:HB2	0.44	1.90	11	1
1:C:41:LEU:O	1:C:43:LYS:N	0.44	2.50	14	1
1:C:64:VAL:HG11	1:C:80:MET:SD	0.44	2.53	21	1
4:C:92:BEP:H181	4:C:92:BEP:C19	0.44	2.43	22	1
1:C:55:GLU:HG2	1:C:56:GLU:N	0.44	2.27	26	1
1:C:27:PHE:CG	1:C:28:VAL:HG13	0.44	2.48	30	2
1:C:5:TYR:OH	1:C:83:ARG:HG3	0.44	2.13	1	1
1:C:45:MET:C	1:C:50:GLN:O	0.44	2.55	29	8
1:C:81:MET:O	1:C:83:ARG:N	0.44	2.51	5	1
1:C:73:ASP:N	1:C:76:GLU:OE2	0.44	2.43	12	1
1:C:16:GLN:O	1:C:19:GLU:OE2	0.44	2.35	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:82:VAL:HA	1:C:85:MET:CG	0.44	2.43	23	1
1:C:15:GLU:O	1:C:19:GLU:CD	0.44	2.56	1	1
1:C:60:MET:SD	4:C:92:BEP:C8	0.44	3.06	1	1
1:C:12:LEU:HB3	1:C:16:GLN:CG	0.44	2.43	22	8
1:C:14:GLU:HG3	1:C:15:GLU:N	0.44	2.28	16	2
1:C:80:MET:HE1	4:C:92:BEP:C4	0.44	2.42	5	1
1:C:48:LEU:CG	2:I:153:MET:HA	0.44	2.43	6	3
1:C:80:MET:HE1	4:C:92:BEP:C22	0.44	2.42	9	1
1:C:13:THR:N	1:C:16:GLN:OE1	0.44	2.43	23	1
1:C:48:LEU:HD23	4:C:92:BEP:H161	0.44	1.90	1	1
1:C:38:THR:OG1	1:C:39:LYS:N	0.44	2.51	19	4
1:C:48:LEU:HD12	1:C:48:LEU:N	0.44	2.27	15	1
1:C:81:MET:O	1:C:85:MET:HG2	0.44	2.13	15	1
1:C:27:PHE:N	1:C:44:VAL:HG21	0.44	2.28	17	1
2:I:154:MET:O	2:I:155:GLN:C	0.44	2.56	27	2
1:C:80:MET:HE2	4:C:92:BEP:C19	0.44	2.43	26	1
1:C:48:LEU:CD2	4:C:92:BEP:H161	0.43	2.43	10	3
1:C:46:ARG:HA	1:C:50:GLN:O	0.43	2.13	4	11
1:C:16:GLN:HA	1:C:19:GLU:CG	0.43	2.43	20	3
1:C:80:MET:HE1	4:C:92:BEP:C3	0.43	2.43	4	1
1:C:27:PHE:CE1	1:C:44:VAL:CB	0.43	3.01	5	1
1:C:33:ASP:OD1	1:C:34:GLY:N	0.43	2.47	11	2
1:C:67:ASP:OD1	1:C:69:SER:CB	0.43	2.65	12	1
1:C:45:MET:HE3	4:C:92:BEP:C18	0.43	2.43	16	1
1:C:24:PHE:CD2	1:C:27:PHE:CE1	0.43	3.05	18	1
1:C:40:GLU:O	1:C:41:LEU:C	0.43	2.57	17	6
1:C:13:THR:O	1:C:14:GLU:C	0.43	2.57	12	4
1:C:9:VAL:HG22	1:C:82:VAL:HG21	0.43	1.89	6	2
1:C:77:PHE:CG	1:C:78:LEU:N	0.43	2.86	8	2
1:C:73:ASP:OD1	1:C:76:GLU:N	0.43	2.42	15	1
1:C:24:PHE:CZ	1:C:78:LEU:CG	0.43	3.01	28	2
1:C:20:PHE:HB3	1:C:24:PHE:CE2	0.43	2.48	28	1
1:C:8:ALA:HB1	1:C:82:VAL:HG11	0.43	1.90	1	1
1:C:18:ASN:O	1:C:21:LYS:N	0.43	2.51	4	1
2:I:153:MET:O	2:I:154:MET:C	0.43	2.57	9	6
1:C:81:MET:CE	4:C:92:BEP:H241	0.43	2.42	6	2
1:C:27:PHE:CB	1:C:36:ILE:HG12	0.43	2.44	9	1
1:C:24:PHE:CZ	1:C:74:PHE:HA	0.43	2.48	11	1
1:C:77:PHE:O	1:C:80:MET:HG3	0.43	2.13	17	1
1:C:79:VAL:O	1:C:81:MET:N	0.43	2.50	27	2
1:C:80:MET:HG3	1:C:81:MET:N	0.43	2.28	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:92:BEP:H171	2:I:153:MET:CE	0.43	2.43	24	1
1:C:24:PHE:CE1	1:C:77:PHE:CD2	0.43	3.07	3	1
1:C:27:PHE:CE1	4:C:92:BEP:C17	0.43	3.02	3	1
1:C:76:GLU:O	1:C:77:PHE:C	0.43	2.57	13	4
1:C:77:PHE:CZ	1:C:81:MET:SD	0.43	3.11	4	1
4:C:92:BEP:H11	2:I:148:ILE:HD13	0.43	1.88	4	1
1:C:32:GLU:OE1	1:C:33:ASP:N	0.43	2.51	9	1
1:C:36:ILE:N	1:C:72:VAL:O	0.43	2.49	28	2
1:C:19:GLU:OE1	1:C:19:GLU:C	0.43	2.57	4	1
1:C:78:LEU:O	1:C:81:MET:HE2	0.43	2.13	7	1
1:C:14:GLU:O	1:C:18:ASN:CG	0.43	2.57	24	4
1:C:16:GLN:O	1:C:17:LYS:C	0.43	2.57	19	3
4:C:92:BEP:C16	2:I:153:MET:CG	0.43	2.97	17	1
1:C:11:GLN:O	1:C:12:LEU:O	0.43	2.36	18	1
1:C:37:SER:O	1:C:41:LEU:N	0.43	2.48	20	1
1:C:60:MET:HE3	4:C:92:BEP:C11	0.43	2.44	22	1
1:C:5:TYR:O	1:C:8:ALA:N	0.43	2.51	25	1
1:C:55:GLU:HG3	1:C:56:GLU:N	0.43	2.27	25	1
1:C:26:ILE:O	1:C:44:VAL:CG2	0.43	2.67	30	1
1:C:61:ILE:HG13	1:C:72:VAL:CG2	0.43	2.44	11	3
1:C:12:LEU:HA	1:C:16:GLN:OE1	0.43	2.14	26	2
1:C:78:LEU:O	1:C:81:MET:CE	0.43	2.67	7	1
1:C:24:PHE:CE1	1:C:74:PHE:HA	0.43	2.49	9	1
1:C:41:LEU:CD1	1:C:57:LEU:CD2	0.43	2.95	16	1
1:C:28:VAL:HB	1:C:31:ALA:CB	0.43	2.43	22	1
1:C:59:GLU:N	1:C:59:GLU:OE1	0.43	2.51	28	1
1:C:21:LYS:O	1:C:22:ALA:C	0.43	2.57	23	3
1:C:46:ARG:NH1	1:C:47:MET:HG2	0.43	2.29	3	1
1:C:18:ASN:O	1:C:19:GLU:C	0.43	2.57	20	11
1:C:44:VAL:O	1:C:45:MET:C	0.43	2.56	23	4
1:C:25:ASP:O	1:C:29:LEU:HB2	0.43	2.13	10	1
1:C:46:ARG:NE	1:C:51:ASN:OD1	0.43	2.52	13	1
1:C:58:GLN:NE2	1:C:62:ASP:OD2	0.43	2.52	13	1
1:C:77:PHE:CD1	4:C:92:BEP:C23	0.43	3.01	18	1
1:C:27:PHE:CZ	4:C:92:BEP:C18	0.43	3.02	19	1
1:C:81:MET:HE1	4:C:92:BEP:H241	0.43	1.90	22	1
1:C:37:SER:O	1:C:38:THR:C	0.43	2.57	5	6
1:C:23:ALA:O	1:C:27:PHE:CE2	0.43	2.72	3	1
4:C:92:BEP:C14	4:C:92:BEP:H201	0.43	2.44	3	1
1:C:61:ILE:CD1	4:C:92:BEP:H211	0.43	2.42	27	4
1:C:29:LEU:HG	1:C:29:LEU:O	0.43	2.13	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:78:LEU:O	1:C:79:VAL:C	0.43	2.57	20	6
1:C:64:VAL:HG12	1:C:80:MET:HG2	0.43	1.90	4	1
1:C:12:LEU:HD22	1:C:16:GLN:CD	0.43	2.34	8	1
4:C:92:BEP:H111	2:I:148:ILE:HD11	0.43	1.89	10	1
1:C:12:LEU:CD1	1:C:16:GLN:NE2	0.43	2.78	12	1
1:C:60:MET:CE	4:C:92:BEP:H201	0.43	2.44	12	1
1:C:56:GLU:OE1	1:C:56:GLU:CA	0.43	2.67	24	1
1:C:58:GLN:OE1	1:C:58:GLN:CA	0.43	2.67	27	1
1:C:5:TYR:O	1:C:6:LYS:C	0.43	2.57	3	4
1:C:65:ASP:OD2	1:C:70:GLY:N	0.43	2.52	6	4
1:C:82:VAL:O	1:C:84:CYS:N	0.43	2.52	7	1
1:C:84:CYS:O	1:C:85:MET:C	0.43	2.57	16	3
4:C:92:BEP:H81	4:C:92:BEP:O1	0.43	2.14	13	1
1:C:80:MET:HE3	4:C:92:BEP:C23	0.43	2.42	17	1
1:C:77:PHE:CD1	4:C:92:BEP:H231	0.43	2.49	18	1
1:C:47:MET:HE3	2:I:156:ALA:HA	0.43	1.89	21	1
1:C:81:MET:CG	2:I:148:ILE:HG21	0.43	2.44	26	1
1:C:72:VAL:HG13	1:C:76:GLU:OE1	0.43	2.14	30	1
1:C:60:MET:CE	4:C:92:BEP:H32	0.42	2.44	7	1
1:C:60:MET:CG	4:C:92:BEP:H201	0.42	2.44	11	1
1:C:60:MET:CE	4:C:92:BEP:H241	0.42	2.43	16	1
1:C:41:LEU:CD2	4:C:92:BEP:H121	0.42	2.43	17	1
1:C:26:ILE:O	1:C:29:LEU:CD2	0.42	2.64	18	1
1:C:66:GLU:OE2	1:C:83:ARG:NH1	0.42	2.52	21	1
4:C:92:BEP:H181	2:I:148:ILE:CD1	0.42	2.43	30	1
1:C:15:GLU:O	1:C:16:GLN:C	0.42	2.57	23	3
1:C:77:PHE:O	1:C:81:MET:HG2	0.42	2.15	11	1
1:C:23:ALA:CB	2:I:153:MET:CE	0.42	2.97	19	2
4:C:92:BEP:H181	4:C:92:BEP:C20	0.42	2.43	14	1
1:C:60:MET:CE	4:C:92:BEP:C11	0.42	2.96	18	1
1:C:61:ILE:HG23	1:C:72:VAL:CG2	0.42	2.44	18	2
1:C:40:GLU:OE1	1:C:40:GLU:C	0.42	2.58	30	1
4:C:92:BEP:C13	4:C:92:BEP:H21	0.42	2.43	15	1
1:C:64:VAL:HG23	1:C:76:GLU:OE1	0.42	2.13	17	1
1:C:73:ASP:C	1:C:73:ASP:OD1	0.42	2.56	19	1
1:C:6:LYS:O	1:C:10:GLU:CB	0.42	2.67	25	1
1:C:16:GLN:OE1	1:C:17:LYS:HA	0.42	2.14	29	1
1:C:26:ILE:O	1:C:29:LEU:N	0.42	2.44	5	1
1:C:81:MET:O	1:C:85:MET:N	0.42	2.43	5	1
1:C:82:VAL:O	1:C:83:ARG:C	0.42	2.56	7	1
2:I:153:MET:HG3	2:I:154:MET:N	0.42	2.29	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:92:BEP:O1	4:C:92:BEP:C11	0.42	2.67	17	2
1:C:41:LEU:HD11	4:C:92:BEP:C22	0.42	2.44	16	1
1:C:17:LYS:O	1:C:20:PHE:HB2	0.42	2.14	24	1
1:C:5:TYR:CD2	1:C:79:VAL:CG1	0.42	3.00	27	1
1:C:26:ILE:HG21	1:C:47:MET:CE	0.42	2.45	19	2
1:C:39:LYS:O	1:C:42:GLY:N	0.42	2.49	4	1
1:C:64:VAL:HG12	1:C:80:MET:CG	0.42	2.44	4	2
1:C:50:GLN:O	1:C:52:PRO:HD3	0.42	2.14	7	4
1:C:12:LEU:HD22	1:C:16:GLN:HE21	0.42	1.71	12	1
1:C:40:GLU:O	1:C:43:LYS:HG2	0.42	2.14	16	1
4:C:92:BEP:H141	4:C:92:BEP:C3	0.42	2.45	3	1
1:C:60:MET:HE2	4:C:92:BEP:N2	0.42	2.30	4	1
1:C:18:ASN:C	1:C:20:PHE:N	0.42	2.73	8	5
1:C:17:LYS:O	1:C:21:LYS:HG3	0.42	2.15	13	1
2:I:153:MET:O	2:I:157:LEU:HG	0.42	2.14	13	3
4:C:92:BEP:C19	4:C:92:BEP:C1	0.42	2.98	17	1
1:C:48:LEU:HD22	4:C:92:BEP:H171	0.42	1.90	21	1
1:C:63:GLU:CB	4:C:92:BEP:H62	0.42	2.44	21	1
1:C:59:GLU:O	1:C:63:GLU:HG3	0.42	2.15	19	1
1:C:84:CYS:SG	4:C:92:BEP:C4	0.42	3.08	19	1
1:C:48:LEU:O	2:I:155:GLN:OE1	0.42	2.38	22	1
1:C:14:GLU:O	1:C:18:ASN:HB2	0.42	2.15	24	1
1:C:6:LYS:O	1:C:10:GLU:HG3	0.42	2.14	26	2
1:C:60:MET:SD	4:C:92:BEP:H111	0.42	2.54	30	1
1:C:80:MET:CE	4:C:92:BEP:C20	0.42	2.98	30	1
1:C:26:ILE:HG13	2:I:157:LEU:CD1	0.42	2.42	12	3
4:C:92:BEP:H112	4:C:92:BEP:H73	0.42	1.90	10	2
1:C:17:LYS:O	1:C:18:ASN:C	0.42	2.57	22	1
1:C:61:ILE:HD13	4:C:92:BEP:H231	0.42	1.90	3	1
1:C:61:ILE:O	1:C:62:ASP:C	0.42	2.58	18	2
1:C:60:MET:CE	4:C:92:BEP:H11	0.42	2.45	17	2
1:C:60:MET:HE1	4:C:92:BEP:C8	0.42	2.45	14	1
1:C:44:VAL:HG11	2:I:153:MET:CE	0.42	2.44	17	1
4:C:92:BEP:C1	4:C:92:BEP:H62	0.42	2.45	19	1
1:C:13:THR:HG22	1:C:14:GLU:N	0.42	2.30	25	1
1:C:48:LEU:CD2	4:C:92:BEP:C16	0.42	2.98	1	2
1:C:57:LEU:O	1:C:58:GLN:C	0.42	2.58	23	4
1:C:45:MET:SD	4:C:92:BEP:H151	0.42	2.54	5	2
1:C:41:LEU:HD22	4:C:92:BEP:C24	0.42	2.45	8	1
1:C:73:ASP:CG	1:C:76:GLU:HG3	0.42	2.35	11	1
1:C:60:MET:HE2	4:C:92:BEP:C12	0.42	2.44	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:59:GLU:O	1:C:63:GLU:OE2	0.42	2.38	17	1
4:C:92:BEP:H62	4:C:92:BEP:H12	0.42	1.92	19	1
1:C:41:LEU:HD21	4:C:92:BEP:C19	0.42	2.45	20	1
2:I:156:ALA:CA	2:I:157:LEU:HD13	0.42	2.45	30	2
1:C:36:ILE:CG2	1:C:41:LEU:HB2	0.42	2.45	27	1
1:C:68:GLY:O	1:C:69:SER:C	0.41	2.59	4	1
1:C:16:GLN:OE1	1:C:17:LYS:HD3	0.41	2.15	5	2
2:I:154:MET:HA	2:I:157:LEU:CD1	0.41	2.45	11	1
1:C:81:MET:O	1:C:84:CYS:SG	0.41	2.75	12	1
4:C:92:BEP:H31	4:C:92:BEP:C14	0.41	2.44	12	1
1:C:72:VAL:HG12	1:C:73:ASP:H	0.41	1.75	15	1
1:C:13:THR:O	1:C:17:LYS:HG2	0.41	2.14	19	1
1:C:14:GLU:CG	1:C:15:GLU:N	0.41	2.82	30	1
1:C:27:PHE:CE1	2:I:153:MET:HE2	0.41	2.50	17	1
1:C:80:MET:HE2	4:C:92:BEP:H31	0.41	1.92	18	1
1:C:36:ILE:HD13	4:C:92:BEP:H211	0.41	1.91	20	1
1:C:7:ALA:O	1:C:11:GLN:HG3	0.41	2.14	21	2
1:C:20:PHE:CE1	1:C:24:PHE:CZ	0.41	3.09	25	1
1:C:23:ALA:HA	2:I:157:LEU:HD21	0.41	1.92	3	1
1:C:28:VAL:O	1:C:31:ALA:CB	0.41	2.69	3	2
1:C:37:SER:C	1:C:39:LYS:N	0.41	2.73	5	1
1:C:27:PHE:CD2	1:C:77:PHE:CE2	0.41	3.08	26	1
1:C:58:GLN:OE1	1:C:58:GLN:HA	0.41	2.16	27	1
2:I:156:ALA:CB	2:I:157:LEU:CD2	0.41	2.96	27	1
1:C:80:MET:SD	1:C:80:MET:C	0.41	2.98	23	2
1:C:23:ALA:O	1:C:26:ILE:HG12	0.41	2.15	25	4
4:C:92:BEP:H112	4:C:92:BEP:C5	0.41	2.45	10	1
1:C:45:MET:O	1:C:46:ARG:C	0.41	2.59	29	1
1:C:41:LEU:HD11	4:C:92:BEP:C20	0.41	2.45	2	1
1:C:73:ASP:OD1	1:C:75:ASP:HB2	0.41	2.16	6	5
1:C:27:PHE:CE1	1:C:44:VAL:HB	0.41	2.50	5	1
1:C:36:ILE:CG2	1:C:37:SER:N	0.41	2.83	9	1
2:I:148:ILE:O	2:I:148:ILE:HG23	0.41	2.14	15	1
1:C:41:LEU:CD2	4:C:92:BEP:H122	0.41	2.43	27	1
1:C:44:VAL:CG1	1:C:48:LEU:CD1	0.41	2.95	1	1
1:C:43:LYS:O	1:C:44:VAL:C	0.41	2.59	2	1
1:C:45:MET:SD	4:C:92:BEP:C14	0.41	3.08	5	1
1:C:81:MET:HB3	1:C:85:MET:HE2	0.41	1.93	11	1
1:C:64:VAL:CB	1:C:72:VAL:HG13	0.41	2.45	14	1
1:C:45:MET:HE1	4:C:92:BEP:C14	0.41	2.46	16	1
1:C:45:MET:HE3	4:C:92:BEP:H141	0.41	1.92	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:C:92:BEP:C14	2:I:153:MET:HE1	0.41	2.45	21	1
4:C:92:BEP:C15	2:I:153:MET:HE2	0.41	2.45	22	1
1:C:21:LYS:HA	1:C:24:PHE:CB	0.41	2.46	24	1
1:C:6:LYS:CA	1:C:9:VAL:CG2	0.41	2.98	25	1
1:C:20:PHE:O	1:C:24:PHE:CG	0.41	2.74	28	1
1:C:36:ILE:O	1:C:71:THR:HA	0.41	2.15	3	1
1:C:85:MET:HG3	1:C:86:LYS:CG	0.41	2.46	5	1
1:C:60:MET:SD	4:C:92:BEP:C1	0.41	3.09	17	1
1:C:61:ILE:HD12	4:C:92:BEP:H211	0.41	1.92	17	1
1:C:53:THR:O	1:C:57:LEU:CB	0.41	2.69	21	1
4:C:92:BEP:N2	2:I:148:ILE:HD13	0.41	2.30	21	1
1:C:81:MET:HE3	4:C:92:BEP:H241	0.41	1.91	6	1
2:I:149:SER:HB3	2:I:151:ASP:OD1	0.41	2.15	6	1
1:C:32:GLU:O	1:C:33:ASP:O	0.41	2.39	9	1
1:C:13:THR:C	1:C:15:GLU:N	0.41	2.74	26	4
1:C:16:GLN:C	1:C:18:ASN:N	0.41	2.74	11	1
1:C:60:MET:HB3	4:C:92:BEP:C23	0.41	2.45	16	1
1:C:58:GLN:CD	1:C:58:GLN:C	0.41	2.79	18	1
1:C:44:VAL:HG13	1:C:45:MET:N	0.41	2.30	22	1
1:C:5:TYR:C	1:C:9:VAL:HG22	0.41	2.33	25	1
1:C:16:GLN:OE1	1:C:17:LYS:CE	0.41	2.69	2	1
1:C:20:PHE:O	1:C:21:LYS:C	0.41	2.57	2	1
1:C:24:PHE:CE2	1:C:74:PHE:CZ	0.41	3.09	3	1
1:C:47:MET:HE1	2:I:156:ALA:O	0.41	2.15	11	1
1:C:10:GLU:O	1:C:11:GLN:C	0.41	2.58	12	1
1:C:27:PHE:O	1:C:40:GLU:HB3	0.41	2.15	12	1
1:C:60:MET:O	1:C:63:GLU:HG3	0.41	2.16	12	2
1:C:41:LEU:CB	1:C:57:LEU:CD2	0.41	2.99	16	1
4:C:92:BEP:H91	4:C:92:BEP:C7	0.41	2.45	20	1
4:C:92:BEP:O1	4:C:92:BEP:H81	0.41	2.15	20	1
1:C:6:LYS:O	1:C:10:GLU:HB2	0.41	2.16	25	1
4:C:92:BEP:H21	4:C:92:BEP:C18	0.41	2.46	25	1
1:C:20:PHE:HB3	1:C:24:PHE:CZ	0.41	2.51	28	1
1:C:24:PHE:CD1	1:C:24:PHE:N	0.41	2.86	28	1
1:C:55:GLU:HG2	1:C:56:GLU:OE1	0.41	2.16	30	1
4:C:92:BEP:C8	2:I:148:ILE:HD11	0.41	2.46	30	1
1:C:67:ASP:OD1	1:C:69:SER:OG	0.41	2.39	5	2
1:C:85:MET:HG3	1:C:86:LYS:HG3	0.41	1.91	5	1
2:I:150:ALA:O	2:I:151:ASP:C	0.41	2.60	8	1
1:C:28:VAL:O	1:C:29:LEU:C	0.41	2.59	10	1
1:C:23:ALA:CA	2:I:157:LEU:HD22	0.41	2.46	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:60:MET:CB	4:C:92:BEP:H241	0.41	2.46	16	1
1:C:77:PHE:CE1	4:C:92:BEP:C24	0.41	3.04	18	1
1:C:20:PHE:CE1	1:C:81:MET:SD	0.41	3.14	19	1
1:C:27:PHE:CD2	1:C:36:ILE:HD13	0.41	2.51	19	1
1:C:67:ASP:OD1	1:C:68:GLY:N	0.41	2.54	20	1
4:C:92:BEP:H112	4:C:92:BEP:C6	0.41	2.46	28	1
4:C:92:BEP:H161	2:I:153:MET:SD	0.40	2.56	3	1
1:C:26:ILE:N	1:C:26:ILE:CD1	0.40	2.81	10	1
1:C:80:MET:SD	1:C:81:MET:HE2	0.40	2.56	15	1
1:C:84:CYS:C	1:C:86:LYS:N	0.40	2.75	16	1
1:C:60:MET:CE	4:C:92:BEP:H91	0.40	2.46	21	1
1:C:60:MET:HE1	4:C:92:BEP:N2	0.40	2.31	2	2
1:C:81:MET:SD	4:C:92:BEP:H51	0.40	2.56	4	1
1:C:48:LEU:HG	2:I:152:ALA:O	0.40	2.16	19	2
1:C:80:MET:O	1:C:83:ARG:HG2	0.40	2.16	8	1
1:C:35:CYS:SG	1:C:73:ASP:HA	0.40	2.57	14	1
2:I:149:SER:O	2:I:153:MET:SD	0.40	2.79	14	1
2:I:148:ILE:O	2:I:148:ILE:HG13	0.40	2.16	15	1
1:C:61:ILE:CD1	4:C:92:BEP:H231	0.40	2.47	16	1
1:C:48:LEU:CD2	2:I:156:ALA:CB	0.40	2.88	17	1
1:C:17:LYS:O	1:C:20:PHE:HB3	0.40	2.17	25	1
1:C:28:VAL:CG1	1:C:34:GLY:C	0.40	2.80	28	1
1:C:45:MET:CE	4:C:92:BEP:H151	0.40	2.47	5	1
1:C:9:VAL:O	1:C:17:LYS:CE	0.40	2.69	14	1
4:C:92:BEP:O1	4:C:92:BEP:H111	0.40	2.15	15	1
1:C:58:GLN:O	1:C:58:GLN:CD	0.40	2.60	18	1
1:C:77:PHE:O	1:C:80:MET:HB3	0.40	2.17	21	1
1:C:23:ALA:O	1:C:26:ILE:N	0.40	2.53	22	2
1:C:25:ASP:O	1:C:29:LEU:HA	0.40	2.16	22	1
1:C:58:GLN:OE1	1:C:58:GLN:O	0.40	2.40	25	1
1:C:20:PHE:CD1	1:C:24:PHE:CZ	0.40	3.09	28	1
1:C:55:GLU:CG	1:C:56:GLU:N	0.40	2.85	1	2
1:C:23:ALA:HA	1:C:26:ILE:HG12	0.40	1.94	3	1
1:C:80:MET:C	1:C:80:MET:SD	0.40	2.99	15	1
1:C:27:PHE:CE1	4:C:92:BEP:C18	0.40	3.05	28	1
1:C:46:ARG:HB3	1:C:51:ASN:OD1	0.40	2.16	28	1
1:C:39:LYS:O	1:C:40:GLU:C	0.40	2.59	2	1
1:C:19:GLU:O	1:C:22:ALA:CB	0.40	2.70	10	1
1:C:27:PHE:CE1	2:I:153:MET:HE1	0.40	2.51	12	1
1:C:47:MET:HE3	2:I:156:ALA:HB1	0.40	1.92	19	1
1:C:41:LEU:HD11	4:C:92:BEP:H122	0.40	1.94	27	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	C	82/89 (92%)	60±4 (73±5%)	19±4 (24±5%)	3±1 (3±1%)	7 38
2	I	10/17 (59%)	7±1 (74±11%)	2±1 (19±9%)	1±1 (7±9%)	2 18
All	All	2760/3180 (87%)	2024 (73%)	637 (23%)	99 (4%)	6 34

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

Mol	Chain	Res	Type	Models (Total)
1	C	73	ASP	21
1	C	77	PHE	12
2	I	150	ALA	9
1	C	49	GLY	7
2	I	148	ILE	6
1	C	33	ASP	4
1	C	79	VAL	4
2	I	149	SER	4
1	C	31	ALA	4
1	C	78	LEU	3
1	C	48	LEU	3
1	C	18	ASN	2
1	C	34	GLY	2
1	C	12	LEU	2
1	C	15	GLU	2
1	C	80	MET	2
1	C	75	ASP	2
1	C	43	LYS	1
1	C	19	GLU	1
1	C	82	VAL	1
1	C	14	GLU	1
1	C	42	GLY	1
1	C	85	MET	1
2	I	154	MET	1
1	C	83	ARG	1
1	C	32	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	C	65	ASP	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	C	71/78 (91%)	51±4 (72±5%)	20±4 (28±5%)	2 18
2	I	7/11 (64%)	4±1 (60±16%)	3±1 (40±16%)	0 5
All	All	2340/2670 (88%)	1650 (71%)	690 (29%)	1 17

All 69 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	C	16	GLN	30
1	C	33	ASP	30
1	C	53	THR	30
2	I	154	MET	28
1	C	26	ILE	25
1	C	20	PHE	24
1	C	65	ASP	23
1	C	29	LEU	21
1	C	24	PHE	19
1	C	75	ASP	18
1	C	37	SER	18
1	C	86	LYS	17
1	C	25	ASP	16
1	C	32	GLU	16
2	I	157	LEU	15
1	C	17	LYS	15
1	C	40	GLU	15
1	C	39	LYS	14
1	C	43	LYS	14
1	C	13	THR	13
1	C	78	LEU	13
1	C	14	GLU	12
1	C	66	GLU	12

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Mol	Chain	Res	Type	Models (Total)
1	C	47	MET	12
1	C	81	MET	11
2	I	149	SER	11
1	C	71	THR	11
1	C	61	ILE	10
1	C	46	ARG	10
1	C	62	ASP	10
2	I	155	GLN	10
2	I	153	MET	10
1	C	19	GLU	8
1	C	59	GLU	8
1	C	69	SER	8
1	C	56	GLU	8
1	C	80	MET	8
1	C	60	MET	8
2	I	151	ASP	7
1	C	83	ARG	7
1	C	76	GLU	7
1	C	48	LEU	7
1	C	67	ASP	6
1	C	73	ASP	6
1	C	51	ASN	5
1	C	45	MET	5
1	C	21	LYS	4
1	C	44	VAL	4
1	C	50	GLN	4
1	C	63	GLU	4
1	C	28	VAL	4
1	C	6	LYS	3
1	C	11	GLN	3
2	I	148	ILE	3
1	C	12	LEU	3
1	C	15	GLU	3
1	C	58	GLN	3
1	C	36	ILE	3
1	C	27	PHE	3
1	C	41	LEU	2
1	C	64	VAL	2
1	C	85	MET	2
1	C	72	VAL	2
1	C	74	PHE	2
1	C	77	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	C	84	CYS	1
1	C	82	VAL	1
1	C	55	GLU	1
1	C	35	CYS	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	BEP	C	92	-	29,29,29	1.25±0.03	4±0 (13±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	BEP	C	92	-	35,37,37	1.38±0.01	5±0 (13±1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BEP	C	92	-	-	0±0,22,29,29	0±0,3,3,3

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
4	C	92	BEP	C19-N3	3.85	1.49	1.38	10	30
4	C	92	BEP	C3-N3	3.30	1.50	1.46	22	30
4	C	92	BEP	C12-N3	2.36	1.49	1.46	5	30
4	C	92	BEP	C12-C13	2.35	1.55	1.51	24	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
4	C	92	BEP	C8-N2-C2	4.91	118.86	114.12	21	30
4	C	92	BEP	C11-N2-C2	4.67	118.63	114.12	15	30
4	C	92	BEP	C12-N3-C19	3.08	115.49	120.78	22	30
4	C	92	BEP	C1-C2-N2	2.92	110.21	115.07	7	30
4	C	92	BEP	C11-N2-C8	2.05	109.84	104.98	1	21

There are no chirality outliers.

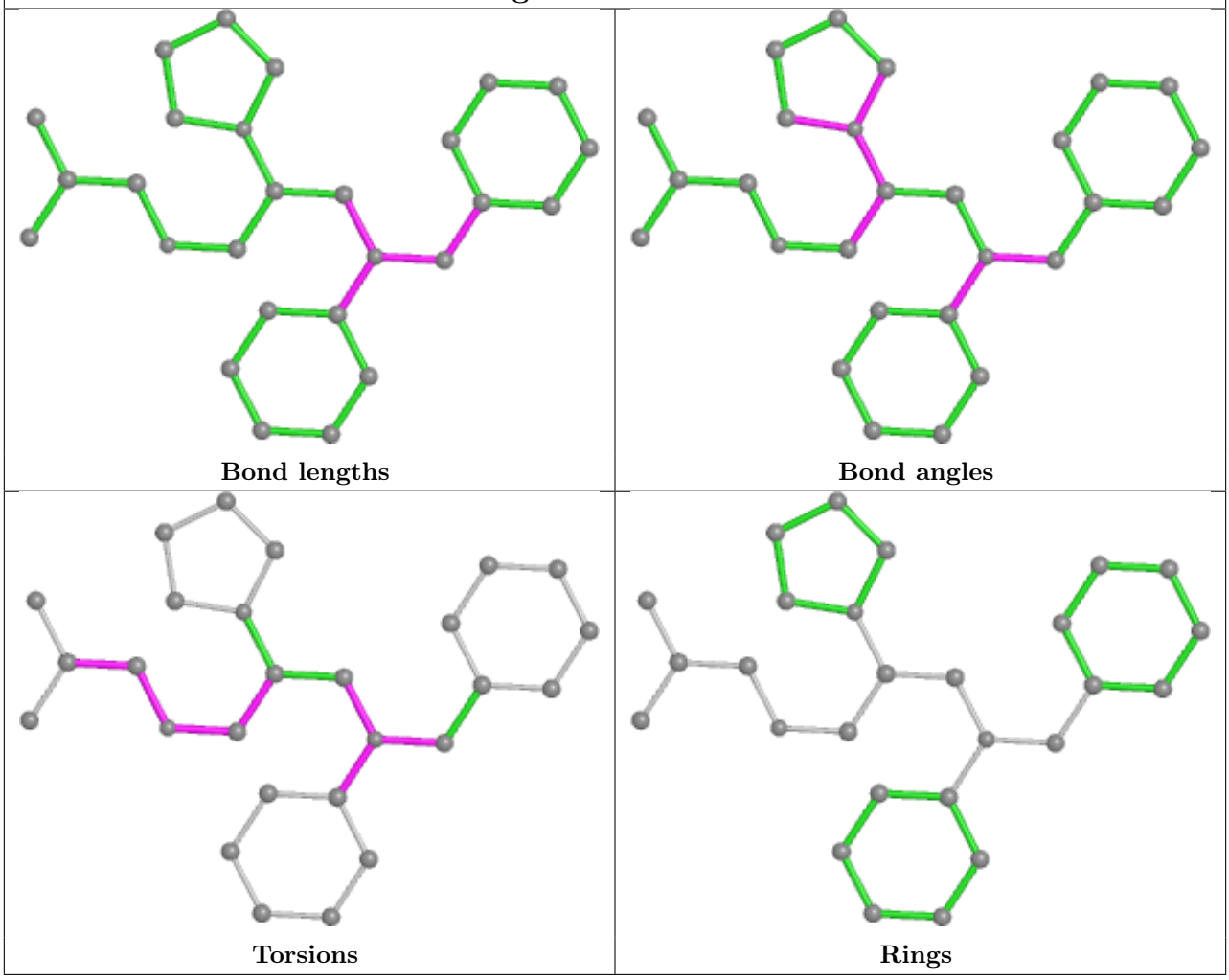
There are no torsion outliers.

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 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 BEP C 92



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