



Full wwPDB NMR Structure Validation Report ⓘ

Aug 10, 2020 – 07:07 AM BST

PDB ID : 1GYA
Title : N-GLYCAN AND POLYPEPTIDE NMR SOLUTION STRUCTURES OF
THE ADHESION DOMAIN OF HUMAN CD2
Authors : Wyss, D.F.; Choi, J.S.; Wagner, G.
Deposited on : 1995-05-26

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
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 : 2.13.1
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

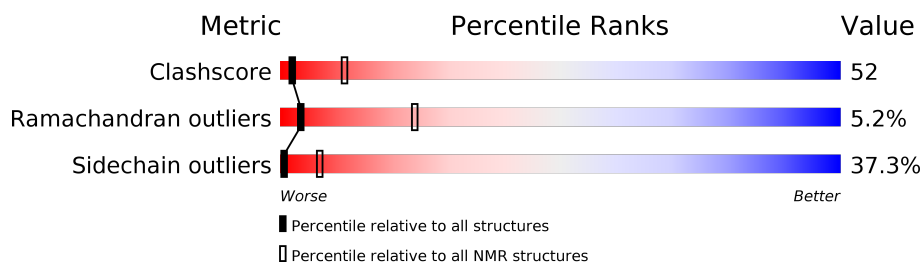
1 Overall quality at a glance i

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	105	 11% 62% 21% 6%
2	B	9	 89% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	B	BMA	3	2	-
2	B	MAN	4	1	-
2	B	MAN	8	1	-
2	B	MAN	9	1	-

2 Ensemble composition and analysis i

This entry contains 18 models. Model 11 is the overall representative, medoid model (most similar to other models).

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:5-A:103 (99)	0.48	11

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	6, 8, 9, 12, 15, 16, 17
2	1, 2, 3, 7, 10, 11, 18
3	5, 13
Single-model clusters	4; 14

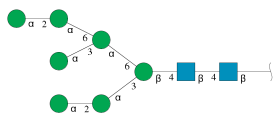
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1976 atoms, of which 994 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HUMAN CD2.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	105	1774	560	897	144	172	1	0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



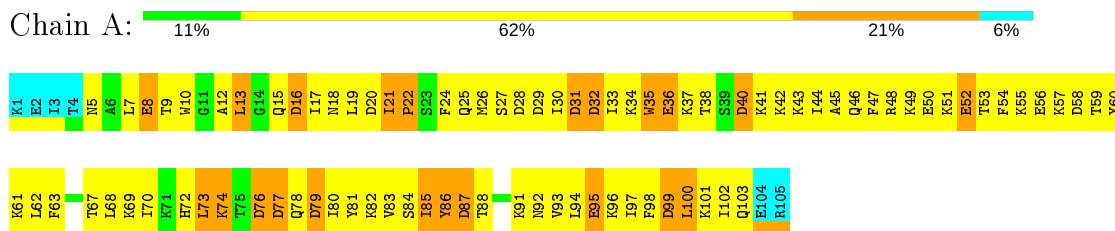
Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	9	202	58	97	2	45	0

4 Residue-property plots

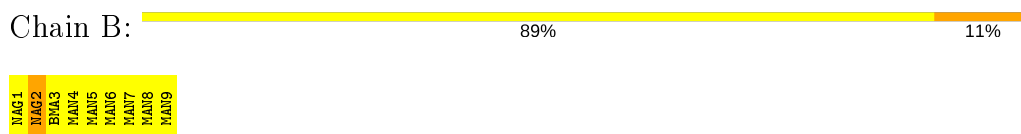
4.1 Average score per residue in the NMR ensemble

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: HUMAN CD2



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

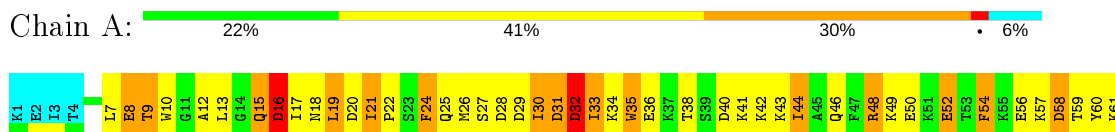


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

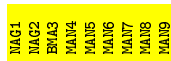
- Molecule 1: HUMAN CD2





- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

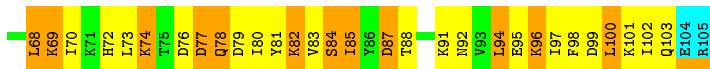
Chain B: 100%



4.2.2 Score per residue for model 2

- Molecule 1: HUMAN CD2

Chain A: 24% 40% 30% 6%



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 89% 11%



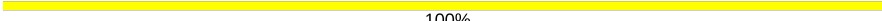
4.2.3 Score per residue for model 3

- Molecule 1: HUMAN CD2

Chain A: 16% 49% 28% 6%




- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  100%

MAG1
MAG2
EMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4.2.4 Score per residue for model 4

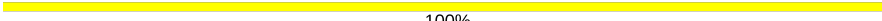
- Molecule 1: HUMAN CD2

Chain A:  20% 40% 32% 6%

K1 E2 I3 T4 N5 A6 L7 E8 T9 W10 G11 A12 L13 G14 Q15 D16 I17 L18 L19 D20 P22 S23 F24 Q25 M26 S27 D28 D29 I30 I31 D32 I33 K34 W35 E36 K37 T38 S39 D40 K41 K42 K43 I44 F47 R48 K49 E50 E51 E52 K55 E56 K57 D58 E59 Y60 K61 L62

F63 K64 L68 K69 I70 K71 H72 L73 K74 T75 D76 D77 Q78 D79 I80 Y81 K82 V83 S84 Y86 D87 T88 K91 N92 V93 L94 K95 I96 K97 I97 F98 D99 K100 K101 I102 Q103 E104 R105


- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  100%

MAG1
MAG2
EMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4.2.5 Score per residue for model 5


- Molecule 1: HUMAN CD2

Chain A:  21% 47% 25% 6%

K1 E2 I3 T4 L7 E8 T9 W10 G11 A12 L13 G14 Q15 D16 I17 L18 L19 D20 P22 S23 M26 S27 D28 D29 I30 I31 D32 I33 K34 W35 E36 K37 T38 S39 D40 K43 I44 A45 Q46 F47 R48 E49 E50 E51 E52 T53 E56 K57 D58 T59 Y60 K61 L62 F63

L68 K69 I70 K71 H72 L73 K74 T75 D76 D77 Q78 I79 I80 Y81 K82 V83 S84 Y86 D87 T88 K91 N92 V93 L94 K95 I96 K97 I97 F98 D99 K100 K101 I102 Q103 E104 R105

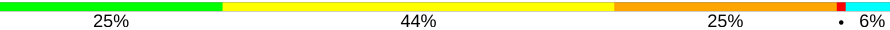
- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4.2.6 Score per residue for model 6

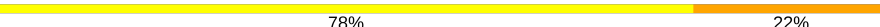
- Molecule 1: HUMAN CD2

Chain A:  25% 44% 25% 6%

K1 E2 I3 T4 N5 A6 L7 L8 E8 T9 M10 G11 A12 A13 L14 G15 Q16 D17 I18 L19 D20 F22 P23 S24 D28 D29 I30 D31 D32 D33 K34 K35 E36 K37 T38 S39 D40 K41 K42 K43 I44 A45 R48 K49 E50 K51 E52 T53 K54 K55 E56 K57 D58 T59 V60 K61 L62 F63

T67 L68 K69 I70 K71 N72 L73 K74 T75 I76 D77 Q78 D79 I80 Y81 K82 V83 S84 I85 Y86 D87 T88 K91 N92 V93 L94 E95 K96 I97 F98 D99 L100 K101 I102 Q103 E104 R105


- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  78% 22%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4.2.7 Score per residue for model 7


- Molecule 1: HUMAN CD2

Chain A:  20% 44% 28% 6%

K1 E2 I3 T4 L7 L8 E8 T9 M10 G11 A12 A13 L14 G15 Q16 D17 I18 L19 D20 F22 P23 S24 D28 D29 I30 D31 D32 D33 K34 K35 E36 K37 T38 S39 D40 K41 K42 K43 I44 A45 K46 F47 R48 K49 K50 E51 E52 T53 E56 K57 D58 T59 V60 K61 L62

F63 T67 L68 K69 I70 K71 N72 L73 K74 T75 I76 D77 Q78 D79 I80 Y81 K82 V83 S84 I85 Y86 D87 T88 K91 N92 V93 L94 E95 K96 I97 F98 D99 L100 K101 I102 Q103 E104 R105

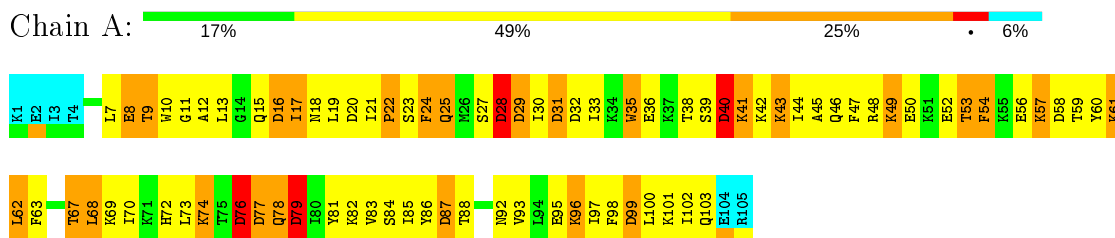
- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  78% 22%

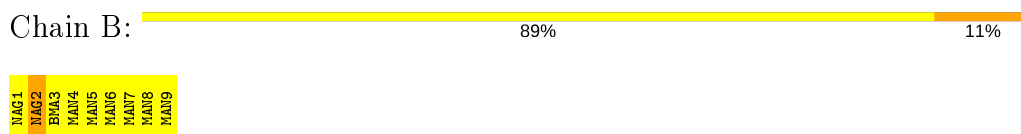
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4.2.8 Score per residue for model 8

- Molecule 1: HUMAN CD2

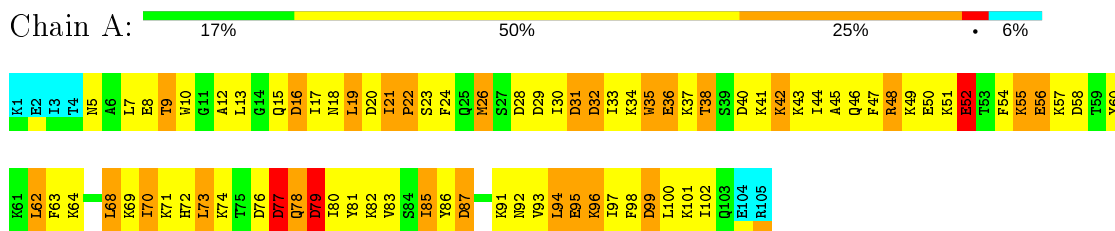


- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

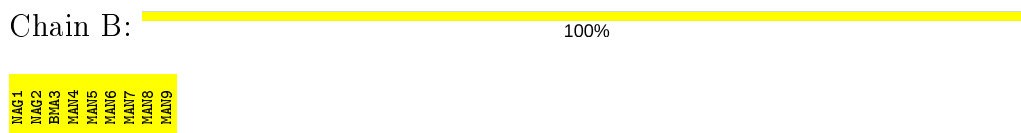


4.2.9 Score per residue for model 9

- Molecule 1: HUMAN CD2

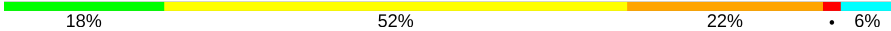


- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4.2.10 Score per residue for model 10

- Molecule 1: HUMAN CD2

Chain A: 




- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

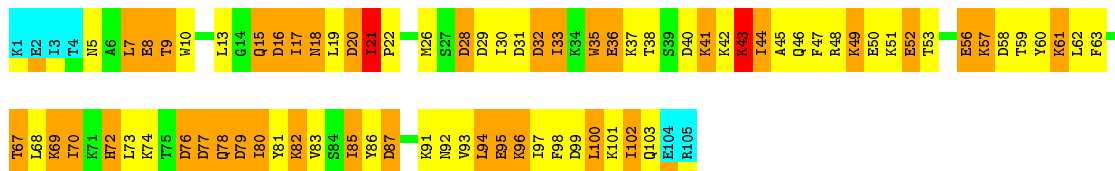
Chain B: 



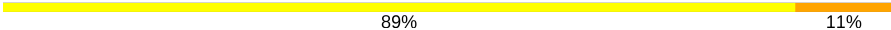
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: HUMAN CD2

Chain A: 



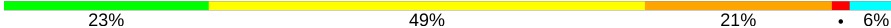
- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 

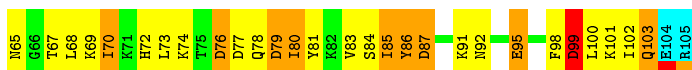


4.2.12 Score per residue for model 12

- Molecule 1: HUMAN CD2

Chain A: 





- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

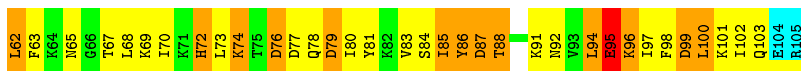
Chain B: 78% 22%



4.2.13 Score per residue for model 13

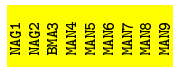
- Molecule 1: HUMAN CD2

Chain A: 15% 50% 25% 6%



- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

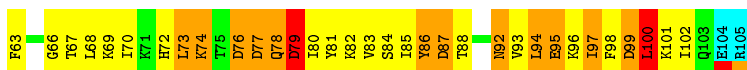
Chain B: 100%




4.2.14 Score per residue for model 14

- Molecule 1: HUMAN CD2

Chain A: 21% 45% 24% 5% 6%




- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4.2.15 Score per residue for model 15


- Molecule 1: HUMAN CD2

Chain A:  13% 51% 30% 6%

K1 E2 I3 T4 N5 A6 L7 E8 T9 W10 G11 A12 L13 G14 Q15 D16 D17 I17 N18 L19 D20 I21 P22 S23 F24 Q25 M26 S27 D28 D29 I30 D31 D32 I33 K34 W35 E36 K37 T38 S39 D40 K41 K42 K43 I44 A45 Q46 F47 R48 K49 E50 K51 E52 T53 F54 K55 E56 K57 T59 Y60

K61 L62 F63 K64 N65 G66 T67 L68 K69 I70 K71 H72 L73 K74 T75 D76 D77 Q78 I80 N81 K82 R83 S84 L85 Y86 D87 T88 I92 N93 L94 E95 K96 I97 F98 D99 L100 K101 I102 Q103 E104 R105

- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  78% 22%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4.2.16 Score per residue for model 16

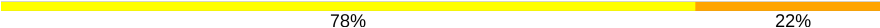
- Molecule 1: HUMAN CD2

Chain A:  23% 48% 23% 6%

K1 E2 I3 T4 N5 A6 L7 E8 T9 W10 G11 A12 L13 G14 Q15 D16 D17 I17 N18 L19 D20 I21 P22 S23 F24 Q25 M26 S27 D28 D29 I30 D31 D32 I33 K34 W35 E36 K37 T38 S39 D40 K41 K42 K43 I44 A45 Q46 F47 R48 K49 E50 K51 E52 T53 F54 K55 E56 K57 T59 Y60

K61 L62 F63 K64 N65 G66 T67 L68 K69 I70 K71 H72 L73 K74 T75 D76 D77 Q78 I80 N81 K82 R83 S84 L85 Y86 D87 T88 I91 N92 Y93 I94 F95 I96 I97 F98 D99 L100 K101 I102 Q103 E104 R105

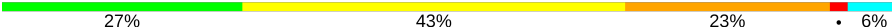
- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  78% 22%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4.2.17 Score per residue for model 17

- Molecule 1: HUMAN CD2

Chain A:  27% 43% 23% 6%

K1 E2 I3 T4 L7 E8 T9 M10 L13 G14 Q15 D16 I17 N18 L19 D20 T21 F22 M26 S27 D28 D29 I30 D31 D32 I33 K34 K35 E36 K37 T38 S39 D40 K41 K42 K43 I44 A45 O46 F47 R48 R49 E50 E52 T53 E56 K57 D58 T59 Y60 W61 L62 F63 T67

I68 K69 I70 K71 H72 L73 K74 T75 D76 D77 Q78 D79 I80 Y81 K82 V83 S84 I85 Y86 D87 K91 N92 V93 L94 E95 K96 I97 F98 D99 L100 K101 I102 Q103 E104 R105

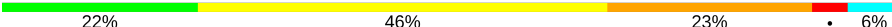
- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4.2.18 Score per residue for model 18

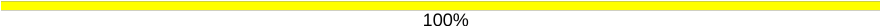
- Molecule 1: HUMAN CD2

Chain A:  22% 46% 23% 6%

K1 E2 I3 T4 N5 A6 L7 E8 T9 M10 G11 A12 L13 G14 Q15 D16 I17 H18 L19 D20 T21 F22 Q25 M26 S27 D28 D29 I30 D31 D32 I33 K34 W35 E36 K37 T38 S39 D40 K41 K42 K43 I44 A45 R48 K49 E50 E52 K55 E56 K57 D58 T59 Y60 W61 L62 F63

K64 T67 L68 K69 I70 L73 K74 T75 D76 D77 Q78 D79 I80 Y81 K82 V83 S84 I85 Y86 D87 T88 K91 N92 V93 L94 E95 K96 I97 F98 D99 L100 K101 I102 Q103 E104 R105

- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry*.

Of the 120 calculated structures, 18 were deposited, based on the following criterion: *PRO-STAT/STRUCT_CHECK*.

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

Software name	Classification	Version
DGII	refinement	
DGII	structure solution	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

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: BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.40±0.00	19±0/837 (2.3± 0.0%)	1.38±0.01	30±1/1120 (2.7± 0.0%)
All	All	1.40	342/15066 (2.3%)	1.38	536/20160 (2.7%)

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
1	A	8	GLU	CD-OE2	10.12	1.36	1.25	7	11
1	A	56	GLU	CD-OE2	10.07	1.36	1.25	18	6
1	A	36	GLU	CD-OE1	10.06	1.36	1.25	2	10
1	A	50	GLU	CD-OE1	10.05	1.36	1.25	10	9
1	A	36	GLU	CD-OE2	10.05	1.36	1.25	6	8
1	A	56	GLU	CD-OE1	10.04	1.36	1.25	6	12
1	A	8	GLU	CD-OE1	10.04	1.36	1.25	9	7
1	A	95	GLU	CD-OE1	10.03	1.36	1.25	9	8
1	A	95	GLU	CD-OE2	10.03	1.36	1.25	5	10
1	A	52	GLU	CD-OE2	10.03	1.36	1.25	12	11
1	A	50	GLU	CD-OE2	10.01	1.36	1.25	12	9
1	A	52	GLU	CD-OE1	9.99	1.36	1.25	10	7
1	A	99	ASP	CG-OD2	5.57	1.38	1.25	12	15
1	A	28	ASP	CG-OD2	5.49	1.38	1.25	8	11
1	A	32	ASP	CG-OD2	5.48	1.38	1.25	9	8
1	A	77	ASP	CG-OD1	5.40	1.37	1.25	16	8
1	A	16	ASP	CG-OD2	5.37	1.37	1.25	8	13
1	A	58	ASP	CG-OD2	5.25	1.37	1.25	16	13
1	A	87	ASP	CG-OD2	5.21	1.37	1.25	9	12
1	A	58	ASP	CG-OD1	5.21	1.37	1.25	14	5
1	A	76	ASP	CG-OD2	5.20	1.37	1.25	15	9
1	A	16	ASP	CG-OD1	5.19	1.37	1.25	18	5
1	A	29	ASP	CG-OD2	5.19	1.37	1.25	16	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	31	ASP	CG-OD2	5.19	1.37	1.25	2	7
1	A	28	ASP	CG-OD1	5.18	1.37	1.25	2	7
1	A	29	ASP	CG-OD1	5.18	1.37	1.25	12	10
1	A	79	ASP	CG-OD2	5.18	1.37	1.25	7	6
1	A	77	ASP	CG-OD2	5.18	1.37	1.25	8	10
1	A	40	ASP	CG-OD2	5.17	1.37	1.25	3	11
1	A	79	ASP	CG-OD1	5.17	1.37	1.25	17	12
1	A	20	ASP	CG-OD2	5.17	1.37	1.25	2	8
1	A	32	ASP	CG-OD1	5.17	1.37	1.25	18	10
1	A	31	ASP	CG-OD1	5.16	1.37	1.25	15	11
1	A	20	ASP	CG-OD1	5.16	1.37	1.25	12	10
1	A	76	ASP	CG-OD1	5.15	1.37	1.25	17	9
1	A	99	ASP	CG-OD1	5.15	1.37	1.25	6	3
1	A	40	ASP	CG-OD1	5.15	1.37	1.25	1	7
1	A	87	ASP	CG-OD1	5.14	1.37	1.25	2	6

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
1	A	48	ARG	NE-CZ-NH1	8.26	124.43	120.30	12	18
1	A	99	ASP	CB-CG-OD1	7.60	125.14	118.30	12	18
1	A	28	ASP	CB-CG-OD1	7.16	124.75	118.30	8	17
1	A	32	ASP	CB-CG-OD1	7.16	124.74	118.30	9	18
1	A	99	ASP	CB-CG-OD2	-7.14	111.88	118.30	12	18
1	A	28	ASP	CB-CG-OD2	-6.92	112.07	118.30	8	17
1	A	32	ASP	CB-CG-OD2	-6.89	112.10	118.30	9	18
1	A	77	ASP	CB-CG-OD1	-6.66	112.31	118.30	16	17
1	A	16	ASP	CB-CG-OD2	-6.60	112.36	118.30	8	18
1	A	77	ASP	CB-CG-OD2	6.54	124.19	118.30	16	17
1	A	16	ASP	CB-CG-OD1	6.46	124.11	118.30	8	18
1	A	29	ASP	CB-CG-OD2	-6.24	112.68	118.30	16	18
1	A	87	ASP	CB-CG-OD2	-6.23	112.69	118.30	14	18
1	A	87	ASP	CB-CG-OD1	-6.18	112.74	118.30	11	18
1	A	20	ASP	CB-CG-OD1	-6.18	112.74	118.30	5	18
1	A	58	ASP	CB-CG-OD1	-6.16	112.75	118.30	5	18
1	A	76	ASP	CB-CG-OD2	-6.16	112.75	118.30	16	18
1	A	79	ASP	CB-CG-OD1	-6.16	112.76	118.30	16	18
1	A	76	ASP	CB-CG-OD1	-6.15	112.77	118.30	14	18
1	A	29	ASP	CB-CG-OD1	-6.15	112.77	118.30	3	18
1	A	58	ASP	CB-CG-OD2	-6.14	112.77	118.30	17	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	31	ASP	CB-CG-OD1	-6.14	112.77	118.30	12	18
1	A	31	ASP	CB-CG-OD2	-6.14	112.77	118.30	2	18
1	A	40	ASP	CB-CG-OD2	-6.13	112.78	118.30	6	18
1	A	79	ASP	CB-CG-OD2	-6.13	112.78	118.30	7	18
1	A	40	ASP	CB-CG-OD1	-6.13	112.79	118.30	5	18
1	A	20	ASP	CB-CG-OD2	-6.12	112.79	118.30	2	18
1	A	10	TRP	CD1-NE1-CE2	-5.75	103.82	109.00	16	18
1	A	48	ARG	NE-CZ-NH2	-5.73	117.44	120.30	3	18
1	A	35	TRP	CD1-NE1-CE2	-5.71	103.86	109.00	5	18

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	823	839	838	96±15
2	B	105	97	88	1±1
All	All	16704	16848	16668	1735

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 52.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:VAL:HG22	1:A:85:ILE:HD11	1.14	1.16	17	9
1:A:73:LEU:HD21	1:A:100:LEU:HD11	1.10	1.19	8	3
1:A:38:THR:HG21	1:A:80:ILE:HG22	1.09	1.23	15	8
1:A:33:ILE:HG23	1:A:85:ILE:HG23	1.06	1.26	6	14
1:A:19:LEU:HD12	1:A:68:LEU:HD22	1.06	1.19	3	2
1:A:12:ALA:HB3	1:A:15:GLN:HG3	1.05	1.19	15	2
1:A:19:LEU:HD12	1:A:68:LEU:HD23	1.04	1.13	6	2
1:A:33:ILE:HG23	1:A:85:ILE:HD13	1.03	1.27	5	3
1:A:19:LEU:HD23	1:A:35:TRP:CZ3	1.02	1.88	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ILE:HG23	1:A:22:PRO:HD3	1.02	1.20	14	4
1:A:21:ILE:HD12	1:A:22:PRO:HD2	1.01	1.30	2	4
1:A:19:LEU:HB3	1:A:35:TRP:CH2	1.00	1.92	8	18
1:A:73:LEU:HB3	1:A:77:ASP:CB	1.00	1.85	15	1
1:A:78:GLN:HG2	1:A:100:LEU:HB2	0.99	1.35	14	1
1:A:19:LEU:HD11	1:A:81:TYR:CD2	0.99	1.93	2	3
1:A:63:PHE:CE2	1:A:69:LYS:HB2	0.98	1.93	1	3
1:A:19:LEU:HD13	1:A:35:TRP:CZ3	0.98	1.93	3	6
1:A:73:LEU:HD23	1:A:100:LEU:HD21	0.98	1.34	6	1
1:A:38:THR:CG2	1:A:80:ILE:HG22	0.98	1.89	14	8
1:A:13:LEU:CD1	1:A:102:ILE:HD12	0.97	1.89	4	1
1:A:73:LEU:HD21	1:A:102:ILE:HD11	0.97	1.37	7	1
1:A:19:LEU:HD22	1:A:70:ILE:HD11	0.97	1.35	15	1
1:A:7:LEU:HD12	1:A:98:PHE:CE2	0.97	1.95	7	9
1:A:13:LEU:HD12	1:A:102:ILE:HG21	0.97	1.31	10	4
1:A:13:LEU:CD1	1:A:102:ILE:HG21	0.96	1.89	4	11
1:A:7:LEU:HD23	1:A:98:PHE:CE2	0.96	1.95	14	5
1:A:19:LEU:HD12	1:A:98:PHE:HD2	0.95	1.21	11	1
1:A:63:PHE:CE1	1:A:69:LYS:HB2	0.95	1.96	15	3
1:A:45:ALA:HB1	1:A:62:LEU:CD1	0.95	1.91	16	3
1:A:83:VAL:HG12	1:A:98:PHE:CE1	0.95	1.96	1	9
1:A:7:LEU:HD23	1:A:98:PHE:CD2	0.95	1.95	11	4
1:A:7:LEU:HD12	1:A:98:PHE:CZ	0.94	1.96	10	6
1:A:73:LEU:HB2	1:A:77:ASP:CB	0.94	1.92	7	5
1:A:83:VAL:HG23	1:A:85:ILE:HD11	0.93	1.36	14	3
1:A:33:ILE:HG23	1:A:85:ILE:CG2	0.93	1.94	6	13
1:A:85:ILE:HD13	1:A:94:LEU:HD23	0.93	1.40	2	1
1:A:21:ILE:HG23	1:A:22:PRO:CD	0.93	1.92	11	4
1:A:17:ILE:CG2	1:A:100:LEU:HD21	0.93	1.94	4	3
1:A:9:THR:HG21	1:A:19:LEU:CD1	0.92	1.93	9	1
1:A:21:ILE:CD1	1:A:22:PRO:HD2	0.91	1.95	13	7
1:A:70:ILE:HD11	1:A:100:LEU:HD21	0.91	1.41	9	1
1:A:73:LEU:HD23	1:A:100:LEU:CD2	0.90	1.96	6	1
1:A:19:LEU:HD12	1:A:35:TRP:CZ3	0.90	2.01	14	3
1:A:21:ILE:CG2	1:A:22:PRO:HD3	0.90	1.96	14	4
1:A:22:PRO:HG3	1:A:94:LEU:HD21	0.90	1.41	15	2
1:A:21:ILE:HD11	1:A:94:LEU:HD21	0.90	1.39	13	4
1:A:83:VAL:HG22	1:A:85:ILE:CD1	0.90	1.96	2	8
1:A:63:PHE:HE1	1:A:69:LYS:HB2	0.90	1.23	15	1
1:A:83:VAL:HG12	1:A:98:PHE:HE1	0.89	1.27	18	7
1:A:83:VAL:CG2	1:A:85:ILE:HD11	0.89	1.98	4	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ALA:HB3	1:A:15:GLN:CG	0.89	1.93	6	1
1:A:81:TYR:HE1	1:A:100:LEU:HB2	0.89	1.28	13	4
1:A:24:PHE:HD2	1:A:94:LEU:HD12	0.89	1.27	4	1
1:A:12:ALA:CB	1:A:15:GLN:HG3	0.88	1.95	6	2
1:A:38:THR:HG21	1:A:80:ILE:CG2	0.88	1.97	13	5
1:A:19:LEU:HD13	1:A:68:LEU:HD23	0.88	1.40	17	1
1:A:21:ILE:HG21	1:A:83:VAL:HG21	0.88	1.44	14	3
1:A:73:LEU:HB2	1:A:77:ASP:HB3	0.88	1.44	7	3
1:A:73:LEU:HD12	1:A:100:LEU:HD21	0.88	1.42	1	1
1:A:33:ILE:HG21	1:A:62:LEU:HD11	0.87	1.45	12	3
1:A:47:PHE:CE1	1:A:53:THR:HG21	0.87	2.04	12	3
1:A:80:ILE:N	1:A:100:LEU:HD12	0.87	1.85	14	1
1:A:73:LEU:HD21	1:A:100:LEU:CD1	0.87	2.00	8	3
1:A:19:LEU:CD1	1:A:68:LEU:HD23	0.86	1.99	6	2
1:A:19:LEU:HD12	1:A:98:PHE:CD2	0.86	2.05	18	5
1:A:73:LEU:CD1	1:A:100:LEU:HD21	0.86	2.00	1	1
1:A:13:LEU:N	1:A:102:ILE:HD13	0.86	1.85	7	1
1:A:13:LEU:HD13	1:A:74:LYS:HB3	0.85	1.48	15	4
1:A:62:LEU:CD1	1:A:68:LEU:HD12	0.85	2.01	9	2
1:A:78:GLN:CD	1:A:100:LEU:HD23	0.85	1.92	14	1
1:A:85:ILE:HD13	1:A:94:LEU:CD2	0.85	2.02	2	1
1:A:63:PHE:CD2	1:A:67:THR:HG22	0.85	2.07	7	6
1:A:17:ILE:HG23	1:A:100:LEU:HD21	0.84	1.47	4	2
1:A:24:PHE:CD2	1:A:94:LEU:HD12	0.84	2.07	4	1
1:A:13:LEU:HD12	1:A:14:GLY:N	0.84	1.87	7	4
1:A:60:TYR:CE1	1:A:81:TYR:HE2	0.84	1.90	7	4
1:A:94:LEU:HD13	1:A:95:GLU:N	0.84	1.88	14	2
1:A:38:THR:HG22	1:A:80:ILE:HB	0.83	1.47	4	1
1:A:21:ILE:HG12	1:A:22:PRO:HD2	0.83	1.49	9	7
1:A:33:ILE:HG23	1:A:85:ILE:HD12	0.83	1.51	9	4
1:A:37:LYS:HB3	1:A:44:ILE:HD11	0.83	1.50	9	1
1:A:45:ALA:HB1	1:A:62:LEU:HD23	0.83	1.50	2	2
1:A:63:PHE:HE2	1:A:69:LYS:HB2	0.82	1.30	1	3
1:A:33:ILE:HA	1:A:85:ILE:HG23	0.82	1.51	18	16
1:A:13:LEU:HD13	1:A:102:ILE:HG21	0.82	1.49	4	2
1:A:44:ILE:HD12	1:A:60:TYR:CD1	0.82	2.10	6	3
1:A:21:ILE:HG13	1:A:22:PRO:HD2	0.82	1.50	7	4
1:A:13:LEU:HD12	1:A:102:ILE:CG2	0.82	2.04	10	9
1:A:63:PHE:CE2	1:A:69:LYS:HB3	0.82	2.10	7	1
1:A:37:LYS:HG2	1:A:42:LYS:HB3	0.81	1.52	3	2
1:A:81:TYR:CE1	1:A:100:LEU:HB2	0.81	2.09	13	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:ASP:C	1:A:100:LEU:HD12	0.81	1.94	14	1
1:A:45:ALA:HB1	1:A:62:LEU:HD13	0.81	1.52	3	5
1:A:7:LEU:HD12	1:A:98:PHE:CE1	0.80	2.11	12	2
1:A:81:TYR:CE2	1:A:100:LEU:HB2	0.80	2.12	2	2
1:A:43:LYS:HB2	1:A:46:GLN:NE2	0.80	1.91	3	1
1:A:19:LEU:HD11	1:A:70:ILE:HD11	0.80	1.53	17	1
1:A:60:TYR:HE2	1:A:81:TYR:HE2	0.80	1.15	17	2
1:A:21:ILE:HD13	1:A:22:PRO:HD2	0.80	1.54	17	2
1:A:21:ILE:HB	1:A:83:VAL:HG11	0.80	1.53	11	3
1:A:17:ILE:HG21	1:A:100:LEU:HD11	0.80	1.53	13	4
1:A:19:LEU:HD12	1:A:68:LEU:CD2	0.79	2.06	3	2
1:A:73:LEU:CD1	1:A:100:LEU:HD23	0.79	2.07	9	2
1:A:33:ILE:CG2	1:A:62:LEU:HD11	0.79	2.07	12	3
1:A:60:TYR:HE1	1:A:81:TYR:HE2	0.79	1.17	7	3
1:A:45:ALA:HB1	1:A:62:LEU:CD2	0.79	2.08	8	5
1:A:37:LYS:CG	1:A:42:LYS:HB3	0.79	2.07	3	2
1:A:15:GLN:O	1:A:73:LEU:HB2	0.78	1.76	11	2
1:A:80:ILE:HG13	1:A:100:LEU:CD1	0.78	2.08	14	1
1:A:68:LEU:HD23	1:A:69:LYS:N	0.78	1.94	2	1
1:A:38:THR:HG21	1:A:80:ILE:CB	0.78	2.08	13	2
1:A:22:PRO:HB3	1:A:94:LEU:HD21	0.78	1.55	10	1
1:A:37:LYS:HB2	1:A:44:ILE:HD11	0.78	1.53	14	1
1:A:44:ILE:HD12	1:A:60:TYR:CE1	0.78	2.13	12	2
1:A:73:LEU:HB3	1:A:77:ASP:CG	0.78	1.97	15	1
1:A:21:ILE:CG1	1:A:83:VAL:HG11	0.78	2.09	1	2
1:A:73:LEU:HB2	1:A:77:ASP:HB2	0.77	1.56	17	4
1:A:33:ILE:HG23	1:A:85:ILE:CD1	0.77	2.10	18	2
1:A:47:PHE:HD1	1:A:62:LEU:HD12	0.77	1.37	10	1
1:A:22:PRO:CG	1:A:94:LEU:HD21	0.77	2.10	15	3
1:A:94:LEU:HD23	1:A:95:GLU:N	0.77	1.93	13	1
1:A:73:LEU:HB2	1:A:77:ASP:CG	0.77	2.00	4	1
1:A:22:PRO:HG2	1:A:94:LEU:HD21	0.77	1.54	6	1
1:A:13:LEU:HD12	1:A:74:LYS:HA	0.76	1.57	4	1
1:A:19:LEU:HD22	1:A:68:LEU:HD23	0.76	1.56	10	1
1:A:73:LEU:HD13	1:A:102:ILE:CD1	0.76	2.11	8	4
1:A:33:ILE:HD13	1:A:85:ILE:CG2	0.76	2.10	4	3
1:A:33:ILE:CG2	1:A:85:ILE:HG23	0.76	2.09	6	13
1:A:47:PHE:CD1	1:A:53:THR:HG21	0.76	2.15	15	2
1:A:9:THR:HG21	1:A:100:LEU:HD22	0.76	1.57	16	2
1:A:19:LEU:CD1	1:A:70:ILE:HD11	0.76	2.11	17	1
1:A:21:ILE:CG1	1:A:22:PRO:HD2	0.76	2.11	9	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:MET:HG2	1:A:30:ILE:HD12	0.76	1.54	4	2
1:A:30:ILE:HD11	1:A:93:VAL:HG21	0.75	1.57	6	3
1:A:73:LEU:CD2	1:A:100:LEU:HD21	0.75	2.11	6	1
1:A:37:LYS:NZ	1:A:40:ASP:HB2	0.75	1.97	13	1
1:A:19:LEU:HD13	1:A:98:PHE:CD2	0.74	2.16	14	1
1:A:100:LEU:O	1:A:101:LYS:HG2	0.74	1.82	14	2
1:A:44:ILE:HD13	1:A:81:TYR:CD2	0.74	2.17	9	2
1:A:60:TYR:HD1	1:A:70:ILE:CG2	0.74	1.95	9	1
1:A:45:ALA:CB	1:A:62:LEU:HD13	0.74	2.12	3	3
1:A:19:LEU:HB2	1:A:68:LEU:HB3	0.74	1.59	18	6
1:A:60:TYR:HE2	1:A:81:TYR:CE1	0.74	2.00	18	1
1:A:9:THR:CG2	1:A:100:LEU:HD22	0.74	2.13	16	2
1:A:12:ALA:O	1:A:15:GLN:HB2	0.73	1.83	8	4
1:A:78:GLN:HG2	1:A:100:LEU:CB	0.73	2.11	14	1
1:A:29:ASP:O	1:A:88:THR:HG23	0.73	1.83	14	5
1:A:60:TYR:HE1	1:A:81:TYR:CE2	0.73	2.00	7	3
1:A:73:LEU:HD13	1:A:73:LEU:O	0.73	1.84	12	2
1:A:78:GLN:HG3	1:A:100:LEU:O	0.73	1.82	11	2
1:A:19:LEU:CD1	1:A:98:PHE:HD2	0.73	1.95	11	1
1:A:60:TYR:HE2	1:A:81:TYR:CE2	0.73	2.00	17	3
1:A:12:ALA:O	1:A:15:GLN:HB3	0.72	1.82	9	5
1:A:61:LYS:O	1:A:68:LEU:HD12	0.72	1.84	1	9
1:A:82:LYS:HG2	1:A:96:LYS:O	0.72	1.84	7	3
1:A:18:ASN:O	1:A:19:LEU:HD22	0.72	1.84	11	2
1:A:13:LEU:HD13	1:A:74:LYS:CB	0.72	2.13	7	4
1:A:19:LEU:CD2	1:A:70:ILE:HD11	0.72	2.11	15	5
1:A:42:LYS:HB3	1:A:42:LYS:NZ	0.72	1.98	4	1
1:A:73:LEU:HD12	1:A:77:ASP:OD1	0.72	1.85	4	1
1:A:15:GLN:HG3	1:A:16:ASP:N	0.72	1.99	13	3
1:A:40:ASP:O	1:A:41:LYS:HG2	0.72	1.85	8	3
1:A:38:THR:HG23	1:A:80:ILE:C	0.72	2.03	11	7
1:A:73:LEU:HB3	1:A:77:ASP:HB3	0.72	1.60	15	1
1:A:19:LEU:HD22	1:A:35:TRP:CZ3	0.72	2.20	17	1
1:A:87:ASP:OD1	1:A:91:LYS:HB2	0.71	1.84	9	6
1:A:73:LEU:HD12	1:A:77:ASP:HB3	0.71	1.63	18	1
1:A:72:HIS:C	1:A:73:LEU:HD22	0.71	2.06	1	1
1:A:51:LYS:O	1:A:52:GLU:HB2	0.71	1.86	18	3
1:A:9:THR:HG21	1:A:19:LEU:HD13	0.71	1.63	9	1
1:A:87:ASP:HB3	1:A:93:VAL:HG11	0.71	1.61	1	4
1:A:70:ILE:HG22	1:A:73:LEU:HD21	0.71	1.62	11	1
1:A:44:ILE:HG23	1:A:60:TYR:CG	0.71	2.21	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:TYR:HE2	1:A:100:LEU:HB2	0.70	1.44	18	2
1:A:13:LEU:HD11	1:A:102:ILE:HG21	0.70	1.61	4	6
1:A:60:TYR:CD1	1:A:70:ILE:CG2	0.70	2.74	9	1
1:A:45:ALA:CB	1:A:62:LEU:HD21	0.70	2.16	10	3
1:A:70:ILE:HD13	1:A:100:LEU:CD2	0.70	2.14	11	1
1:A:82:LYS:HG3	1:A:96:LYS:O	0.70	1.86	18	6
1:A:21:ILE:CD1	1:A:85:ILE:HG13	0.70	2.16	18	1
1:A:18:ASN:O	1:A:19:LEU:HD23	0.70	1.85	16	2
1:A:19:LEU:CD1	1:A:68:LEU:HD22	0.70	2.16	16	2
1:A:13:LEU:HD12	1:A:13:LEU:C	0.70	2.06	15	3
1:A:13:LEU:HD22	1:A:102:ILE:HG21	0.70	1.61	17	2
1:A:32:ASP:O	1:A:33:ILE:HD13	0.70	1.87	3	1
1:A:43:LYS:HD2	1:A:54:PHE:CD2	0.70	2.21	8	1
1:A:38:THR:HG21	1:A:80:ILE:HB	0.69	1.62	5	2
1:A:63:PHE:HE1	1:A:69:LYS:CB	0.69	2.00	15	1
1:A:32:ASP:C	1:A:33:ILE:HD12	0.69	2.06	1	2
1:A:7:LEU:HD23	1:A:98:PHE:CZ	0.69	2.22	14	2
1:A:81:TYR:CE1	1:A:100:LEU:HD22	0.69	2.22	9	1
1:A:35:TRP:HB3	1:A:68:LEU:HD22	0.69	1.63	15	1
1:A:22:PRO:HG2	1:A:96:LYS:HG3	0.69	1.65	13	1
1:A:33:ILE:CA	1:A:85:ILE:HG23	0.69	2.18	7	13
1:A:33:ILE:CG2	1:A:85:ILE:HD12	0.69	2.18	14	2
1:A:9:THR:HG23	1:A:99:ASP:O	0.69	1.86	8	1
1:A:45:ALA:HB1	1:A:62:LEU:HD21	0.69	1.65	10	3
1:A:19:LEU:HD21	1:A:100:LEU:HD13	0.69	1.64	12	2
1:A:44:ILE:HD12	1:A:60:TYR:CD2	0.69	2.21	1	2
1:A:19:LEU:HB3	1:A:35:TRP:CZ2	0.69	2.23	11	3
1:A:79:ASP:O	1:A:100:LEU:HB3	0.69	1.88	14	3
1:A:12:ALA:HB3	1:A:15:GLN:NE2	0.68	2.04	18	2
1:A:21:ILE:HD12	1:A:94:LEU:HD11	0.68	1.64	14	1
1:A:60:TYR:CE2	1:A:81:TYR:HE2	0.68	2.04	17	3
1:A:33:ILE:CB	1:A:85:ILE:HG23	0.68	2.18	13	9
1:A:36:GLU:C	1:A:44:ILE:HD12	0.68	2.08	9	2
1:A:73:LEU:HD13	1:A:102:ILE:HD11	0.68	1.66	8	2
1:A:35:TRP:CG	1:A:68:LEU:HD12	0.68	2.23	5	2
1:A:73:LEU:HD12	1:A:100:LEU:HD23	0.68	1.65	11	2
1:A:44:ILE:HD12	1:A:60:TYR:CE2	0.68	2.22	1	1
1:A:21:ILE:HD13	1:A:22:PRO:N	0.68	2.03	9	3
1:A:19:LEU:HB2	1:A:68:LEU:O	0.68	1.89	1	6
1:A:5:ASN:HB3	1:A:97:ILE:HD12	0.68	1.64	10	1
1:A:63:PHE:CZ	1:A:69:LYS:HB2	0.67	2.24	5	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LYS:HB3	1:A:44:ILE:HG23	0.67	1.64	5	1
1:A:38:THR:HG23	1:A:81:TYR:N	0.67	2.04	2	6
1:A:13:LEU:HD13	1:A:102:ILE:CG2	0.67	2.18	4	1
1:A:13:LEU:HD13	1:A:74:LYS:HA	0.67	1.65	5	2
1:A:100:LEU:HD22	1:A:100:LEU:O	0.67	1.88	14	1
1:A:43:LYS:O	1:A:43:LYS:HD3	0.67	1.90	12	1
1:A:40:ASP:C	1:A:41:LYS:HG3	0.67	2.10	4	1
1:A:13:LEU:C	1:A:13:LEU:HD12	0.67	2.09	7	1
1:A:73:LEU:HD12	1:A:77:ASP:O	0.67	1.90	9	2
1:A:48:ARG:O	1:A:52:GLU:HB3	0.67	1.89	18	1
1:A:73:LEU:CD2	1:A:100:LEU:HD11	0.67	2.11	8	3
1:A:9:THR:HG21	1:A:19:LEU:HD23	0.67	1.67	6	1
1:A:35:TRP:CH2	1:A:98:PHE:CE2	0.67	2.83	8	3
1:A:81:TYR:CZ	1:A:100:LEU:HD22	0.67	2.24	9	1
1:A:73:LEU:HD22	1:A:77:ASP:O	0.67	1.90	16	2
1:A:24:PHE:O	1:A:94:LEU:HD22	0.67	1.89	16	1
1:A:47:PHE:CE1	1:A:53:THR:HG22	0.66	2.25	8	2
1:A:70:ILE:HD13	1:A:100:LEU:HD22	0.66	1.65	11	1
1:A:45:ALA:HB1	1:A:62:LEU:HG	0.66	1.66	18	2
1:A:80:ILE:HG12	1:A:99:ASP:CG	0.66	2.10	14	1
1:A:19:LEU:HD21	1:A:100:LEU:CD1	0.66	2.20	7	3
1:A:73:LEU:O	1:A:102:ILE:HD11	0.66	1.88	11	1
1:A:47:PHE:CD1	1:A:53:THR:HG22	0.66	2.25	8	2
1:A:18:ASN:O	1:A:19:LEU:HD12	0.66	1.90	10	1
1:A:73:LEU:CD1	1:A:102:ILE:HD11	0.66	2.20	10	2
1:A:80:ILE:HG12	1:A:99:ASP:OD2	0.66	1.90	13	1
1:A:7:LEU:HD12	1:A:98:PHE:CD2	0.66	2.26	7	3
1:A:35:TRP:CB	1:A:68:LEU:HD22	0.66	2.21	15	1
1:A:26:MET:CG	1:A:30:ILE:HD12	0.66	2.21	4	1
1:A:70:ILE:HD11	1:A:81:TYR:CE2	0.65	2.25	7	2
1:A:13:LEU:HD12	1:A:102:ILE:HD12	0.65	1.65	4	1
1:A:13:LEU:HG	1:A:102:ILE:HD12	0.65	1.66	11	1
1:A:73:LEU:HD12	1:A:73:LEU:O	0.65	1.90	16	1
1:A:21:ILE:HG13	1:A:22:PRO:HD3	0.65	1.67	11	1
1:A:7:LEU:HD23	1:A:98:PHE:CD1	0.65	2.27	3	1
1:A:70:ILE:HD11	1:A:100:LEU:CD2	0.65	2.21	9	3
1:A:85:ILE:HD12	1:A:94:LEU:HD12	0.65	1.67	15	1
1:A:37:LYS:CB	1:A:44:ILE:HD11	0.65	2.22	14	2
1:A:12:ALA:N	1:A:73:LEU:HD12	0.65	2.06	13	1
1:A:13:LEU:HD13	1:A:102:ILE:HD12	0.65	1.69	4	1
1:A:17:ILE:CG2	1:A:73:LEU:HD23	0.65	2.22	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:LEU:HD12	1:A:73:LEU:C	0.65	2.11	16	1
1:A:63:PHE:HE2	1:A:69:LYS:HB3	0.65	1.48	7	1
1:A:9:THR:HG22	1:A:100:LEU:HA	0.64	1.70	1	6
1:A:38:THR:HG23	1:A:81:TYR:C	0.64	2.12	17	5
1:A:15:GLN:HG3	1:A:16:ASP:H	0.64	1.52	13	1
1:A:33:ILE:HB	1:A:62:LEU:HD21	0.64	1.67	5	2
1:A:21:ILE:HD12	1:A:21:ILE:C	0.64	2.13	11	1
1:A:13:LEU:HD12	1:A:74:LYS:CA	0.64	2.22	4	1
1:A:59:THR:O	1:A:70:ILE:HG23	0.64	1.93	17	9
1:A:30:ILE:HG23	1:A:86:TYR:O	0.64	1.92	13	3
1:A:15:GLN:O	1:A:73:LEU:HB3	0.64	1.93	3	4
1:A:21:ILE:HD13	1:A:21:ILE:C	0.64	2.13	1	1
1:A:19:LEU:HD11	1:A:81:TYR:CG	0.64	2.28	2	3
1:A:68:LEU:CD2	1:A:70:ILE:CG2	0.64	2.76	9	1
1:A:35:TRP:CH2	1:A:98:PHE:CD2	0.64	2.86	8	2
1:A:21:ILE:HD13	1:A:83:VAL:HG11	0.64	1.68	5	1
1:A:21:ILE:HD12	1:A:22:PRO:CD	0.64	2.23	5	3
1:A:21:ILE:HG21	1:A:65:ASN:O	0.64	1.93	12	3
1:A:72:HIS:O	1:A:73:LEU:HD22	0.63	1.92	1	2
1:A:100:LEU:HD13	1:A:101:LYS:N	0.63	2.08	5	2
1:A:19:LEU:HD13	1:A:68:LEU:CD2	0.63	2.22	17	1
1:A:94:LEU:HD13	1:A:94:LEU:C	0.63	2.13	15	1
1:A:60:TYR:CE1	1:A:70:ILE:HG23	0.63	2.27	10	6
1:A:80:ILE:HG13	1:A:100:LEU:HD11	0.63	1.71	14	1
1:A:16:ASP:HA	1:A:73:LEU:HD23	0.63	1.68	1	1
1:A:37:LYS:HB3	1:A:44:ILE:CD1	0.63	2.21	9	1
1:A:38:THR:HG23	1:A:81:TYR:CA	0.63	2.24	14	5
1:A:19:LEU:HD22	1:A:68:LEU:CD2	0.63	2.24	10	1
1:A:78:GLN:HG3	1:A:101:LYS:HA	0.62	1.69	17	4
1:A:80:ILE:HG23	1:A:98:PHE:O	0.62	1.93	13	5
1:A:45:ALA:CB	1:A:62:LEU:HD23	0.62	2.22	2	1
1:A:22:PRO:CB	1:A:94:LEU:HD21	0.62	2.23	7	3
1:A:78:GLN:CG	1:A:100:LEU:HD23	0.62	2.24	14	1
2:B:2:NAG:H83	2:B:7:MAN:H3	0.62	1.70	16	1
1:A:86:TYR:CD1	1:A:86:TYR:N	0.62	2.67	6	5
1:A:35:TRP:CZ3	1:A:98:PHE:HD2	0.62	2.11	8	2
1:A:73:LEU:C	1:A:73:LEU:HD23	0.62	2.14	7	1
1:A:37:LYS:CD	1:A:42:LYS:HB3	0.62	2.25	9	1
1:A:62:LEU:HD23	1:A:68:LEU:HD12	0.62	1.70	10	1
1:A:7:LEU:CD2	1:A:98:PHE:CD2	0.62	2.83	2	1
1:A:61:LYS:HE3	1:A:63:PHE:HE1	0.62	1.52	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:LEU:C	1:A:63:PHE:HD1	0.62	1.98	4	2
1:A:43:LYS:HD3	1:A:46:GLN:HB3	0.61	1.71	8	1
1:A:57:LYS:CG	1:A:59:THR:HG22	0.61	2.25	17	2
1:A:68:LEU:C	1:A:68:LEU:HD23	0.61	2.15	2	1
1:A:85:ILE:O	1:A:93:VAL:HG23	0.61	1.96	3	1
1:A:5:ASN:O	1:A:97:ILE:HD12	0.61	1.94	18	4
1:A:73:LEU:O	1:A:73:LEU:HD22	0.61	1.95	6	1
1:A:11:GLY:HA3	1:A:73:LEU:HD11	0.61	1.73	13	1
1:A:74:LYS:O	1:A:102:ILE:HD12	0.61	1.95	7	1
1:A:19:LEU:HD21	1:A:81:TYR:CD2	0.61	2.31	15	1
1:A:70:ILE:HD12	1:A:100:LEU:CD1	0.61	2.26	17	1
1:A:22:PRO:HG2	1:A:96:LYS:CD	0.61	2.26	17	1
1:A:83:VAL:CG1	1:A:98:PHE:CE1	0.61	2.82	7	10
1:A:33:ILE:HG23	1:A:85:ILE:HG12	0.61	1.73	13	2
1:A:35:TRP:CB	1:A:68:LEU:HD12	0.61	2.26	2	3
1:A:83:VAL:CG1	1:A:98:PHE:HE1	0.61	2.09	9	4
1:A:21:ILE:CG2	1:A:22:PRO:CD	0.61	2.72	11	3
1:A:85:ILE:N	1:A:85:ILE:HD12	0.60	2.11	2	1
1:A:35:TRP:CD1	1:A:62:LEU:HD11	0.60	2.31	3	2
1:A:21:ILE:CD1	1:A:94:LEU:HD11	0.60	2.26	14	1
1:A:57:LYS:HG3	1:A:59:THR:HG22	0.60	1.72	10	3
1:A:37:LYS:HB2	1:A:44:ILE:CD1	0.60	2.25	14	1
1:A:78:GLN:HA	1:A:100:LEU:HD12	0.60	1.71	8	1
1:A:44:ILE:HG23	1:A:60:TYR:CD2	0.60	2.31	15	1
1:A:60:TYR:HE2	1:A:81:TYR:HE1	0.60	1.36	18	1
1:A:13:LEU:HD13	1:A:74:LYS:CA	0.60	2.26	5	2
1:A:24:PHE:CD1	1:A:94:LEU:HD23	0.60	2.32	7	1
1:A:19:LEU:HD12	1:A:35:TRP:HZ3	0.60	1.54	14	1
1:A:33:ILE:CG2	1:A:85:ILE:HD13	0.60	2.15	5	1
1:A:31:ASP:CG	1:A:88:THR:HG22	0.60	2.16	2	1
1:A:79:ASP:N	1:A:100:LEU:HB3	0.60	2.10	14	1
1:A:60:TYR:CE2	1:A:81:TYR:HE1	0.60	2.13	18	1
1:A:80:ILE:HG12	1:A:99:ASP:OD1	0.60	1.97	16	2
1:A:73:LEU:HB2	1:A:77:ASP:OD2	0.60	1.97	4	1
1:A:37:LYS:HB3	1:A:44:ILE:CG2	0.60	2.27	5	1
1:A:73:LEU:HB3	1:A:77:ASP:HB2	0.60	1.72	14	1
1:A:19:LEU:HD22	1:A:70:ILE:CD1	0.60	2.19	15	1
1:A:94:LEU:C	1:A:94:LEU:HD13	0.60	2.17	14	2
1:A:22:PRO:HG3	1:A:96:LYS:HE2	0.60	1.73	6	1
1:A:70:ILE:CD1	1:A:100:LEU:HD21	0.60	2.23	9	2
1:A:17:ILE:HG22	1:A:73:LEU:HD23	0.60	1.74	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LEU:CD2	1:A:98:PHE:CE2	0.59	2.85	2	5
1:A:84:SER:HB2	1:A:86:TYR:HE1	0.59	1.57	14	1
1:A:63:PHE:CD1	1:A:67:THR:HG22	0.59	2.33	11	2
1:A:63:PHE:HD2	1:A:67:THR:HG22	0.59	1.57	12	2
1:A:38:THR:HG22	1:A:81:TYR:C	0.59	2.18	2	2
1:A:47:PHE:CD1	1:A:62:LEU:HD12	0.59	2.27	10	1
1:A:63:PHE:CE1	1:A:69:LYS:HB3	0.59	2.31	11	1
1:A:17:ILE:CD1	1:A:70:ILE:HD13	0.59	2.27	12	1
1:A:73:LEU:HD22	1:A:77:ASP:CG	0.59	2.17	15	1
1:A:45:ALA:C	1:A:46:GLN:HG3	0.59	2.18	3	1
1:A:21:ILE:CB	1:A:22:PRO:HD3	0.59	2.27	11	2
1:A:19:LEU:HD13	1:A:98:PHE:HD2	0.59	1.51	14	1
1:A:45:ALA:HB1	1:A:62:LEU:HD11	0.59	1.68	16	1
1:A:60:TYR:CE1	1:A:70:ILE:CG2	0.59	2.86	10	6
1:A:80:ILE:HD13	1:A:80:ILE:N	0.59	2.13	12	1
1:A:35:TRP:CH2	1:A:98:PHE:CE1	0.59	2.90	7	1
1:A:7:LEU:HD12	1:A:7:LEU:C	0.59	2.18	2	1
1:A:17:ILE:HG21	1:A:100:LEU:HD21	0.58	1.71	4	4
1:A:7:LEU:CD1	1:A:98:PHE:CZ	0.58	2.86	5	7
1:A:73:LEU:HD12	1:A:102:ILE:CD1	0.58	2.29	10	1
1:A:80:ILE:HG23	1:A:99:ASP:OD2	0.58	1.98	17	2
1:A:7:LEU:CD1	1:A:98:PHE:CE2	0.58	2.87	16	8
1:A:73:LEU:CD1	1:A:73:LEU:C	0.58	2.71	16	1
1:A:86:TYR:N	1:A:86:TYR:CD1	0.58	2.71	1	3
1:A:21:ILE:HG13	1:A:83:VAL:HG11	0.58	1.74	1	1
1:A:44:ILE:HD12	1:A:68:LEU:HD21	0.58	1.75	6	1
1:A:44:ILE:HD11	1:A:81:TYR:CD2	0.58	2.33	12	1
1:A:19:LEU:CB	1:A:35:TRP:CH2	0.58	2.85	17	10
1:A:13:LEU:H	1:A:13:LEU:HD23	0.58	1.57	2	2
1:A:19:LEU:CD1	1:A:35:TRP:CZ3	0.58	2.87	2	5
1:A:73:LEU:HD12	1:A:77:ASP:CB	0.58	2.29	18	1
1:A:35:TRP:CH2	1:A:98:PHE:CZ	0.58	2.92	7	1
1:A:13:LEU:HD22	1:A:102:ILE:CG2	0.58	2.28	17	1
1:A:86:TYR:HD1	1:A:86:TYR:N	0.58	1.95	6	2
1:A:13:LEU:CD1	1:A:102:ILE:CG2	0.58	2.81	14	7
1:A:44:ILE:HD13	1:A:81:TYR:CE2	0.58	2.33	9	1
1:A:73:LEU:HD22	1:A:77:ASP:OD1	0.58	1.99	15	1
1:A:84:SER:CB	1:A:86:TYR:HE1	0.57	2.11	1	3
1:A:45:ALA:O	1:A:46:GLN:HG3	0.57	1.99	3	1
1:A:19:LEU:HG	1:A:70:ILE:HD11	0.57	1.75	13	1
1:A:31:ASP:OD1	1:A:88:THR:HG22	0.57	1.99	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:LYS:CE	1:A:63:PHE:HE1	0.57	2.13	14	2
1:A:81:TYR:HE1	1:A:100:LEU:CB	0.57	2.09	13	2
1:A:70:ILE:HG22	1:A:77:ASP:OD2	0.57	1.99	14	1
1:A:63:PHE:CE1	1:A:69:LYS:CB	0.57	2.80	15	1
1:A:60:TYR:CE2	1:A:81:TYR:CE1	0.57	2.89	18	1
1:A:30:ILE:HD11	1:A:93:VAL:CG2	0.57	2.29	6	2
1:A:21:ILE:HD13	1:A:83:VAL:CG1	0.57	2.29	5	2
1:A:86:TYR:HD1	1:A:92:ASN:HA	0.57	1.60	18	2
1:A:45:ALA:HB3	1:A:68:LEU:CD1	0.57	2.30	17	3
1:A:19:LEU:CD1	1:A:98:PHE:CD2	0.57	2.87	1	2
1:A:83:VAL:HG23	1:A:85:ILE:CD1	0.57	2.21	14	1
1:A:73:LEU:HD23	1:A:100:LEU:HD11	0.57	1.77	2	1
1:A:12:ALA:HA	1:A:102:ILE:HG23	0.56	1.77	5	2
1:A:19:LEU:O	1:A:67:THR:HG23	0.56	2.00	6	3
1:A:37:LYS:HZ3	1:A:40:ASP:HB2	0.56	1.58	13	1
1:A:37:LYS:HB3	1:A:42:LYS:O	0.56	2.00	14	2
1:A:85:ILE:O	1:A:93:VAL:HG22	0.56	1.98	9	3
1:A:44:ILE:CD1	1:A:81:TYR:CD2	0.56	2.88	9	3
1:A:21:ILE:CG1	1:A:22:PRO:HD3	0.56	2.29	11	2
1:A:33:ILE:HG22	1:A:62:LEU:HD11	0.56	1.75	14	1
1:A:70:ILE:CD1	1:A:81:TYR:CE2	0.56	2.88	14	2
1:A:19:LEU:HD12	1:A:98:PHE:CG	0.56	2.35	18	1
1:A:60:TYR:CD2	1:A:70:ILE:CG2	0.56	2.88	4	1
1:A:12:ALA:C	1:A:102:ILE:HD13	0.56	2.20	7	1
1:A:101:LYS:O	1:A:102:ILE:HD13	0.56	2.01	17	1
1:A:47:PHE:HD1	1:A:53:THR:HG21	0.56	1.58	15	1
1:A:57:LYS:HB2	1:A:59:THR:HG22	0.56	1.77	1	3
1:A:19:LEU:HD12	1:A:35:TRP:CH2	0.56	2.36	14	3
1:A:13:LEU:HD12	1:A:74:LYS:C	0.56	2.21	4	1
1:A:60:TYR:HD1	1:A:70:ILE:HG21	0.56	1.60	9	1
1:A:44:ILE:CD1	1:A:81:TYR:CE2	0.56	2.88	12	1
1:A:24:PHE:HD1	1:A:25:GLN:N	0.56	1.98	13	2
1:A:26:MET:HE1	1:A:85:ILE:HG21	0.56	1.78	17	1
1:A:45:ALA:CB	1:A:62:LEU:CD1	0.56	2.84	9	4
1:A:74:LYS:CE	1:A:76:ASP:HB3	0.56	2.29	8	1
1:A:78:GLN:HB2	1:A:102:ILE:HD11	0.56	1.78	14	2
1:A:73:LEU:CB	1:A:77:ASP:CB	0.56	2.74	15	5
1:A:83:VAL:CG1	1:A:98:PHE:CE2	0.56	2.88	8	1
1:A:103:GLN:HG2	1:A:103:GLN:O	0.56	2.01	13	1
1:A:44:ILE:HD11	1:A:81:TYR:HD2	0.55	1.61	12	1
1:A:35:TRP:CZ3	1:A:98:PHE:CD2	0.55	2.95	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:VAL:HG12	1:A:98:PHE:CZ	0.55	2.35	1	1
1:A:73:LEU:O	1:A:73:LEU:HD13	0.55	2.02	3	3
1:A:13:LEU:HB2	1:A:74:LYS:CB	0.55	2.31	17	1
1:A:40:ASP:OD2	1:A:42:LYS:HB2	0.55	2.01	7	2
1:A:44:ILE:CG2	1:A:60:TYR:CG	0.55	2.89	15	1
1:A:21:ILE:CB	1:A:83:VAL:HG11	0.55	2.27	10	3
1:A:41:LYS:O	1:A:41:LYS:HD2	0.55	2.02	3	1
1:A:60:TYR:CE1	1:A:81:TYR:CE2	0.55	2.95	11	2
1:A:73:LEU:HD12	1:A:102:ILE:HD11	0.55	1.78	10	1
1:A:94:LEU:HD23	1:A:94:LEU:C	0.55	2.20	13	1
1:A:100:LEU:HD22	1:A:100:LEU:C	0.55	2.22	14	1
1:A:19:LEU:HD23	1:A:70:ILE:HD11	0.55	1.79	18	2
1:A:97:ILE:C	1:A:98:PHE:HD1	0.55	2.04	2	2
1:A:38:THR:HG23	1:A:80:ILE:O	0.55	2.02	5	2
1:A:100:LEU:HD13	1:A:100:LEU:C	0.55	2.22	8	2
1:A:34:LYS:CG	1:A:46:GLN:HG3	0.55	2.31	10	1
1:A:73:LEU:HD13	1:A:74:LYS:O	0.55	2.01	16	1
1:A:42:LYS:HB3	1:A:42:LYS:HZ2	0.55	1.61	4	1
1:A:42:LYS:O	1:A:44:ILE:HG23	0.55	2.02	17	3
1:A:35:TRP:HB3	1:A:68:LEU:HD12	0.55	1.78	2	1
1:A:78:GLN:CG	1:A:100:LEU:HB2	0.55	2.24	14	1
1:A:81:TYR:CE1	1:A:100:LEU:CB	0.54	2.90	8	2
1:A:62:LEU:CD1	1:A:68:LEU:CD1	0.54	2.85	13	1
1:A:73:LEU:HD21	1:A:100:LEU:HG	0.54	1.79	16	1
1:A:19:LEU:HD22	1:A:35:TRP:HZ3	0.54	1.61	17	1
1:A:9:THR:HG22	1:A:100:LEU:HD12	0.54	1.78	1	1
1:A:83:VAL:HG22	1:A:85:ILE:CG1	0.54	2.32	7	4
1:A:35:TRP:CB	1:A:68:LEU:CD1	0.54	2.85	5	3
1:A:36:GLU:OE2	1:A:41:LYS:HG2	0.54	2.02	9	2
1:A:21:ILE:C	1:A:21:ILE:HD13	0.54	2.21	14	1
1:A:47:PHE:CE1	1:A:53:THR:CG2	0.54	2.90	8	3
1:A:37:LYS:CG	1:A:42:LYS:CB	0.54	2.84	3	1
1:A:30:ILE:HD13	1:A:87:ASP:HB3	0.54	1.78	11	2
1:A:81:TYR:OH	1:A:100:LEU:HD22	0.54	2.03	9	2
1:A:57:LYS:HB3	1:A:59:THR:HG22	0.54	1.77	13	3
1:A:63:PHE:CD2	1:A:67:THR:CG2	0.54	2.90	12	5
1:A:100:LEU:HD13	1:A:100:LEU:N	0.54	2.17	14	1
1:A:21:ILE:HD13	1:A:21:ILE:O	0.54	2.02	14	1
1:A:38:THR:OG1	1:A:80:ILE:HG22	0.54	2.03	10	8
1:A:19:LEU:HD13	1:A:35:TRP:CE3	0.54	2.37	6	1
1:A:34:LYS:HG3	1:A:46:GLN:HG2	0.54	1.78	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:LEU:HD22	1:A:77:ASP:C	0.54	2.22	16	1
1:A:33:ILE:CD1	1:A:85:ILE:CG2	0.54	2.85	3	4
1:A:85:ILE:CD1	1:A:94:LEU:HD23	0.54	2.27	2	1
1:A:70:ILE:CG2	1:A:73:LEU:HD21	0.54	2.33	11	1
1:A:17:ILE:HG22	1:A:73:LEU:CD1	0.54	2.33	1	1
1:A:21:ILE:HG21	1:A:66:GLY:O	0.54	2.02	3	1
1:A:99:ASP:O	1:A:101:LYS:HG3	0.54	2.03	8	1
1:A:22:PRO:HG2	1:A:94:LEU:CD2	0.54	2.32	6	1
1:A:70:ILE:HD13	1:A:81:TYR:OH	0.54	2.02	13	1
1:A:17:ILE:HG21	1:A:100:LEU:CD1	0.53	2.33	1	2
1:A:87:ASP:CG	1:A:91:LYS:HB2	0.53	2.22	2	1
1:A:83:VAL:HG11	1:A:98:PHE:HE1	0.53	1.63	5	1
1:A:26:MET:HB3	1:A:30:ILE:HG21	0.53	1.78	7	2
1:A:68:LEU:HD23	1:A:70:ILE:CG2	0.53	2.33	9	1
1:A:13:LEU:HA	1:A:74:LYS:HA	0.53	1.80	15	1
1:A:13:LEU:CD1	1:A:74:LYS:HB3	0.53	2.30	7	2
1:A:33:ILE:CG2	1:A:62:LEU:HD21	0.53	2.33	17	1
1:A:73:LEU:CD1	1:A:100:LEU:HD12	0.53	2.34	18	1
1:A:35:TRP:CB	1:A:68:LEU:HD13	0.53	2.33	12	4
1:A:17:ILE:HG13	1:A:100:LEU:HD11	0.53	1.80	12	1
1:A:7:LEU:CD1	1:A:98:PHE:CE1	0.53	2.88	12	1
1:A:30:ILE:HD13	1:A:31:ASP:N	0.53	2.18	1	1
1:A:7:LEU:HD23	1:A:98:PHE:CG	0.53	2.37	3	2
1:A:63:PHE:HD2	1:A:67:THR:CG2	0.53	2.17	12	1
1:A:22:PRO:HG3	1:A:96:LYS:HE3	0.53	1.80	7	2
1:A:44:ILE:HD11	1:A:68:LEU:CD2	0.53	2.34	1	1
1:A:44:ILE:HD11	1:A:68:LEU:HD21	0.53	1.80	1	1
1:A:35:TRP:CG	1:A:68:LEU:CD1	0.53	2.91	5	2
1:A:19:LEU:HD21	1:A:70:ILE:HD11	0.53	1.80	11	1
1:A:37:LYS:CA	1:A:44:ILE:HD11	0.53	2.33	14	1
1:A:22:PRO:HG3	1:A:96:LYS:HG3	0.53	1.81	6	1
1:A:24:PHE:CD1	1:A:94:LEU:HD12	0.53	2.38	13	1
1:A:34:LYS:HG3	1:A:46:GLN:HG3	0.52	1.80	1	1
1:A:94:LEU:HD22	1:A:95:GLU:H	0.52	1.63	5	2
1:A:63:PHE:CZ	1:A:69:LYS:HB3	0.52	2.39	11	3
1:A:47:PHE:HE1	1:A:53:THR:HG21	0.52	1.64	13	1
1:A:33:ILE:O	1:A:62:LEU:HD21	0.52	2.03	14	1
1:A:44:ILE:HD12	1:A:60:TYR:HD2	0.52	1.60	17	1
1:A:21:ILE:CG1	1:A:83:VAL:CG1	0.52	2.87	1	2
1:A:61:LYS:HE3	1:A:63:PHE:CE1	0.52	2.37	14	2
1:A:62:LEU:HD12	1:A:63:PHE:H	0.52	1.64	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ILE:HD12	1:A:93:VAL:HG21	0.52	1.80	8	1
1:A:45:ALA:CB	1:A:62:LEU:HD11	0.52	2.35	9	2
1:A:73:LEU:CD2	1:A:100:LEU:CD1	0.52	2.87	13	3
1:A:73:LEU:CD1	1:A:100:LEU:CD2	0.52	2.87	11	2
1:A:63:PHE:CE2	1:A:67:THR:HG22	0.52	2.40	10	1
1:A:73:LEU:HD12	1:A:77:ASP:C	0.52	2.23	18	1
1:A:41:LYS:HG3	1:A:41:LYS:O	0.52	2.04	11	3
1:A:21:ILE:HD13	1:A:22:PRO:CD	0.52	2.34	9	1
1:A:37:LYS:HD3	1:A:42:LYS:HB3	0.52	1.82	15	2
1:A:37:LYS:HE3	1:A:42:LYS:HB2	0.52	1.82	16	1
1:A:60:TYR:CD1	1:A:70:ILE:HG23	0.52	2.38	15	4
1:A:17:ILE:CG2	1:A:73:LEU:CD2	0.52	2.88	13	1
1:A:45:ALA:CB	1:A:68:LEU:CD1	0.52	2.87	7	3
1:A:21:ILE:C	1:A:21:ILE:CD1	0.51	2.78	14	3
1:A:45:ALA:HB1	1:A:62:LEU:HB2	0.51	1.82	6	2
1:A:33:ILE:CG1	1:A:85:ILE:CG2	0.51	2.87	7	2
1:A:19:LEU:CG	1:A:35:TRP:CH2	0.51	2.94	11	1
1:A:35:TRP:HB3	1:A:68:LEU:HD13	0.51	1.82	3	1
1:A:37:LYS:HB2	1:A:44:ILE:CG2	0.51	2.35	10	1
1:A:79:ASP:C	1:A:100:LEU:HB3	0.51	2.26	14	1
1:A:36:GLU:O	1:A:44:ILE:HD12	0.51	2.04	9	2
1:A:80:ILE:CG1	1:A:100:LEU:CD1	0.51	2.87	14	1
1:A:95:GLU:HG2	1:A:96:LYS:N	0.51	2.21	14	2
1:A:80:ILE:HG23	1:A:99:ASP:OD1	0.51	2.06	15	2
1:A:79:ASP:O	1:A:100:LEU:HB2	0.51	2.05	9	1
1:A:22:PRO:HG2	1:A:96:LYS:CE	0.51	2.36	17	1
1:A:21:ILE:HG13	1:A:83:VAL:CG1	0.51	2.36	1	2
1:A:83:VAL:CG1	1:A:98:PHE:CZ	0.51	2.93	1	1
1:A:73:LEU:CD1	1:A:102:ILE:CD1	0.51	2.88	10	3
1:A:83:VAL:HG12	1:A:98:PHE:CE2	0.51	2.41	8	1
1:A:43:LYS:HD3	1:A:46:GLN:CB	0.51	2.34	8	1
1:A:79:ASP:N	1:A:100:LEU:CB	0.51	2.73	14	1
1:A:85:ILE:HD12	1:A:94:LEU:CD1	0.51	2.35	15	1
1:A:70:ILE:CD1	1:A:100:LEU:CD1	0.51	2.89	17	1
1:A:21:ILE:HG12	1:A:22:PRO:CD	0.51	2.35	6	4
1:A:70:ILE:CD1	1:A:100:LEU:CD2	0.51	2.89	11	2
1:A:51:LYS:O	1:A:52:GLU:CB	0.51	2.59	18	1
1:A:73:LEU:HD21	1:A:100:LEU:CD2	0.50	2.36	2	1
1:A:17:ILE:HG22	1:A:73:LEU:HD13	0.50	1.81	7	1
1:A:33:ILE:HD13	1:A:85:ILE:HG22	0.50	1.82	6	1
1:A:32:ASP:O	1:A:33:ILE:HD12	0.50	2.06	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:LEU:CG	1:A:70:ILE:HD11	0.50	2.36	13	1
1:A:33:ILE:HG21	1:A:66:GLY:HA2	0.50	1.83	14	1
1:A:33:ILE:HG23	1:A:85:ILE:HG21	0.50	1.82	16	2
1:A:60:TYR:CD2	1:A:70:ILE:HG22	0.50	2.40	4	1
1:A:45:ALA:HB1	1:A:62:LEU:CG	0.50	2.36	11	2
1:A:33:ILE:CD1	1:A:33:ILE:N	0.50	2.75	1	2
1:A:13:LEU:CD1	1:A:75:THR:N	0.50	2.75	4	1
1:A:13:LEU:CD1	1:A:13:LEU:C	0.50	2.79	7	1
1:A:19:LEU:HG	1:A:68:LEU:HD23	0.50	1.82	14	1
1:A:44:ILE:HD13	1:A:81:TYR:CD1	0.50	2.42	14	1
1:A:44:ILE:CD1	1:A:68:LEU:HD21	0.50	2.36	1	2
1:A:85:ILE:C	1:A:86:TYR:HD1	0.50	2.10	6	2
1:A:38:THR:CG2	1:A:81:TYR:N	0.50	2.75	11	4
1:A:44:ILE:CG2	1:A:60:TYR:CD2	0.50	2.95	3	1
1:A:24:PHE:CE1	1:A:94:LEU:HD23	0.50	2.42	7	1
1:A:94:LEU:C	1:A:94:LEU:HD23	0.50	2.27	17	1
1:A:45:ALA:HB3	1:A:68:LEU:HD13	0.50	1.84	7	2
1:A:19:LEU:CD2	1:A:70:ILE:CD1	0.49	2.90	18	3
1:A:70:ILE:HG22	1:A:73:LEU:HD12	0.49	1.83	17	1
1:A:81:TYR:CD1	1:A:81:TYR:N	0.49	2.80	1	2
1:A:83:VAL:CG2	1:A:85:ILE:CD1	0.49	2.85	9	2
1:A:73:LEU:HD21	1:A:100:LEU:HD12	0.49	1.82	10	1
1:A:94:LEU:C	1:A:94:LEU:CD1	0.49	2.80	14	1
1:A:61:LYS:HB3	1:A:63:PHE:HE1	0.49	1.67	4	1
1:A:21:ILE:CB	1:A:22:PRO:CD	0.49	2.91	11	2
1:A:85:ILE:CD1	1:A:94:LEU:HD12	0.49	2.38	15	1
1:A:21:ILE:CG1	1:A:22:PRO:CD	0.49	2.88	17	8
1:A:94:LEU:HD22	1:A:95:GLU:N	0.49	2.22	5	2
1:A:81:TYR:HE1	1:A:100:LEU:HB3	0.49	1.66	8	1
1:A:22:PRO:HG2	1:A:96:LYS:HD2	0.49	1.83	17	2
1:A:38:THR:CG2	1:A:80:ILE:CG2	0.49	2.87	5	1
1:A:11:GLY:HA3	1:A:73:LEU:HD12	0.49	1.85	12	2
1:A:17:ILE:HG21	1:A:73:LEU:CD2	0.49	2.37	13	1
1:A:46:GLN:N	1:A:62:LEU:HD12	0.49	2.22	1	1
1:A:78:GLN:HG2	1:A:100:LEU:O	0.49	2.08	16	3
1:A:34:LYS:HG2	1:A:46:GLN:HG3	0.49	1.85	15	2
1:A:60:TYR:HE1	1:A:81:TYR:CE1	0.49	2.25	14	1
1:A:80:ILE:C	1:A:81:TYR:CD1	0.49	2.87	1	2
1:A:54:PHE:CD1	1:A:54:PHE:C	0.49	2.87	16	3
1:A:60:TYR:HA	1:A:70:ILE:HG22	0.49	1.84	9	2
1:A:73:LEU:HD13	1:A:102:ILE:HD13	0.49	1.84	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ILE:HD12	1:A:47:PHE:CD2	0.49	2.42	13	1
1:A:22:PRO:HG3	1:A:96:LYS:CG	0.48	2.38	6	1
1:A:78:GLN:HG3	1:A:101:LYS:C	0.48	2.29	14	1
1:A:22:PRO:HD3	1:A:96:LYS:HD3	0.48	1.85	15	1
1:A:30:ILE:CD1	1:A:93:VAL:HG21	0.48	2.38	11	2
1:A:44:ILE:CD1	1:A:60:TYR:CE1	0.48	2.92	12	1
1:A:94:LEU:CD2	1:A:94:LEU:C	0.48	2.81	13	1
1:A:17:ILE:HD13	1:A:18:ASN:N	0.48	2.22	11	1
1:A:96:LYS:HB3	1:A:98:PHE:HE1	0.48	1.67	15	1
1:A:37:LYS:CA	1:A:44:ILE:CD1	0.48	2.92	14	1
1:A:46:GLN:HG2	1:A:47:PHE:N	0.48	2.22	5	2
2:B:2:NAG:H83	2:B:7:MAN:O2	0.48	2.09	10	4
1:A:7:LEU:CD2	1:A:98:PHE:CZ	0.48	2.96	14	1
1:A:80:ILE:N	1:A:80:ILE:CD1	0.48	2.77	6	1
1:A:22:PRO:HG3	1:A:96:LYS:CD	0.48	2.39	13	1
1:A:19:LEU:HD11	1:A:70:ILE:CD1	0.48	2.35	17	1
1:A:17:ILE:HG22	1:A:73:LEU:HD11	0.48	1.83	1	2
1:A:11:GLY:O	1:A:102:ILE:HG23	0.48	2.09	8	1
1:A:13:LEU:CB	1:A:74:LYS:HA	0.48	2.39	17	1
1:A:9:THR:HG23	1:A:99:ASP:C	0.48	2.28	8	1
1:A:74:LYS:NZ	1:A:76:ASP:HB3	0.48	2.23	8	1
1:A:21:ILE:CD1	1:A:22:PRO:CD	0.48	2.92	9	2
1:A:35:TRP:CG	1:A:68:LEU:HD22	0.48	2.44	15	1
1:A:37:LYS:HA	1:A:44:ILE:HD11	0.47	1.86	14	1
1:A:15:GLN:O	1:A:73:LEU:CB	0.47	2.62	3	1
1:A:26:MET:CE	1:A:85:ILE:HG21	0.47	2.39	17	2
1:A:59:THR:HG23	1:A:60:TYR:HD1	0.47	1.68	18	1
1:A:24:PHE:CD1	1:A:24:PHE:C	0.47	2.88	8	1
1:A:35:TRP:CD1	1:A:62:LEU:HD22	0.47	2.43	10	1
1:A:60:TYR:CE2	1:A:81:TYR:CE2	0.47	3.01	1	2
1:A:19:LEU:HD12	1:A:35:TRP:HH2	0.47	1.68	11	2
1:A:13:LEU:HB3	1:A:74:LYS:HA	0.47	1.86	2	2
1:A:73:LEU:CA	1:A:77:ASP:HB2	0.47	2.39	6	3
1:A:45:ALA:CB	1:A:62:LEU:CD2	0.47	2.87	8	3
1:A:33:ILE:HG22	1:A:62:LEU:HD21	0.47	1.86	17	2
1:A:74:LYS:O	1:A:102:ILE:HD11	0.47	2.10	17	2
2:B:1:NAG:H62	2:B:2:NAG:H82	0.47	1.87	10	1
1:A:80:ILE:HG23	1:A:99:ASP:HB3	0.47	1.87	12	1
1:A:21:ILE:N	1:A:22:PRO:CD	0.47	2.77	1	1
1:A:26:MET:HB3	1:A:30:ILE:HD12	0.47	1.86	4	1
1:A:33:ILE:CG2	1:A:85:ILE:CG2	0.47	2.88	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LYS:CG	1:A:46:GLN:HG2	0.47	2.39	13	1
1:A:99:ASP:OD1	1:A:100:LEU:HD13	0.47	2.09	14	1
1:A:46:GLN:CB	1:A:54:PHE:CE1	0.47	2.98	1	1
1:A:81:TYR:HE2	1:A:100:LEU:CB	0.47	2.22	15	2
1:A:5:ASN:O	1:A:6:ALA:HB2	0.47	2.10	10	2
1:A:60:TYR:CD1	1:A:70:ILE:HG21	0.47	2.40	9	1
1:A:21:ILE:HD13	1:A:22:PRO:O	0.47	2.10	12	1
1:A:17:ILE:CG2	1:A:100:LEU:HD11	0.47	2.34	13	1
1:A:61:LYS:HE2	1:A:63:PHE:CE1	0.47	2.45	2	1
1:A:86:TYR:CD2	1:A:92:ASN:HA	0.47	2.44	10	2
1:A:62:LEU:O	1:A:63:PHE:HD1	0.47	1.91	8	1
1:A:15:GLN:CG	1:A:16:ASP:N	0.47	2.74	13	1
1:A:19:LEU:CD1	1:A:70:ILE:CD1	0.47	2.93	10	2
1:A:19:LEU:CD1	1:A:70:ILE:HD12	0.47	2.39	10	1
1:A:50:GLU:C	1:A:51:LYS:HG2	0.47	2.31	18	1
1:A:46:GLN:HB2	1:A:54:PHE:HE1	0.47	1.70	1	1
1:A:61:LYS:HE2	1:A:63:PHE:HE1	0.47	1.68	2	1
1:A:96:LYS:CB	1:A:98:PHE:HE1	0.47	2.23	6	1
1:A:73:LEU:CD1	1:A:102:ILE:HD13	0.46	2.41	8	2
1:A:37:LYS:HB2	1:A:44:ILE:HG21	0.46	1.85	10	1
1:A:50:GLU:O	1:A:51:LYS:HG2	0.46	2.10	18	1
1:A:30:ILE:HD12	1:A:33:ILE:HD11	0.46	1.88	1	1
1:A:44:ILE:HG21	1:A:60:TYR:CD2	0.46	2.45	3	1
1:A:62:LEU:HD12	1:A:63:PHE:N	0.46	2.25	17	2
1:A:72:HIS:O	1:A:73:LEU:HD23	0.46	2.10	17	2
1:A:19:LEU:HD21	1:A:100:LEU:HD12	0.46	1.88	7	1
1:A:21:ILE:HG23	1:A:22:PRO:HD2	0.46	1.81	11	2
1:A:48:ARG:H	1:A:53:THR:HG22	0.46	1.70	15	1
1:A:87:ASP:OD2	1:A:93:VAL:HG12	0.46	2.10	11	1
1:A:78:GLN:HG2	1:A:100:LEU:HD23	0.46	1.86	14	1
1:A:38:THR:HG22	1:A:82:LYS:HB2	0.46	1.85	8	1
1:A:73:LEU:HD23	1:A:100:LEU:CD1	0.46	2.41	3	1
1:A:80:ILE:CD1	1:A:80:ILE:N	0.46	2.79	12	1
1:A:38:THR:CG2	1:A:81:TYR:CA	0.46	2.94	14	1
1:A:81:TYR:CE2	1:A:100:LEU:CB	0.46	2.99	15	1
1:A:13:LEU:CD1	1:A:14:GLY:N	0.46	2.71	7	1
1:A:60:TYR:CE1	1:A:70:ILE:HD11	0.46	2.45	7	1
1:A:97:ILE:C	1:A:98:PHE:CD1	0.46	2.89	15	2
1:A:73:LEU:HD11	1:A:100:LEU:HD12	0.46	1.88	18	1
1:A:63:PHE:N	1:A:63:PHE:CD1	0.46	2.84	4	2
1:A:80:ILE:N	1:A:80:ILE:HD12	0.46	2.26	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:LEU:CB	1:A:77:ASP:HB2	0.46	2.37	17	4
1:A:72:HIS:C	1:A:73:LEU:CD2	0.46	2.83	1	1
1:A:19:LEU:N	1:A:68:LEU:O	0.46	2.49	2	11
1:A:35:TRP:CH2	1:A:98:PHE:HD2	0.46	2.29	3	1
1:A:86:TYR:HA	1:A:93:VAL:HG23	0.46	1.88	3	1
1:A:96:LYS:HB3	1:A:98:PHE:CE1	0.46	2.46	6	1
1:A:83:VAL:HG22	1:A:85:ILE:HG13	0.46	1.86	7	1
1:A:62:LEU:HD13	1:A:68:LEU:HD12	0.46	1.80	9	1
1:A:19:LEU:HD13	1:A:70:ILE:HD12	0.46	1.86	10	1
1:A:61:LYS:HZ1	1:A:63:PHE:HD1	0.45	1.51	3	1
1:A:19:LEU:HD13	1:A:35:TRP:HZ3	0.45	1.69	7	2
1:A:26:MET:CE	1:A:33:ILE:HD11	0.45	2.40	13	1
1:A:100:LEU:N	1:A:100:LEU:CD1	0.45	2.79	14	1
1:A:73:LEU:HD23	1:A:102:ILE:HD11	0.45	1.89	5	1
1:A:7:LEU:HD23	1:A:98:PHE:HD2	0.45	1.62	6	1
1:A:38:THR:CB	1:A:80:ILE:HG22	0.45	2.40	14	1
1:A:63:PHE:HE2	2:B:2:NAG:H82	0.45	1.72	15	1
1:A:19:LEU:HG	1:A:35:TRP:CZ3	0.45	2.47	11	3
1:A:73:LEU:HD12	1:A:77:ASP:CG	0.45	2.31	4	1
1:A:22:PRO:HB2	1:A:94:LEU:HD21	0.45	1.88	6	1
1:A:73:LEU:CD2	1:A:73:LEU:C	0.45	2.85	7	1
1:A:21:ILE:HG21	1:A:83:VAL:CG2	0.45	2.30	14	1
1:A:84:SER:HB2	1:A:86:TYR:CE1	0.45	2.46	6	6
1:A:62:LEU:C	1:A:63:PHE:CD1	0.45	2.89	5	3
1:A:22:PRO:HG3	1:A:96:LYS:CE	0.45	2.41	13	1
1:A:100:LEU:CD2	1:A:100:LEU:C	0.45	2.85	14	1
1:A:39:SER:O	1:A:41:LYS:HG3	0.45	2.12	4	1
1:A:67:THR:CG2	1:A:68:LEU:N	0.45	2.79	6	2
1:A:74:LYS:CE	1:A:76:ASP:CB	0.45	2.94	8	1
1:A:46:GLN:N	1:A:62:LEU:HD21	0.45	2.26	9	1
1:A:7:LEU:C	1:A:7:LEU:HD12	0.45	2.32	11	1
1:A:43:LYS:CD	1:A:43:LYS:N	0.45	2.78	12	1
1:A:12:ALA:H	1:A:73:LEU:HD12	0.45	1.71	13	1
1:A:98:PHE:CD1	1:A:98:PHE:N	0.45	2.85	1	1
1:A:73:LEU:CD2	1:A:100:LEU:HD13	0.45	2.42	3	1
1:A:26:MET:CB	1:A:30:ILE:HD12	0.45	2.42	4	1
1:A:33:ILE:CB	1:A:62:LEU:HD21	0.45	2.41	5	2
1:A:38:THR:CG2	1:A:81:TYR:C	0.45	2.85	16	5
1:A:74:LYS:HE2	1:A:76:ASP:CB	0.45	2.42	8	1
1:A:12:ALA:N	1:A:73:LEU:CD1	0.45	2.80	13	1
1:A:38:THR:CG2	1:A:80:ILE:C	0.45	2.85	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:LEU:CD2	1:A:68:LEU:C	0.44	2.85	2	1
1:A:24:PHE:CD1	1:A:94:LEU:CD2	0.44	3.00	7	1
1:A:17:ILE:HD11	1:A:70:ILE:HD12	0.44	1.89	8	1
1:A:73:LEU:C	1:A:73:LEU:CD1	0.44	2.86	10	1
1:A:13:LEU:HA	1:A:74:LYS:CA	0.44	2.42	15	1
1:A:83:VAL:HG11	1:A:98:PHE:CE1	0.44	2.47	5	1
1:A:11:GLY:O	1:A:102:ILE:HD13	0.44	2.12	8	1
1:A:81:TYR:N	1:A:81:TYR:CD1	0.44	2.85	10	1
1:A:63:PHE:HD2	1:A:67:THR:HB	0.44	1.72	14	1
1:A:87:ASP:OD2	1:A:91:LYS:HB2	0.44	2.13	2	1
1:A:13:LEU:HD11	1:A:75:THR:N	0.44	2.27	4	1
1:A:12:ALA:C	1:A:102:ILE:CD1	0.44	2.85	7	1
1:A:86:TYR:CD1	1:A:92:ASN:HA	0.44	2.46	18	6
1:A:43:LYS:HB2	1:A:46:GLN:CD	0.44	2.33	11	1
1:A:24:PHE:CD1	1:A:25:GLN:N	0.44	2.84	13	1
1:A:22:PRO:HG3	1:A:96:LYS:HD2	0.44	1.88	13	1
1:A:81:TYR:CE1	1:A:100:LEU:HB3	0.44	2.47	8	1
1:A:37:LYS:N	1:A:44:ILE:HD12	0.44	2.28	9	1
1:A:9:THR:HG21	1:A:19:LEU:HD12	0.44	1.81	9	1
1:A:81:TYR:CE2	1:A:100:LEU:HB3	0.44	2.48	15	1
1:A:44:ILE:CD1	1:A:60:TYR:CD1	0.44	2.95	6	1
1:A:9:THR:HG21	1:A:100:LEU:HD12	0.44	1.88	11	1
1:A:78:GLN:HG3	1:A:100:LEU:C	0.44	2.32	11	1
1:A:19:LEU:HD23	1:A:68:LEU:HD23	0.44	1.89	18	1
1:A:13:LEU:CB	1:A:74:LYS:CB	0.44	2.95	17	1
1:A:15:GLN:HB3	1:A:73:LEU:HB3	0.44	1.89	2	1
1:A:102:ILE:CG2	1:A:103:GLN:N	0.44	2.80	7	1
1:A:24:PHE:CE2	1:A:30:ILE:HD11	0.44	2.48	7	1
1:A:60:TYR:HE1	1:A:81:TYR:OH	0.44	1.96	8	1
1:A:73:LEU:HD12	1:A:100:LEU:CD2	0.44	2.39	11	1
1:A:7:LEU:HB3	1:A:98:PHE:CD1	0.44	2.47	3	2
1:A:13:LEU:CD1	1:A:74:LYS:C	0.44	2.86	4	1
1:A:70:ILE:HD13	1:A:81:TYR:CZ	0.44	2.48	13	1
1:A:13:LEU:HD23	1:A:74:LYS:HB3	0.44	1.89	14	2
1:A:78:GLN:HG3	1:A:102:ILE:HG12	0.43	1.90	14	1
1:A:71:LYS:HG3	1:A:72:HIS:N	0.43	2.28	15	1
1:A:13:LEU:HG	1:A:74:LYS:CB	0.43	2.43	6	2
1:A:13:LEU:C	1:A:13:LEU:CD1	0.43	2.78	15	2
1:A:73:LEU:CD2	1:A:77:ASP:CG	0.43	2.86	15	1
1:A:35:TRP:CE2	1:A:68:LEU:HB2	0.43	2.48	1	2
1:A:7:LEU:HD11	1:A:96:LYS:HD2	0.43	1.90	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:PHE:CD2	1:A:67:THR:HB	0.43	2.49	14	1
1:A:34:LYS:HG3	1:A:86:TYR:CE2	0.43	2.48	18	1
1:A:33:ILE:O	1:A:34:LYS:HG2	0.43	2.14	2	1
1:A:37:LYS:HG3	1:A:42:LYS:HB3	0.43	1.88	3	1
1:A:54:PHE:C	1:A:54:PHE:CD1	0.43	2.91	8	2
1:A:60:TYR:HE1	1:A:81:TYR:HH	0.43	1.57	8	1
1:A:34:LYS:N	1:A:84:SER:O	0.43	2.52	2	1
1:A:87:ASP:CG	1:A:93:VAL:CG1	0.43	2.87	6	3
1:A:68:LEU:HD21	1:A:70:ILE:CG2	0.43	2.43	9	1
1:A:91:LYS:O	1:A:93:VAL:HG13	0.43	2.14	16	2
1:A:17:ILE:CG2	1:A:73:LEU:HD13	0.43	2.44	7	1
1:A:37:LYS:HB3	1:A:44:ILE:HD13	0.43	1.91	7	1
1:A:73:LEU:HD23	1:A:100:LEU:HD23	0.43	1.89	12	1
1:A:46:GLN:HB2	1:A:54:PHE:CE1	0.43	2.49	1	1
1:A:84:SER:CB	1:A:86:TYR:CE1	0.43	2.99	1	3
1:A:21:ILE:HG12	1:A:22:PRO:N	0.43	2.29	3	2
1:A:47:PHE:CD1	1:A:53:THR:CG2	0.43	3.02	11	1
1:A:78:GLN:HG2	1:A:100:LEU:CG	0.43	2.43	14	1
1:A:60:TYR:CD2	1:A:70:ILE:HG21	0.43	2.49	4	1
1:A:73:LEU:HA	1:A:77:ASP:HB2	0.43	1.91	6	1
1:A:6:ALA:HB1	1:A:99:ASP:OD1	0.43	2.14	10	1
1:A:73:LEU:O	1:A:73:LEU:CD1	0.43	2.63	12	1
1:A:37:LYS:HG3	1:A:44:ILE:HD11	0.43	1.91	15	1
1:A:33:ILE:HG13	1:A:85:ILE:CG2	0.42	2.43	12	2
1:A:12:ALA:HB3	1:A:15:GLN:OE1	0.42	2.14	4	1
1:A:37:LYS:HD3	1:A:42:LYS:CB	0.42	2.44	9	1
1:A:73:LEU:HA	1:A:77:ASP:CB	0.42	2.44	11	1
1:A:22:PRO:CG	1:A:96:LYS:CD	0.42	2.96	13	1
1:A:54:PHE:HD1	1:A:54:PHE:C	0.42	2.17	16	1
1:A:83:VAL:HG13	1:A:96:LYS:HB2	0.42	1.91	3	1
1:A:86:TYR:HD2	1:A:92:ASN:N	0.42	2.12	7	1
2:B:2:NAG:O7	2:B:2:NAG:C3	0.42	2.68	11	1
1:A:13:LEU:CD1	1:A:74:LYS:HA	0.42	2.37	4	1
1:A:100:LEU:CD1	1:A:100:LEU:C	0.42	2.86	8	1
1:A:26:MET:SD	1:A:30:ILE:HG21	0.42	2.54	15	1
1:A:63:PHE:CE2	2:B:2:NAG:H82	0.42	2.49	15	1
2:B:2:NAG:C3	2:B:2:NAG:O7	0.42	2.67	2	2
1:A:21:ILE:CB	1:A:22:PRO:HD2	0.42	2.45	3	1
1:A:19:LEU:HD23	1:A:70:ILE:CD1	0.42	2.44	8	1
1:A:44:ILE:CG2	1:A:60:TYR:CD1	0.42	3.03	14	1
1:A:19:LEU:HD22	1:A:70:ILE:HD13	0.42	1.91	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:LYS:HG2	1:A:83:VAL:N	0.42	2.28	10	1
1:A:26:MET:CB	1:A:30:ILE:CG2	0.42	2.97	16	1
1:A:35:TRP:HB3	1:A:68:LEU:CD1	0.42	2.45	16	1
1:A:21:ILE:HD13	1:A:22:PRO:HA	0.42	1.90	1	1
1:A:31:ASP:CB	1:A:88:THR:HG22	0.42	2.45	2	1
1:A:60:TYR:CZ	1:A:81:TYR:HE2	0.42	2.33	11	1
1:A:9:THR:CG2	1:A:100:LEU:CD1	0.42	2.97	1	1
1:A:60:TYR:CD1	1:A:70:ILE:HG12	0.42	2.50	2	2
1:A:94:LEU:CD1	1:A:94:LEU:C	0.42	2.86	15	1
1:A:21:ILE:HD11	1:A:94:LEU:CD2	0.42	2.45	1	1
1:A:21:ILE:HG13	1:A:22:PRO:CD	0.42	2.41	11	4
1:A:73:LEU:HD23	1:A:102:ILE:CD1	0.42	2.44	5	1
1:A:35:TRP:CZ3	1:A:98:PHE:CE1	0.42	3.08	7	1
1:A:86:TYR:CD2	1:A:92:ASN:CA	0.42	3.03	10	2
1:A:78:GLN:NE2	1:A:102:ILE:CG1	0.42	2.83	11	1
1:A:32:ASP:C	1:A:33:ILE:CD1	0.42	2.87	11	1
1:A:57:LYS:HG2	1:A:59:THR:HG22	0.42	1.92	17	1
1:A:63:PHE:CZ	1:A:69:LYS:CB	0.42	3.03	10	1
1:A:21:ILE:CG2	1:A:83:VAL:HG21	0.42	2.43	11	1
1:A:37:LYS:O	1:A:38:THR:C	0.42	2.58	12	1
1:A:79:ASP:C	1:A:80:ILE:HD13	0.42	2.35	12	1
1:A:24:PHE:HB3	1:A:94:LEU:CD1	0.42	2.44	13	1
1:A:19:LEU:HB3	1:A:35:TRP:HH2	0.42	1.62	14	1
1:A:17:ILE:HG22	1:A:73:LEU:CG	0.42	2.45	1	1
1:A:83:VAL:HG21	1:A:85:ILE:HD11	0.42	1.90	1	1
1:A:9:THR:CG2	1:A:100:LEU:HA	0.41	2.45	8	1
1:A:63:PHE:HD2	1:A:67:THR:O	0.41	1.98	1	1
1:A:87:ASP:OD1	1:A:93:VAL:HG13	0.41	2.15	5	1
1:A:17:ILE:HD11	1:A:70:ILE:HD13	0.41	1.91	12	1
1:A:38:THR:HG23	1:A:81:TYR:HA	0.41	1.90	14	1
1:A:74:LYS:C	1:A:102:ILE:CD1	0.41	2.89	2	1
1:A:13:LEU:HG	1:A:74:LYS:HB3	0.41	1.92	4	1
1:A:24:PHE:HD2	1:A:94:LEU:HD13	0.41	1.75	9	1
1:A:60:TYR:CE2	1:A:70:ILE:HG21	0.41	2.51	4	1
1:A:13:LEU:HG	1:A:74:LYS:CA	0.41	2.45	6	1
1:A:10:TRP:O	1:A:17:ILE:HD12	0.41	2.16	6	1
1:A:38:THR:CG2	1:A:80:ILE:HB	0.41	2.41	13	1
1:A:30:ILE:CD1	1:A:33:ILE:CD1	0.41	2.98	1	1
1:A:44:ILE:HG21	1:A:60:TYR:CE2	0.41	2.50	3	1
1:A:33:ILE:HD12	1:A:85:ILE:CG2	0.41	2.45	3	1
1:A:60:TYR:CE1	1:A:70:ILE:HG13	0.41	2.51	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ILE:HG12	1:A:85:ILE:CG2	0.41	2.46	17	2
1:A:7:LEU:HD11	1:A:96:LYS:HD3	0.41	1.93	9	1
1:A:19:LEU:HD13	1:A:70:ILE:CD1	0.41	2.46	10	1
1:A:70:ILE:HD13	1:A:100:LEU:HD21	0.41	1.92	11	1
1:A:57:LYS:O	1:A:61:LYS:HB2	0.41	2.15	15	1
1:A:47:PHE:CD2	1:A:53:THR:HG21	0.41	2.51	16	1
1:A:85:ILE:C	1:A:86:TYR:CD1	0.41	2.94	17	1
1:A:17:ILE:CG2	1:A:73:LEU:HD22	0.41	2.45	18	1
1:A:35:TRP:HD1	1:A:62:LEU:HD21	0.41	1.75	2	1
1:A:79:ASP:HB2	1:A:81:TYR:CZ	0.41	2.51	7	1
1:A:35:TRP:HD1	1:A:62:LEU:HD11	0.41	1.75	13	1
1:A:44:ILE:CD1	1:A:60:TYR:CD2	0.41	3.02	1	1
1:A:45:ALA:CB	1:A:68:LEU:HD13	0.41	2.46	6	1
1:A:73:LEU:HD13	1:A:77:ASP:O	0.41	2.15	11	1
1:A:61:LYS:HB2	1:A:69:LYS:HB3	0.41	1.90	12	1
1:A:35:TRP:CD1	1:A:62:LEU:CD1	0.41	3.04	3	1
1:A:21:ILE:HG13	1:A:83:VAL:HG13	0.41	1.91	14	1
1:A:24:PHE:C	1:A:24:PHE:CD1	0.41	2.94	1	1
1:A:86:TYR:HA	1:A:93:VAL:CG2	0.41	2.45	3	1
1:A:30:ILE:CG2	1:A:31:ASP:N	0.41	2.84	5	1
1:A:35:TRP:CH2	1:A:98:PHE:HE2	0.41	2.30	8	1
1:A:63:PHE:HE2	1:A:69:LYS:CB	0.41	2.28	9	1
1:A:77:ASP:OD1	1:A:100:LEU:HD21	0.41	2.16	15	1
1:A:70:ILE:CD1	1:A:81:TYR:HE2	0.41	2.27	16	1
1:A:83:VAL:HG22	1:A:85:ILE:HG12	0.41	1.91	9	2
1:A:47:PHE:HD1	1:A:48:ARG:N	0.41	2.14	4	1
1:A:79:ASP:HB2	1:A:81:TYR:CE1	0.41	2.50	4	1
1:A:21:ILE:HD12	1:A:83:VAL:CG2	0.41	2.45	18	1
1:A:21:ILE:HD11	1:A:94:LEU:HD23	0.40	1.93	1	1
1:A:61:LYS:HB3	1:A:61:LYS:HE3	0.40	1.48	12	1
1:A:33:ILE:HD12	1:A:33:ILE:N	0.40	2.31	1	1
1:A:60:TYR:CE1	1:A:70:ILE:HG12	0.40	2.52	11	1
1:A:21:ILE:HG12	1:A:85:ILE:HD11	0.40	1.94	11	1
1:A:32:ASP:O	1:A:85:ILE:HG22	0.40	2.17	16	1
1:A:35:TRP:HB2	1:A:68:LEU:HD13	0.40	1.94	17	1
1:A:21:ILE:CG2	1:A:66:GLY:O	0.40	2.70	3	1
1:A:97:ILE:O	1:A:98:PHE:HD1	0.40	1.99	3	1
1:A:19:LEU:HD23	1:A:70:ILE:HD12	0.40	1.93	8	1
1:A:60:TYR:HD1	1:A:70:ILE:HG22	0.40	1.75	9	1
1:A:57:LYS:HG3	1:A:59:THR:CG2	0.40	2.47	11	1
2:B:1:NAG:H62	2:B:2:NAG:C7	0.40	2.47	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:LEU:CD2	1:A:102:ILE:HD11	0.40	2.26	7	1
1:A:37:LYS:HA	1:A:44:ILE:CD1	0.40	2.47	14	1

6.3 Torsion angles [\(i\)](#)

6.3.1 Protein backbone [\(i\)](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	99/105 (94%)	79±2 (80±2%)	15±2 (15±2%)	5±1 (5±1%)	4	24
All	All	1782/1890 (94%)	1424 (80%)	265 (15%)	93 (5%)	4	24

All 17 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	72	HIS	16
1	A	22	PRO	14
1	A	27	SER	12
1	A	52	GLU	12
1	A	43	LYS	7
1	A	49	LYS	6
1	A	92	ASN	6
1	A	39	SER	4
1	A	8	GLU	3
1	A	55	LYS	2
1	A	38	THR	2
1	A	20	ASP	2
1	A	21	ILE	2
1	A	28	ASP	2
1	A	57	LYS	1
1	A	44	ILE	1
1	A	100	LEU	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	92/98 (94%)	58±4 (63±5%)	34±4 (37±5%)	1 7
All	All	1656/1764 (94%)	1038 (63%)	618 (37%)	1 7

All 82 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	16	ASP	18
1	A	74	LYS	17
1	A	78	GLN	16
1	A	9	THR	16
1	A	31	ASP	15
1	A	85	ILE	14
1	A	21	ILE	13
1	A	76	ASP	12
1	A	86	TYR	12
1	A	96	LYS	11
1	A	100	LEU	11
1	A	94	LEU	11
1	A	49	LYS	10
1	A	17	ILE	10
1	A	40	ASP	10
1	A	51	LYS	10
1	A	15	GLN	10
1	A	77	ASP	10
1	A	61	LYS	10
1	A	57	LYS	9
1	A	13	LEU	9
1	A	69	LYS	9
1	A	25	GLN	9
1	A	103	GLN	9
1	A	73	LEU	9
1	A	30	ILE	9
1	A	43	LYS	9
1	A	18	ASN	8
1	A	55	LYS	8

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Mol	Chain	Res	Type	Models (Total)
1	A	95	GLU	8
1	A	62	LEU	8
1	A	97	ILE	8
1	A	5	ASN	8
1	A	88	THR	8
1	A	26	MET	8
1	A	47	PHE	8
1	A	91	LYS	8
1	A	92	ASN	8
1	A	79	ASP	8
1	A	99	ASP	7
1	A	82	LYS	7
1	A	56	GLU	7
1	A	42	LYS	7
1	A	41	LYS	7
1	A	8	GLU	7
1	A	19	LEU	7
1	A	84	SER	7
1	A	23	SER	7
1	A	54	PHE	7
1	A	44	ILE	7
1	A	64	LYS	7
1	A	67	THR	7
1	A	36	GLU	6
1	A	68	LEU	6
1	A	33	ILE	6
1	A	20	ASP	6
1	A	53	THR	6
1	A	37	LYS	6
1	A	101	LYS	6
1	A	24	PHE	6
1	A	34	LYS	6
1	A	71	LYS	6
1	A	70	ILE	5
1	A	46	GLN	5
1	A	80	ILE	5
1	A	32	ASP	5
1	A	52	GLU	5
1	A	28	ASP	4
1	A	48	ARG	4
1	A	58	ASP	3
1	A	7	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	39	SER	3
1	A	50	GLU	3
1	A	81	TYR	3
1	A	27	SER	3
1	A	98	PHE	2
1	A	72	HIS	2
1	A	63	PHE	2
1	A	87	ASP	2
1	A	93	VAL	2
1	A	38	THR	1
1	A	102	ILE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

9 monosaccharides are modelled in this entry.

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
2	NAG	B	1	1,2	14,14,15	1.37±0.00	0±0 (0±0%)
2	NAG	B	2	2	14,14,15	1.32±0.00	0±0 (0±0%)
2	BMA	B	3	2	11,11,12	1.37±0.00	0±0 (0±0%)
2	MAN	B	4	2	11,11,12	1.33±0.00	0±0 (0±0%)
2	MAN	B	5	2	11,11,12	1.29±0.00	0±0 (0±0%)
2	MAN	B	6	2	11,11,12	1.26±0.00	0±0 (0±0%)
2	MAN	B	7	2	11,11,12	1.23±0.00	0±0 (0±0%)
2	MAN	B	8	2	11,11,12	1.32±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	MAN	B	9	2	11,11,12	1.25±0.00	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	NAG	B	1	1,2	17,19,21	1.09±0.00	0±0 (0±0%)
2	NAG	B	2	2	17,19,21	1.06±0.00	0±0 (0±0%)
2	BMA	B	3	2	15,15,17	0.95±0.00	0±0 (0±0%)
2	MAN	B	4	2	15,15,17	1.01±0.00	0±0 (0±0%)
2	MAN	B	5	2	15,15,17	1.05±0.00	0±0 (0±0%)
2	MAN	B	6	2	15,15,17	1.16±0.00	0±0 (0±0%)
2	MAN	B	7	2	15,15,17	1.13±0.00	0±0 (0±0%)
2	MAN	B	8	2	15,15,17	1.06±0.00	0±0 (0±0%)
2	MAN	B	9	2	15,15,17	1.11±0.00	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	0±0,6,23,26	0±0,1,1,1
2	NAG	B	2	2	-	0±0,6,23,26	0±0,1,1,1
2	BMA	B	3	2	-	0±0,2,19,22	0±0,1,1,1
2	MAN	B	4	2	-	0±0,2,19,22	0±0,1,1,1
2	MAN	B	5	2	-	0±0,2,19,22	0±0,1,1,1
2	MAN	B	6	2	-	0±0,2,19,22	0±0,1,1,1
2	MAN	B	7	2	-	0±0,2,19,22	0±0,1,1,1
2	MAN	B	8	2	-	0±0,2,19,22	0±0,1,1,1
2	MAN	B	9	2	-	0±0,2,19,22	0±0,1,1,1

There are no bond-length outliers.

There are no bond-angle outliers.

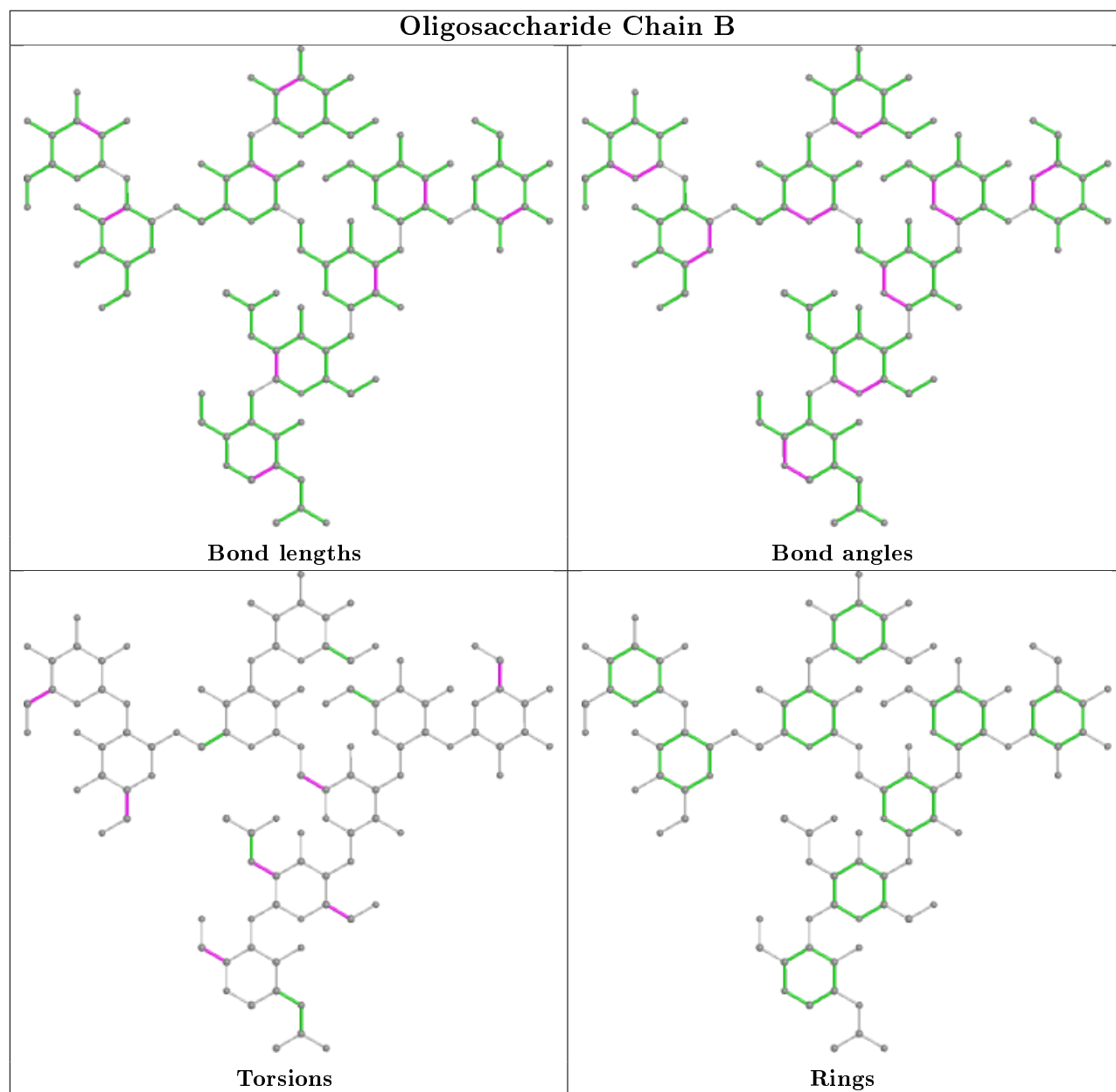
All unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	3	BMA	C1	2
2	B	8	MAN	C1	1
2	B	9	MAN	C1	1
2	B	4	MAN	C1	1

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 oligosaccharide.



6.6 Ligand geometry [i](#)

There are no ligands in this entry.

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