



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 03:18 PM UTC

PDB ID : 1HD4 / pdb_00001hd4
Title : SOLUTION STRUCTURE OF THE A-SUBUNIT OF HUMAN CHORIONIC GONADOTROPIN [MODELED WITH DIANTENNARY GLYCAN AT ASN78]
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Deposited on : 2000-11-07

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

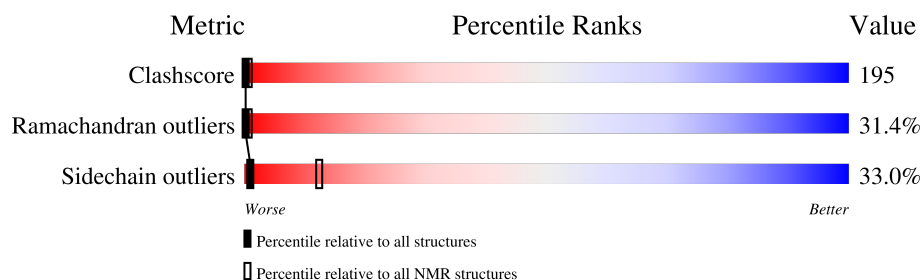
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	92	
2	B	9	

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	NAG	2	1	-
2	B	NAG	5	1	-

2 Ensemble composition and analysis

This entry contains 26 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:11-A:29, A:61-A:83 (42)	0.59	3

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 1 single-model cluster was found.

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

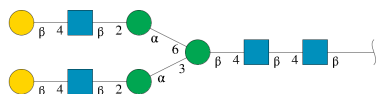
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1595 atoms, of which 778 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CHORIONIC GONADOTROPIN.

Mol	Chain	Residues	Atoms						Trace
1	A	92	Total	C	H	N	O	S	0
			1381	437	675	122	134	13	

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



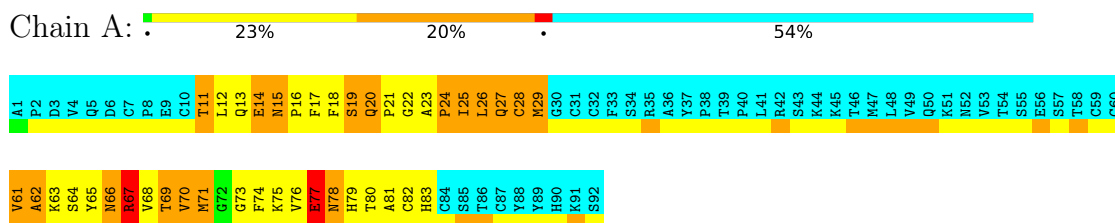
Mol	Chain	Residues	Atoms					Trace
2	B	9	Total	C	H	N	O	0
			214	62	103	4	45	

4 Residue-property plots

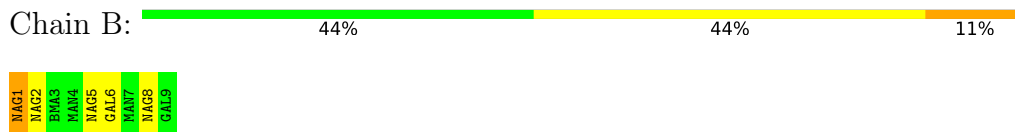
4.1 Average score per residue in the NMR ensemble

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: CHORIONIC GONADOTROPIN



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

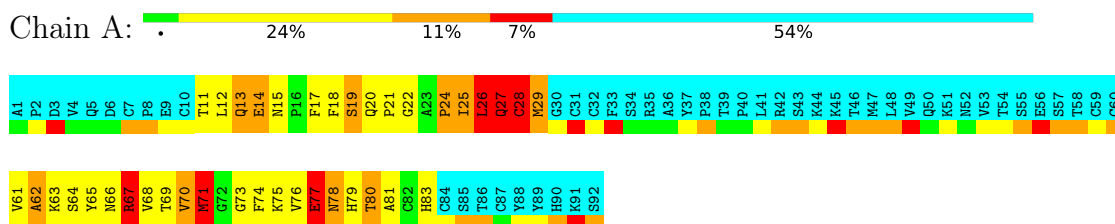


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

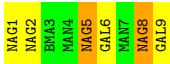
4.2.1 Score per residue for model 1

• Molecule 1: CHORIONIC GONADOTROPIN



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

Chain B: 



4.2.2 Score per residue for model 2

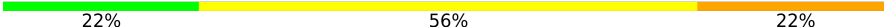
- Molecule 1: CHORIONIC GONADOTROPIN

Chain A: 





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

Chain B: 



4.2.3 Score per residue for model 3 (medoid)

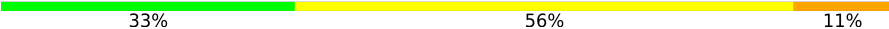
- Molecule 1: CHORIONIC GONADOTROPIN

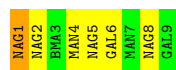
Chain A: 





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

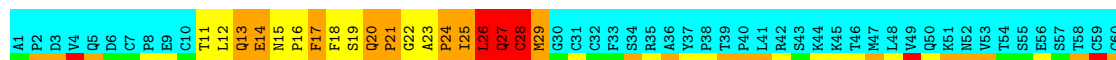
Chain B:  33% 56% 11%



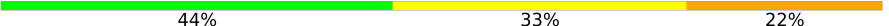
4.2.4 Score per residue for model 4

- Molecule 1: CHORIONIC GONADOTROPIN

Chain A:  23% 15% 7% 54%



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

Chain B:  44% 33% 22%



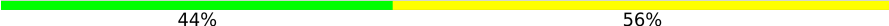
4.2.5 Score per residue for model 5

- Molecule 1: CHORIONIC GONADOTROPIN

Chain A:  21% 20% 54%



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

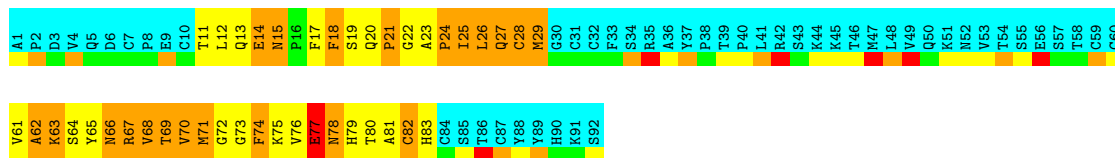
Chain B:  44% 56%



4.2.6 Score per residue for model 6

- Molecule 1: CHORIONIC GONADOTROPIN

Chain A: . 21% 23% 54%



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

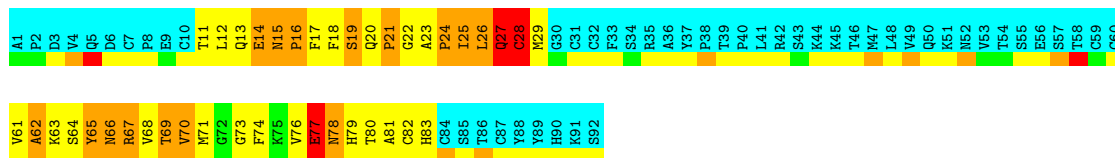
Chain B: 33% 44% 22%



4.2.7 Score per residue for model 7

- Molecule 1: CHORIONIC GONADOTROPIN

Chain A: . 24% 16% 54%



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

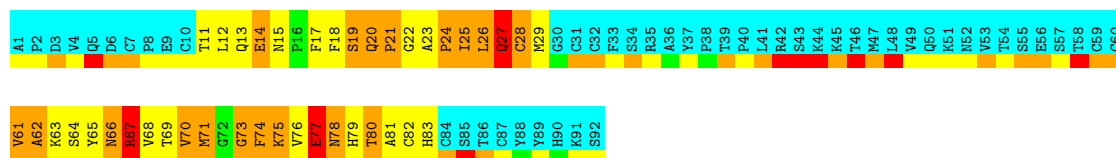
Chain B: 44% 44% 11%



4.2.8 Score per residue for model 8

- Molecule 1: CHORIONIC GONADOTROPIN

Chain A: . 21% 20% 54%



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

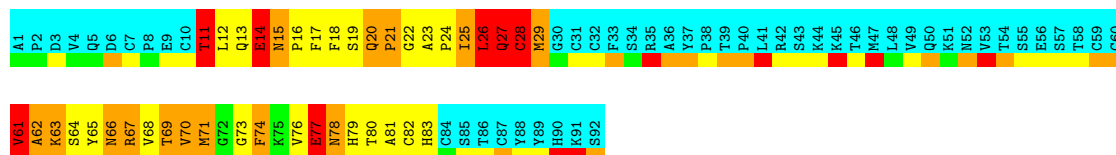
Chain B: 11% 44% 44%



4.2.9 Score per residue for model 9

- Molecule 1: CHORIONIC GONADOTROPIN

Chain A: 21% 15% 8% 54%



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

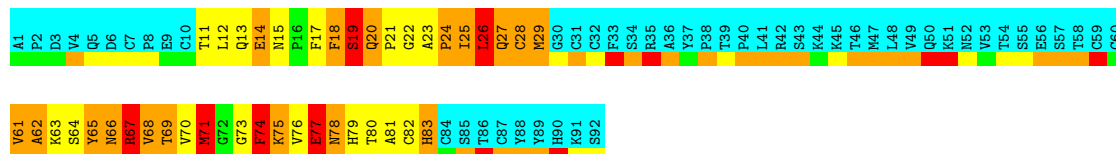
Chain B: 33% 67%



4.2.10 Score per residue for model 10

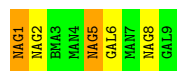
- Molecule 1: CHORIONIC GONADOTROPIN

Chain A: 18% 18% 7% 54%



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

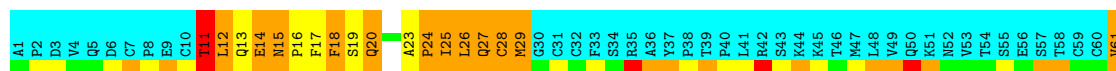
Chain B: 



4.2.11 Score per residue for model 11

- Molecule 1: CHORIONIC GONADOTROPIN

Chain A: 



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

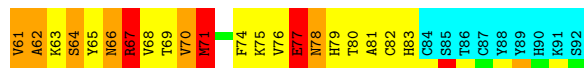
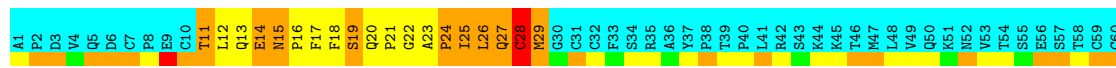
Chain B: 



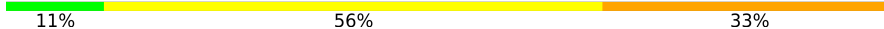
4.2.12 Score per residue for model 12

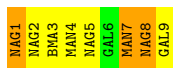
- Molecule 1: CHORIONIC GONADOTROPIN

Chain A: 



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

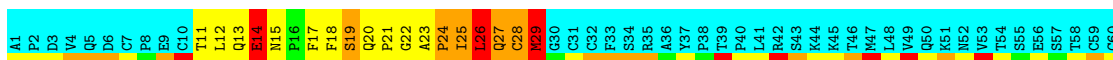
Chain B:  11% 56% 33%



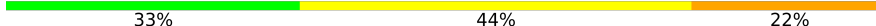
4.2.13 Score per residue for model 13

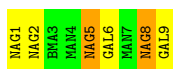
- Molecule 1: CHORIONIC GONADOTROPIN

Chain A:  23% 13% 7% 54%



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

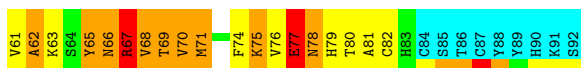
Chain B:  33% 44% 22%



4.2.14 Score per residue for model 14

- Molecule 1: CHORIONIC GONADOTROPIN

Chain A:  5% 15% 22% 54%



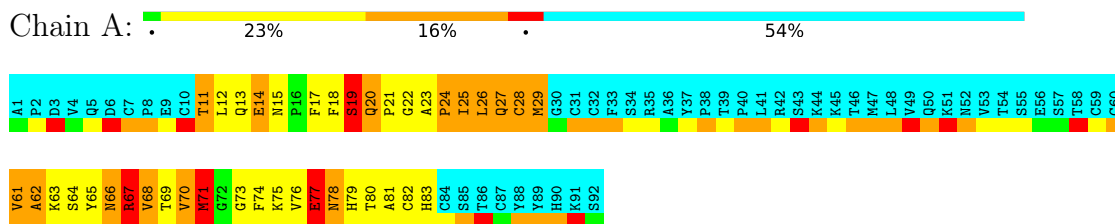
- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  44% 33% 22%

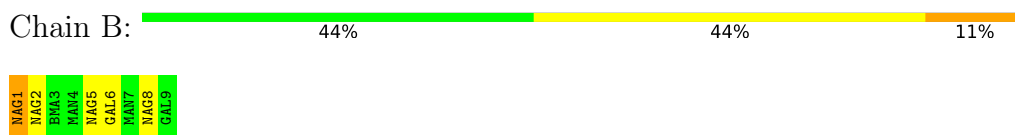


4.2.15 Score per residue for model 15

- Molecule 1: CHORIONIC GONADOTROPIN

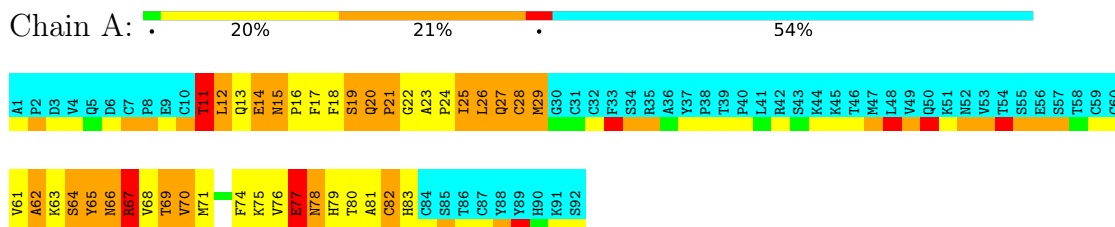


- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

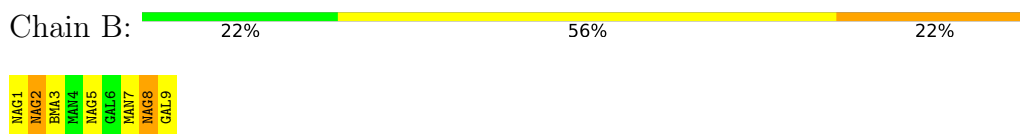


4.2.16 Score per residue for model 16

- Molecule 1: CHORIONIC GONADOTROPIN



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



4.2.17 Score per residue for model 17

- Molecule 1: CHORIONIC GONADOTROPIN

Chain A: 18% 20% 54%



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

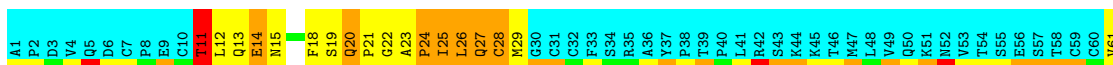
Chain B: 44% 44% 11%



4.2.18 Score per residue for model 18

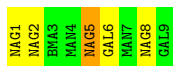
- Molecule 1: CHORIONIC GONADOTROPIN

Chain A: 21% 18% 54%



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

Chain B: 44% 44% 11%



4.2.19 Score per residue for model 19

- Molecule 1: CHORIONIC GONADOTROPIN

Chain A: 16% 24% 54%





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

Chain B: 22% 56% 22%



4.2.20 Score per residue for model 20

- Molecule 1: CHORIONIC GONADOTROPIN

Chain A: 23% 15% 5% 54%



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

Chain B: 11% 67% 22%



4.2.21 Score per residue for model 21

- Molecule 1: CHORIONIC GONADOTROPIN

Chain A: 22% 18% 54%



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

nose-(1-2)-alpha-D-mannopyranose-(1-6)]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%

NAG1
NAG2
BMA3
MAN4
NAG5
GAL6
MAN7
NAG8
GAL9

4.2.22 Score per residue for model 22

• Molecule 1: CHORIONIC GONADOTROPIN

Chain A:  22% 20% 54%

A1 P2 D3 V4 Q5 D6 C7 P8 E9 C10 T11 L12 Q13 E14 N15 P16 F17 F18 S19 Q20 P21 G22 A23 P24 I25 L26 Q27 C28 C29 N29 G30 C31 C32 F33 S34 R35 A36 Y37 P38 T39 P40 L41 L42 S43 S44 K44 K45 T46 M47 L48 V49 Q50 K51 N52 V53 T54 S55 E56 S57 T58 C59 C60

V61 A62 K63 S64 N65 N66 N67 V68 T69 V70 M71 G72 G73 F74 V75 V76 E77 N78 H79 T80 A81 C82 H83 C84 S85 T86 C87 Y88 Y89 H90 K91 S92

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

Chain B:  56% 33% 11%

NAG1
NAG2
BMA3
MAN4
NAG5
GAL6
MAN7
NAG8
GAL9

4.2.23 Score per residue for model 23

• Molecule 1: CHORIONIC GONADOTROPIN

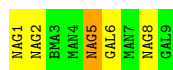
Chain A:  21% 18% 54%

A1 P2 D3 V4 Q5 D6 C7 P8 E9 C10 T11 L12 Q13 E14 N15 P16 F17 F18 S19 Q20 P21 G22 A23 P24 I25 L26 Q27 C28 C29 N29 G30 C31 C32 F33 S34 R35 A36 Y37 P38 T39 P40 L41 L42 S43 S44 K44 K45 T46 M47 L48 V49 Q50 K51 N52 V53 T54 S55 E56 S57 T58 C59 C60

V61 A62 K63 S64 N65 N66 N67 V68 T69 V70 M71 F74 K75 V76 E77 N78 H79 T80 A81 C82 H83 C84 S85 T86 C87 Y88 Y89 H90 K91 S92

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

Chain B:  44% 44% 11%



4.2.24 Score per residue for model 24

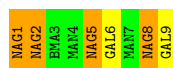
- Molecule 1: CHORIONIC GONADOTROPIN

Chain A: 24% 17% 54%



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

Chain B: 33% 22% 44%



4.2.25 Score per residue for model 25

- Molecule 1: CHORIONIC GONADOTROPIN

Chain A: 22% 16% 54%



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

Chain B: 33% 44% 22%



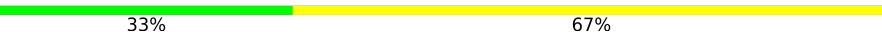
4.2.26 Score per residue for model 26

• Molecule 1: CHORIONIC GONADOTROPIN

Chain A: 



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

Chain B: 



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *DG/SA*.

Of the 150 calculated structures, 26 were deposited, based on the following criterion: ?.

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

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

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, BMA, GAL

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	0.60±0.03	0±0/333 (0.0± 0.0%)	0.96±0.03	0±0/452 (0.1± 0.1%)
All	All	0.60	0/8658 (0.0%)	0.96	12/11752 (0.1%)

There are no bond-length outliers.

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	26	LEU	N-CA-C	5.84	115.80	108.45	26	10
1	A	16	PRO	N-CA-C	-5.07	109.41	114.68	7	2

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	324	313	313	159±11
2	B	111	103	94	10±4
All	All	11310	10816	10582	4279

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 195.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ILE:CG2	1:A:76:VAL:HG21	1.21	1.65	10	26
1:A:12:LEU:HD21	1:A:79:HIS:O	1.20	1.34	22	26
1:A:25:ILE:HG23	1:A:76:VAL:HG21	1.12	1.16	8	26
1:A:18:PHE:CD1	1:A:70:VAL:HG12	1.11	1.80	20	4
1:A:23:ALA:CB	2:B:1:NAG:H83	1.11	1.76	16	13
1:A:18:PHE:CD2	1:A:70:VAL:HG13	1.08	1.84	4	9
1:A:12:LEU:HD23	1:A:26:LEU:HD13	1.07	1.25	6	22
1:A:23:ALA:HB1	2:B:1:NAG:H83	1.06	1.17	5	21
1:A:63:LYS:N	1:A:81:ALA:O	1.05	1.88	21	26
1:A:25:ILE:HD11	2:B:1:NAG:H82	1.04	1.30	26	24
1:A:26:LEU:HD12	1:A:79:HIS:N	1.03	1.68	2	25
1:A:18:PHE:CG	1:A:70:VAL:HG21	1.02	1.89	7	12
1:A:12:LEU:HD21	1:A:26:LEU:HD13	1.01	1.32	11	8
1:A:25:ILE:CD1	1:A:68:VAL:HG21	1.00	1.86	8	26
1:A:12:LEU:CD2	1:A:26:LEU:HD13	0.99	1.87	6	18
1:A:26:LEU:HD11	1:A:78:ASN:OD1	0.97	1.59	10	4
1:A:25:ILE:HG23	1:A:76:VAL:CG2	0.97	1.89	12	26
1:A:25:ILE:O	1:A:26:LEU:HD23	0.95	1.60	24	21
1:A:12:LEU:HD23	1:A:26:LEU:HB3	0.95	1.35	11	6
1:A:26:LEU:HD12	1:A:78:ASN:C	0.95	1.86	11	26
1:A:25:ILE:HG13	1:A:68:VAL:HG21	0.95	1.37	1	25
1:A:25:ILE:CG1	1:A:68:VAL:HG21	0.94	1.91	1	25
1:A:23:ALA:HB1	2:B:1:NAG:C8	0.94	1.92	22	12
1:A:25:ILE:C	1:A:26:LEU:HG	0.93	1.89	9	14
1:A:63:LYS:HB2	1:A:83:HIS:CD2	0.91	2.01	13	2
1:A:25:ILE:CD1	1:A:68:VAL:HG11	0.91	1.95	2	24
1:A:15:ASN:ND2	1:A:70:VAL:HG11	0.90	1.81	20	2
1:A:15:ASN:ND2	1:A:76:VAL:HG11	0.90	1.81	18	18
1:A:17:PHE:CE1	1:A:71:MET:HE2	0.90	2.02	17	1
1:A:18:PHE:CD1	1:A:70:VAL:HG21	0.89	2.02	16	7
1:A:66:ASN:CB	1:A:78:ASN:HB3	0.89	1.98	10	26
1:A:18:PHE:CE2	1:A:68:VAL:HG23	0.88	2.03	15	3
1:A:68:VAL:HG13	1:A:78:ASN:HB2	0.88	1.45	5	21
1:A:71:MET:HE3	1:A:74:PHE:CE2	0.87	2.05	13	1
1:A:25:ILE:HD11	1:A:68:VAL:HG21	0.87	1.46	7	12
1:A:25:ILE:HG22	1:A:26:LEU:N	0.86	1.84	15	26
1:A:24:PRO:O	1:A:25:ILE:O	0.86	1.92	9	26
1:A:25:ILE:HG22	1:A:26:LEU:H	0.86	1.30	16	26
1:A:26:LEU:HD13	1:A:79:HIS:O	0.86	1.70	8	25
1:A:12:LEU:HD23	1:A:26:LEU:CB	0.86	1.99	19	9
1:A:25:ILE:CG2	1:A:76:VAL:HG11	0.86	1.99	12	23

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ILE:C	1:A:26:LEU:HD23	0.86	1.96	13	16
1:A:12:LEU:HD12	1:A:82:CYS:SG	0.85	2.11	16	6
1:A:25:ILE:HG21	1:A:76:VAL:HG21	0.85	1.48	10	17
2:B:3:BMA:H62	2:B:7:MAN:H5	0.85	1.48	21	2
1:A:11:THR:OG1	1:A:12:LEU:N	0.85	2.08	11	18
1:A:25:ILE:CG2	1:A:76:VAL:CG2	0.84	2.54	21	26
1:A:12:LEU:CD2	1:A:79:HIS:O	0.84	2.24	22	26
1:A:12:LEU:HD23	1:A:26:LEU:CD1	0.84	2.02	6	5
1:A:63:LYS:HG3	1:A:81:ALA:C	0.83	1.97	20	4
1:A:68:VAL:HG22	1:A:76:VAL:CG2	0.83	2.04	26	21
1:A:11:THR:O	1:A:29:MET:N	0.83	2.11	22	18
1:A:25:ILE:HD11	1:A:68:VAL:HG11	0.83	1.48	1	26
1:A:18:PHE:CD2	1:A:70:VAL:HG21	0.83	2.08	14	9
1:A:66:ASN:CA	1:A:78:ASN:HB3	0.83	2.04	11	18
1:A:25:ILE:HG21	1:A:76:VAL:HG11	0.83	1.48	12	19
1:A:18:PHE:CE2	1:A:70:VAL:HG13	0.82	2.09	6	6
1:A:82:CYS:C	1:A:83:HIS:CD2	0.82	2.57	24	2
1:A:25:ILE:CD1	2:B:1:NAG:H82	0.82	2.04	14	16
1:A:68:VAL:O	1:A:70:VAL:HG22	0.82	1.73	19	8
1:A:77:GLU:O	1:A:79:HIS:N	0.81	2.13	12	26
1:A:68:VAL:HG11	2:B:1:NAG:H82	0.81	1.52	7	2
1:A:17:PHE:CZ	1:A:71:MET:HE2	0.81	2.11	17	4
1:A:25:ILE:CG2	1:A:26:LEU:H	0.80	1.89	7	26
1:A:68:VAL:O	1:A:68:VAL:HG23	0.80	1.76	10	24
2:B:5:NAG:H3	2:B:6:GAL:O2	0.80	1.77	13	3
1:A:18:PHE:CE2	1:A:70:VAL:HG21	0.79	2.12	17	3
1:A:15:ASN:CG	1:A:76:VAL:HG11	0.79	2.01	4	8
2:B:8:NAG:H4	2:B:9:GAL:O2	0.79	1.78	21	4
1:A:20:GLN:O	1:A:22:GLY:N	0.79	2.16	12	23
1:A:18:PHE:HB3	1:A:25:ILE:CG1	0.79	2.08	18	12
1:A:66:ASN:C	1:A:78:ASN:HB3	0.79	2.02	11	26
1:A:61:VAL:O	1:A:61:VAL:HG12	0.78	1.77	16	4
1:A:61:VAL:HG12	1:A:61:VAL:O	0.78	1.78	26	4
1:A:63:LYS:HG3	1:A:81:ALA:CB	0.78	2.09	23	4
1:A:25:ILE:CG2	1:A:26:LEU:N	0.77	2.46	7	26
1:A:66:ASN:HB3	1:A:78:ASN:HB3	0.77	1.55	25	26
1:A:68:VAL:O	1:A:68:VAL:CG2	0.77	2.31	10	15
1:A:77:GLU:O	1:A:78:ASN:C	0.77	2.27	19	26
1:A:18:PHE:CD1	1:A:70:VAL:CG1	0.77	2.68	25	7
1:A:11:THR:O	1:A:12:LEU:HD12	0.77	1.79	24	3
2:B:2:NAG:O7	2:B:2:NAG:C3	0.76	2.33	18	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ASN:HD22	1:A:76:VAL:HG11	0.76	1.38	26	5
1:A:61:VAL:HG22	1:A:61:VAL:O	0.76	1.80	25	2
1:A:68:VAL:HG23	1:A:78:ASN:HB2	0.76	1.55	12	1
1:A:62:ALA:HB2	1:A:79:HIS:CG	0.76	2.15	17	23
1:A:65:TYR:HB3	1:A:77:GLU:HB2	0.76	1.58	16	17
1:A:65:TYR:CB	1:A:77:GLU:O	0.76	2.34	10	26
2:B:5:NAG:C1	2:B:5:NAG:O7	0.76	2.34	25	1
2:B:8:NAG:C3	2:B:8:NAG:O7	0.75	2.34	18	2
1:A:69:THR:HG23	1:A:73:GLY:C	0.74	2.07	10	7
1:A:76:VAL:O	1:A:78:ASN:N	0.74	2.20	14	26
2:B:3:BMA:H62	2:B:7:MAN:C5	0.74	2.13	21	2
1:A:15:ASN:OD1	1:A:17:PHE:CZ	0.74	2.41	4	2
1:A:28:CYS:SG	1:A:79:HIS:HB3	0.74	2.22	18	4
1:A:15:ASN:H	1:A:25:ILE:C	0.74	1.90	16	25
1:A:76:VAL:O	1:A:77:GLU:C	0.74	2.31	20	26
2:B:5:NAG:C3	2:B:5:NAG:O7	0.74	2.34	5	1
1:A:12:LEU:HD21	1:A:79:HIS:CB	0.73	2.13	9	15
1:A:78:ASN:O	1:A:80:THR:HG23	0.73	1.82	21	9
1:A:11:THR:C	1:A:12:LEU:HD12	0.73	2.08	18	4
1:A:13:GLN:O	1:A:14:GLU:O	0.73	2.06	26	26
1:A:11:THR:O	1:A:28:CYS:HA	0.73	1.84	22	21
1:A:15:ASN:HD22	1:A:25:ILE:HG21	0.73	1.42	2	11
1:A:25:ILE:CD1	1:A:68:VAL:CG2	0.73	2.66	7	26
1:A:15:ASN:ND2	1:A:25:ILE:HG21	0.73	1.99	2	8
1:A:15:ASN:CG	1:A:18:PHE:CD2	0.72	2.67	7	8
1:A:14:GLU:HA	1:A:25:ILE:O	0.72	1.85	9	26
2:B:8:NAG:H3	2:B:8:NAG:O7	0.72	1.81	19	1
1:A:63:LYS:CB	1:A:83:HIS:CD2	0.72	2.71	13	2
2:B:3:BMA:H62	2:B:7:MAN:H3	0.72	1.59	12	2
1:A:15:ASN:OD1	1:A:17:PHE:CG	0.71	2.42	26	1
1:A:26:LEU:CD1	1:A:79:HIS:O	0.71	2.39	7	22
1:A:68:VAL:HG12	1:A:68:VAL:O	0.71	1.84	12	1
1:A:18:PHE:CD2	1:A:70:VAL:CG1	0.71	2.73	8	9
1:A:18:PHE:HD2	1:A:25:ILE:HG21	0.71	1.45	9	12
1:A:77:GLU:CG	1:A:79:HIS:HE2	0.71	1.98	10	3
1:A:18:PHE:CD1	1:A:70:VAL:HG11	0.71	2.21	3	6
1:A:77:GLU:O	1:A:79:HIS:HD2	0.71	1.68	12	22
1:A:63:LYS:CB	1:A:81:ALA:O	0.70	2.39	1	1
1:A:18:PHE:CD1	1:A:70:VAL:CG2	0.70	2.73	16	4
1:A:61:VAL:HG13	1:A:83:HIS:NE2	0.70	2.00	25	2
1:A:25:ILE:HD12	1:A:68:VAL:CG1	0.70	2.17	10	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:VAL:O	1:A:69:THR:C	0.70	2.35	7	24
1:A:18:PHE:CD2	1:A:25:ILE:HG13	0.70	2.22	20	8
1:A:19:SER:HA	1:A:24:PRO:HA	0.70	1.64	15	13
1:A:65:TYR:CG	1:A:77:GLU:CG	0.70	2.75	20	9
1:A:63:LYS:CG	1:A:81:ALA:C	0.70	2.65	23	4
1:A:12:LEU:CD2	1:A:79:HIS:HB2	0.69	2.18	12	15
1:A:24:PRO:HD2	2:B:1:NAG:H3	0.69	1.62	22	8
1:A:18:PHE:CG	1:A:25:ILE:HG13	0.69	2.23	13	13
1:A:76:VAL:C	1:A:78:ASN:N	0.69	2.50	12	26
1:A:70:VAL:HG22	1:A:74:PHE:HB2	0.69	1.64	10	4
1:A:18:PHE:CE1	1:A:70:VAL:HB	0.68	2.24	3	5
1:A:63:LYS:CE	1:A:83:HIS:CE1	0.68	2.77	24	1
2:B:8:NAG:H5	2:B:9:GAL:C2	0.68	2.18	6	2
1:A:15:ASN:CB	1:A:25:ILE:HB	0.68	2.18	6	26
1:A:12:LEU:HD21	1:A:79:HIS:C	0.68	2.13	24	18
1:A:18:PHE:CD2	1:A:25:ILE:HG21	0.68	2.23	14	12
1:A:13:GLN:O	1:A:14:GLU:C	0.68	2.36	23	26
1:A:15:ASN:HB2	1:A:25:ILE:HG22	0.68	1.64	26	25
1:A:64:SER:O	1:A:80:THR:N	0.68	2.27	20	13
1:A:78:ASN:OD1	1:A:78:ASN:O	0.68	2.12	17	5
1:A:15:ASN:OD1	1:A:17:PHE:CE2	0.68	2.47	4	2
1:A:63:LYS:HE3	1:A:81:ALA:HB1	0.67	1.66	20	1
1:A:61:VAL:HG13	1:A:83:HIS:CE1	0.67	2.24	25	1
2:B:3:BMA:H62	2:B:7:MAN:C3	0.67	2.19	12	2
1:A:64:SER:HB3	1:A:80:THR:OG1	0.67	1.90	25	8
2:B:3:BMA:O2	2:B:4:MAN:C5	0.67	2.43	8	2
1:A:25:ILE:CD1	1:A:68:VAL:CG1	0.67	2.71	15	21
1:A:27:GLN:O	1:A:28:CYS:O	0.67	2.13	25	4
1:A:61:VAL:O	1:A:62:ALA:C	0.67	2.38	4	24
1:A:70:VAL:CG2	1:A:74:PHE:HB2	0.67	2.19	20	4
1:A:25:ILE:HD12	1:A:68:VAL:HG21	0.67	1.64	8	7
2:B:8:NAG:H3	2:B:9:GAL:O2	0.67	1.89	14	1
1:A:15:ASN:ND2	1:A:76:VAL:CG1	0.67	2.57	6	19
1:A:26:LEU:O	1:A:76:VAL:HB	0.67	1.90	8	26
1:A:63:LYS:HD3	1:A:83:HIS:HB3	0.67	1.65	23	1
1:A:25:ILE:HG13	1:A:68:VAL:CG2	0.66	2.19	13	22
2:B:8:NAG:H5	2:B:9:GAL:H2	0.66	1.67	6	2
1:A:15:ASN:N	1:A:25:ILE:O	0.66	2.29	23	17
1:A:18:PHE:N	1:A:18:PHE:CD1	0.66	2.60	14	5
1:A:18:PHE:CE2	1:A:68:VAL:CG2	0.66	2.79	15	2
1:A:13:GLN:CG	1:A:29:MET:HA	0.66	2.20	23	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:PHE:CE1	1:A:70:VAL:HG12	0.66	2.26	25	3
1:A:12:LEU:HD12	1:A:28:CYS:SG	0.66	2.30	21	5
2:B:8:NAG:H5	2:B:9:GAL:O5	0.66	1.90	17	1
1:A:26:LEU:O	1:A:76:VAL:CG1	0.66	2.44	10	22
1:A:78:ASN:O	1:A:78:ASN:OD1	0.66	2.13	21	4
1:A:61:VAL:O	1:A:61:VAL:HG13	0.66	1.89	15	4
1:A:16:PRO:HD2	1:A:17:PHE:CE1	0.66	2.25	26	3
1:A:15:ASN:OD1	1:A:18:PHE:CD2	0.65	2.49	22	13
1:A:25:ILE:CG2	1:A:76:VAL:CG1	0.65	2.73	19	13
1:A:25:ILE:HD12	1:A:68:VAL:CG2	0.65	2.22	8	18
1:A:77:GLU:HG3	1:A:79:HIS:NE2	0.65	2.07	9	5
1:A:18:PHE:CE1	1:A:70:VAL:HG21	0.65	2.26	3	3
1:A:12:LEU:CD1	1:A:82:CYS:SG	0.65	2.85	8	8
2:B:3:BMA:C6	2:B:7:MAN:H5	0.65	2.21	12	1
1:A:61:VAL:O	1:A:62:ALA:O	0.65	2.14	24	19
1:A:78:ASN:O	1:A:80:THR:CG2	0.65	2.45	19	9
1:A:14:GLU:CD	1:A:24:PRO:HB2	0.65	2.17	14	12
1:A:20:GLN:CG	1:A:23:ALA:HB3	0.65	2.21	19	1
1:A:25:ILE:HD11	1:A:68:VAL:CG1	0.65	2.22	12	5
1:A:27:GLN:O	1:A:28:CYS:C	0.65	2.39	8	23
1:A:18:PHE:CE1	1:A:70:VAL:CG2	0.64	2.80	3	2
1:A:82:CYS:C	1:A:83:HIS:HD2	0.64	2.01	24	2
1:A:25:ILE:HG21	1:A:76:VAL:CG1	0.64	2.23	19	10
1:A:62:ALA:HB1	1:A:64:SER:O	0.64	1.92	25	7
2:B:3:BMA:C6	2:B:7:MAN:H3	0.64	2.22	21	2
1:A:14:GLU:HG3	1:A:26:LEU:HD23	0.64	1.69	16	1
1:A:62:ALA:HB2	1:A:79:HIS:CD2	0.64	2.28	1	9
1:A:68:VAL:HG22	1:A:76:VAL:HG21	0.64	1.68	26	11
1:A:15:ASN:HB2	1:A:25:ILE:CB	0.64	2.23	24	22
1:A:65:TYR:CG	1:A:77:GLU:HG2	0.64	2.28	20	8
2:B:8:NAG:H3	2:B:9:GAL:H2	0.64	1.68	1	2
2:B:5:NAG:H5	2:B:6:GAL:O2	0.64	1.92	24	3
2:B:8:NAG:O7	2:B:8:NAG:C3	0.64	2.46	19	1
1:A:70:VAL:HG22	1:A:74:PHE:CB	0.64	2.23	10	4
1:A:71:MET:O	1:A:74:PHE:CD2	0.64	2.51	9	3
1:A:62:ALA:HA	1:A:81:ALA:O	0.64	1.93	16	18
1:A:20:GLN:HG3	1:A:23:ALA:HB3	0.64	1.70	11	3
1:A:15:ASN:HD21	1:A:70:VAL:HG11	0.64	1.50	20	1
1:A:12:LEU:CD2	1:A:79:HIS:CB	0.63	2.76	9	11
1:A:26:LEU:HD12	1:A:78:ASN:CA	0.63	2.23	19	5
1:A:18:PHE:CD2	1:A:25:ILE:CG1	0.63	2.80	25	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LEU:CD1	1:A:78:ASN:C	0.63	2.71	16	25
1:A:63:LYS:HG3	1:A:81:ALA:HB1	0.63	1.68	23	4
1:A:13:GLN:HG3	1:A:29:MET:HA	0.63	1.70	1	4
1:A:65:TYR:HB2	1:A:77:GLU:C	0.63	2.19	12	13
2:B:8:NAG:C3	2:B:9:GAL:O5	0.63	2.46	1	3
1:A:15:ASN:OD1	1:A:18:PHE:CG	0.63	2.52	21	4
1:A:18:PHE:CZ	1:A:70:VAL:HG21	0.63	2.28	17	1
1:A:18:PHE:CD2	1:A:70:VAL:CG2	0.63	2.81	21	4
1:A:18:PHE:CD1	1:A:70:VAL:CB	0.63	2.82	16	4
1:A:20:GLN:N	1:A:23:ALA:O	0.63	2.30	9	3
2:B:8:NAG:O7	2:B:8:NAG:H3	0.63	1.94	18	3
1:A:15:ASN:HB3	1:A:25:ILE:HB	0.63	1.70	16	17
1:A:25:ILE:C	1:A:26:LEU:CG	0.63	2.72	16	20
1:A:25:ILE:HD11	1:A:68:VAL:CG2	0.63	2.20	7	2
1:A:25:ILE:HD12	1:A:68:VAL:HG11	0.63	1.71	21	6
1:A:65:TYR:CD1	1:A:65:TYR:N	0.63	2.66	23	3
1:A:65:TYR:CB	1:A:77:GLU:CG	0.62	2.77	20	9
1:A:74:PHE:C	1:A:75:LYS:HG2	0.62	2.18	3	1
1:A:69:THR:HA	1:A:74:PHE:O	0.62	1.94	24	25
1:A:70:VAL:HG23	1:A:71:MET:HG2	0.62	1.72	10	2
1:A:71:MET:SD	1:A:74:PHE:CZ	0.62	2.92	10	1
1:A:65:TYR:CB	1:A:77:GLU:CB	0.62	2.78	14	23
1:A:25:ILE:C	1:A:26:LEU:CD2	0.62	2.73	13	12
1:A:11:THR:O	1:A:82:CYS:SG	0.62	2.57	18	3
1:A:83:HIS:O	1:A:83:HIS:CD2	0.61	2.53	18	10
2:B:1:NAG:O4	2:B:2:NAG:O7	0.61	2.18	4	10
1:A:15:ASN:ND2	1:A:25:ILE:CG2	0.61	2.63	15	7
1:A:18:PHE:CE1	1:A:70:VAL:CB	0.61	2.83	3	3
1:A:25:ILE:CD1	1:A:68:VAL:CB	0.61	2.78	12	1
1:A:15:ASN:OD1	1:A:17:PHE:CD2	0.61	2.53	26	1
1:A:18:PHE:CG	1:A:25:ILE:CG1	0.61	2.84	15	9
1:A:66:ASN:CB	1:A:78:ASN:CB	0.61	2.77	17	9
1:A:25:ILE:CG2	1:A:76:VAL:CB	0.61	2.78	19	14
1:A:17:PHE:CZ	1:A:71:MET:SD	0.61	2.93	19	3
1:A:66:ASN:HB3	1:A:78:ASN:HD22	0.61	1.56	25	3
1:A:66:ASN:O	1:A:67:ARG:C	0.61	2.44	3	26
1:A:68:VAL:O	1:A:68:VAL:HG22	0.61	1.94	15	1
1:A:26:LEU:CD1	1:A:79:HIS:N	0.61	2.62	5	12
2:B:5:NAG:H4	2:B:6:GAL:O2	0.61	1.96	20	8
1:A:70:VAL:HG23	1:A:74:PHE:CB	0.61	2.25	2	1
1:A:68:VAL:HG23	1:A:78:ASN:CB	0.61	2.26	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:5:NAG:H3	2:B:5:NAG:O7	0.61	1.95	5	1
1:A:64:SER:CB	1:A:80:THR:OG1	0.61	2.48	26	11
1:A:17:PHE:CE2	1:A:71:MET:SD	0.61	2.94	23	1
1:A:28:CYS:HB2	1:A:79:HIS:HD1	0.61	1.56	9	7
1:A:12:LEU:CD1	1:A:12:LEU:N	0.61	2.64	26	2
1:A:77:GLU:HG2	1:A:79:HIS:HE2	0.61	1.54	10	2
1:A:18:PHE:HB3	1:A:25:ILE:HG12	0.60	1.72	25	6
1:A:12:LEU:HD12	1:A:12:LEU:N	0.60	2.12	20	3
2:B:2:NAG:O7	2:B:2:NAG:H3	0.60	1.97	10	9
1:A:64:SER:HB2	1:A:80:THR:HG1	0.60	1.56	1	1
1:A:78:ASN:OD1	1:A:80:THR:HG22	0.60	1.95	11	6
1:A:11:THR:O	1:A:28:CYS:SG	0.60	2.59	24	2
1:A:78:ASN:O	1:A:80:THR:N	0.60	2.34	11	4
2:B:3:BMA:C2	2:B:4:MAN:O5	0.60	2.49	8	2
1:A:18:PHE:O	1:A:20:GLN:N	0.60	2.34	1	11
2:B:5:NAG:O7	2:B:5:NAG:O3	0.60	2.20	11	3
1:A:66:ASN:O	1:A:67:ARG:O	0.60	2.20	18	20
1:A:15:ASN:OD1	1:A:18:PHE:CE2	0.60	2.55	22	10
1:A:65:TYR:CD2	1:A:77:GLU:HG2	0.60	2.31	6	3
1:A:11:THR:HG1	1:A:12:LEU:H	0.60	1.39	16	1
1:A:15:ASN:CG	1:A:17:PHE:CE2	0.60	2.80	24	2
1:A:18:PHE:O	1:A:20:GLN:CG	0.60	2.50	18	3
1:A:78:ASN:OD1	2:B:1:NAG:O5	0.59	2.18	2	6
1:A:14:GLU:O	1:A:16:PRO:HD3	0.59	1.96	21	11
1:A:65:TYR:CG	1:A:77:GLU:HG3	0.59	2.32	17	8
1:A:18:PHE:CD2	1:A:68:VAL:CG2	0.59	2.85	15	4
1:A:15:ASN:HD22	1:A:25:ILE:CG2	0.59	2.10	2	10
1:A:12:LEU:CD1	1:A:28:CYS:SG	0.59	2.90	21	3
1:A:19:SER:HA	1:A:23:ALA:O	0.59	1.97	16	3
1:A:61:VAL:O	1:A:61:VAL:HG23	0.59	1.98	13	2
1:A:65:TYR:HB3	1:A:77:GLU:HB3	0.59	1.73	6	9
1:A:14:GLU:HG2	1:A:24:PRO:HB2	0.59	1.73	9	2
1:A:28:CYS:HB2	1:A:79:HIS:CE1	0.59	2.32	1	4
1:A:77:GLU:CG	1:A:79:HIS:NE2	0.59	2.65	11	7
1:A:66:ASN:HB3	1:A:78:ASN:CB	0.59	2.27	19	9
1:A:11:THR:O	1:A:28:CYS:CB	0.59	2.51	16	4
1:A:78:ASN:OD1	1:A:78:ASN:C	0.59	2.46	15	3
1:A:63:LYS:HE2	1:A:83:HIS:CE1	0.59	2.32	24	1
1:A:12:LEU:N	1:A:12:LEU:HD12	0.59	2.12	26	5
1:A:18:PHE:CD1	1:A:70:VAL:HB	0.59	2.32	7	2
1:A:18:PHE:CD2	1:A:68:VAL:HG23	0.59	2.32	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ASN:HB2	1:A:25:ILE:CG2	0.59	2.27	12	26
2:B:2:NAG:O7	2:B:2:NAG:O3	0.59	2.19	20	7
1:A:65:TYR:CB	1:A:77:GLU:HB2	0.59	2.28	9	11
1:A:15:ASN:CG	1:A:18:PHE:CE2	0.59	2.81	7	6
1:A:26:LEU:O	1:A:27:GLN:HB2	0.58	1.96	7	15
1:A:27:GLN:O	1:A:27:GLN:HG2	0.58	1.97	14	8
1:A:17:PHE:CD1	1:A:17:PHE:N	0.58	2.70	24	3
1:A:12:LEU:HD11	1:A:82:CYS:SG	0.58	2.38	12	6
1:A:75:LYS:CD	1:A:75:LYS:N	0.58	2.65	23	1
1:A:71:MET:HB2	1:A:74:PHE:CD1	0.58	2.33	12	9
1:A:18:PHE:CB	1:A:25:ILE:CG1	0.58	2.81	15	12
1:A:66:ASN:HB2	1:A:80:THR:CG2	0.58	2.29	11	8
1:A:61:VAL:O	1:A:61:VAL:CG1	0.58	2.50	26	5
2:B:5:NAG:H5	2:B:6:GAL:O5	0.58	1.98	19	2
1:A:65:TYR:CD2	1:A:77:GLU:HG3	0.58	2.33	22	5
1:A:11:THR:O	1:A:28:CYS:CA	0.58	2.52	11	8
1:A:13:GLN:HG3	1:A:29:MET:CB	0.58	2.29	16	6
1:A:18:PHE:HB3	1:A:25:ILE:HB	0.58	1.74	26	9
1:A:70:VAL:O	1:A:71:MET:C	0.58	2.45	25	22
1:A:61:VAL:O	1:A:83:HIS:CD2	0.58	2.56	9	2
1:A:63:LYS:HE3	1:A:83:HIS:CE1	0.58	2.34	24	1
1:A:17:PHE:CZ	1:A:71:MET:CE	0.58	2.87	12	2
1:A:15:ASN:HB2	1:A:25:ILE:HB	0.58	1.76	24	12
1:A:18:PHE:CZ	1:A:70:VAL:CG2	0.58	2.86	17	2
1:A:64:SER:OG	1:A:81:ALA:HB3	0.58	1.98	23	3
2:B:4:MAN:O2	2:B:5:NAG:O7	0.57	2.22	21	4
1:A:11:THR:C	1:A:82:CYS:SG	0.57	2.87	11	2
1:A:17:PHE:CD2	1:A:71:MET:SD	0.57	2.96	20	2
1:A:26:LEU:HG	1:A:78:ASN:OD1	0.57	1.99	13	6
1:A:61:VAL:HG23	1:A:83:HIS:O	0.57	2.00	9	1
1:A:67:ARG:HB3	1:A:77:GLU:HA	0.57	1.76	4	13
1:A:12:LEU:CD2	1:A:26:LEU:HD22	0.57	2.29	19	2
1:A:27:GLN:O	1:A:27:GLN:CG	0.57	2.52	25	10
1:A:12:LEU:CD2	1:A:26:LEU:CD1	0.57	2.76	16	5
1:A:18:PHE:CE2	1:A:76:VAL:HG13	0.57	2.34	21	3
2:B:3:BMA:C6	2:B:7:MAN:C5	0.57	2.81	12	2
2:B:3:BMA:O2	2:B:4:MAN:H5	0.57	2.00	19	1
1:A:71:MET:SD	1:A:74:PHE:CD2	0.57	2.98	1	1
1:A:15:ASN:C	1:A:17:PHE:H	0.57	2.08	12	11
1:A:74:PHE:O	1:A:75:LYS:HG3	0.57	2.00	19	6
1:A:13:GLN:CD	1:A:29:MET:CB	0.56	2.78	26	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ALA:HB2	1:A:79:HIS:ND1	0.56	2.13	16	5
1:A:71:MET:HG3	1:A:74:PHE:CD2	0.56	2.35	24	3
1:A:17:PHE:CE1	1:A:71:MET:SD	0.56	2.98	22	2
1:A:65:TYR:HB3	1:A:77:GLU:CB	0.56	2.30	7	14
1:A:26:LEU:HD12	1:A:78:ASN:HA	0.56	1.77	19	1
1:A:14:GLU:OE2	1:A:24:PRO:CB	0.56	2.53	26	7
1:A:18:PHE:HB3	1:A:25:ILE:CB	0.56	2.31	4	8
1:A:68:VAL:HG22	1:A:76:VAL:HG22	0.56	1.76	17	9
1:A:25:ILE:CG1	1:A:68:VAL:CG2	0.56	2.83	7	6
1:A:14:GLU:HG3	1:A:25:ILE:O	0.56	2.01	13	5
2:B:8:NAG:H5	2:B:9:GAL:O2	0.56	2.01	14	1
1:A:26:LEU:CD1	1:A:78:ASN:OD1	0.56	2.49	15	3
1:A:14:GLU:CD	1:A:24:PRO:HG2	0.56	2.26	16	1
1:A:76:VAL:O	1:A:79:HIS:CD2	0.56	2.59	6	7
2:B:3:BMA:H4	2:B:7:MAN:C5	0.56	2.31	7	1
1:A:65:TYR:HB2	1:A:77:GLU:O	0.56	2.01	12	14
2:B:8:NAG:H3	2:B:9:GAL:C2	0.56	2.30	1	2
1:A:15:ASN:HB2	1:A:25:ILE:C	0.56	2.26	24	15
1:A:74:PHE:O	1:A:75:LYS:HG2	0.56	2.00	2	4
1:A:12:LEU:HD21	1:A:79:HIS:HB3	0.56	1.78	9	5
1:A:63:LYS:HB3	1:A:81:ALA:CB	0.55	2.30	11	10
1:A:70:VAL:O	1:A:74:PHE:N	0.55	2.36	25	11
1:A:13:GLN:CG	1:A:29:MET:HB2	0.55	2.30	13	4
1:A:20:GLN:CB	1:A:21:PRO:CD	0.55	2.83	3	3
2:B:3:BMA:C6	2:B:7:MAN:C3	0.55	2.85	21	2
1:A:70:VAL:HG23	1:A:74:PHE:HB2	0.55	1.78	2	4
1:A:71:MET:HG3	1:A:74:PHE:CG	0.55	2.37	13	2
1:A:17:PHE:CE2	1:A:71:MET:HE3	0.55	2.37	1	1
1:A:28:CYS:HB2	1:A:79:HIS:ND1	0.55	2.17	5	11
1:A:69:THR:CG2	1:A:73:GLY:HA2	0.55	2.32	15	13
1:A:17:PHE:CZ	1:A:71:MET:HG2	0.55	2.37	8	1
1:A:67:ARG:CA	1:A:77:GLU:HA	0.55	2.32	18	23
1:A:12:LEU:N	1:A:12:LEU:CD1	0.55	2.70	20	5
1:A:83:HIS:O	1:A:83:HIS:CG	0.55	2.59	23	8
1:A:18:PHE:HB2	1:A:25:ILE:CG1	0.55	2.32	22	12
1:A:67:ARG:CZ	1:A:77:GLU:OE2	0.55	2.55	19	1
1:A:14:GLU:CD	1:A:26:LEU:CD2	0.55	2.80	9	1
1:A:12:LEU:HA	1:A:28:CYS:HA	0.54	1.79	3	21
2:B:5:NAG:O3	2:B:5:NAG:O7	0.54	2.22	9	1
1:A:19:SER:O	1:A:19:SER:OG	0.54	2.26	26	7
1:A:17:PHE:CD2	1:A:18:PHE:CE1	0.54	2.95	21	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:SER:HB2	1:A:80:THR:OG1	0.54	2.02	24	13
1:A:12:LEU:HB3	1:A:26:LEU:HB3	0.54	1.80	6	1
1:A:17:PHE:CZ	1:A:71:MET:HG3	0.54	2.37	25	2
1:A:83:HIS:CD2	1:A:83:HIS:N	0.54	2.76	24	2
1:A:25:ILE:O	1:A:26:LEU:CD2	0.54	2.52	16	1
1:A:28:CYS:H	1:A:79:HIS:CE1	0.54	2.21	13	2
1:A:13:GLN:OE1	1:A:29:MET:HE2	0.54	2.02	21	2
1:A:12:LEU:HG	1:A:79:HIS:HB2	0.54	1.80	23	12
1:A:18:PHE:O	1:A:23:ALA:O	0.54	2.26	10	5
1:A:71:MET:O	1:A:74:PHE:CD1	0.54	2.61	4	1
1:A:18:PHE:HE2	1:A:76:VAL:HG13	0.54	1.62	21	3
1:A:68:VAL:CG2	1:A:78:ASN:HB2	0.54	2.31	12	1
1:A:18:PHE:CE2	1:A:70:VAL:CG2	0.54	2.88	17	3
1:A:70:VAL:HG23	1:A:71:MET:N	0.54	2.17	25	1
2:B:8:NAG:O3	2:B:9:GAL:O5	0.54	2.26	2	3
1:A:68:VAL:HG13	1:A:78:ASN:CB	0.54	2.30	9	2
1:A:68:VAL:O	1:A:70:VAL:CG2	0.54	2.56	12	2
1:A:19:SER:CA	1:A:24:PRO:HA	0.54	2.33	9	2
1:A:13:GLN:CG	1:A:29:MET:O	0.54	2.56	15	1
1:A:13:GLN:OE1	1:A:29:MET:CE	0.54	2.55	18	1
1:A:68:VAL:O	1:A:69:THR:O	0.53	2.26	20	6
1:A:20:GLN:CB	1:A:21:PRO:HD2	0.53	2.34	25	2
1:A:18:PHE:HB2	1:A:25:ILE:HB	0.53	1.81	19	3
1:A:26:LEU:O	1:A:76:VAL:CB	0.53	2.57	10	14
1:A:70:VAL:O	1:A:73:GLY:N	0.53	2.39	21	10
1:A:68:VAL:HG11	2:B:1:NAG:C8	0.53	2.30	7	1
2:B:3:BMA:O2	2:B:4:MAN:O5	0.53	2.26	8	1
1:A:77:GLU:HG2	1:A:79:HIS:NE2	0.53	2.18	11	1
1:A:14:GLU:OE2	1:A:24:PRO:HB2	0.53	2.03	6	6
1:A:75:LYS:HB3	1:A:77:GLU:OE1	0.53	2.03	11	1
1:A:25:ILE:CG1	1:A:68:VAL:HG11	0.53	2.33	12	1
1:A:70:VAL:N	1:A:74:PHE:O	0.53	2.35	25	5
1:A:74:PHE:O	1:A:75:LYS:CG	0.53	2.56	6	2
2:B:8:NAG:O3	2:B:9:GAL:C1	0.53	2.57	2	2
1:A:65:TYR:N	1:A:65:TYR:CD1	0.53	2.75	11	3
2:B:8:NAG:O7	2:B:8:NAG:O3	0.53	2.27	20	3
1:A:63:LYS:CE	1:A:81:ALA:HB1	0.53	2.34	20	1
1:A:62:ALA:C	1:A:81:ALA:O	0.53	2.52	16	9
1:A:63:LYS:HA	1:A:83:HIS:CD2	0.53	2.39	10	3
1:A:25:ILE:HA	1:A:78:ASN:OD1	0.53	2.04	12	10
1:A:65:TYR:CD2	1:A:77:GLU:CG	0.53	2.91	22	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:MET:HE2	1:A:74:PHE:CE1	0.53	2.39	16	1
1:A:12:LEU:HD11	1:A:79:HIS:O	0.53	2.04	11	1
1:A:17:PHE:CE2	1:A:71:MET:HG3	0.53	2.39	25	2
1:A:68:VAL:CG2	1:A:68:VAL:O	0.53	2.57	7	2
1:A:62:ALA:CA	1:A:81:ALA:O	0.52	2.57	16	8
1:A:12:LEU:HD23	1:A:26:LEU:CG	0.52	2.34	16	4
1:A:18:PHE:O	1:A:20:GLN:HG3	0.52	2.04	13	5
1:A:67:ARG:HG3	1:A:77:GLU:HA	0.52	1.82	19	2
1:A:29:MET:O	1:A:29:MET:SD	0.52	2.67	18	1
1:A:64:SER:O	1:A:80:THR:OG1	0.52	2.27	20	2
1:A:14:GLU:HG3	1:A:24:PRO:O	0.52	2.04	21	14
1:A:65:TYR:HB3	1:A:77:GLU:O	0.52	2.05	14	9
1:A:24:PRO:C	1:A:25:ILE:O	0.52	2.53	9	17
1:A:71:MET:SD	1:A:74:PHE:CE2	0.52	3.03	10	2
2:B:5:NAG:O6	2:B:6:GAL:C1	0.52	2.58	13	1
1:A:15:ASN:O	1:A:19:SER:HB3	0.52	2.05	26	2
1:A:76:VAL:HG23	1:A:78:ASN:H	0.52	1.64	6	15
1:A:66:ASN:CB	1:A:78:ASN:CG	0.52	2.83	21	3
1:A:13:GLN:OE1	1:A:29:MET:CB	0.52	2.58	2	1
1:A:28:CYS:N	1:A:79:HIS:HD1	0.52	2.02	8	3
1:A:71:MET:CG	1:A:74:PHE:CD2	0.52	2.93	11	1
2:B:8:NAG:C6	2:B:9:GAL:O5	0.52	2.58	13	1
1:A:77:GLU:HB3	1:A:79:HIS:CD2	0.52	2.40	22	4
1:A:13:GLN:HG2	1:A:29:MET:HB2	0.51	1.82	5	5
1:A:24:PRO:O	1:A:26:LEU:HD23	0.51	2.05	18	8
1:A:69:THR:OG1	1:A:75:LYS:CD	0.51	2.58	11	2
1:A:63:LYS:HD2	1:A:83:HIS:HB3	0.51	1.82	20	2
1:A:18:PHE:CE2	1:A:76:VAL:CG1	0.51	2.93	7	3
1:A:62:ALA:CB	1:A:79:HIS:CG	0.51	2.91	22	3
1:A:13:GLN:CD	1:A:29:MET:HB2	0.51	2.30	2	1
1:A:66:ASN:C	1:A:78:ASN:CB	0.51	2.80	11	9
1:A:77:GLU:O	1:A:79:HIS:CD2	0.51	2.58	12	1
1:A:25:ILE:HG21	1:A:76:VAL:CG2	0.51	2.29	14	3
1:A:62:ALA:HB2	1:A:79:HIS:CE1	0.51	2.40	16	1
2:B:3:BMA:H2	2:B:4:MAN:C5	0.51	2.35	12	1
1:A:14:GLU:HG2	1:A:24:PRO:HG2	0.51	1.83	9	1
1:A:23:ALA:HB2	2:B:1:NAG:H83	0.51	1.78	9	1
2:B:5:NAG:H3	2:B:6:GAL:O5	0.51	2.05	15	1
1:A:63:LYS:CG	1:A:82:CYS:N	0.51	2.74	20	2
1:A:15:ASN:OD1	1:A:17:PHE:N	0.51	2.40	26	1
1:A:70:VAL:O	1:A:71:MET:O	0.51	2.28	9	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:GLN:HG2	1:A:29:MET:CB	0.51	2.36	25	2
1:A:20:GLN:OE1	1:A:21:PRO:N	0.51	2.44	8	1
1:A:14:GLU:CG	1:A:24:PRO:HG2	0.51	2.35	9	2
1:A:63:LYS:HG3	1:A:82:CYS:N	0.51	2.20	20	1
1:A:61:VAL:O	1:A:61:VAL:CG2	0.51	2.53	25	1
1:A:12:LEU:CD2	1:A:26:LEU:CB	0.51	2.86	11	1
1:A:27:GLN:CD	1:A:27:GLN:O	0.51	2.54	13	1
2:B:5:NAG:C3	2:B:6:GAL:O2	0.51	2.56	13	3
1:A:12:LEU:HD21	1:A:26:LEU:CD1	0.51	2.23	11	2
1:A:13:GLN:CG	1:A:29:MET:CA	0.50	2.89	5	3
1:A:13:GLN:CD	1:A:29:MET:O	0.50	2.54	15	1
1:A:14:GLU:CD	1:A:24:PRO:CG	0.50	2.84	16	1
1:A:71:MET:CE	1:A:74:PHE:CE2	0.50	2.90	13	1
1:A:63:LYS:HG2	1:A:82:CYS:CA	0.50	2.36	23	3
1:A:24:PRO:O	1:A:25:ILE:C	0.50	2.54	9	2
1:A:67:ARG:CG	1:A:77:GLU:HA	0.50	2.36	3	8
1:A:18:PHE:CB	1:A:25:ILE:HG13	0.50	2.36	18	5
1:A:13:GLN:CG	1:A:29:MET:HB3	0.50	2.37	8	2
1:A:17:PHE:HB3	1:A:18:PHE:CD1	0.50	2.42	14	1
1:A:70:VAL:CG2	1:A:74:PHE:CB	0.50	2.86	25	3
1:A:63:LYS:CA	1:A:81:ALA:O	0.50	2.60	1	1
1:A:27:GLN:O	1:A:27:GLN:CD	0.50	2.55	25	2
1:A:14:GLU:CD	1:A:26:LEU:HD23	0.50	2.32	9	1
1:A:65:TYR:CA	1:A:77:GLU:O	0.50	2.60	6	12
1:A:17:PHE:CD1	1:A:70:VAL:HB	0.50	2.42	10	1
1:A:63:LYS:HE2	1:A:83:HIS:CG	0.50	2.42	13	1
1:A:64:SER:OG	1:A:81:ALA:CB	0.50	2.59	23	1
1:A:14:GLU:HG2	1:A:24:PRO:O	0.50	2.07	16	1
1:A:64:SER:OG	1:A:80:THR:OG1	0.50	2.26	23	2
1:A:13:GLN:NE2	1:A:29:MET:HB3	0.50	2.22	26	1
1:A:63:LYS:HB3	1:A:81:ALA:O	0.49	2.06	1	1
1:A:73:GLY:O	1:A:74:PHE:O	0.49	2.30	6	4
1:A:13:GLN:HG3	1:A:29:MET:HB2	0.49	1.84	11	3
1:A:12:LEU:CG	1:A:79:HIS:HB2	0.49	2.37	12	8
1:A:83:HIS:CG	1:A:83:HIS:O	0.49	2.65	16	2
1:A:63:LYS:CD	1:A:83:HIS:HB3	0.49	2.36	23	3
1:A:26:LEU:O	1:A:27:GLN:CB	0.49	2.61	2	19
1:A:78:ASN:O	1:A:79:HIS:C	0.49	2.56	17	11
1:A:28:CYS:CB	1:A:79:HIS:HD1	0.49	2.21	8	1
1:A:11:THR:C	1:A:28:CYS:HA	0.49	2.33	17	4
1:A:66:ASN:HB2	1:A:78:ASN:OD1	0.49	2.08	21	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:8:NAG:C5	2:B:9:GAL:O5	0.49	2.61	17	1
2:B:3:BMA:H4	2:B:7:MAN:O5	0.49	2.08	20	1
1:A:66:ASN:OD1	2:B:1:NAG:O7	0.49	2.30	1	1
1:A:71:MET:HG3	1:A:74:PHE:CE2	0.49	2.43	24	1
1:A:18:PHE:CD2	1:A:68:VAL:HG21	0.49	2.43	10	1
1:A:11:THR:O	1:A:13:GLN:HG2	0.49	2.07	15	1
1:A:15:ASN:N	1:A:24:PRO:O	0.49	2.46	16	2
2:B:8:NAG:H3	2:B:9:GAL:O5	0.49	2.06	6	2
1:A:65:TYR:CB	1:A:77:GLU:HG3	0.49	2.38	25	6
2:B:7:MAN:H62	2:B:8:NAG:H82	0.48	1.84	8	1
1:A:13:GLN:NE2	1:A:29:MET:SD	0.48	2.86	23	1
1:A:62:ALA:CB	1:A:79:HIS:CD2	0.48	2.95	1	2
1:A:13:GLN:CD	1:A:29:MET:HB3	0.48	2.33	8	3
1:A:19:SER:HB2	1:A:24:PRO:HA	0.48	1.85	16	1
1:A:71:MET:CE	1:A:74:PHE:CZ	0.48	2.96	16	1
1:A:14:GLU:HG2	1:A:24:PRO:CB	0.48	2.38	9	2
1:A:75:LYS:O	1:A:77:GLU:OE2	0.48	2.32	12	1
1:A:71:MET:CE	1:A:74:PHE:CE1	0.48	2.97	16	1
2:B:4:MAN:C1	2:B:5:NAG:O7	0.48	2.62	25	1
1:A:67:ARG:HA	1:A:77:GLU:CA	0.48	2.39	12	11
1:A:78:ASN:C	1:A:78:ASN:OD1	0.48	2.57	2	2
1:A:15:ASN:ND2	1:A:17:PHE:CE2	0.48	2.82	24	3
1:A:82:CYS:O	1:A:83:HIS:CD2	0.48	2.66	24	1
1:A:18:PHE:HD2	1:A:70:VAL:HG13	0.48	1.55	4	1
1:A:70:VAL:HG23	1:A:71:MET:CG	0.48	2.37	10	2
1:A:17:PHE:HB2	1:A:71:MET:CE	0.48	2.39	15	1
1:A:63:LYS:HD3	1:A:82:CYS:C	0.48	2.33	26	3
1:A:66:ASN:O	1:A:66:ASN:CG	0.48	2.57	13	2
1:A:77:GLU:C	1:A:79:HIS:N	0.48	2.71	19	14
1:A:11:THR:C	1:A:28:CYS:SG	0.48	2.96	19	3
1:A:14:GLU:HG3	1:A:24:PRO:HB2	0.48	1.84	3	3
1:A:14:GLU:OE2	1:A:19:SER:OG	0.48	2.32	19	1
1:A:14:GLU:OE2	1:A:24:PRO:HB3	0.48	2.09	26	1
1:A:67:ARG:HG3	1:A:77:GLU:OE1	0.47	2.08	10	1
1:A:67:ARG:NE	1:A:77:GLU:OE2	0.47	2.47	19	1
1:A:11:THR:HA	1:A:28:CYS:SG	0.47	2.49	3	2
1:A:64:SER:HB2	1:A:81:ALA:HB3	0.47	1.85	10	1
1:A:71:MET:O	1:A:74:PHE:N	0.47	2.43	6	2
1:A:83:HIS:CD2	1:A:83:HIS:O	0.47	2.68	20	1
2:B:8:NAG:C4	2:B:9:GAL:O2	0.47	2.58	21	2
1:A:13:GLN:NE2	1:A:29:MET:HG2	0.47	2.24	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:5:NAG:C6	2:B:6:GAL:O5	0.47	2.62	8	1
1:A:13:GLN:OE1	1:A:29:MET:SD	0.47	2.73	13	2
1:A:61:VAL:HG23	1:A:83:HIS:CD2	0.47	2.45	20	1
1:A:20:GLN:HB3	1:A:21:PRO:HD2	0.47	1.86	10	3
1:A:12:LEU:HG	1:A:28:CYS:SG	0.47	2.49	16	2
1:A:13:GLN:HG3	1:A:29:MET:O	0.47	2.09	15	1
2:B:5:NAG:C5	2:B:6:GAL:O5	0.47	2.61	19	1
1:A:19:SER:CB	1:A:24:PRO:HA	0.47	2.39	9	2
1:A:68:VAL:O	1:A:68:VAL:CG1	0.47	2.56	12	1
1:A:15:ASN:ND2	1:A:17:PHE:CD2	0.47	2.82	26	1
1:A:15:ASN:O	1:A:19:SER:CB	0.47	2.63	4	1
1:A:15:ASN:CB	1:A:25:ILE:CB	0.47	2.93	18	6
1:A:77:GLU:HB2	1:A:79:HIS:CD2	0.47	2.44	8	3
1:A:14:GLU:HG2	1:A:24:PRO:CG	0.47	2.40	9	1
1:A:77:GLU:CD	1:A:79:HIS:NE2	0.47	2.73	16	1
1:A:25:ILE:HG22	1:A:76:VAL:HG11	0.47	1.83	19	7
1:A:15:ASN:C	1:A:17:PHE:N	0.47	2.73	19	3
1:A:28:CYS:SG	1:A:79:HIS:CB	0.47	2.98	18	1
1:A:18:PHE:CE2	1:A:68:VAL:O	0.47	2.68	13	3
1:A:28:CYS:N	1:A:79:HIS:ND1	0.47	2.62	19	6
1:A:25:ILE:HD11	1:A:68:VAL:CB	0.47	2.40	12	1
1:A:20:GLN:HB2	1:A:21:PRO:CD	0.46	2.39	3	2
1:A:65:TYR:HB2	1:A:77:GLU:CA	0.46	2.40	12	7
1:A:79:HIS:N	1:A:79:HIS:CD2	0.46	2.82	10	8
1:A:27:GLN:O	1:A:27:GLN:HG3	0.46	2.10	17	5
1:A:17:PHE:CD2	1:A:70:VAL:HG21	0.46	2.45	4	1
1:A:15:ASN:OD1	1:A:17:PHE:HB3	0.46	2.11	5	7
1:A:14:GLU:CA	1:A:25:ILE:O	0.46	2.60	9	2
1:A:21:PRO:HA	2:B:9:GAL:O2	0.46	2.09	9	1
1:A:77:GLU:HG3	1:A:79:HIS:HE2	0.46	1.69	21	1
2:B:8:NAG:H62	2:B:9:GAL:O5	0.46	2.10	13	1
1:A:63:LYS:HD3	1:A:83:HIS:CB	0.46	2.39	23	1
1:A:70:VAL:HG22	1:A:74:PHE:HB3	0.46	1.87	25	1
1:A:64:SER:O	1:A:80:THR:HG23	0.46	2.11	1	2
1:A:14:GLU:CG	1:A:24:PRO:HB2	0.46	2.40	23	8
1:A:68:VAL:CG1	1:A:78:ASN:HB2	0.46	2.39	15	3
1:A:26:LEU:HD11	1:A:78:ASN:CG	0.46	2.36	18	1
1:A:66:ASN:N	1:A:78:ASN:O	0.46	2.48	21	4
1:A:20:GLN:HG3	1:A:21:PRO:CD	0.46	2.41	4	1
1:A:18:PHE:O	1:A:19:SER:C	0.46	2.59	8	2
1:A:12:LEU:HD12	1:A:28:CYS:HA	0.46	1.87	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:ARG:CB	1:A:77:GLU:HA	0.46	2.40	2	15
1:A:17:PHE:C	1:A:17:PHE:CD1	0.46	2.94	1	3
1:A:71:MET:C	1:A:73:GLY:N	0.46	2.73	6	7
1:A:20:GLN:O	1:A:23:ALA:N	0.46	2.41	6	2
1:A:13:GLN:NE2	1:A:29:MET:CB	0.46	2.78	26	1
1:A:64:SER:O	1:A:80:THR:CB	0.45	2.65	20	2
1:A:70:VAL:HG12	1:A:71:MET:H	0.45	1.71	5	4
1:A:11:THR:CG2	1:A:29:MET:HE3	0.45	2.41	23	1
2:B:3:BMA:H2	2:B:4:MAN:O5	0.45	2.11	19	2
1:A:65:TYR:CB	1:A:77:GLU:HB3	0.45	2.41	18	1
1:A:26:LEU:HD12	1:A:79:HIS:CA	0.45	2.38	2	2
1:A:71:MET:HB2	1:A:74:PHE:CE1	0.45	2.47	13	3
1:A:76:VAL:HG23	1:A:78:ASN:N	0.45	2.27	15	9
1:A:75:LYS:N	1:A:75:LYS:HD3	0.45	2.26	8	1
1:A:25:ILE:HD12	1:A:68:VAL:CB	0.45	2.40	12	1
1:A:13:GLN:NE2	1:A:29:MET:O	0.45	2.49	16	1
1:A:15:ASN:OD1	1:A:18:PHE:N	0.45	2.42	26	1
1:A:66:ASN:N	1:A:78:ASN:HB3	0.45	2.25	18	4
1:A:69:THR:OG1	1:A:75:LYS:HD2	0.45	2.12	24	2
1:A:29:MET:SD	1:A:29:MET:C	0.45	3.00	13	1
1:A:28:CYS:SG	1:A:79:HIS:ND1	0.45	2.89	22	1
1:A:16:PRO:CD	1:A:17:PHE:CE1	0.45	2.98	26	1
1:A:67:ARG:HA	1:A:77:GLU:HA	0.45	1.89	10	3
2:B:1:NAG:C6	2:B:2:NAG:C1	0.45	2.95	17	4
1:A:11:THR:CA	1:A:28:CYS:SG	0.45	3.05	3	2
1:A:71:MET:O	1:A:73:GLY:N	0.45	2.50	25	3
1:A:15:ASN:OD1	1:A:18:PHE:CD1	0.45	2.70	11	1
1:A:25:ILE:HD12	1:A:68:VAL:HB	0.45	1.89	12	1
1:A:12:LEU:HD21	1:A:79:HIS:HB2	0.45	1.86	14	1
2:B:5:NAG:H61	2:B:6:GAL:O2	0.45	2.12	21	1
1:A:11:THR:O	1:A:28:CYS:C	0.45	2.60	22	1
1:A:11:THR:O	1:A:28:CYS:HB3	0.45	2.11	11	2
1:A:71:MET:HG3	1:A:74:PHE:CD1	0.44	2.46	3	1
1:A:15:ASN:HB2	1:A:26:LEU:N	0.44	2.27	26	2
1:A:18:PHE:HD2	1:A:25:ILE:CG2	0.44	2.24	7	5
2:B:3:BMA:C2	2:B:4:MAN:H5	0.44	2.43	12	1
1:A:66:ASN:HB3	1:A:78:ASN:CG	0.44	2.38	21	2
1:A:26:LEU:O	1:A:76:VAL:HG12	0.44	2.12	1	2
1:A:65:TYR:HB2	1:A:77:GLU:CB	0.44	2.42	23	5
1:A:71:MET:SD	1:A:74:PHE:CE1	0.44	3.10	10	1
1:A:14:GLU:O	1:A:16:PRO:CD	0.44	2.65	11	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:THR:HG23	1:A:29:MET:CE	0.44	2.42	23	1
2:B:3:BMA:O4	2:B:4:MAN:H3	0.44	2.13	20	1
1:A:74:PHE:C	1:A:75:LYS:CG	0.44	2.90	23	1
1:A:13:GLN:HG3	1:A:29:MET:HB3	0.44	1.88	9	2
1:A:61:VAL:O	1:A:83:HIS:NE2	0.44	2.51	20	3
1:A:15:ASN:N	1:A:26:LEU:HA	0.44	2.27	26	1
1:A:18:PHE:CG	1:A:25:ILE:HG12	0.44	2.47	15	1
1:A:14:GLU:CD	1:A:19:SER:OG	0.44	2.60	19	1
2:B:2:NAG:O6	2:B:3:BMA:C1	0.43	2.65	4	1
1:A:69:THR:HG23	1:A:74:PHE:O	0.43	2.13	10	1
2:B:3:BMA:C4	2:B:7:MAN:C1	0.43	2.95	16	1
1:A:15:ASN:CG	1:A:18:PHE:H	0.43	2.21	26	1
1:A:74:PHE:C	1:A:75:LYS:HG3	0.43	2.37	23	1
2:B:3:BMA:C5	2:B:7:MAN:H5	0.43	2.43	12	1
1:A:15:ASN:O	1:A:19:SER:HB2	0.43	2.13	9	2
1:A:67:ARG:CG	1:A:77:GLU:OE1	0.43	2.67	10	1
1:A:17:PHE:CB	1:A:71:MET:HE2	0.43	2.43	15	1
1:A:20:GLN:CD	1:A:23:ALA:HB3	0.43	2.39	19	1
1:A:17:PHE:CD1	1:A:17:PHE:C	0.43	2.97	20	1
1:A:13:GLN:NE2	1:A:29:MET:CG	0.43	2.81	26	1
1:A:16:PRO:HG2	1:A:17:PHE:CE1	0.43	2.48	26	1
1:A:66:ASN:HB3	1:A:78:ASN:O	0.43	2.14	1	1
2:B:5:NAG:O3	2:B:6:GAL:H2	0.43	2.14	3	1
1:A:20:GLN:HG3	1:A:21:PRO:N	0.43	2.29	4	1
1:A:68:VAL:HG23	1:A:70:VAL:CG2	0.43	2.44	19	1
1:A:17:PHE:HD2	1:A:70:VAL:HG21	0.43	1.73	4	1
1:A:63:LYS:HB3	1:A:81:ALA:HB1	0.43	1.89	17	2
1:A:71:MET:SD	1:A:71:MET:N	0.43	2.92	11	1
1:A:65:TYR:HB2	1:A:77:GLU:HG3	0.42	1.91	25	1
1:A:70:VAL:HG23	1:A:74:PHE:HB3	0.42	1.92	2	1
1:A:14:GLU:HA	1:A:26:LEU:HD23	0.42	1.90	9	1
1:A:64:SER:N	1:A:81:ALA:HB3	0.42	2.29	10	2
1:A:66:ASN:O	1:A:68:VAL:HG12	0.42	2.14	10	1
1:A:66:ASN:OD1	1:A:78:ASN:ND2	0.42	2.51	13	1
1:A:63:LYS:HG2	1:A:82:CYS:C	0.42	2.39	20	1
1:A:27:GLN:NE2	1:A:28:CYS:O	0.42	2.53	13	1
1:A:15:ASN:CG	1:A:17:PHE:CD2	0.42	2.97	26	1
1:A:18:PHE:CB	1:A:70:VAL:HG21	0.42	2.41	7	1
2:B:4:MAN:O3	2:B:8:NAG:H5	0.42	2.14	26	1
1:A:18:PHE:CZ	1:A:74:PHE:CB	0.42	3.02	12	1
1:A:68:VAL:HG12	1:A:70:VAL:HG22	0.42	1.89	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ASN:HD22	1:A:18:PHE:HB2	0.42	1.75	4	1
1:A:65:TYR:HA	1:A:77:GLU:O	0.42	2.15	11	1
1:A:67:ARG:HG3	1:A:77:GLU:CA	0.42	2.44	19	1
1:A:17:PHE:HE1	1:A:71:MET:HE1	0.42	1.75	3	1
1:A:18:PHE:HD1	1:A:70:VAL:HG11	0.42	1.70	3	2
1:A:20:GLN:O	1:A:21:PRO:C	0.42	2.62	6	2
1:A:18:PHE:HE2	1:A:76:VAL:CG1	0.42	2.26	7	1
1:A:61:VAL:CG1	1:A:83:HIS:CE1	0.42	3.02	25	1
1:A:27:GLN:O	1:A:27:GLN:OE1	0.42	2.37	1	1
1:A:28:CYS:O	1:A:29:MET:O	0.42	2.38	19	1
1:A:66:ASN:HB2	1:A:80:THR:HG22	0.41	1.90	11	1
1:A:18:PHE:CE2	1:A:70:VAL:HG23	0.41	2.49	14	2
1:A:68:VAL:O	1:A:70:VAL:HG23	0.41	2.15	12	1
1:A:12:LEU:HD22	1:A:26:LEU:HD22	0.41	1.90	19	1
1:A:73:GLY:O	1:A:75:LYS:HD2	0.41	2.15	21	1
1:A:13:GLN:HG2	1:A:29:MET:CA	0.41	2.46	23	1
1:A:71:MET:O	1:A:72:GLY:C	0.41	2.62	6	1
1:A:18:PHE:HB2	1:A:25:ILE:CB	0.41	2.45	12	2
1:A:15:ASN:ND2	1:A:70:VAL:HG21	0.41	2.30	15	1
1:A:63:LYS:HD3	1:A:83:HIS:N	0.41	2.29	23	1
1:A:67:ARG:NH1	1:A:77:GLU:OE2	0.41	2.54	25	1
1:A:13:GLN:O	1:A:13:GLN:HG3	0.41	2.14	26	1
1:A:17:PHE:CD2	1:A:71:MET:HE3	0.41	2.50	1	1
1:A:13:GLN:OE1	1:A:29:MET:HG2	0.41	2.15	3	1
1:A:18:PHE:CG	1:A:70:VAL:CG2	0.41	2.80	7	1
1:A:28:CYS:H	1:A:79:HIS:HD1	0.41	1.56	7	2
1:A:20:GLN:CD	1:A:21:PRO:HD2	0.41	2.41	9	1
1:A:18:PHE:O	1:A:20:GLN:HG2	0.41	2.13	18	2
1:A:15:ASN:HD22	1:A:70:VAL:HG11	0.41	1.71	20	1
1:A:69:THR:HG23	1:A:73:GLY:HA2	0.41	1.92	7	1
1:A:62:ALA:HA	1:A:82:CYS:HA	0.41	1.91	16	3
1:A:65:TYR:C	1:A:80:THR:HG23	0.41	2.41	16	1
1:A:64:SER:C	1:A:80:THR:HG1	0.41	2.24	18	1
1:A:14:GLU:CG	1:A:24:PRO:O	0.41	2.68	21	1
2:B:5:NAG:C4	2:B:6:GAL:O2	0.41	2.69	21	1
1:A:17:PHE:CZ	1:A:71:MET:CG	0.41	3.03	25	1
1:A:18:PHE:HD2	1:A:25:ILE:CG1	0.41	2.27	25	1
1:A:18:PHE:O	1:A:18:PHE:CD1	0.41	2.73	26	1
2:B:3:BMA:H2	2:B:4:MAN:H5	0.41	1.92	12	1
1:A:13:GLN:CD	1:A:29:MET:HG2	0.41	2.41	20	1
1:A:63:LYS:NZ	1:A:81:ALA:HB1	0.41	2.31	25	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:1:NAG:H61	2:B:2:NAG:N2	0.41	2.31	23	1
1:A:66:ASN:HB3	1:A:78:ASN:ND2	0.41	2.27	25	1
1:A:20:GLN:OE1	1:A:21:PRO:CD	0.40	2.70	8	1
1:A:66:ASN:HB2	1:A:78:ASN:CG	0.40	2.40	21	1
1:A:73:GLY:C	1:A:74:PHE:O	0.40	2.62	6	1
2:B:8:NAG:C3	2:B:9:GAL:H2	0.40	2.39	1	1
1:A:26:LEU:CG	1:A:78:ASN:OD1	0.40	2.67	13	1
1:A:20:GLN:HB2	1:A:21:PRO:HD2	0.40	1.93	16	1
1:A:61:VAL:O	1:A:61:VAL:HG22	0.40	2.16	2	1
1:A:71:MET:HE3	1:A:71:MET:HA	0.40	1.93	11	1
1:A:17:PHE:CD2	1:A:18:PHE:HE1	0.40	2.34	12	1
1:A:18:PHE:HD2	1:A:70:VAL:CG1	0.40	2.28	13	1
1:A:14:GLU:HG2	1:A:25:ILE:O	0.40	2.16	23	1
1:A:83:HIS:H	1:A:83:HIS:CD2	0.40	2.34	25	1
1:A:26:LEU:CD1	1:A:79:HIS:C	0.40	2.95	2	1
2:B:1:NAG:O4	2:B:2:NAG:C7	0.40	2.69	4	1
1:A:63:LYS:HB3	1:A:81:ALA:HB3	0.40	1.92	5	1
2:B:8:NAG:C5	2:B:9:GAL:C2	0.40	2.93	6	1
1:A:13:GLN:CG	1:A:29:MET:CB	0.40	3.00	7	1
1:A:66:ASN:HB2	1:A:78:ASN:O	0.40	2.17	9	1
1:A:12:LEU:HD23	1:A:26:LEU:HD22	0.40	1.94	19	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	42/92 (46%)	16±2 (38±4%)	13±2 (30±5%)	13±1 (31±3%)	0	1
All	All	1092/2392 (46%)	420 (38%)	329 (30%)	343 (31%)	0	1

All 21 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	14	GLU	26

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Mol	Chain	Res	Type	Models (Total)
1	A	25	ILE	26
1	A	27	GLN	26
1	A	62	ALA	26
1	A	67	ARG	26
1	A	77	GLU	26
1	A	78	ASN	26
1	A	24	PRO	24
1	A	28	CYS	24
1	A	69	THR	22
1	A	19	SER	19
1	A	21	PRO	18
1	A	71	MET	16
1	A	61	VAL	10
1	A	74	PHE	8
1	A	11	THR	7
1	A	79	HIS	5
1	A	29	MET	4
1	A	83	HIS	2
1	A	73	GLY	1
1	A	72	GLY	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	36/83 (43%)	24±2 (67±6%)	12±2 (33±6%)	1	12
All	All	936/2158 (43%)	627 (67%)	309 (33%)	1	12

All 28 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	26	LEU	26
1	A	77	GLU	26
1	A	70	VAL	22
1	A	66	ASN	22
1	A	67	ARG	19

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Mol	Chain	Res	Type	Models (Total)
1	A	75	LYS	16
1	A	71	MET	14
1	A	15	ASN	14
1	A	29	MET	14
1	A	19	SER	13
1	A	20	GLN	13
1	A	11	THR	13
1	A	82	CYS	12
1	A	27	GLN	10
1	A	65	TYR	10
1	A	68	VAL	10
1	A	28	CYS	9
1	A	18	PHE	7
1	A	63	LYS	7
1	A	12	LEU	7
1	A	61	VAL	6
1	A	80	THR	4
1	A	14	GLU	4
1	A	13	GLN	3
1	A	17	PHE	3
1	A	64	SER	3
1	A	74	PHE	1
1	A	83	HIS	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	2,1	14,14,15	0.38±0.02	0±0 (0±0%)
2	NAG	B	2	2	14,14,15	0.39±0.04	0±0 (0±0%)
2	BMA	B	3	2	11,11,12	0.34±0.04	0±0 (0±0%)
2	MAN	B	4	2	11,11,12	0.28±0.02	0±0 (0±0%)
2	NAG	B	5	2	14,14,15	0.45±0.03	0±0 (0±0%)
2	GAL	B	6	2	11,11,12	0.25±0.02	0±0 (0±0%)
2	MAN	B	7	2	11,11,12	0.26±0.04	0±0 (0±0%)
2	NAG	B	8	2	14,14,15	0.46±0.03	0±0 (0±0%)
2	GAL	B	9	2	11,11,12	0.24±0.02	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	2,1	17,19,21	0.71±0.04	0±0 (2±2%)
2	NAG	B	2	2	17,19,21	0.71±0.08	0±0 (2±2%)
2	BMA	B	3	2	15,15,17	0.39±0.04	0±0 (0±0%)
2	MAN	B	4	2	15,15,17	0.56±0.04	0±0 (0±0%)
2	NAG	B	5	2	17,19,21	0.70±0.04	1±0 (3±2%)
2	GAL	B	6	2	15,15,17	0.36±0.02	0±0 (0±0%)
2	MAN	B	7	2	15,15,17	0.65±0.17	0±0 (1±2%)
2	NAG	B	8	2	17,19,21	0.78±0.05	1±0 (4±2%)
2	GAL	B	9	2	15,15,17	0.36±0.02	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	2,1	-	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

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

There are no bond-length outliers.

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
2	B	7	MAN	C1-O5-C5	3.99	117.54	112.19	12	4
2	B	8	NAG	C2-N2-C7	3.00	118.88	122.90	16	19
2	B	2	NAG	C2-N2-C7	2.82	119.13	122.90	25	9
2	B	5	NAG	C2-N2-C7	2.43	119.64	122.90	23	15
2	B	1	NAG	C2-N2-C7	2.30	119.82	122.90	14	13

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

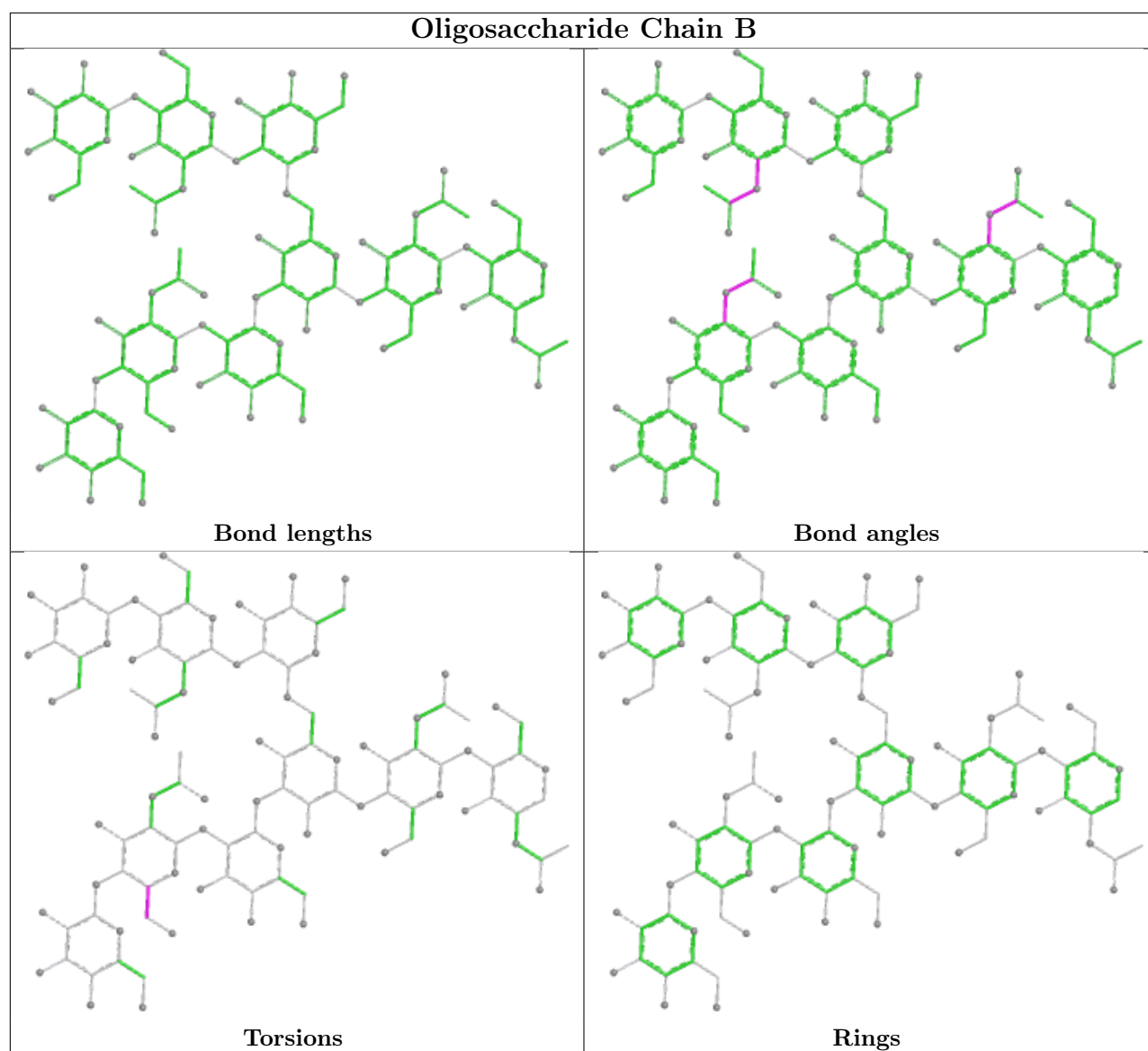
Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	2	NAG	C1	1
2	B	5	NAG	C1	1

All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	5	NAG	C1-C2-N2-C7	1

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