



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 12:44 PM UTC

PDB ID : 2LS6 / pdb_00002ls6
BMRB ID : 17694
Title : Solution NMR Structure of a Non-canonical galactose-binding CBM32 from *Clostridium perfringens*
Authors : Grondin, J.M.; Chitayat, S.; Ficko-Blean, E.; Boraston, A.B.; Smith, S.P.
Deposited on : 2012-04-20

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
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

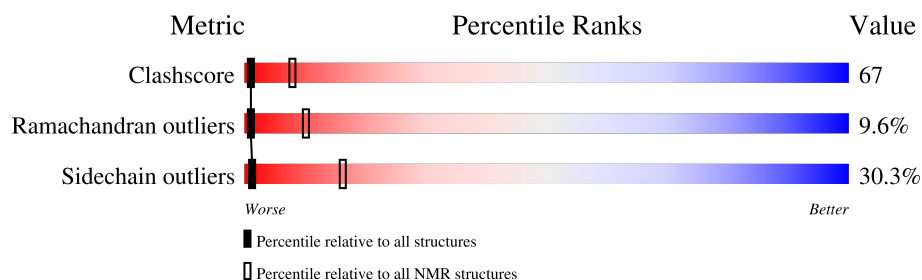
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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	164	18% 48% 14% 20%

2 Ensemble composition and analysis

This entry contains 21 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:28-A:159 (132)	0.69	7

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 3, 4, 5, 7, 8, 11, 13, 14, 15, 17, 18, 19, 20, 21
2	1, 12, 16
3	6, 9, 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2540 atoms, of which 1251 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hyaluronoglucosaminidase.

Mol	Chain	Residues	Atoms						Trace
1	A	164	Total	C	H	N	O	S	0
			2540	793	1251	236	255	5	

There are 23 discrepancies between the modelled and reference sequences:

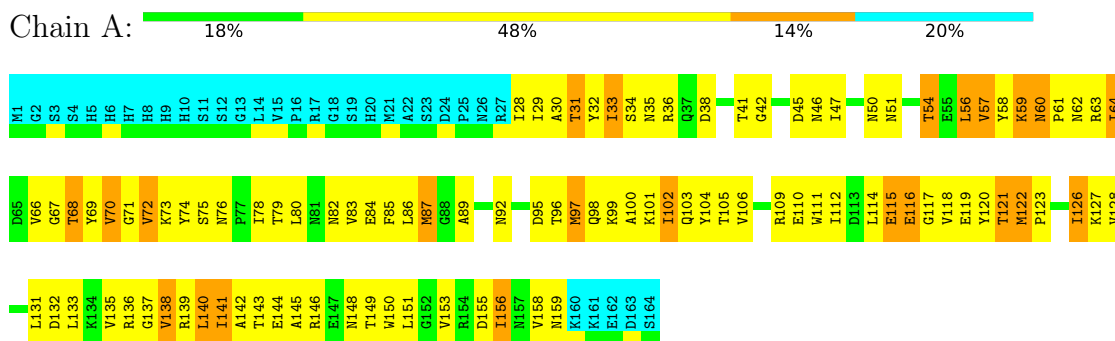
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q0TUP2
A	2	GLY	-	expression tag	UNP Q0TUP2
A	3	SER	-	expression tag	UNP Q0TUP2
A	4	SER	-	expression tag	UNP Q0TUP2
A	5	HIS	-	expression tag	UNP Q0TUP2
A	6	HIS	-	expression tag	UNP Q0TUP2
A	7	HIS	-	expression tag	UNP Q0TUP2
A	8	HIS	-	expression tag	UNP Q0TUP2
A	9	HIS	-	expression tag	UNP Q0TUP2
A	10	HIS	-	expression tag	UNP Q0TUP2
A	11	SER	-	expression tag	UNP Q0TUP2
A	12	SER	-	expression tag	UNP Q0TUP2
A	13	GLY	-	expression tag	UNP Q0TUP2
A	14	LEU	-	expression tag	UNP Q0TUP2
A	15	VAL	-	expression tag	UNP Q0TUP2
A	16	PRO	-	expression tag	UNP Q0TUP2
A	17	ARG	-	expression tag	UNP Q0TUP2
A	18	GLY	-	expression tag	UNP Q0TUP2
A	19	SER	-	expression tag	UNP Q0TUP2
A	20	HIS	-	expression tag	UNP Q0TUP2
A	21	MET	-	expression tag	UNP Q0TUP2
A	22	ALA	-	expression tag	UNP Q0TUP2
A	23	SER	-	expression tag	UNP Q0TUP2

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: Hyaluronoglucosaminidase

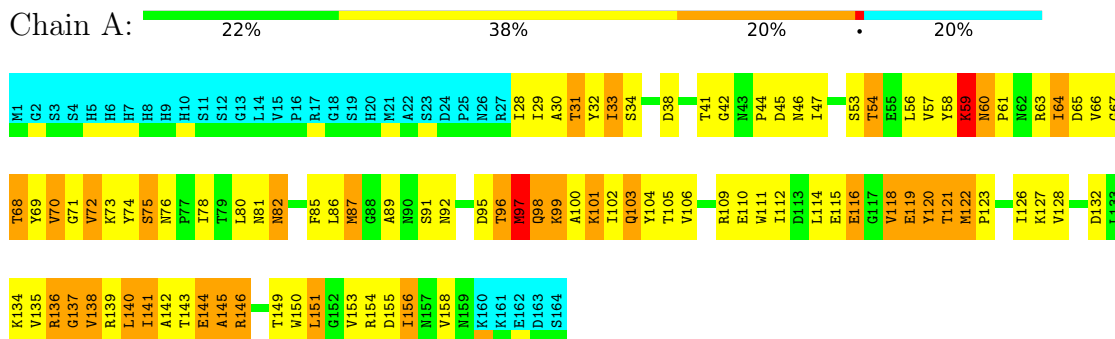


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

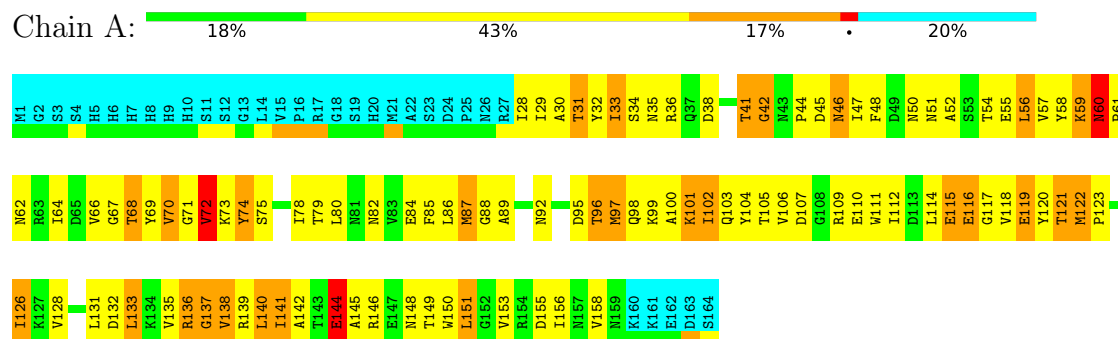
4.2.1 Score per residue for model 1

- Molecule 1: Hyaluronoglucosaminidase



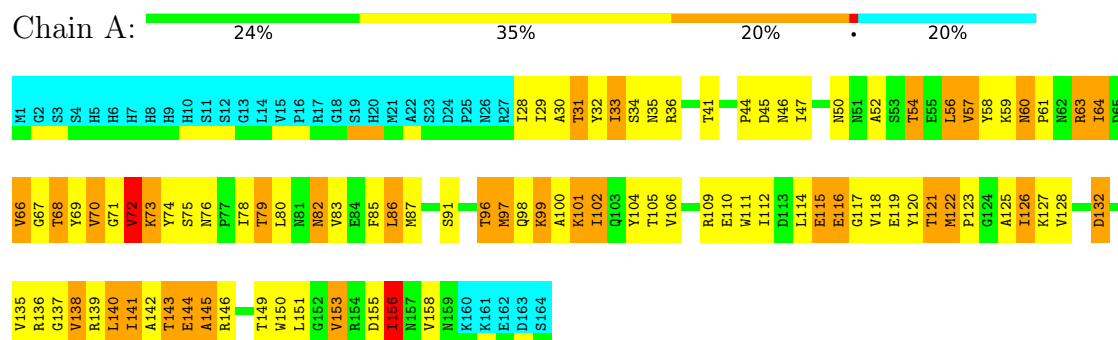
4.2.5 Score per residue for model 5

- Molecule 1: Hyaluronoglucosaminidase



4.2.6 Score per residue for model 6

- Molecule 1: Hyaluronoglucosaminidase



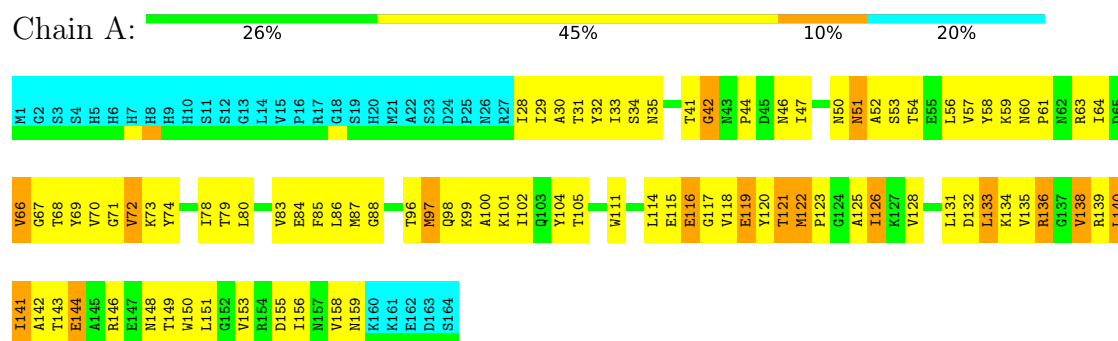
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Hyaluronoglucosaminidase



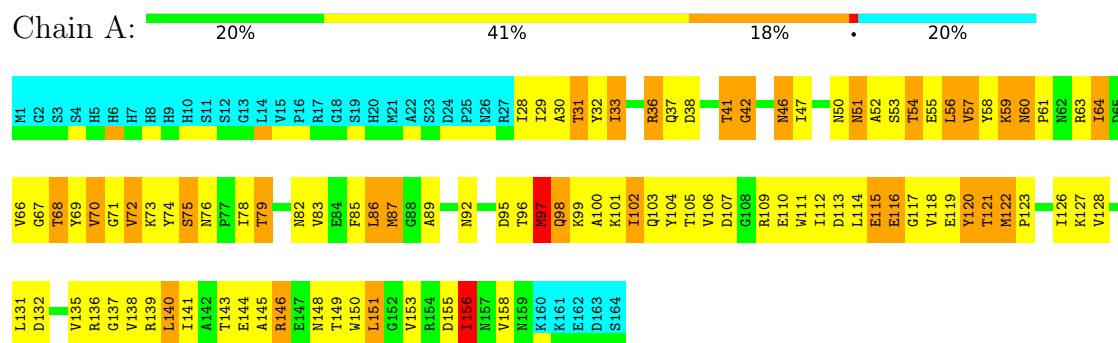
4.2.8 Score per residue for model 8

- Molecule 1: Hyaluronoglucosaminidase



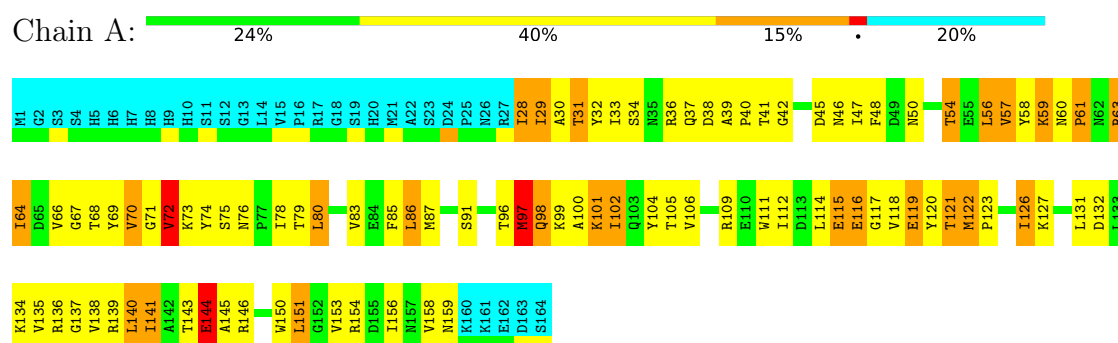
4.2.9 Score per residue for model 9

- Molecule 1: Hyaluronoglucosaminidase



4.2.10 Score per residue for model 10

- Molecule 1: Hyaluronoglucosaminidase



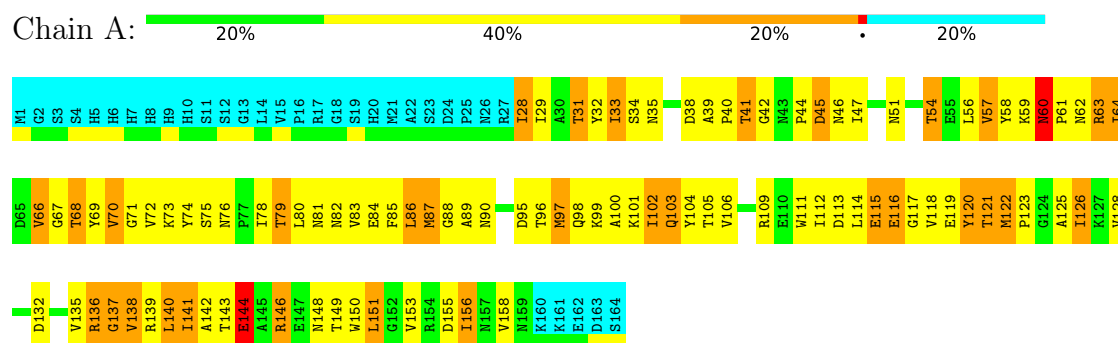
4.2.11 Score per residue for model 11

- Molecule 1: Hyaluronoglucosaminidase



4.2.12 Score per residue for model 12

- Molecule 1: Hyaluronoglucosaminidase



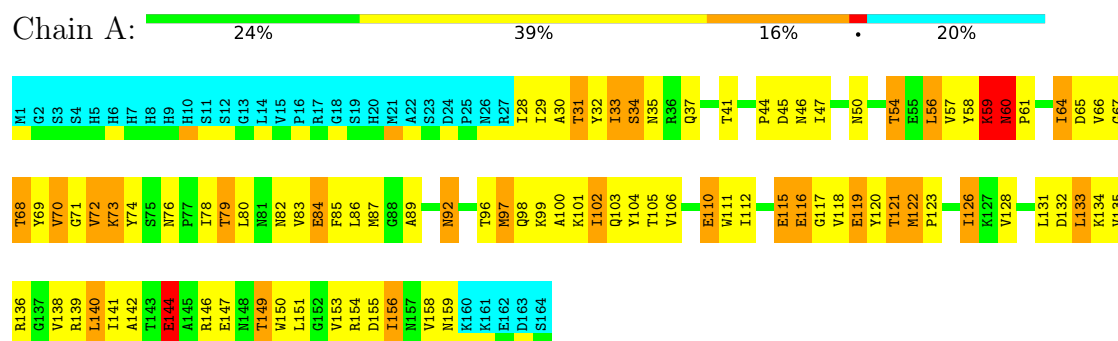
4.2.13 Score per residue for model 13

- Molecule 1: Hyaluronoglucosaminidase



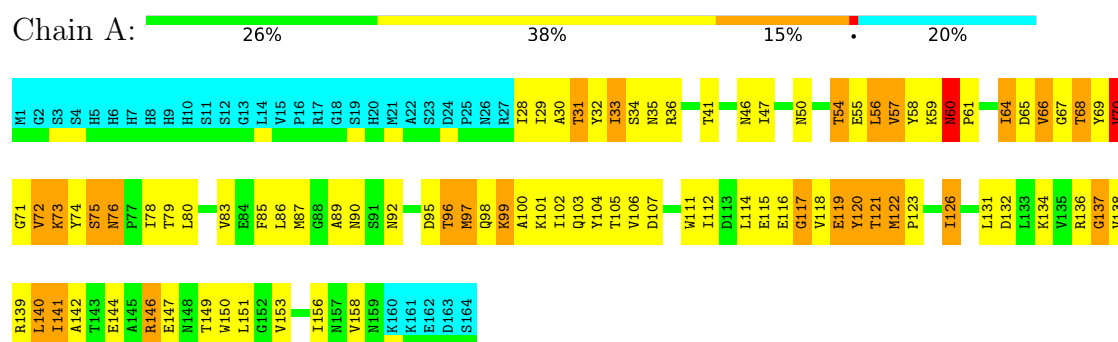
4.2.14 Score per residue for model 14

- Molecule 1: Hyaluronoglucosaminidase



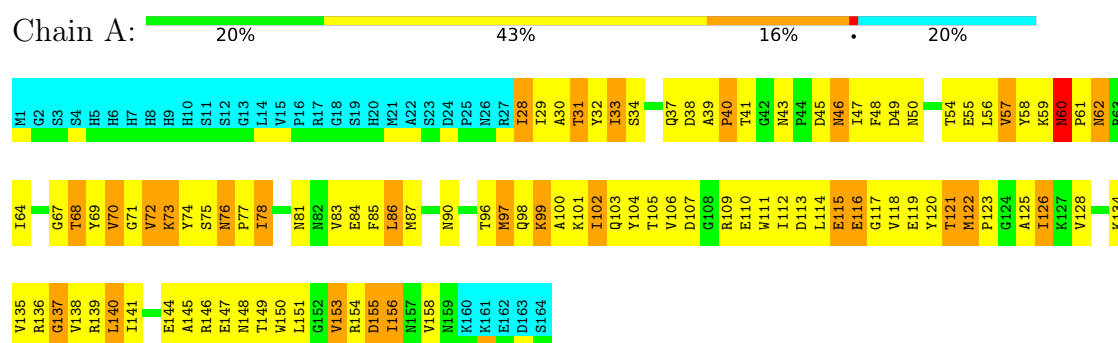
4.2.15 Score per residue for model 15

- Molecule 1: Hyaluronoglucosaminidase



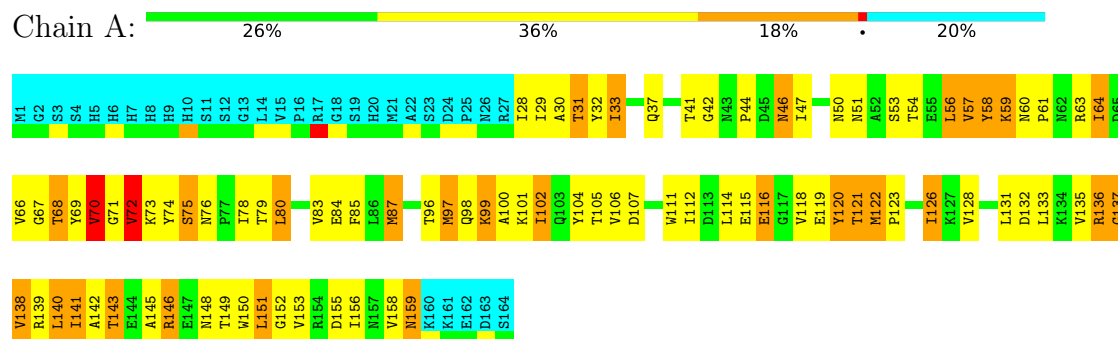
4.2.16 Score per residue for model 16

- Molecule 1: Hyaluronoglucosaminidase



4.2.17 Score per residue for model 17

- Molecule 1: Hyaluronoglucosaminidase



4.2.18 Score per residue for model 18

- Molecule 1: Hyaluronoglucosaminidase



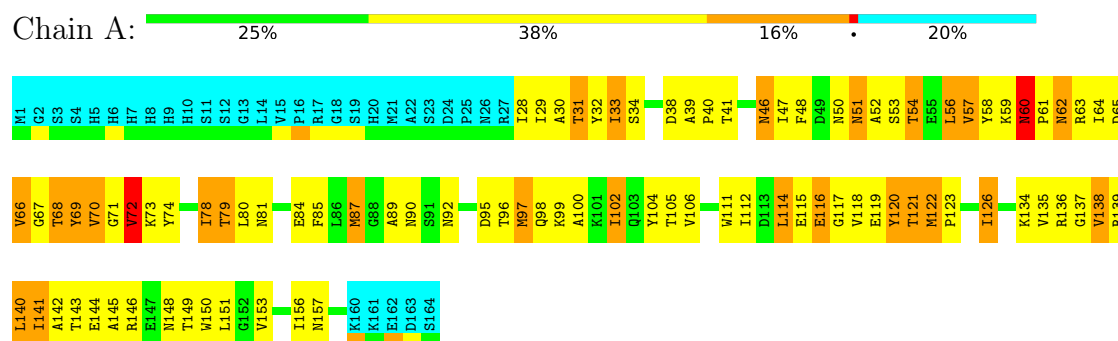
4.2.19 Score per residue for model 19

- Molecule 1: Hyaluronoglucosaminidase



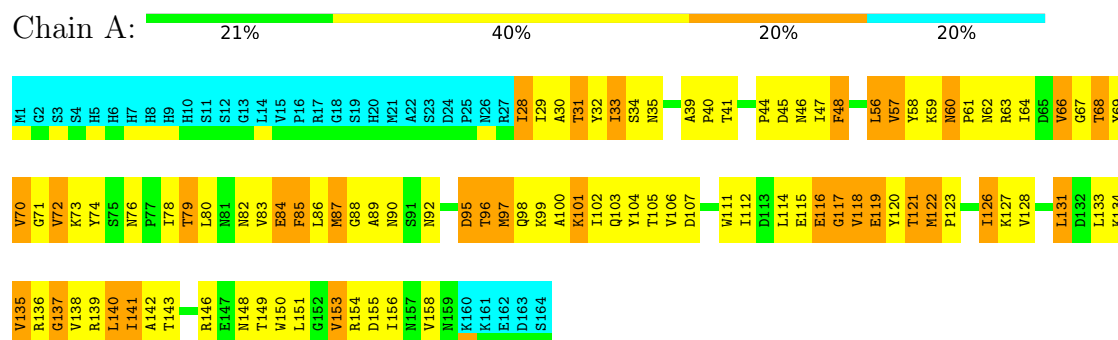
4.2.20 Score per residue for model 20

- Molecule 1: Hyaluronoglucosaminidase



4.2.21 Score per residue for model 21

- Molecule 1: Hyaluronoglucosaminidase



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 21 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1735
Number of shifts mapped to atoms	1735
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1041	1020	1020	139±12
All	All	21861	21420	21420	2912

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 67.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:MET:HE3	1:A:140:LEU:HD22	0.92	1.40	12	16
1:A:83:VAL:HG23	1:A:158:VAL:HG12	0.90	1.44	12	4
1:A:59:LYS:HB3	1:A:150:TRP:CG	0.89	2.01	4	9
1:A:85:PHE:CE1	1:A:102:ILE:HD13	0.86	2.04	15	2
1:A:46:ASN:ND2	1:A:54:THR:HG23	0.85	1.85	7	16
1:A:59:LYS:HG3	1:A:150:TRP:CE2	0.84	2.07	18	8
1:A:64:ILE:HD12	1:A:145:ALA:HB1	0.84	1.48	19	2
1:A:120:TYR:CZ	1:A:126:ILE:CG2	0.83	2.61	20	3
1:A:100:ALA:HB1	1:A:141:ILE:O	0.82	1.73	13	21
1:A:28:ILE:CG2	1:A:78:ILE:HD13	0.82	2.05	15	3
1:A:114:LEU:CD2	1:A:128:VAL:HG21	0.82	2.03	2	5
1:A:28:ILE:HG13	1:A:78:ILE:HG21	0.81	1.52	1	3
1:A:116:GLU:O	1:A:118:VAL:N	0.81	2.13	21	21
1:A:121:THR:O	1:A:122:MET:HE3	0.81	1.76	13	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:ILE:CD1	1:A:145:ALA:HB1	0.81	2.04	16	4
1:A:120:TYR:CE1	1:A:126:ILE:HG23	0.81	2.11	2	19
1:A:72:VAL:HG13	1:A:138:VAL:CG2	0.80	2.06	13	21
1:A:72:VAL:HG12	1:A:156:ILE:HD11	0.80	1.51	19	4
1:A:47:ILE:CG1	1:A:156:ILE:HG23	0.79	2.08	14	2
1:A:46:ASN:CG	1:A:54:THR:HG23	0.79	2.03	18	15
1:A:32:TYR:OH	1:A:153:VAL:HG11	0.79	1.78	3	2
1:A:118:VAL:HG11	1:A:120:TYR:CE1	0.78	2.13	10	20
1:A:32:TYR:OH	1:A:70:VAL:HG21	0.78	1.77	6	21
1:A:115:GLU:CD	1:A:128:VAL:HG22	0.78	2.03	19	4
1:A:96:THR:HG23	1:A:121:THR:O	0.78	1.79	12	15
1:A:102:ILE:HG13	1:A:120:TYR:CE2	0.77	2.14	21	18
1:A:83:VAL:HG11	1:A:114:LEU:HD11	0.77	1.55	8	7
1:A:115:GLU:OE1	1:A:128:VAL:HG22	0.76	1.80	6	5
1:A:32:TYR:OH	1:A:153:VAL:HG21	0.75	1.81	8	13
1:A:87:MET:SD	1:A:151:LEU:HD11	0.75	2.22	2	6
1:A:44:PRO:CB	1:A:47:ILE:HD11	0.75	2.12	11	1
1:A:140:LEU:O	1:A:141:ILE:HD12	0.74	1.81	12	1
1:A:72:VAL:CG1	1:A:156:ILE:HD11	0.74	2.11	19	5
1:A:114:LEU:HD21	1:A:128:VAL:HG11	0.74	1.59	19	4
1:A:28:ILE:HD13	1:A:78:ILE:HG22	0.74	1.60	8	11
1:A:96:THR:HG21	1:A:123:PRO:HD2	0.74	1.60	13	6
1:A:28:ILE:HG21	1:A:78:ILE:HD13	0.74	1.60	11	3
1:A:47:ILE:HG23	1:A:156:ILE:HD13	0.74	1.57	6	2
1:A:68:THR:O	1:A:142:ALA:HB2	0.73	1.84	3	15
1:A:114:LEU:HD22	1:A:128:VAL:HG21	0.73	1.57	21	4
1:A:33:ILE:HD11	1:A:138:VAL:O	0.73	1.84	21	10
1:A:29:ILE:HG22	1:A:75:SER:HB2	0.72	1.60	17	8
1:A:97:MET:CE	1:A:140:LEU:HD22	0.72	2.14	15	11
1:A:64:ILE:HD12	1:A:68:THR:HB	0.72	1.61	1	1
1:A:102:ILE:HG13	1:A:120:TYR:CD2	0.72	2.18	21	2
1:A:102:ILE:HB	1:A:120:TYR:CE2	0.72	2.19	20	1
1:A:85:PHE:CE1	1:A:102:ILE:HG21	0.72	2.20	13	12
1:A:80:LEU:CD2	1:A:131:LEU:HD23	0.72	2.14	11	4
1:A:56:LEU:HD13	1:A:153:VAL:CG2	0.71	2.15	3	2
1:A:52:ALA:HB2	1:A:155:ASP:CG	0.71	2.09	6	1
1:A:28:ILE:HD11	1:A:75:SER:HB3	0.71	1.60	9	1
1:A:80:LEU:HD12	1:A:158:VAL:HG23	0.71	1.59	11	2
1:A:115:GLU:OE2	1:A:128:VAL:HG13	0.71	1.85	13	4
1:A:64:ILE:HD13	1:A:65:ASP:N	0.71	1.99	1	1
1:A:83:VAL:HG21	1:A:138:VAL:HG11	0.71	1.62	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:146:ARG:HG3	1:A:149:THR:HG21	0.70	1.63	6	9
1:A:59:LYS:HG3	1:A:150:TRP:CZ2	0.70	2.21	5	1
1:A:70:VAL:HG23	1:A:71:GLY:N	0.70	2.01	3	20
1:A:120:TYR:C	1:A:123:PRO:HD3	0.70	2.11	1	21
1:A:28:ILE:HB	1:A:78:ILE:HG21	0.70	1.62	12	12
1:A:28:ILE:CB	1:A:78:ILE:HG21	0.70	2.16	9	6
1:A:102:ILE:HG23	1:A:140:LEU:HG	0.70	1.62	12	10
1:A:30:ALA:HB1	1:A:72:VAL:CG2	0.70	2.16	1	14
1:A:104:TYR:HB3	1:A:114:LEU:HD12	0.70	1.63	20	16
1:A:101:LYS:O	1:A:140:LEU:HD23	0.70	1.86	11	10
1:A:56:LEU:C	1:A:56:LEU:HD22	0.70	2.12	9	7
1:A:69:TYR:CE2	1:A:141:ILE:HD13	0.70	2.22	6	3
1:A:29:ILE:HD13	1:A:30:ALA:N	0.70	2.02	10	1
1:A:64:ILE:HG21	1:A:68:THR:OG1	0.70	1.86	1	2
1:A:146:ARG:HB3	1:A:149:THR:HG21	0.69	1.63	14	4
1:A:80:LEU:HD11	1:A:158:VAL:HG21	0.69	1.63	14	1
1:A:59:LYS:HG3	1:A:150:TRP:CD2	0.69	2.22	15	5
1:A:72:VAL:O	1:A:138:VAL:HG22	0.69	1.87	15	19
1:A:74:TYR:OH	1:A:158:VAL:HG11	0.69	1.87	16	7
1:A:103:GLN:OE1	1:A:141:ILE:HD13	0.69	1.87	18	3
1:A:105:THR:O	1:A:135:VAL:HG22	0.69	1.87	14	12
1:A:97:MET:SD	1:A:142:ALA:HB2	0.69	2.28	12	2
1:A:47:ILE:CG2	1:A:156:ILE:HD13	0.69	2.18	9	2
1:A:85:PHE:HA	1:A:156:ILE:HB	0.68	1.65	18	8
1:A:47:ILE:HG23	1:A:156:ILE:HB	0.68	1.66	20	10
1:A:96:THR:HG22	1:A:121:THR:O	0.68	1.88	21	6
1:A:47:ILE:HD13	1:A:56:LEU:HD12	0.68	1.64	2	7
1:A:80:LEU:HD23	1:A:131:LEU:HD21	0.68	1.64	18	2
1:A:122:MET:N	1:A:123:PRO:HD3	0.68	2.04	21	21
1:A:118:VAL:HG11	1:A:120:TYR:CZ	0.68	2.23	2	13
1:A:36:ARG:NH1	1:A:64:ILE:HG23	0.68	2.04	9	1
1:A:41:THR:HG21	1:A:57:VAL:HG22	0.68	1.65	16	1
1:A:47:ILE:HG23	1:A:156:ILE:HG23	0.67	1.65	6	3
1:A:28:ILE:HD11	1:A:75:SER:OG	0.67	1.89	15	1
1:A:82:ASN:O	1:A:158:VAL:HG23	0.67	1.89	21	1
1:A:80:LEU:HD13	1:A:135:VAL:HG12	0.67	1.64	14	2
1:A:72:VAL:O	1:A:138:VAL:CG2	0.67	2.43	15	21
1:A:98:GLN:C	1:A:121:THR:HB	0.67	2.14	9	21
1:A:59:LYS:O	1:A:60:ASN:C	0.67	2.38	14	6
1:A:105:THR:HG23	1:A:136:ARG:O	0.67	1.90	2	20
1:A:96:THR:HG23	1:A:97:MET:N	0.67	2.05	18	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:TYR:CE2	1:A:126:ILE:HG21	0.67	2.24	20	1
1:A:56:LEU:HD21	1:A:58:TYR:CE1	0.67	2.24	1	9
1:A:59:LYS:CB	1:A:150:TRP:CG	0.67	2.78	13	10
1:A:86:LEU:CD1	1:A:125:ALA:HB1	0.67	2.20	16	6
1:A:72:VAL:HG13	1:A:138:VAL:HG23	0.66	1.66	1	12
1:A:66:VAL:HG22	1:A:144:GLU:HA	0.66	1.66	19	4
1:A:66:VAL:HG12	1:A:144:GLU:CA	0.66	2.20	5	1
1:A:120:TYR:CE1	1:A:126:ILE:CG2	0.66	2.79	15	8
1:A:80:LEU:HD12	1:A:158:VAL:CG2	0.66	2.20	11	3
1:A:116:GLU:O	1:A:117:GLY:C	0.66	2.37	21	2
1:A:102:ILE:HB	1:A:120:TYR:HE2	0.66	1.50	20	1
1:A:32:TYR:CD2	1:A:47:ILE:HD13	0.66	2.25	5	4
1:A:80:LEU:HD23	1:A:131:LEU:HD23	0.66	1.66	5	1
1:A:41:THR:HG22	1:A:57:VAL:H	0.66	1.48	17	17
1:A:76:ASN:O	1:A:78:ILE:HG23	0.66	1.90	15	6
1:A:114:LEU:CD2	1:A:128:VAL:HG11	0.65	2.22	19	3
1:A:132:ASP:C	1:A:133:LEU:HD23	0.65	2.15	14	2
1:A:122:MET:HE3	1:A:122:MET:HA	0.65	1.66	8	2
1:A:80:LEU:CD1	1:A:158:VAL:HG23	0.65	2.21	11	3
1:A:59:LYS:CB	1:A:150:TRP:CD2	0.65	2.79	10	9
1:A:64:ILE:HD12	1:A:64:ILE:O	0.65	1.91	16	6
1:A:64:ILE:N	1:A:64:ILE:HD13	0.65	2.07	10	3
1:A:69:TYR:HB2	1:A:140:LEU:O	0.65	1.92	1	15
1:A:31:THR:O	1:A:72:VAL:HG23	0.65	1.92	10	5
1:A:66:VAL:HG22	1:A:143:THR:O	0.65	1.92	11	1
1:A:31:THR:C	1:A:72:VAL:HG23	0.65	2.17	6	6
1:A:29:ILE:O	1:A:29:ILE:HG23	0.64	1.92	3	2
1:A:66:VAL:HG12	1:A:144:GLU:N	0.64	2.06	5	1
1:A:28:ILE:HD11	1:A:75:SER:CB	0.64	2.22	9	1
1:A:36:ARG:NH2	1:A:64:ILE:HG21	0.64	2.07	18	1
1:A:122:MET:N	1:A:123:PRO:CD	0.64	2.60	20	21
1:A:99:LYS:O	1:A:143:THR:HG22	0.64	1.91	4	4
1:A:28:ILE:CD1	1:A:78:ILE:HG22	0.64	2.21	5	3
1:A:64:ILE:HD13	1:A:68:THR:HG21	0.64	1.68	19	1
1:A:56:LEU:HD13	1:A:153:VAL:HG21	0.64	1.69	3	2
1:A:87:MET:HB2	1:A:153:VAL:HG13	0.64	1.69	17	8
1:A:64:ILE:HD12	1:A:145:ALA:CB	0.63	2.21	19	1
1:A:115:GLU:CG	1:A:128:VAL:HG22	0.63	2.24	8	2
1:A:28:ILE:CG2	1:A:78:ILE:HG21	0.63	2.23	9	2
1:A:30:ALA:HB1	1:A:72:VAL:HG21	0.63	1.68	1	9
1:A:57:VAL:HG23	1:A:151:LEU:O	0.63	1.93	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:MET:HE3	1:A:97:MET:HA	0.63	1.70	19	1
1:A:86:LEU:HD11	1:A:125:ALA:HB1	0.63	1.69	16	4
1:A:89:ALA:HB1	1:A:95:ASP:HB2	0.63	1.69	20	7
1:A:65:ASP:OD1	1:A:66:VAL:HG23	0.63	1.94	15	1
1:A:59:LYS:O	1:A:60:ASN:O	0.63	2.17	16	8
1:A:28:ILE:HG21	1:A:78:ILE:HG12	0.63	1.69	9	1
1:A:146:ARG:NE	1:A:149:THR:HG21	0.63	2.08	1	1
1:A:115:GLU:HG3	1:A:128:VAL:HG22	0.63	1.69	8	1
1:A:30:ALA:HB1	1:A:72:VAL:HG22	0.62	1.71	4	6
1:A:80:LEU:HD22	1:A:135:VAL:HG11	0.62	1.68	18	3
1:A:151:LEU:CD1	1:A:153:VAL:HG13	0.62	2.24	3	1
1:A:69:TYR:CE2	1:A:141:ILE:HD12	0.62	2.29	13	5
1:A:83:VAL:CG2	1:A:158:VAL:HG12	0.62	2.24	16	2
1:A:120:TYR:CZ	1:A:126:ILE:HG21	0.62	2.30	21	3
1:A:102:ILE:HD11	1:A:126:ILE:HG21	0.62	1.72	4	8
1:A:66:VAL:HG22	1:A:144:GLU:CA	0.62	2.25	6	3
1:A:47:ILE:HG12	1:A:156:ILE:HG23	0.62	1.69	18	3
1:A:115:GLU:OE2	1:A:128:VAL:HG22	0.62	1.95	17	3
1:A:32:TYR:CD2	1:A:47:ILE:HG21	0.62	2.29	8	5
1:A:66:VAL:HG13	1:A:143:THR:O	0.62	1.95	13	1
1:A:83:VAL:HG12	1:A:131:LEU:CD2	0.62	2.25	11	2
1:A:47:ILE:N	1:A:47:ILE:HD12	0.61	2.10	18	12
1:A:80:LEU:HD21	1:A:131:LEU:HD23	0.61	1.71	11	2
1:A:41:THR:HG21	1:A:55:GLU:HG2	0.61	1.71	4	1
1:A:46:ASN:ND2	1:A:54:THR:O	0.61	2.34	19	10
1:A:80:LEU:CD1	1:A:158:VAL:HG21	0.61	2.24	21	3
1:A:59:LYS:HB3	1:A:150:TRP:CD2	0.61	2.29	4	7
1:A:151:LEU:C	1:A:151:LEU:HD13	0.61	2.20	3	11
1:A:28:ILE:CG1	1:A:78:ILE:HG21	0.61	2.26	1	4
1:A:85:PHE:HD1	1:A:156:ILE:HD12	0.61	1.56	14	2
1:A:59:LYS:HB2	1:A:150:TRP:CE2	0.60	2.31	10	6
1:A:80:LEU:HD23	1:A:80:LEU:O	0.60	1.95	19	3
1:A:146:ARG:CG	1:A:149:THR:HG21	0.60	2.25	17	5
1:A:39:ALA:HB1	1:A:40:PRO:HD2	0.60	1.73	20	7
1:A:47:ILE:HG13	1:A:156:ILE:HG23	0.60	1.73	14	3
1:A:80:LEU:HD23	1:A:81:ASN:N	0.60	2.11	20	1
1:A:59:LYS:CB	1:A:150:TRP:CD1	0.60	2.84	9	6
1:A:102:ILE:CG1	1:A:120:TYR:CE2	0.60	2.85	19	20
1:A:87:MET:HE2	1:A:126:ILE:HD11	0.60	1.73	1	1
1:A:31:THR:N	1:A:73:LYS:O	0.60	2.35	21	12
1:A:116:GLU:O	1:A:118:VAL:HG23	0.60	1.96	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:TYR:CD1	1:A:135:VAL:HG23	0.60	2.32	7	3
1:A:29:ILE:HG22	1:A:75:SER:HB3	0.59	1.72	15	2
1:A:56:LEU:HD22	1:A:56:LEU:O	0.59	1.97	19	6
1:A:47:ILE:HG23	1:A:156:ILE:O	0.59	1.98	18	1
1:A:105:THR:HG22	1:A:111:TRP:CZ2	0.59	2.32	18	19
1:A:69:TYR:CG	1:A:140:LEU:O	0.59	2.55	7	19
1:A:151:LEU:HD12	1:A:153:VAL:HG23	0.59	1.74	19	1
1:A:85:PHE:HA	1:A:156:ILE:HG23	0.59	1.73	11	8
1:A:66:VAL:HG12	1:A:143:THR:O	0.59	1.97	21	2
1:A:56:LEU:HD23	1:A:57:VAL:N	0.58	2.13	16	5
1:A:64:ILE:HD13	1:A:64:ILE:C	0.58	2.23	1	1
1:A:151:LEU:HD13	1:A:151:LEU:O	0.58	1.98	21	2
1:A:140:LEU:HD23	1:A:140:LEU:N	0.58	2.13	20	1
1:A:83:VAL:HG11	1:A:114:LEU:CD1	0.58	2.27	8	2
1:A:56:LEU:HD13	1:A:153:VAL:CG1	0.58	2.28	13	1
1:A:31:THR:O	1:A:73:LYS:N	0.58	2.36	12	19
1:A:118:VAL:HG12	1:A:120:TYR:CD1	0.58	2.34	1	1
1:A:89:ALA:HB1	1:A:92:ASN:O	0.58	1.97	3	6
1:A:80:LEU:O	1:A:80:LEU:HD13	0.58	1.98	12	1
1:A:80:LEU:HD23	1:A:131:LEU:CD1	0.58	2.29	21	1
1:A:28:ILE:HG21	1:A:78:ILE:HG21	0.58	1.76	9	5
1:A:146:ARG:HG2	1:A:149:THR:HG21	0.58	1.75	12	3
1:A:32:TYR:CE2	1:A:153:VAL:HG11	0.58	2.33	10	5
1:A:85:PHE:CD2	1:A:156:ILE:HG13	0.58	2.34	6	1
1:A:47:ILE:CG2	1:A:156:ILE:HD12	0.58	2.29	5	4
1:A:28:ILE:HD13	1:A:28:ILE:N	0.58	2.14	3	1
1:A:87:MET:HG2	1:A:153:VAL:HG13	0.57	1.76	9	1
1:A:72:VAL:CG1	1:A:138:VAL:HG23	0.57	2.29	2	17
1:A:41:THR:HG23	1:A:42:GLY:N	0.57	2.15	5	5
1:A:100:ALA:O	1:A:118:VAL:O	0.57	2.21	9	19
1:A:85:PHE:CD1	1:A:156:ILE:HD12	0.57	2.34	14	2
1:A:28:ILE:HD13	1:A:78:ILE:CG2	0.57	2.28	12	11
1:A:158:VAL:HG13	1:A:158:VAL:O	0.57	2.00	10	3
1:A:45:ASP:HB2	1:A:54:THR:HG21	0.57	1.75	1	2
1:A:72:VAL:HB	1:A:156:ILE:HD11	0.57	1.77	1	4
1:A:28:ILE:HG22	1:A:74:TYR:HB3	0.57	1.75	3	1
1:A:102:ILE:O	1:A:114:LEU:N	0.57	2.37	15	12
1:A:115:GLU:OE2	1:A:118:VAL:HG21	0.57	1.99	12	1
1:A:29:ILE:HG22	1:A:75:SER:CB	0.57	2.30	17	3
1:A:96:THR:CG2	1:A:121:THR:O	0.57	2.53	19	12
1:A:155:ASP:C	1:A:156:ILE:HG22	0.57	2.25	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:PHE:CE1	1:A:102:ILE:HD11	0.57	2.35	20	1
1:A:28:ILE:HG21	1:A:78:ILE:CG2	0.57	2.30	5	1
1:A:85:PHE:CD1	1:A:102:ILE:HD13	0.57	2.34	15	2
1:A:72:VAL:CG1	1:A:138:VAL:CG2	0.56	2.83	2	20
1:A:98:GLN:O	1:A:121:THR:HG21	0.56	1.99	19	19
1:A:36:ARG:NH2	1:A:64:ILE:HD13	0.56	2.15	3	1
1:A:104:TYR:CB	1:A:114:LEU:HD12	0.56	2.31	20	1
1:A:80:LEU:HD11	1:A:83:VAL:HB	0.56	1.76	13	6
1:A:87:MET:HG3	1:A:153:VAL:HG22	0.56	1.77	4	2
1:A:86:LEU:HD22	1:A:86:LEU:N	0.56	2.16	11	2
1:A:44:PRO:HA	1:A:47:ILE:HD12	0.56	1.76	6	4
1:A:57:VAL:HG23	1:A:151:LEU:C	0.56	2.26	9	1
1:A:104:TYR:CD2	1:A:114:LEU:HD13	0.56	2.35	9	2
1:A:31:THR:HG22	1:A:48:PHE:CE1	0.56	2.36	21	1
1:A:114:LEU:C	1:A:114:LEU:HD23	0.56	2.26	17	14
1:A:80:LEU:HD11	1:A:158:VAL:CG2	0.56	2.31	17	1
1:A:103:GLN:HG2	1:A:113:ASP:HA	0.56	1.78	2	1
1:A:80:LEU:HD23	1:A:131:LEU:CD2	0.56	2.30	5	1
1:A:97:MET:HE3	1:A:140:LEU:CD2	0.56	2.29	21	2
1:A:98:GLN:O	1:A:121:THR:CG2	0.56	2.54	19	9
1:A:66:VAL:HG13	1:A:143:THR:HA	0.56	1.77	18	3
1:A:44:PRO:O	1:A:47:ILE:N	0.56	2.37	6	3
1:A:47:ILE:HG23	1:A:156:ILE:HD12	0.55	1.76	5	1
1:A:80:LEU:HD12	1:A:158:VAL:HG21	0.55	1.77	21	1
1:A:60:ASN:CB	1:A:61:PRO:CD	0.55	2.84	2	6
1:A:59:LYS:HB2	1:A:150:TRP:NE1	0.55	2.17	9	1
1:A:46:ASN:HB3	1:A:51:ASN:O	0.55	2.01	9	3
1:A:64:ILE:HD12	1:A:64:ILE:N	0.55	2.16	9	1
1:A:119:GLU:C	1:A:121:THR:H	0.55	2.09	20	20
1:A:114:LEU:HD21	1:A:128:VAL:HG21	0.55	1.73	2	2
1:A:44:PRO:HB3	1:A:47:ILE:HD11	0.55	1.79	11	1
1:A:140:LEU:HD23	1:A:141:ILE:N	0.55	2.17	21	3
1:A:96:THR:OG1	1:A:97:MET:N	0.55	2.39	15	15
1:A:118:VAL:CG1	1:A:119:GLU:N	0.55	2.70	1	20
1:A:158:VAL:HG22	1:A:159:ASN:OD1	0.55	2.02	11	1
1:A:87:MET:HB2	1:A:153:VAL:HA	0.55	1.77	10	2
1:A:98:GLN:O	1:A:99:LYS:CG	0.55	2.55	18	8
1:A:58:TYR:CZ	1:A:70:VAL:HG11	0.55	2.36	17	1
1:A:83:VAL:HG22	1:A:85:PHE:CE1	0.55	2.35	21	1
1:A:97:MET:O	1:A:121:THR:HA	0.55	2.02	19	18
1:A:89:ALA:HB3	1:A:93:PRO:HA	0.55	1.78	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:ILE:O	1:A:156:ILE:HG12	0.55	2.01	14	3
1:A:96:THR:HA	1:A:151:LEU:HD22	0.55	1.79	12	3
1:A:59:LYS:HB2	1:A:150:TRP:CD1	0.55	2.37	9	5
1:A:102:ILE:HD12	1:A:115:GLU:OE1	0.55	2.02	9	3
1:A:114:LEU:HD23	1:A:114:LEU:O	0.55	2.02	20	1
1:A:32:TYR:HH	1:A:70:VAL:HG21	0.55	1.59	6	1
1:A:47:ILE:HG13	1:A:156:ILE:HG13	0.54	1.79	2	1
1:A:133:LEU:HD23	1:A:133:LEU:N	0.54	2.16	14	1
1:A:66:VAL:O	1:A:66:VAL:HG13	0.54	2.01	8	1
1:A:102:ILE:HD11	1:A:126:ILE:CG2	0.54	2.33	18	13
1:A:28:ILE:HG22	1:A:78:ILE:HD13	0.54	1.80	15	1
1:A:46:ASN:HA	1:A:51:ASN:HB3	0.54	1.78	17	1
1:A:60:ASN:HB3	1:A:61:PRO:CD	0.54	2.33	2	4
1:A:67:GLY:O	1:A:69:TYR:CD2	0.53	2.61	7	20
1:A:102:ILE:HG22	1:A:139:ARG:O	0.53	2.02	4	4
1:A:141:ILE:HD13	1:A:142:ALA:N	0.53	2.19	20	2
1:A:60:ASN:CG	1:A:61:PRO:HD3	0.53	2.28	2	3
1:A:60:ASN:CB	1:A:61:PRO:HD2	0.53	2.32	11	9
1:A:151:LEU:HD13	1:A:151:LEU:C	0.53	2.28	21	1
1:A:151:LEU:HD12	1:A:153:VAL:HG22	0.53	1.79	5	1
1:A:104:TYR:HA	1:A:111:TRP:CZ3	0.53	2.38	11	20
1:A:47:ILE:HD11	1:A:56:LEU:HD11	0.53	1.80	17	3
1:A:100:ALA:O	1:A:120:TYR:CD2	0.53	2.62	19	9
1:A:99:LYS:O	1:A:100:ALA:HB2	0.53	2.04	15	19
1:A:56:LEU:HD21	1:A:153:VAL:HB	0.53	1.80	8	2
1:A:102:ILE:HG12	1:A:120:TYR:CE2	0.53	2.39	3	14
1:A:59:LYS:O	1:A:61:PRO:N	0.53	2.42	21	5
1:A:32:TYR:CD1	1:A:33:ILE:N	0.53	2.77	12	11
1:A:83:VAL:HG12	1:A:131:LEU:HD22	0.53	1.80	11	1
1:A:60:ASN:CB	1:A:61:PRO:HD3	0.53	2.34	2	9
1:A:138:VAL:HG21	1:A:158:VAL:HG11	0.53	1.80	12	1
1:A:128:VAL:HG11	1:A:131:LEU:HD22	0.53	1.79	13	1
1:A:47:ILE:HG23	1:A:156:ILE:HG12	0.52	1.79	1	4
1:A:70:VAL:CG2	1:A:71:GLY:N	0.52	2.71	18	9
1:A:32:TYR:CE1	1:A:33:ILE:O	0.52	2.62	14	13
1:A:87:MET:HB3	1:A:153:VAL:HG12	0.52	1.79	3	1
1:A:44:PRO:HA	1:A:56:LEU:HD12	0.52	1.81	1	2
1:A:118:VAL:CG1	1:A:120:TYR:CE1	0.52	2.90	4	13
1:A:41:THR:HG23	1:A:57:VAL:O	0.52	2.04	16	1
1:A:71:GLY:HA2	1:A:85:PHE:CE2	0.52	2.39	16	4
1:A:74:TYR:OH	1:A:158:VAL:HG21	0.52	2.05	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:LEU:HD11	1:A:131:LEU:HD21	0.52	1.81	9	1
1:A:120:TYR:CD2	1:A:140:LEU:HD21	0.52	2.40	6	3
1:A:28:ILE:HG12	1:A:78:ILE:HG23	0.52	1.81	17	2
1:A:85:PHE:CD1	1:A:156:ILE:HG13	0.52	2.39	9	1
1:A:58:TYR:CE2	1:A:70:VAL:HG11	0.52	2.39	17	1
1:A:32:TYR:CD1	1:A:33:ILE:O	0.52	2.63	21	15
1:A:104:TYR:CD1	1:A:135:VAL:CG2	0.52	2.92	7	4
1:A:83:VAL:HA	1:A:158:VAL:HG12	0.52	1.81	9	1
1:A:58:TYR:CD1	1:A:58:TYR:N	0.52	2.78	17	1
1:A:85:PHE:HD2	1:A:156:ILE:HD13	0.52	1.65	15	8
1:A:47:ILE:CG2	1:A:156:ILE:HG23	0.52	2.34	9	3
1:A:85:PHE:HE1	1:A:102:ILE:HG21	0.52	1.61	13	4
1:A:158:VAL:HG23	1:A:158:VAL:O	0.52	2.04	7	1
1:A:86:LEU:N	1:A:155:ASP:O	0.52	2.43	18	13
1:A:151:LEU:HD12	1:A:153:VAL:CG2	0.52	2.35	5	1
1:A:74:TYR:HH	1:A:158:VAL:HG11	0.52	1.64	16	2
1:A:32:TYR:HE2	1:A:153:VAL:HG11	0.51	1.65	7	2
1:A:83:VAL:HG21	1:A:85:PHE:CZ	0.51	2.39	9	1
1:A:72:VAL:O	1:A:138:VAL:HG23	0.51	2.04	1	5
1:A:102:ILE:HA	1:A:140:LEU:HG	0.51	1.82	2	2
1:A:43:ASN:OD1	1:A:54:THR:HG21	0.51	2.05	4	1
1:A:79:THR:HG23	1:A:79:THR:O	0.51	2.06	6	4
1:A:151:LEU:C	1:A:151:LEU:HD12	0.51	2.30	17	1
1:A:80:LEU:HD13	1:A:80:LEU:C	0.51	2.30	12	1
1:A:103:GLN:CB	1:A:141:ILE:HD13	0.51	2.36	12	1
1:A:100:ALA:O	1:A:120:TYR:CD1	0.51	2.64	1	1
1:A:100:ALA:O	1:A:120:TYR:HD1	0.51	1.89	1	1
1:A:115:GLU:CG	1:A:120:TYR:OH	0.51	2.59	15	12
1:A:111:TRP:CZ3	1:A:139:ARG:CB	0.51	2.94	4	18
1:A:84:GLU:O	1:A:156:ILE:HG23	0.51	2.06	20	3
1:A:47:ILE:HG22	1:A:156:ILE:HG13	0.51	1.82	11	1
1:A:87:MET:CG	1:A:153:VAL:HG22	0.51	2.36	8	1
1:A:58:TYR:O	1:A:58:TYR:CD1	0.51	2.64	9	1
1:A:80:LEU:HD11	1:A:158:VAL:HG23	0.51	1.82	17	1
1:A:120:TYR:CD1	1:A:126:ILE:HD13	0.50	2.41	19	17
1:A:41:THR:HG22	1:A:56:LEU:HA	0.50	1.81	13	3
1:A:56:LEU:HD13	1:A:153:VAL:HG11	0.50	1.81	13	1
1:A:72:VAL:HG13	1:A:138:VAL:HG21	0.50	1.83	5	2
1:A:144:GLU:O	1:A:145:ALA:HB3	0.50	2.07	18	2
1:A:85:PHE:O	1:A:126:ILE:HG13	0.50	2.06	1	5
1:A:57:VAL:HG23	1:A:59:LYS:CE	0.50	2.36	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LYS:CG	1:A:150:TRP:CE2	0.50	2.95	11	3
1:A:140:LEU:HD23	1:A:141:ILE:H	0.50	1.67	16	3
1:A:66:VAL:HG12	1:A:143:THR:C	0.50	2.31	20	1
1:A:56:LEU:HD23	1:A:56:LEU:C	0.50	2.32	1	2
1:A:60:ASN:CG	1:A:61:PRO:HD2	0.50	2.32	11	4
1:A:141:ILE:HD13	1:A:142:ALA:H	0.50	1.65	20	1
1:A:34:SER:CB	1:A:58:TYR:CE2	0.50	2.95	13	13
1:A:32:TYR:HD2	1:A:47:ILE:HG21	0.50	1.65	6	3
1:A:47:ILE:HD11	1:A:56:LEU:CD1	0.50	2.37	17	2
1:A:131:LEU:CD1	1:A:133:LEU:HD21	0.50	2.37	14	1
1:A:68:THR:HG22	1:A:68:THR:O	0.50	2.07	12	4
1:A:69:TYR:CD1	1:A:139:ARG:CD	0.50	2.95	13	2
1:A:56:LEU:CD2	1:A:56:LEU:C	0.50	2.85	10	6
1:A:47:ILE:HG21	1:A:156:ILE:HD12	0.50	1.83	4	5
1:A:66:VAL:HG22	1:A:144:GLU:N	0.50	2.22	6	2
1:A:103:GLN:N	1:A:139:ARG:O	0.49	2.41	21	4
1:A:51:ASN:O	1:A:53:SER:N	0.49	2.44	8	5
1:A:120:TYR:CE1	1:A:126:ILE:HG21	0.49	2.42	15	1
1:A:80:LEU:HD23	1:A:80:LEU:C	0.49	2.32	19	1
1:A:83:VAL:HG23	1:A:158:VAL:CG1	0.49	2.33	16	5
1:A:87:MET:O	1:A:87:MET:HE3	0.49	2.07	2	1
1:A:46:ASN:HB2	1:A:47:ILE:HD12	0.49	1.84	21	6
1:A:90:ASN:ND2	1:A:150:TRP:CE3	0.49	2.80	21	6
1:A:158:VAL:HG22	1:A:159:ASN:ND2	0.49	2.21	19	2
1:A:33:ILE:O	1:A:70:VAL:HB	0.49	2.07	17	2
1:A:46:ASN:HD21	1:A:54:THR:C	0.49	2.15	11	4
1:A:28:ILE:CG2	1:A:74:TYR:HB3	0.49	2.37	2	6
1:A:69:TYR:CD1	1:A:69:TYR:C	0.49	2.91	11	10
1:A:69:TYR:CB	1:A:140:LEU:O	0.49	2.60	17	13
1:A:85:PHE:CD1	1:A:102:ILE:CD1	0.49	2.95	21	2
1:A:115:GLU:HG3	1:A:116:GLU:N	0.49	2.23	15	2
1:A:89:ALA:C	1:A:152:GLY:HA3	0.49	2.33	2	1
1:A:80:LEU:HD21	1:A:83:VAL:HB	0.49	1.83	7	2
1:A:61:PRO:O	1:A:62:ASN:C	0.49	2.55	20	7
1:A:64:ILE:HG13	1:A:145:ALA:HB1	0.49	1.83	18	2
1:A:102:ILE:CG1	1:A:140:LEU:HG	0.49	2.38	15	2
1:A:29:ILE:HG22	1:A:30:ALA:N	0.49	2.23	4	9
1:A:105:THR:CG2	1:A:111:TRP:CE2	0.49	2.96	14	12
1:A:46:ASN:OD1	1:A:47:ILE:HD12	0.49	2.07	9	1
1:A:80:LEU:HD12	1:A:159:ASN:OD1	0.49	2.08	7	1
1:A:100:ALA:CB	1:A:141:ILE:O	0.49	2.61	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ILE:HG22	1:A:115:GLU:N	0.49	2.23	20	1
1:A:118:VAL:HB	1:A:120:TYR:CE1	0.48	2.43	1	1
1:A:141:ILE:O	1:A:141:ILE:CG2	0.48	2.61	8	7
1:A:80:LEU:O	1:A:131:LEU:O	0.48	2.31	5	4
1:A:64:ILE:HG23	1:A:68:THR:OG1	0.48	2.08	14	1
1:A:60:ASN:HB3	1:A:61:PRO:HD3	0.48	1.85	2	7
1:A:151:LEU:CD1	1:A:153:VAL:HG22	0.48	2.38	2	3
1:A:56:LEU:HD22	1:A:153:VAL:HG22	0.48	1.85	3	1
1:A:28:ILE:CG1	1:A:78:ILE:CG2	0.48	2.91	5	11
1:A:74:TYR:CD1	1:A:137:GLY:HA2	0.48	2.43	15	14
1:A:97:MET:O	1:A:121:THR:CB	0.48	2.61	20	13
1:A:121:THR:O	1:A:122:MET:CE	0.48	2.61	1	12
1:A:86:LEU:HD23	1:A:86:LEU:N	0.48	2.22	13	2
1:A:57:VAL:HG23	1:A:59:LYS:HE2	0.48	1.86	5	1
1:A:96:THR:CG2	1:A:97:MET:N	0.48	2.74	18	5
1:A:36:ARG:HH11	1:A:64:ILE:HG23	0.48	1.68	9	1
1:A:69:TYR:CD2	1:A:141:ILE:HD12	0.48	2.43	14	2
1:A:85:PHE:CE1	1:A:102:ILE:CD1	0.48	2.96	20	1
1:A:35:ASN:ND2	1:A:69:TYR:CZ	0.48	2.81	8	5
1:A:74:TYR:CZ	1:A:158:VAL:HG11	0.48	2.43	14	2
1:A:28:ILE:HD11	1:A:76:ASN:OD1	0.48	2.08	21	1
1:A:59:LYS:HB3	1:A:150:TRP:CD1	0.48	2.43	9	4
1:A:74:TYR:CD1	1:A:74:TYR:N	0.48	2.81	17	18
1:A:104:TYR:C	1:A:104:TYR:CD1	0.48	2.91	19	5
1:A:59:LYS:HG3	1:A:150:TRP:CG	0.48	2.43	11	3
1:A:97:MET:CB	1:A:120:TYR:O	0.48	2.62	10	18
1:A:34:SER:CB	1:A:58:TYR:CD2	0.48	2.97	6	2
1:A:131:LEU:HD12	1:A:133:LEU:HD21	0.48	1.84	14	1
1:A:69:TYR:C	1:A:70:VAL:CG1	0.48	2.86	17	4
1:A:64:ILE:HD13	1:A:68:THR:CB	0.48	2.39	16	1
1:A:32:TYR:OH	1:A:70:VAL:CG2	0.48	2.62	12	8
1:A:56:LEU:C	1:A:56:LEU:CD2	0.48	2.86	1	6
1:A:115:GLU:HG2	1:A:128:VAL:HG22	0.48	1.85	4	1
1:A:59:LYS:C	1:A:60:ASN:O	0.48	2.57	16	9
1:A:66:VAL:H	1:A:145:ALA:HB3	0.48	1.69	6	1
1:A:80:LEU:HD21	1:A:158:VAL:CG2	0.48	2.38	10	1
1:A:151:LEU:HD12	1:A:152:GLY:N	0.48	2.23	17	1
1:A:79:THR:HA	1:A:134:LYS:HA	0.48	1.85	2	1
1:A:32:TYR:CE2	1:A:56:LEU:CD1	0.48	2.96	7	4
1:A:64:ILE:HD13	1:A:68:THR:OG1	0.48	2.09	17	3
1:A:111:TRP:HZ3	1:A:139:ARG:N	0.47	2.07	1	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:TYR:CD2	1:A:47:ILE:HD12	0.47	2.44	11	1
1:A:32:TYR:CE2	1:A:47:ILE:HD12	0.47	2.44	11	1
1:A:94:ASN:OD1	1:A:122:MET:HE1	0.47	2.09	19	1
1:A:72:VAL:O	1:A:138:VAL:N	0.47	2.46	21	9
1:A:59:LYS:HG2	1:A:150:TRP:CD2	0.47	2.44	2	1
1:A:59:LYS:HB2	1:A:150:TRP:CD2	0.47	2.42	10	3
1:A:68:THR:CG2	1:A:68:THR:O	0.47	2.63	1	1
1:A:66:VAL:HG12	1:A:144:GLU:HA	0.47	1.86	5	1
1:A:56:LEU:O	1:A:56:LEU:HD13	0.47	2.09	9	1
1:A:101:LYS:HA	1:A:118:VAL:HG12	0.47	1.85	21	1
1:A:47:ILE:HG13	1:A:156:ILE:CG1	0.47	2.39	2	1
1:A:80:LEU:HD21	1:A:83:VAL:N	0.47	2.24	4	1
1:A:140:LEU:C	1:A:141:ILE:HD12	0.47	2.34	12	1
1:A:46:ASN:N	1:A:46:ASN:OD1	0.47	2.47	19	2
1:A:29:ILE:O	1:A:74:TYR:HA	0.47	2.09	5	4
1:A:127:LYS:O	1:A:128:VAL:HG13	0.47	2.10	9	1
1:A:101:LYS:HD2	1:A:141:ILE:HG22	0.47	1.86	10	1
1:A:116:GLU:C	1:A:118:VAL:N	0.47	2.73	21	2
1:A:102:ILE:CG1	1:A:140:LEU:HD22	0.47	2.38	20	1
1:A:47:ILE:N	1:A:47:ILE:CD1	0.47	2.78	13	10
1:A:115:GLU:HG2	1:A:120:TYR:OH	0.47	2.10	2	4
1:A:105:THR:HB	1:A:111:TRP:CD1	0.47	2.44	14	11
1:A:111:TRP:CZ3	1:A:139:ARG:HB2	0.47	2.44	13	8
1:A:87:MET:CG	1:A:88:GLY:N	0.47	2.78	12	6
1:A:64:ILE:N	1:A:64:ILE:CD1	0.47	2.77	12	3
1:A:111:TRP:CZ3	1:A:139:ARG:N	0.47	2.82	21	10
1:A:66:VAL:HG23	1:A:144:GLU:N	0.47	2.23	8	1
1:A:158:VAL:HG13	1:A:159:ASN:ND2	0.47	2.25	19	1
1:A:56:LEU:CD1	1:A:56:LEU:N	0.47	2.78	17	5
1:A:32:TYR:CD1	1:A:58:TYR:OH	0.47	2.68	8	5
1:A:97:MET:HB2	1:A:120:TYR:O	0.47	2.10	9	9
1:A:69:TYR:CE1	1:A:139:ARG:NE	0.47	2.83	14	4
1:A:31:THR:O	1:A:72:VAL:HA	0.47	2.10	20	2
1:A:69:TYR:O	1:A:70:VAL:HG12	0.47	2.10	17	1
1:A:118:VAL:CG1	1:A:120:TYR:CD1	0.47	2.97	20	1
1:A:72:VAL:CG1	1:A:156:ILE:HD13	0.47	2.40	11	1
1:A:85:PHE:CD1	1:A:85:PHE:N	0.47	2.82	21	2
1:A:104:TYR:HB3	1:A:114:LEU:CD1	0.46	2.40	2	1
1:A:105:THR:CG2	1:A:111:TRP:CZ2	0.46	2.99	4	11
1:A:131:LEU:C	1:A:133:LEU:HD23	0.46	2.34	11	2
1:A:46:ASN:O	1:A:51:ASN:N	0.46	2.49	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:VAL:HG11	1:A:120:TYR:CD1	0.46	2.43	21	2
1:A:84:GLU:CB	1:A:127:LYS:HA	0.46	2.41	2	1
1:A:36:ARG:HB3	1:A:60:ASN:CG	0.46	2.35	5	1
1:A:69:TYR:CE1	1:A:139:ARG:CD	0.46	2.99	3	4
1:A:44:PRO:O	1:A:47:ILE:HD12	0.46	2.11	5	1
1:A:41:THR:HG22	1:A:57:VAL:N	0.46	2.26	14	6
1:A:137:GLY:O	1:A:138:VAL:HG13	0.46	2.10	6	3
1:A:81:ASN:OD1	1:A:159:ASN:HA	0.46	2.10	2	1
1:A:151:LEU:CD1	1:A:151:LEU:C	0.46	2.89	3	3
1:A:61:PRO:O	1:A:63:ARG:N	0.46	2.49	18	3
1:A:87:MET:HB2	1:A:153:VAL:HG22	0.46	1.86	19	1
1:A:103:GLN:CD	1:A:141:ILE:HD12	0.46	2.35	3	1
1:A:44:PRO:CA	1:A:47:ILE:HD12	0.46	2.41	5	2
1:A:141:ILE:O	1:A:141:ILE:HG23	0.46	2.10	13	1
1:A:96:THR:HB	1:A:151:LEU:HD13	0.46	1.87	17	1
1:A:115:GLU:OE1	1:A:128:VAL:HG21	0.46	2.09	1	2
1:A:115:GLU:OE1	1:A:128:VAL:HG13	0.46	2.11	18	2
1:A:111:TRP:CH2	1:A:139:ARG:HB2	0.46	2.46	3	5
1:A:59:LYS:CE	1:A:59:LYS:N	0.46	2.79	5	1
1:A:143:THR:HG22	1:A:143:THR:O	0.46	2.11	18	2
1:A:78:ILE:HD12	1:A:159:ASN:OD1	0.46	2.11	14	1
1:A:70:VAL:O	1:A:140:LEU:N	0.46	2.48	21	2
1:A:41:THR:CG2	1:A:57:VAL:O	0.46	2.64	16	1
1:A:83:VAL:CG2	1:A:138:VAL:HG11	0.45	2.40	11	2
1:A:87:MET:HB3	1:A:153:VAL:HG22	0.45	1.87	9	1
1:A:102:ILE:CG2	1:A:103:GLN:N	0.45	2.78	15	2
1:A:58:TYR:CE1	1:A:151:LEU:HB3	0.45	2.46	17	1
1:A:84:GLU:HB2	1:A:126:ILE:O	0.45	2.11	2	2
1:A:58:TYR:N	1:A:58:TYR:CD1	0.45	2.84	19	4
1:A:68:THR:O	1:A:68:THR:HG22	0.45	2.10	17	2
1:A:58:TYR:CE1	1:A:151:LEU:O	0.45	2.69	17	1
1:A:85:PHE:CZ	1:A:138:VAL:HB	0.45	2.46	2	1
1:A:97:MET:HG2	1:A:100:ALA:HB3	0.45	1.88	2	3
1:A:58:TYR:CE1	1:A:70:VAL:CG1	0.45	2.99	9	1
1:A:151:LEU:CD1	1:A:153:VAL:HG23	0.45	2.42	19	1
1:A:97:MET:CG	1:A:120:TYR:O	0.45	2.65	1	1
1:A:102:ILE:HD12	1:A:115:GLU:CD	0.45	2.37	14	2
1:A:84:GLU:CD	1:A:86:LEU:HD21	0.45	2.37	21	1
1:A:118:VAL:HB	1:A:120:TYR:HE1	0.45	1.72	1	1
1:A:120:TYR:O	1:A:123:PRO:HG3	0.45	2.12	1	3
1:A:29:ILE:CG2	1:A:30:ALA:N	0.45	2.79	20	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:LEU:HD23	1:A:131:LEU:HD12	0.45	1.87	21	1
1:A:102:ILE:HG12	1:A:140:LEU:HG	0.45	1.89	21	1
1:A:104:TYR:CD1	1:A:104:TYR:C	0.45	2.95	7	14
1:A:79:THR:HG22	1:A:132:ASP:OD1	0.45	2.11	7	1
1:A:58:TYR:O	1:A:150:TRP:HB3	0.45	2.12	16	1
1:A:62:ASN:HB3	1:A:148:ASN:HA	0.45	1.87	16	1
1:A:36:ARG:HD3	1:A:64:ILE:HG21	0.45	1.89	2	1
1:A:60:ASN:N	1:A:61:PRO:CD	0.45	2.79	10	3
1:A:30:ALA:O	1:A:48:PHE:CD1	0.45	2.70	10	4
1:A:97:MET:HB3	1:A:121:THR:HA	0.45	1.88	20	1
1:A:52:ALA:HB2	1:A:155:ASP:HB2	0.45	1.88	2	1
1:A:86:LEU:HD12	1:A:125:ALA:HB1	0.45	1.88	7	1
1:A:64:ILE:HG21	1:A:68:THR:HG21	0.45	1.89	13	1
1:A:45:ASP:O	1:A:49:ASP:N	0.45	2.50	16	1
1:A:56:LEU:HD11	1:A:153:VAL:HB	0.44	1.89	5	1
1:A:69:TYR:CD1	1:A:140:LEU:O	0.44	2.70	11	2
1:A:32:TYR:CE1	1:A:58:TYR:CE2	0.44	3.05	1	1
1:A:80:LEU:HD13	1:A:135:VAL:HG11	0.44	1.88	1	2
1:A:35:ASN:HB2	1:A:69:TYR:CD1	0.44	2.47	13	7
1:A:38:ASP:OD1	1:A:58:TYR:CD1	0.44	2.70	4	1
1:A:90:ASN:OD1	1:A:150:TRP:CZ3	0.44	2.71	20	1
1:A:65:ASP:O	1:A:66:VAL:C	0.44	2.60	2	2
1:A:87:MET:CB	1:A:153:VAL:HA	0.44	2.42	2	1
1:A:64:ILE:HD12	1:A:68:THR:CB	0.44	2.41	3	1
1:A:135:VAL:HG22	1:A:136:ARG:N	0.44	2.27	7	3
1:A:56:LEU:O	1:A:153:VAL:N	0.44	2.51	21	3
1:A:101:LYS:HB3	1:A:116:GLU:O	0.44	2.12	13	1
1:A:35:ASN:N	1:A:69:TYR:O	0.44	2.50	8	2
1:A:83:VAL:CG2	1:A:85:PHE:CE1	0.44	3.01	21	1
1:A:34:SER:HB3	1:A:58:TYR:CE2	0.44	2.48	14	8
1:A:97:MET:HB2	1:A:120:TYR:C	0.44	2.38	1	1
1:A:30:ALA:O	1:A:48:PHE:HA	0.44	2.12	2	1
1:A:85:PHE:CD2	1:A:156:ILE:HD13	0.44	2.48	15	4
1:A:97:MET:CE	1:A:140:LEU:HD13	0.44	2.43	6	2
1:A:43:ASN:O	1:A:54:THR:CG2	0.44	2.66	11	2
1:A:47:ILE:HG12	1:A:48:PHE:CD1	0.44	2.48	11	1
1:A:115:GLU:CG	1:A:128:VAL:HG11	0.44	2.43	12	1
1:A:156:ILE:O	1:A:156:ILE:CG1	0.44	2.66	1	2
1:A:33:ILE:HG13	1:A:72:VAL:N	0.44	2.27	17	5
1:A:102:ILE:HG13	1:A:115:GLU:HB2	0.44	1.90	8	4
1:A:66:VAL:HG23	1:A:143:THR:C	0.44	2.38	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:ASN:ND2	1:A:150:TRP:CZ3	0.44	2.85	18	1
1:A:68:THR:CG2	1:A:145:ALA:HB2	0.44	2.42	1	1
1:A:78:ILE:O	1:A:134:LYS:HA	0.44	2.12	1	1
1:A:41:THR:O	1:A:42:GLY:C	0.44	2.60	19	2
1:A:44:PRO:O	1:A:45:ASP:C	0.44	2.60	6	6
1:A:28:ILE:HD12	1:A:78:ILE:CG2	0.44	2.42	7	3
1:A:151:LEU:CD1	1:A:153:VAL:CG2	0.44	2.96	20	4
1:A:104:TYR:CD1	1:A:104:TYR:O	0.44	2.71	1	3
1:A:141:ILE:O	1:A:141:ILE:HG22	0.44	2.13	19	3
1:A:64:ILE:CG2	1:A:68:THR:CB	0.44	2.96	14	1
1:A:83:VAL:HG12	1:A:131:LEU:HD23	0.44	1.90	15	1
1:A:76:ASN:O	1:A:78:ILE:CG2	0.44	2.66	16	1
1:A:58:TYR:OH	1:A:153:VAL:CG2	0.44	2.66	17	1
1:A:67:GLY:H	1:A:142:ALA:HB3	0.44	1.72	17	2
1:A:57:VAL:HG21	1:A:90:ASN:CG	0.44	2.38	19	1
1:A:118:VAL:CG1	1:A:120:TYR:CE2	0.44	3.01	2	1
1:A:121:THR:C	1:A:123:PRO:HD3	0.44	2.37	2	6
1:A:32:TYR:CE2	1:A:56:LEU:HD13	0.44	2.48	7	1
1:A:74:TYR:CE1	1:A:138:VAL:HG22	0.44	2.48	14	5
1:A:83:VAL:HG22	1:A:84:GLU:N	0.44	2.28	14	2
1:A:64:ILE:CG2	1:A:68:THR:OG1	0.44	2.66	21	1
1:A:102:ILE:HG13	1:A:120:TYR:CZ	0.43	2.49	1	1
1:A:126:ILE:CD1	1:A:140:LEU:HD11	0.43	2.43	1	1
1:A:69:TYR:CE2	1:A:141:ILE:CD1	0.43	2.99	6	2
1:A:56:LEU:HD21	1:A:58:TYR:CZ	0.43	2.48	15	2
1:A:64:ILE:C	1:A:64:ILE:CD1	0.43	2.90	1	1
1:A:89:ALA:CB	1:A:92:ASN:O	0.43	2.66	11	7
1:A:103:GLN:NE2	1:A:141:ILE:HD12	0.43	2.28	3	1
1:A:111:TRP:CH2	1:A:138:VAL:C	0.43	2.96	19	6
1:A:46:ASN:OD1	1:A:46:ASN:N	0.43	2.51	20	2
1:A:104:TYR:CE2	1:A:113:ASP:O	0.43	2.72	18	3
1:A:118:VAL:CG1	1:A:120:TYR:CZ	0.43	3.01	14	2
1:A:119:GLU:C	1:A:121:THR:N	0.43	2.75	20	5
1:A:151:LEU:C	1:A:151:LEU:CD1	0.43	2.91	1	4
1:A:111:TRP:CZ3	1:A:139:ARG:HB3	0.43	2.48	8	3
1:A:101:LYS:HA	1:A:120:TYR:CE2	0.43	2.49	6	2
1:A:47:ILE:HB	1:A:156:ILE:HD12	0.43	1.89	11	1
1:A:69:TYR:CE1	1:A:139:ARG:HD3	0.43	2.48	3	1
1:A:59:LYS:C	1:A:60:ASN:ND2	0.43	2.77	5	1
1:A:85:PHE:CD2	1:A:156:ILE:HD12	0.43	2.48	16	1
1:A:102:ILE:HD12	1:A:128:VAL:CG2	0.43	2.44	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:MET:HE3	1:A:122:MET:CA	0.43	2.39	8	2
1:A:115:GLU:HG2	1:A:128:VAL:HG11	0.43	1.89	5	2
1:A:86:LEU:O	1:A:155:ASP:N	0.43	2.48	12	3
1:A:71:GLY:HA2	1:A:85:PHE:CE1	0.43	2.49	9	2
1:A:34:SER:OG	1:A:58:TYR:CE2	0.43	2.71	14	2
1:A:56:LEU:H	1:A:56:LEU:HD13	0.43	1.74	19	1
1:A:56:LEU:HB3	1:A:153:VAL:HG23	0.43	1.89	3	1
1:A:70:VAL:HG11	1:A:151:LEU:CD1	0.43	2.43	7	1
1:A:104:TYR:CD2	1:A:114:LEU:HD12	0.43	2.48	12	1
1:A:84:GLU:O	1:A:156:ILE:HA	0.43	2.13	18	1
1:A:156:ILE:HG12	1:A:156:ILE:O	0.43	2.12	1	1
1:A:69:TYR:CE1	1:A:139:ARG:HD2	0.43	2.49	5	1
1:A:89:ALA:HB3	1:A:93:PRO:CA	0.43	2.43	11	1
1:A:132:ASP:N	1:A:133:LEU:HD23	0.43	2.29	14	1
1:A:46:ASN:OD1	1:A:54:THR:HG23	0.43	2.13	16	1
1:A:114:LEU:CD2	1:A:114:LEU:C	0.43	2.91	16	1
1:A:100:ALA:CB	1:A:142:ALA:HA	0.43	2.43	6	2
1:A:56:LEU:C	1:A:57:VAL:CG1	0.43	2.92	17	10
1:A:54:THR:CG2	1:A:55:GLU:N	0.43	2.81	5	1
1:A:100:ALA:HB2	1:A:142:ALA:HA	0.43	1.91	7	1
1:A:64:ILE:HD13	1:A:68:THR:HB	0.43	1.91	16	1
1:A:115:GLU:CB	1:A:120:TYR:OH	0.43	2.67	1	1
1:A:105:THR:CG2	1:A:136:ARG:O	0.43	2.67	6	9
1:A:30:ALA:HA	1:A:73:LYS:O	0.43	2.14	15	1
1:A:56:LEU:N	1:A:56:LEU:HD13	0.42	2.29	8	3
1:A:28:ILE:HD11	1:A:76:ASN:HB2	0.42	1.91	10	1
1:A:84:GLU:HB3	1:A:126:ILE:O	0.42	2.14	17	3
1:A:38:ASP:OD2	1:A:58:TYR:CD1	0.42	2.71	1	1
1:A:118:VAL:HG11	1:A:120:TYR:CE2	0.42	2.49	2	1
1:A:58:TYR:CD2	1:A:70:VAL:HG11	0.42	2.49	13	1
1:A:46:ASN:HB3	1:A:154:ARG:O	0.42	2.14	16	1
1:A:28:ILE:N	1:A:28:ILE:CD1	0.42	2.79	3	1
1:A:87:MET:HG3	1:A:152:GLY:O	0.42	2.13	7	1
1:A:74:TYR:CZ	1:A:158:VAL:HG21	0.42	2.49	9	2
1:A:89:ALA:HB1	1:A:95:ASP:CB	0.42	2.43	21	2
1:A:119:GLU:HB3	1:A:121:THR:HG22	0.42	1.90	17	1
1:A:69:TYR:CE1	1:A:139:ARG:CZ	0.42	3.02	1	1
1:A:97:MET:HA	1:A:97:MET:CE	0.42	2.43	1	1
1:A:104:TYR:CD1	1:A:135:VAL:HG21	0.42	2.49	19	3
1:A:32:TYR:CD2	1:A:56:LEU:CD1	0.42	3.02	7	1
1:A:89:ALA:CB	1:A:93:PRO:HA	0.42	2.44	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:GLY:O	1:A:69:TYR:CG	0.42	2.73	10	1
1:A:69:TYR:CD1	1:A:139:ARG:HD3	0.42	2.50	13	1
1:A:64:ILE:HD12	1:A:68:THR:HG21	0.42	1.90	3	1
1:A:103:GLN:HB2	1:A:141:ILE:HD13	0.42	1.90	12	1
1:A:52:ALA:HB2	1:A:155:ASP:CB	0.42	2.44	2	1
1:A:69:TYR:CD1	1:A:139:ARG:HD2	0.42	2.49	18	3
1:A:100:ALA:C	1:A:118:VAL:O	0.42	2.63	7	5
1:A:87:MET:SD	1:A:153:VAL:HG22	0.42	2.54	8	1
1:A:102:ILE:HG12	1:A:140:LEU:HA	0.42	1.90	20	1
1:A:102:ILE:HG23	1:A:140:LEU:CG	0.42	2.45	2	1
1:A:35:ASN:OD1	1:A:69:TYR:CZ	0.42	2.73	15	7
1:A:151:LEU:HD11	1:A:153:VAL:CG1	0.42	2.44	3	1
1:A:28:ILE:CD1	1:A:78:ILE:CG2	0.42	2.98	7	3
1:A:63:ARG:O	1:A:64:ILE:HG23	0.42	2.15	12	1
1:A:51:ASN:ND2	1:A:53:SER:CB	0.42	2.83	17	1
1:A:59:LYS:O	1:A:61:PRO:CD	0.42	2.68	9	1
1:A:102:ILE:CD1	1:A:120:TYR:CE2	0.42	3.02	15	1
1:A:155:ASP:C	1:A:156:ILE:CG2	0.42	2.92	19	2
1:A:102:ILE:HG22	1:A:115:GLU:CB	0.42	2.44	20	1
1:A:84:GLU:CG	1:A:86:LEU:HD21	0.42	2.45	21	1
1:A:111:TRP:CZ3	1:A:138:VAL:C	0.42	2.98	2	1
1:A:64:ILE:C	1:A:64:ILE:HD12	0.42	2.40	5	1
1:A:87:MET:HG2	1:A:88:GLY:N	0.42	2.29	5	1
1:A:46:ASN:CG	1:A:54:THR:CG2	0.42	2.93	19	1
1:A:105:THR:HB	1:A:111:TRP:CD2	0.41	2.50	2	1
1:A:120:TYR:CD2	1:A:140:LEU:HD11	0.41	2.49	3	2
1:A:131:LEU:O	1:A:133:LEU:N	0.41	2.53	3	3
1:A:47:ILE:HG12	1:A:156:ILE:CG2	0.41	2.45	6	2
1:A:33:ILE:C	1:A:34:SER:OG	0.41	2.62	8	1
1:A:76:ASN:CB	1:A:77:PRO:HD2	0.41	2.45	16	1
1:A:87:MET:CG	1:A:152:GLY:O	0.41	2.68	17	1
1:A:159:ASN:OD1	1:A:159:ASN:N	0.41	2.53	17	1
1:A:105:THR:CB	1:A:110:GLU:O	0.41	2.68	14	3
1:A:59:LYS:HD2	1:A:150:TRP:CH2	0.41	2.50	6	1
1:A:38:ASP:CB	1:A:60:ASN:HB2	0.41	2.45	10	1
1:A:44:PRO:HB2	1:A:47:ILE:HD11	0.41	1.90	11	1
1:A:58:TYR:O	1:A:58:TYR:CG	0.41	2.73	9	1
1:A:59:LYS:HD2	1:A:150:TRP:CZ3	0.41	2.50	16	2
1:A:139:ARG:C	1:A:140:LEU:HD23	0.41	2.40	20	1
1:A:89:ALA:HB1	1:A:95:ASP:HB3	0.41	1.92	21	1
1:A:29:ILE:O	1:A:29:ILE:CG2	0.41	2.68	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:ASP:C	1:A:145:ALA:HB3	0.41	2.41	3	1
1:A:34:SER:HB2	1:A:58:TYR:CE2	0.41	2.50	4	2
1:A:36:ARG:NE	1:A:36:ARG:CA	0.41	2.84	6	1
1:A:35:ASN:CG	1:A:69:TYR:CZ	0.41	2.98	8	1
1:A:66:VAL:HG13	1:A:144:GLU:N	0.41	2.29	14	1
1:A:56:LEU:HD13	1:A:56:LEU:N	0.41	2.30	19	1
1:A:84:GLU:CB	1:A:126:ILE:O	0.41	2.68	3	1
1:A:46:ASN:OD1	1:A:54:THR:N	0.41	2.52	10	1
1:A:32:TYR:CD2	1:A:47:ILE:CD1	0.41	3.03	11	1
1:A:33:ILE:HD12	1:A:139:ARG:NE	0.41	2.31	12	1
1:A:136:ARG:CD	1:A:136:ARG:N	0.41	2.82	17	1
1:A:111:TRP:CE2	1:A:139:ARG:NH2	0.41	2.88	21	1
1:A:38:ASP:OD1	1:A:58:TYR:CG	0.41	2.73	1	1
1:A:102:ILE:HD11	1:A:120:TYR:CE2	0.41	2.50	1	1
1:A:60:ASN:ND2	1:A:61:PRO:HD3	0.41	2.31	2	1
1:A:74:TYR:N	1:A:74:TYR:CD1	0.41	2.87	2	1
1:A:46:ASN:O	1:A:50:ASN:HA	0.41	2.15	5	1
1:A:38:ASP:HB3	1:A:60:ASN:HB2	0.41	1.92	2	1
1:A:86:LEU:N	1:A:86:LEU:CD2	0.41	2.83	11	1
1:A:155:ASP:OD1	1:A:156:ILE:N	0.41	2.54	11	2
1:A:97:MET:HB3	1:A:120:TYR:O	0.41	2.15	13	1
1:A:33:ILE:CD1	1:A:138:VAL:O	0.41	2.64	21	1
1:A:85:PHE:O	1:A:126:ILE:CB	0.41	2.68	1	1
1:A:151:LEU:CD1	1:A:153:VAL:CG1	0.41	2.99	3	1
1:A:38:ASP:OD2	1:A:58:TYR:CG	0.41	2.74	4	1
1:A:38:ASP:CB	1:A:60:ASN:OD1	0.41	2.69	5	1
1:A:62:ASN:O	1:A:148:ASN:N	0.41	2.54	5	1
1:A:59:LYS:O	1:A:61:PRO:HD2	0.41	2.16	9	1
1:A:38:ASP:HB3	1:A:60:ASN:CB	0.41	2.46	10	1
1:A:56:LEU:N	1:A:56:LEU:CD1	0.41	2.83	11	1
1:A:103:GLN:NE2	1:A:141:ILE:HD13	0.41	2.31	13	1
1:A:72:VAL:N	1:A:138:VAL:HG23	0.41	2.31	17	1
1:A:158:VAL:HG13	1:A:159:ASN:HD22	0.41	1.75	19	1
1:A:46:ASN:CB	1:A:47:ILE:HD12	0.41	2.46	21	1
1:A:46:ASN:ND2	1:A:54:THR:HB	0.41	2.30	5	1
1:A:80:LEU:CD1	1:A:158:VAL:CG2	0.41	2.99	5	1
1:A:29:ILE:CD1	1:A:30:ALA:N	0.41	2.82	10	1
1:A:46:ASN:OD1	1:A:54:THR:CG2	0.41	2.69	11	1
1:A:96:THR:O	1:A:97:MET:C	0.41	2.64	20	2
1:A:32:TYR:CE1	1:A:58:TYR:OH	0.40	2.68	12	2
1:A:69:TYR:CD2	1:A:141:ILE:HD13	0.40	2.50	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ILE:CG1	1:A:48:PHE:CD1	0.40	3.03	11	1
1:A:59:LYS:HG2	1:A:150:TRP:CE2	0.40	2.51	11	1
1:A:86:LEU:CB	1:A:155:ASP:O	0.40	2.69	14	1
1:A:47:ILE:HG21	1:A:156:ILE:HD13	0.40	1.91	18	1
1:A:68:THR:HG22	1:A:97:MET:HE1	0.40	1.93	19	1
1:A:85:PHE:HB2	1:A:126:ILE:HD12	0.40	1.92	1	1
1:A:46:ASN:O	1:A:50:ASN:N	0.40	2.54	11	1
1:A:64:ILE:CG1	1:A:145:ALA:HB1	0.40	2.46	13	1
1:A:60:ASN:HB3	1:A:61:PRO:HD2	0.40	1.92	15	1
1:A:69:TYR:C	1:A:69:TYR:CD1	0.40	2.98	17	1
1:A:108:GLY:CA	1:A:136:ARG:CD	0.40	2.99	4	1
1:A:35:ASN:CB	1:A:67:GLY:O	0.40	2.69	7	1
1:A:86:LEU:O	1:A:155:ASP:O	0.40	2.40	9	1
1:A:46:ASN:ND2	1:A:54:THR:CG2	0.40	2.85	19	1
1:A:158:VAL:O	1:A:159:ASN:CB	0.40	2.70	19	1
1:A:31:THR:HA	1:A:48:PHE:CE1	0.40	2.50	21	1
1:A:105:THR:HB	1:A:111:TRP:CE2	0.40	2.52	2	1
1:A:87:MET:HE3	1:A:87:MET:HB2	0.40	1.84	3	1
1:A:80:LEU:CD2	1:A:131:LEU:CD2	0.40	3.00	8	1
1:A:43:ASN:ND2	1:A:43:ASN:N	0.40	2.69	11	1
1:A:74:TYR:CE1	1:A:158:VAL:HG21	0.40	2.51	12	1
1:A:30:ALA:O	1:A:48:PHE:CE1	0.40	2.74	16	1
1:A:81:ASN:ND2	1:A:159:ASN:ND2	0.40	2.69	18	1
1:A:85:PHE:CZ	1:A:102:ILE:HD11	0.40	2.51	20	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	132/164 (80%)	89±3 (67±2%)	31±3 (23±2%)	13±3 (10±2%)	1	10
All	All	2772/3444 (80%)	1863 (67%)	642 (23%)	267 (10%)	1	10

All 34 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	VAL	20
1	A	117	GLY	19
1	A	116	GLU	18
1	A	66	VAL	17
1	A	97	MET	17
1	A	60	ASN	15
1	A	137	GLY	14
1	A	50	ASN	14
1	A	79	THR	14
1	A	132	ASP	13
1	A	144	GLU	13
1	A	120	TYR	9
1	A	42	GLY	9
1	A	148	ASN	9
1	A	63	ARG	8
1	A	82	ASN	7
1	A	52	ALA	7
1	A	145	ALA	6
1	A	51	ASN	5
1	A	62	ASN	5
1	A	61	PRO	4
1	A	70	VAL	4
1	A	45	ASP	4
1	A	156	ILE	3
1	A	68	THR	3
1	A	59	LYS	2
1	A	93	PRO	1
1	A	38	ASP	1
1	A	95	ASP	1
1	A	41	THR	1
1	A	113	ASP	1
1	A	28	ILE	1
1	A	40	PRO	1
1	A	155	ASP	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	115/143 (80%)	78±12 (68±10%)	34±6 (29±5%)	1	18
All	All	2340/3003 (78%)	1631 (70%)	709 (30%)	1	16

All 94 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	121	THR	21
1	A	122	MET	21
1	A	140	LEU	21
1	A	31	THR	20
1	A	33	ILE	20
1	A	70	VAL	20
1	A	106	VAL	20
1	A	112	ILE	20
1	A	87	MET	19
1	A	68	THR	18
1	A	126	ILE	18
1	A	101	LYS	17
1	A	56	LEU	17
1	A	102	ILE	17
1	A	141	ILE	15
1	A	54	THR	14
1	A	57	VAL	14
1	A	64	ILE	12
1	A	109	ARG	12
1	A	138	VAL	12
1	A	60	ASN	12
1	A	127	LYS	11
1	A	115	GLU	11
1	A	151	LEU	10
1	A	73	LYS	10
1	A	59	LYS	9
1	A	75	SER	9
1	A	96	THR	9
1	A	144	GLU	9
1	A	46	ASN	9
1	A	63	ARG	9
1	A	133	LEU	9
1	A	107	ASP	9
1	A	99	LYS	8
1	A	110	GLU	8
1	A	119	GLU	8

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Mol	Chain	Res	Type	Models (Total)
1	A	146	ARG	8
1	A	156	ILE	8
1	A	72	VAL	8
1	A	79	THR	8
1	A	86	LEU	8
1	A	134	LYS	8
1	A	136	ARG	7
1	A	38	ASP	7
1	A	37	GLN	7
1	A	103	GLN	6
1	A	36	ARG	6
1	A	76	ASN	6
1	A	91	SER	5
1	A	95	ASP	5
1	A	98	GLN	5
1	A	154	ARG	5
1	A	28	ILE	5
1	A	84	GLU	5
1	A	81	ASN	4
1	A	82	ASN	4
1	A	157	ASN	4
1	A	153	VAL	4
1	A	55	GLU	4
1	A	78	ILE	4
1	A	159	ASN	4
1	A	147	GLU	4
1	A	53	SER	3
1	A	97	MET	3
1	A	29	ILE	3
1	A	45	ASP	3
1	A	50	ASN	3
1	A	43	ASN	3
1	A	116	GLU	3
1	A	34	SER	3
1	A	41	THR	3
1	A	143	THR	3
1	A	80	LEU	3
1	A	148	ASN	3
1	A	118	VAL	2
1	A	132	ASP	2
1	A	74	TYR	2
1	A	47	ILE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	128	VAL	2
1	A	135	VAL	2
1	A	129	GLU	1
1	A	51	ASN	1
1	A	65	ASP	1
1	A	92	ASN	1
1	A	149	THR	1
1	A	58	TYR	1
1	A	155	ASP	1
1	A	83	VAL	1
1	A	69	TYR	1
1	A	114	LEU	1
1	A	48	PHE	1
1	A	62	ASN	1
1	A	85	PHE	1
1	A	131	LEU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1735
Number of shifts mapped to atoms	1735
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	14

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	143	-0.24 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	134	-0.20 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}'$	134	0.26 ± 0.21	None needed (< 0.5 ppm)
^{15}N	136	0.26 ± 0.58	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 1616 atoms were assigned a chemical shift out of a possible 1792. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	650/657 (99%)	267/267 (100%)	257/264 (97%)	126/126 (100%)
Sidechain	914/1037 (88%)	621/669 (93%)	274/321 (85%)	19/47 (40%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	52/98 (53%)	26/46 (57%)	24/50 (48%)	2/2 (100%)
Overall	1616/1792 (90%)	914/982 (93%)	555/635 (87%)	147/175 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1735 atoms were assigned a chemical shift out of a possible 2198. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	701/816 (86%)	288/332 (87%)	277/328 (84%)	136/156 (87%)
Sidechain	982/1228 (80%)	666/792 (84%)	296/380 (78%)	20/56 (36%)
Aromatic	52/154 (34%)	26/74 (35%)	24/64 (38%)	2/16 (12%)
Overall	1735/2198 (79%)	980/1198 (82%)	597/772 (77%)	158/228 (69%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	139	ARG	HD3	-0.69	1.81 – 4.39	-14.7
1	A	139	ARG	HD2	0.81	1.97 – 4.26	-10.1
1	A	87	MET	CG	20.44	25.46 – 38.60	-8.8
1	A	59	LYS	HG3	-0.91	0.04 – 2.67	-8.6
1	A	59	LYS	HE3	1.30	1.92 – 3.89	-8.2
1	A	105	THR	HB	1.61	2.57 – 5.77	-8.0
1	A	105	THR	HG21	-0.19	0.08 – 2.19	-6.3
1	A	105	THR	HG22	-0.19	0.08 – 2.19	-6.3
1	A	105	THR	HG23	-0.19	0.08 – 2.19	-6.3
1	A	59	LYS	HD3	0.44	0.54 – 2.65	-5.5
1	A	140	LEU	HB3	-0.39	-0.26 – 3.31	-5.4
1	A	36	ARG	HG3	0.11	0.15 – 2.94	-5.2
1	A	90	ASN	H	11.42	5.28 – 11.36	5.1
1	A	40	PRO	HB2	0.36	0.37 – 3.78	-5.0

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble

composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

