Full wwPDB NMR Structure Validation Report (i)

Jun 17, 2024 – 07:54 AM EDT

PDB ID	:	5MMU
BMRB ID	:	25968
Title	:	NMR solution structure of the major apple allergen Mal d 1
Authors	:	Ahammer, L.; Grutsch, S.; Kamenik, A.S.; Liedl, K.R.; Tollinger, M.
Deposited on	:	2016-12-12

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

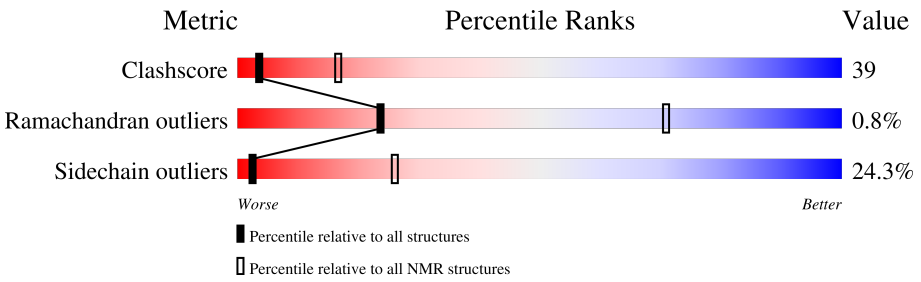
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	158	47% 42% 10% •

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:2-A:158 (157)	0.54	10

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 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2462 atoms, of which 1223 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major allergen Mal d 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	158	2462	792	1223	200	246	1	0

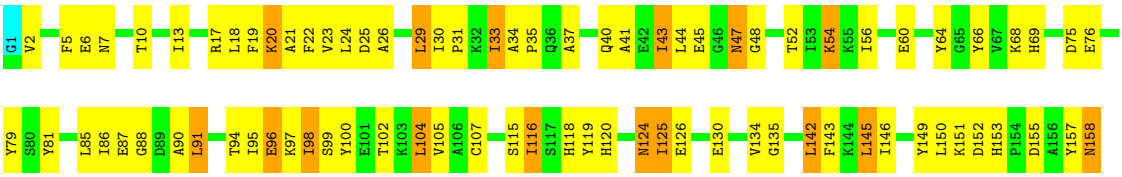
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Major allergen Mal d 1

Chain A: 47% 42% 10%



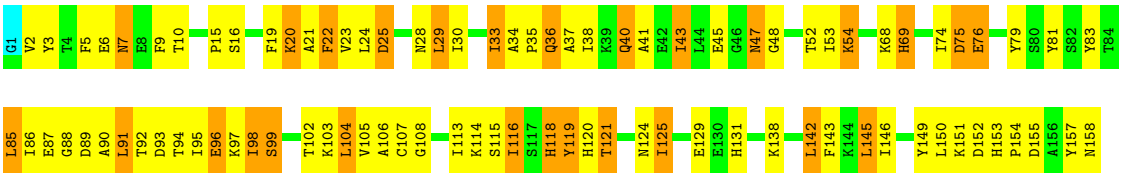
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Major allergen Mal d 1

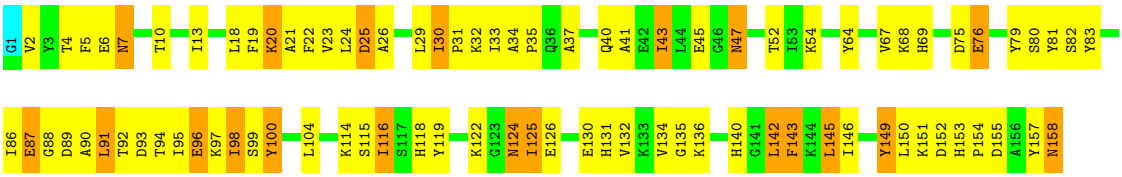
Chain A: 42% 40% 17%



4.2.2 Score per residue for model 2

• Molecule 1: Major allergen Mal d 1

Chain A: 44% 42% 13%



4.2.3 Score per residue for model 3

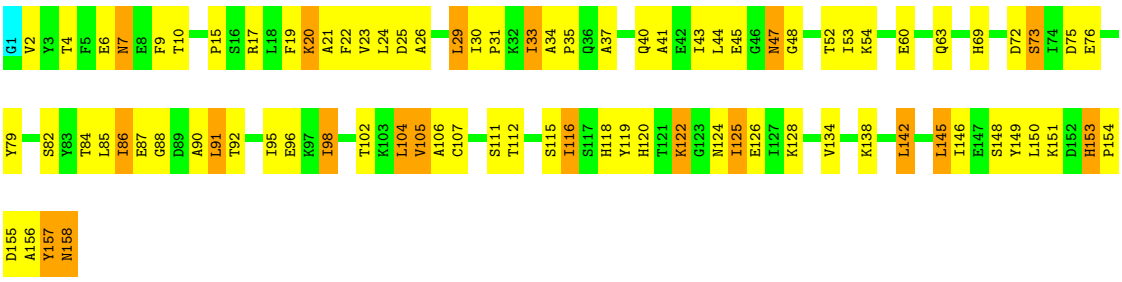
• Molecule 1: Major allergen Mal d 1

Chain A: 44% 42% 14%

4.2.4 Score per residue for model 4

• Molecule 1: Major allergen Mal d 1

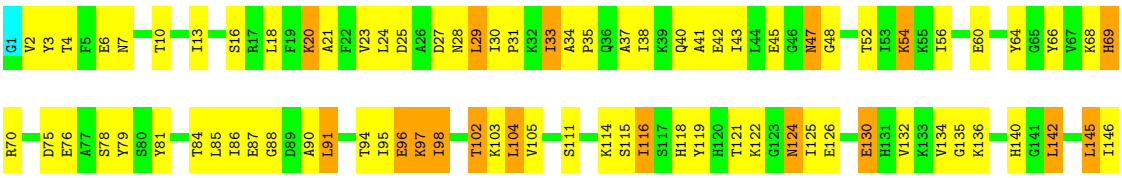
Chain A: 46% 42% 12%

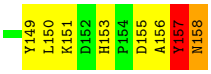


4.2.5 Score per residue for model 5

• Molecule 1: Major allergen Mal d 1

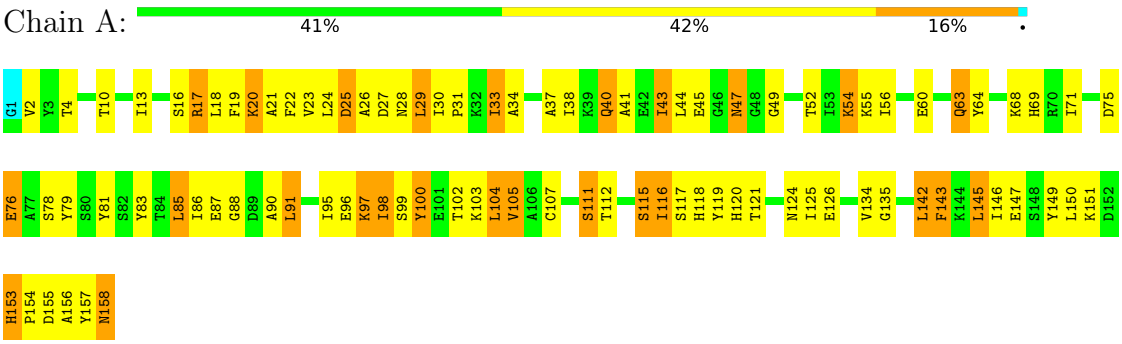
Chain A: 43% 44% 11%





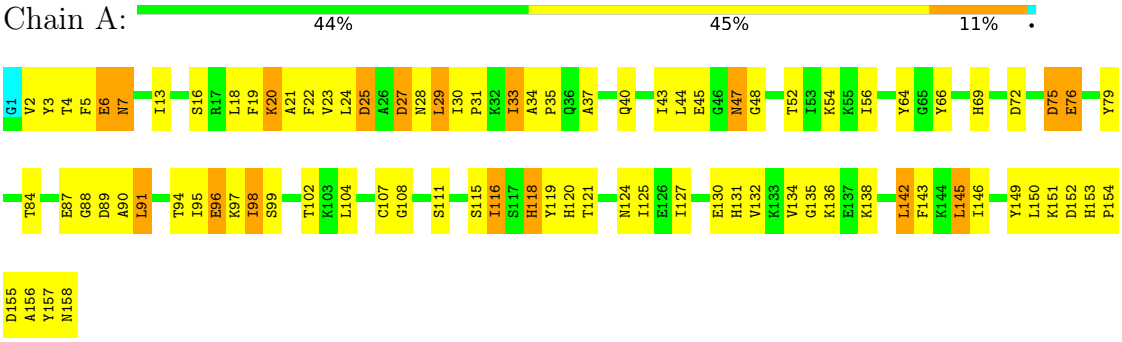
4.2.6 Score per residue for model 6

• Molecule 1: Major allergen Mal d 1



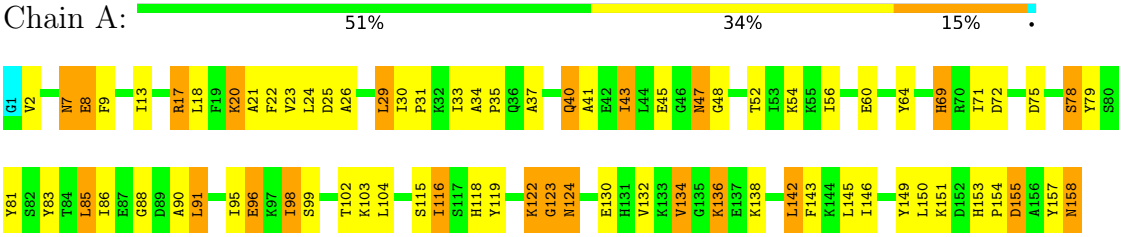
4.2.7 Score per residue for model 7

• Molecule 1: Major allergen Mal d 1



4.2.8 Score per residue for model 8

• Molecule 1: Major allergen Mal d 1



4.2.9 Score per residue for model 9

- Molecule 1: Major allergen Mal d 1

Chain A: 49% 34% 16%

G1 V2 F5 E6 N7 E8 F9 T10 F19 K20 A21 F22 V23 L24 D25 A26 D27 N28 L29 I30 P31 K32 I33 A34 P35 Q36 A37 Q40 I43 L44 E45 G46 N47 G48 T52 I53 K54 K55 F58 Y64 K68 D75 E76 Y79 S80 Y81 T84 L85 I86

E87 G88 D89 A90 L91 T94 I95 E96 K97 I98 S99 Y100 E101 T102 K103 L104 V105 S115 I116 S117 H118 Y119 H120 N124 I125 E126 E130 V134 H140 G141 L142 F143 K144 L145 I146 Y149 L150 K151 D152 H153 P154 D155 A156 Y157 N158

4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Major allergen Mal d 1

Chain A: 42% 43% 15%

G1 V2 F5 E8 P15 S16 R17 L18 F19 K20 A21 F22 V23 L24 D25 A26 L29 I30 P31 K32 I33 A34 P35 Q36 A37 I38 K39 Q40 A41 E42 I43 L44 E45 G46 N47 G48 T52 I53 K54 K55 I56 G59 S62 Q63 Y64 G65 Y66 H69 D72 S73 I74

D75 E76 Y79 S80 Y81 S82 Y83 T84 L85 I86 E87 G88 D89 A90 L91 T92 D93 T94 I95 E96 K97 I98 S99 T102 K103 L104 V105 A106 C107 G108 S115 I116 Y119 N124 I125 E126 E130 H131 V134 G135 K138 A139 H140 G141 L142 L145 I146 Y149 L150 K151

D152 H153 P154 D155 A156 Y157 N158

4.2.11 Score per residue for model 11

- Molecule 1: Major allergen Mal d 1

Chain A: 42% 43% 14%

G1 V2 Y3 T4 P15 S16 R17 L18 F19 K20 A21 F22 V23 L24 D25 A26 D27 N28 L29 I30 P31 K32 I33 A34 P35 I38 K39 Q40 A41 E42 I43 L44 E45 G46 N47 G48 T52 I53 K54 K55 I56 E60 G61 S62 Q63 Y64 G65 Y66 V67 K68 H69 D72 S73 I74 D75

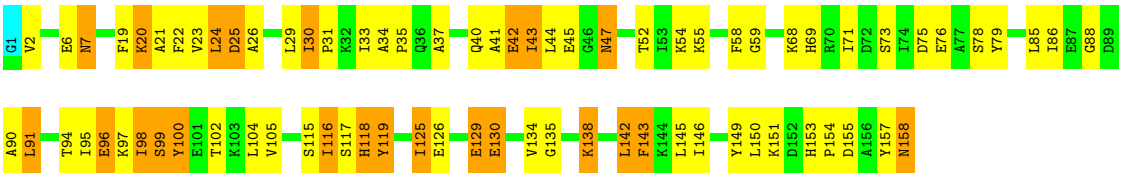
E76 Y79 S80 Y81 S82 Y83 T84 L85 I86 E87 G88 D89 A90 L91 T92 I95 E96 K97 I98 S99 T102 K103 L104 V105 A106 T112 S115 I116 S117 H118 Y119 K122 I125 E126 E130 K133 V134 E137 K138 L142 F143 K144 L145 I146 Y149 L150 K151 D152

H153 P154 D155 A156 Y157 N158

4.2.12 Score per residue for model 12

- Molecule 1: Major allergen Mal d 1

Chain A: 51% 34% 15%



4.2.13 Score per residue for model 13

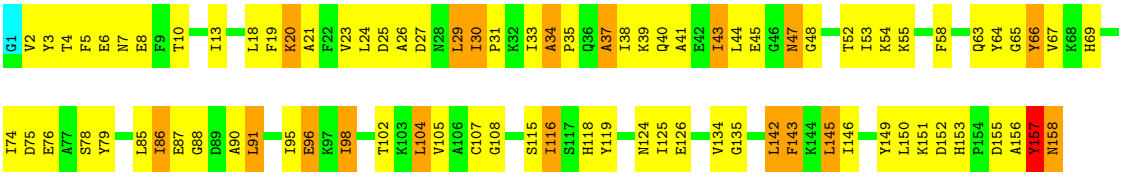
- Molecule 1: Major allergen Mal d 1

Chain A: 47% 44% 9%

4.2.14 Score per residue for model 14

- Molecule 1: Major allergen Mal d 1

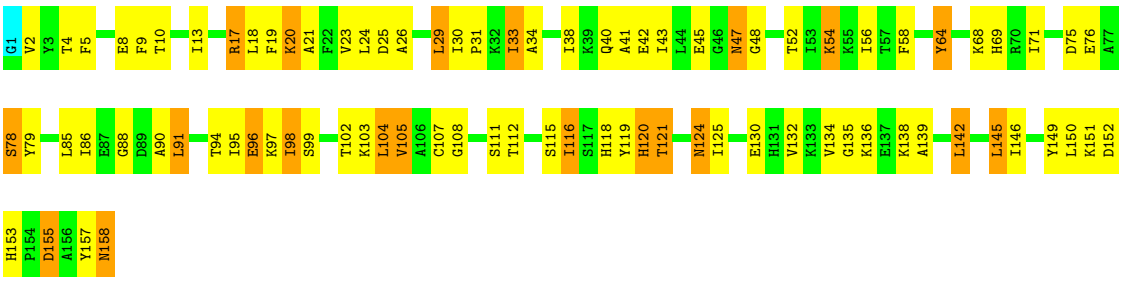
Chain A: 45% 42% 11%



4.2.15 Score per residue for model 15

- Molecule 1: Major allergen Mal d 1

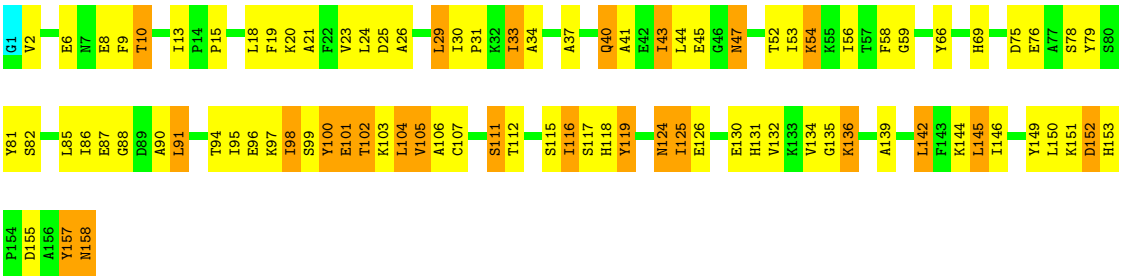
Chain A: 45% 41% 13%



4.2.16 Score per residue for model 16

- Molecule 1: Major allergen Mal d 1

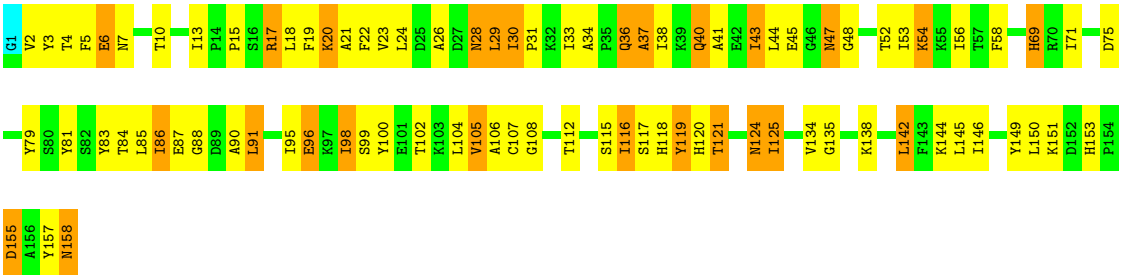
Chain A: 42% 41% 16%



4.2.17 Score per residue for model 17

- Molecule 1: Major allergen Mal d 1

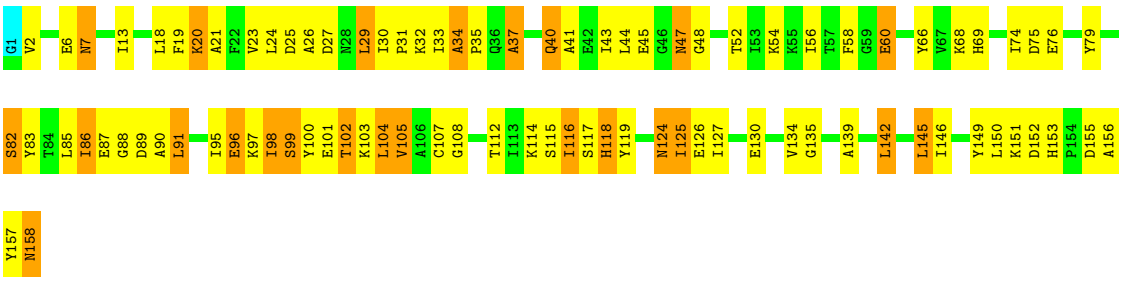
Chain A: 44% 39% 16%



4.2.18 Score per residue for model 18

- Molecule 1: Major allergen Mal d 1

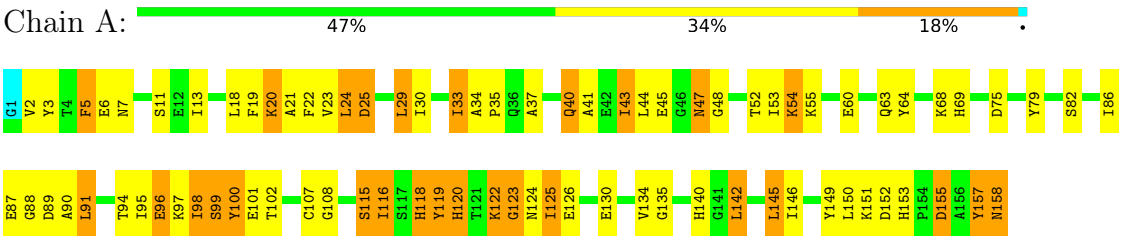
Chain A: 43% 41% 15%



4.2.19 Score per residue for model 19

- Molecule 1: Major allergen Mal d 1

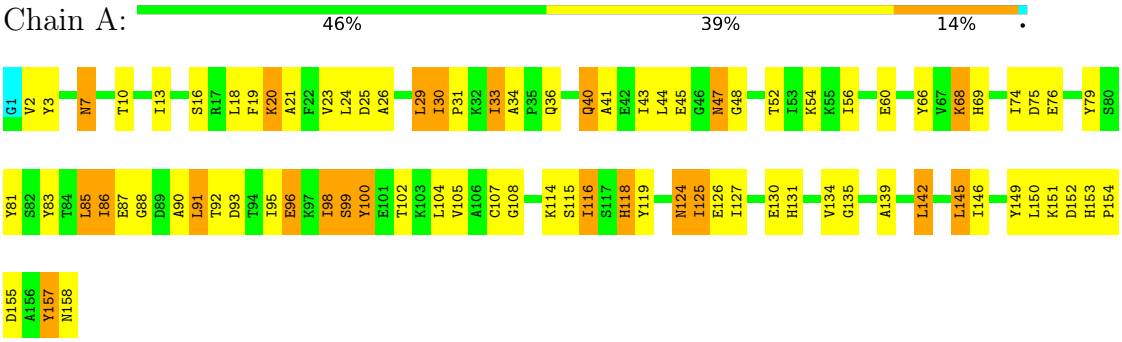
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Major allergen Mal d 1

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 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**
Amber	refinement	
Xplor-NIH	structure calculation	2.42

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	1680
Number of shifts mapped to atoms	1680
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1235	1218	1218	96±11
All	All	24700	24360	24360	1930

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:LEU:HD12	1:A:25:ASP:N	0.94	1.77	14	8
1:A:2:VAL:HG21	1:A:118:HIS:CD2	0.90	2.01	1	2
1:A:45:GLU:O	1:A:52:THR:HG23	0.89	1.66	17	20
1:A:116:ILE:HD13	1:A:116:ILE:N	0.88	1.83	20	20
1:A:24:LEU:H	1:A:24:LEU:HD13	0.86	1.29	19	1
1:A:91:LEU:N	1:A:91:LEU:HD22	0.85	1.87	17	17
1:A:26:ALA:O	1:A:30:ILE:HG22	0.85	1.70	13	1
1:A:21:ALA:HB2	1:A:150:LEU:HD11	0.83	1.49	6	20
1:A:2:VAL:HG21	1:A:118:HIS:CG	0.80	2.11	1	1
1:A:104:LEU:N	1:A:104:LEU:HD23	0.80	1.91	6	11
1:A:29:LEU:HD13	1:A:146:ILE:HG23	0.80	1.54	16	4
1:A:91:LEU:HD23	1:A:91:LEU:N	0.80	1.91	18	3
1:A:24:LEU:HD23	1:A:157:TYR:CD2	0.79	2.12	17	5
1:A:23:VAL:HG23	1:A:24:LEU:CD1	0.79	2.07	13	12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:PHE:O	1:A:23:VAL:HG22	0.79	1.77	6	18
1:A:115:SER:C	1:A:116:ILE:HD13	0.77	2.00	15	20
1:A:24:LEU:HD13	1:A:24:LEU:N	0.77	1.95	19	2
1:A:2:VAL:HG23	1:A:119:TYR:C	0.76	2.01	12	20
1:A:44:LEU:HD12	1:A:44:LEU:N	0.76	1.95	13	4
1:A:24:LEU:HD23	1:A:157:TYR:CD1	0.76	2.16	9	6
1:A:20:LYS:CB	1:A:24:LEU:HD21	0.76	2.11	12	2
1:A:118:HIS:O	1:A:118:HIS:ND1	0.75	2.19	1	1
1:A:23:VAL:HG23	1:A:24:LEU:HD13	0.75	1.58	12	12
1:A:150:LEU:H	1:A:150:LEU:HD22	0.75	1.41	20	11
1:A:29:LEU:HD12	1:A:146:ILE:HG23	0.75	1.58	5	6
1:A:34:ALA:HB2	1:A:145:LEU:CG	0.74	2.12	15	15
1:A:95:ILE:HG21	1:A:98:ILE:CD1	0.73	2.13	4	17
1:A:56:ILE:HD13	1:A:69:HIS:CD2	0.73	2.18	7	2
1:A:24:LEU:HD13	1:A:157:TYR:CD1	0.73	2.18	5	2
1:A:42:GLU:C	1:A:54:LYS:HZ1	0.73	1.87	11	1
1:A:24:LEU:HD22	1:A:25:ASP:N	0.73	1.99	19	2
1:A:56:ILE:HD12	1:A:56:ILE:N	0.72	2.00	6	10
1:A:29:LEU:HD21	1:A:149:TYR:CD2	0.72	2.19	10	4
1:A:34:ALA:HB2	1:A:145:LEU:HG	0.72	1.60	17	11
1:A:41:ALA:HB1	1:A:54:LYS:NZ	0.71	2.01	15	2
1:A:34:ALA:HB1	1:A:37:ALA:HB3	0.70	1.62	12	12
1:A:24:LEU:HD13	1:A:24:LEU:H	0.70	1.45	12	1
1:A:90:ALA:C	1:A:91:LEU:HD23	0.70	2.07	20	3
1:A:29:LEU:HD21	1:A:149:TYR:CG	0.70	2.20	15	4
1:A:34:ALA:HB2	1:A:145:LEU:HD22	0.70	1.60	6	1
1:A:25:ASP:O	1:A:29:LEU:HB2	0.69	1.87	10	8
1:A:5:PHE:CE2	1:A:7:ASN:ND2	0.69	2.61	19	1
1:A:116:ILE:N	1:A:116:ILE:CD1	0.68	2.56	12	20
1:A:149:TYR:O	1:A:153:HIS:N	0.68	2.27	17	20
1:A:83:TYR:CE2	1:A:100:TYR:CD1	0.68	2.81	20	1
1:A:124:ASN:H	1:A:124:ASN:HD22	0.68	1.32	16	7
1:A:142:LEU:N	1:A:142:LEU:HD23	0.68	2.04	14	19
1:A:119:TYR:N	1:A:119:TYR:CD2	0.68	2.61	9	4
1:A:146:ILE:O	1:A:150:LEU:HD22	0.67	1.89	3	20
1:A:34:ALA:HB2	1:A:145:LEU:CD2	0.67	2.18	6	10
1:A:20:LYS:CB	1:A:24:LEU:HD11	0.67	2.20	18	8
1:A:30:ILE:HG23	1:A:31:PRO:HD3	0.66	1.64	13	1
1:A:91:LEU:HD22	1:A:91:LEU:H	0.66	1.50	17	17
1:A:100:TYR:CD1	1:A:100:TYR:N	0.66	2.63	20	1
1:A:21:ALA:O	1:A:26:ALA:HB2	0.66	1.90	2	11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ILE:HD12	1:A:145:LEU:C	0.66	2.11	13	14
1:A:119:TYR:CD1	1:A:119:TYR:N	0.66	2.62	16	5
1:A:34:ALA:N	1:A:145:LEU:HD11	0.66	2.05	20	3
1:A:43:ILE:HA	1:A:54:LYS:HB2	0.65	1.66	9	1
1:A:155:ASP:O	1:A:158:ASN:ND2	0.65	2.30	13	17
1:A:150:LEU:HD22	1:A:150:LEU:H	0.65	1.50	9	9
1:A:69:HIS:N	1:A:69:HIS:ND1	0.65	2.43	11	1
1:A:103:LYS:C	1:A:104:LEU:HD23	0.65	2.12	15	9
1:A:39:LYS:H	1:A:39:LYS:CD	0.64	2.06	13	1
1:A:95:ILE:HD11	1:A:127:ILE:HD12	0.64	1.69	7	3
1:A:33:ILE:HD12	1:A:145:LEU:HB3	0.64	1.70	9	12
1:A:150:LEU:HD22	1:A:150:LEU:N	0.64	2.08	20	20
1:A:34:ALA:HB2	1:A:145:LEU:HD23	0.64	1.68	1	7
1:A:81:TYR:CE2	1:A:83:TYR:CD1	0.64	2.86	13	2
1:A:91:LEU:N	1:A:91:LEU:CD2	0.63	2.61	1	20
1:A:81:TYR:CE2	1:A:83:TYR:CD2	0.63	2.85	6	2
1:A:17:ARG:N	1:A:17:ARG:CD	0.63	2.61	17	2
1:A:20:LYS:HB3	1:A:24:LEU:HD21	0.63	1.69	12	2
1:A:34:ALA:HB2	1:A:145:LEU:CD1	0.63	2.23	15	4
1:A:17:ARG:N	1:A:17:ARG:HE	0.63	1.92	15	2
1:A:24:LEU:HD12	1:A:24:LEU:N	0.63	2.08	20	1
1:A:85:LEU:HD13	1:A:90:ALA:HB1	0.63	1.69	14	9
1:A:75:ASP:O	1:A:79:TYR:N	0.62	2.31	14	20
1:A:24:LEU:HD23	1:A:157:TYR:CG	0.62	2.28	16	4
1:A:44:LEU:HD11	1:A:55:LYS:CB	0.62	2.24	14	3
1:A:21:ALA:O	1:A:146:ILE:HG21	0.62	1.95	20	5
1:A:24:LEU:CD1	1:A:24:LEU:N	0.62	2.63	13	10
1:A:42:GLU:CA	1:A:54:LYS:HZ1	0.62	2.08	11	1
1:A:22:PHE:CE1	1:A:143:PHE:CE2	0.61	2.88	12	2
1:A:40:GLN:NE2	1:A:41:ALA:N	0.61	2.48	18	4
1:A:121:THR:HG21	1:A:126:GLU:HA	0.61	1.73	5	2
1:A:40:GLN:HE21	1:A:41:ALA:N	0.61	1.94	16	8
1:A:20:LYS:HB2	1:A:24:LEU:HD11	0.61	1.72	2	8
1:A:134:VAL:HG13	1:A:135:GLY:N	0.61	2.10	2	1
1:A:39:LYS:H	1:A:39:LYS:HD2	0.61	1.55	13	1
1:A:33:ILE:HG13	1:A:145:LEU:HD12	0.61	1.71	16	2
1:A:81:TYR:CE1	1:A:83:TYR:CD2	0.61	2.89	8	1
1:A:13:ILE:O	1:A:18:LEU:HD11	0.61	1.96	20	13
1:A:69:HIS:CE1	1:A:83:TYR:CD1	0.61	2.89	18	2
1:A:24:LEU:N	1:A:24:LEU:HD12	0.61	2.09	13	9
1:A:86:ILE:HD13	1:A:87:GLU:N	0.61	2.11	17	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:LEU:HD13	1:A:157:TYR:CG	0.60	2.31	4	4
1:A:29:LEU:HD22	1:A:33:ILE:HD11	0.60	1.73	15	3
1:A:47:ASN:H	1:A:47:ASN:HD22	0.60	1.38	19	12
1:A:124:ASN:H	1:A:124:ASN:ND2	0.60	1.94	16	7
1:A:69:HIS:CE1	1:A:83:TYR:CD2	0.60	2.89	20	1
1:A:99:SER:OG	1:A:118:HIS:CE1	0.60	2.55	1	1
1:A:37:ALA:HB2	1:A:142:LEU:HD22	0.60	1.73	14	5
1:A:21:ALA:CB	1:A:150:LEU:HD11	0.60	2.25	6	4
1:A:40:GLN:NE2	1:A:41:ALA:H	0.59	1.95	12	8
1:A:34:ALA:HB2	1:A:145:LEU:HD11	0.59	1.73	16	3
1:A:63:GLN:NE2	1:A:63:GLN:H	0.59	1.95	10	2
1:A:29:LEU:HD21	1:A:149:TYR:CD1	0.59	2.33	15	3
1:A:69:HIS:CE1	1:A:85:LEU:CD2	0.59	2.86	16	4
1:A:44:LEU:N	1:A:44:LEU:CD1	0.59	2.66	13	5
1:A:2:VAL:HG23	1:A:119:TYR:O	0.59	1.98	5	20
1:A:104:LEU:N	1:A:104:LEU:CD2	0.58	2.62	15	8
1:A:37:ALA:CB	1:A:142:LEU:HD22	0.58	2.27	14	3
1:A:52:THR:C	1:A:53:ILE:HD12	0.58	2.18	17	5
1:A:7:ASN:ND2	1:A:7:ASN:N	0.58	2.52	12	6
1:A:146:ILE:HG22	1:A:150:LEU:HD21	0.58	1.76	5	7
1:A:30:ILE:HG13	1:A:146:ILE:HD11	0.58	1.76	1	6
1:A:21:ALA:HB1	1:A:146:ILE:CG2	0.57	2.29	16	10
1:A:4:THR:HG23	1:A:118:HIS:CE1	0.57	2.34	4	4
1:A:157:TYR:CG	1:A:157:TYR:O	0.57	2.57	20	4
1:A:33:ILE:HD12	1:A:145:LEU:O	0.57	1.98	20	3
1:A:29:LEU:CD2	1:A:33:ILE:HD11	0.57	2.29	15	1
1:A:56:ILE:N	1:A:56:ILE:CD1	0.57	2.67	7	9
1:A:30:ILE:O	1:A:34:ALA:HB3	0.56	2.00	17	5
1:A:88:GLY:C	1:A:90:ALA:H	0.56	2.04	8	20
1:A:30:ILE:N	1:A:31:PRO:HD2	0.56	2.15	20	14
1:A:20:LYS:HD3	1:A:156:ALA:O	0.56	2.00	5	2
1:A:81:TYR:CE1	1:A:83:TYR:CD1	0.56	2.94	11	2
1:A:4:THR:HG23	1:A:118:HIS:NE2	0.56	2.16	17	2
1:A:41:ALA:HB1	1:A:54:LYS:HE2	0.56	1.77	11	1
1:A:121:THR:HG21	1:A:125:ILE:O	0.56	1.99	17	3
1:A:30:ILE:N	1:A:31:PRO:CD	0.56	2.68	15	8
1:A:47:ASN:ND2	1:A:47:ASN:N	0.56	2.54	19	6
1:A:42:GLU:N	1:A:54:LYS:NZ	0.56	2.54	15	3
1:A:38:ILE:HD12	1:A:38:ILE:N	0.56	2.16	14	3
1:A:24:LEU:HD12	1:A:25:ASP:H	0.56	1.60	4	6
1:A:153:HIS:CD2	1:A:155:ASP:OD1	0.56	2.59	3	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ASN:H	1:A:47:ASN:ND2	0.55	1.99	19	7
1:A:95:ILE:HG21	1:A:98:ILE:HD13	0.55	1.78	7	5
1:A:153:HIS:CG	1:A:155:ASP:OD1	0.55	2.59	12	1
1:A:107:CYS:SG	1:A:108:GLY:N	0.55	2.79	19	9
1:A:17:ARG:N	1:A:17:ARG:NE	0.55	2.54	15	2
1:A:130:GLU:N	1:A:130:GLU:OE1	0.55	2.40	16	2
1:A:63:GLN:NE2	1:A:64:TYR:CE2	0.55	2.74	14	1
1:A:146:ILE:O	1:A:150:LEU:CD2	0.55	2.55	2	20
1:A:24:LEU:N	1:A:24:LEU:CD1	0.55	2.70	19	1
1:A:44:LEU:HD11	1:A:55:LYS:HB3	0.55	1.79	14	3
1:A:29:LEU:O	1:A:33:ILE:CG1	0.55	2.55	19	4
1:A:96:GLU:OE2	1:A:120:HIS:CE1	0.55	2.60	19	3
1:A:4:THR:OG1	1:A:118:HIS:CE1	0.54	2.60	7	5
1:A:29:LEU:HD13	1:A:149:TYR:CD1	0.54	2.37	11	1
1:A:16:SER:C	1:A:20:LYS:HZ2	0.54	2.06	13	1
1:A:86:ILE:HD13	1:A:87:GLU:H	0.54	1.62	20	1
1:A:119:TYR:CD2	1:A:119:TYR:N	0.54	2.75	19	2
1:A:153:HIS:CE1	1:A:155:ASP:OD2	0.54	2.60	3	1
1:A:22:PHE:CE2	1:A:143:PHE:CE2	0.54	2.95	7	1
1:A:36:GLN:HE21	1:A:37:ALA:N	0.54	1.99	17	1
1:A:15:PRO:CG	1:A:106:ALA:HB2	0.54	2.33	16	2
1:A:23:VAL:HG23	1:A:24:LEU:N	0.54	2.17	14	7
1:A:95:ILE:CD1	1:A:127:ILE:HD12	0.54	2.33	7	1
1:A:5:PHE:CD1	1:A:7:ASN:ND2	0.54	2.76	9	1
1:A:142:LEU:O	1:A:145:LEU:HB2	0.54	2.02	15	3
1:A:6:GLU:C	1:A:7:ASN:HD22	0.54	2.06	19	9
1:A:72:ASP:OD1	1:A:73:SER:N	0.54	2.41	4	1
1:A:43:ILE:HG23	1:A:54:LYS:HG2	0.54	1.80	14	9
1:A:24:LEU:HD12	1:A:24:LEU:C	0.54	2.22	14	8
1:A:33:ILE:HD12	1:A:145:LEU:HB2	0.53	1.79	6	1
1:A:157:TYR:O	1:A:157:TYR:CD1	0.53	2.61	13	1
1:A:156:ALA:HB1	1:A:157:TYR:CE1	0.53	2.38	7	2
1:A:20:LYS:NZ	1:A:156:ALA:O	0.53	2.41	9	1
1:A:47:ASN:HD22	1:A:48:GLY:N	0.53	2.02	3	15
1:A:69:HIS:NE2	1:A:83:TYR:CD2	0.53	2.76	10	1
1:A:154:PRO:O	1:A:158:ASN:ND2	0.53	2.41	20	2
1:A:24:LEU:HD22	1:A:25:ASP:H	0.53	1.63	19	2
1:A:124:ASN:HD22	1:A:125:ILE:N	0.53	2.00	17	1
1:A:25:ASP:CB	1:A:157:TYR:CZ	0.53	2.91	6	2
1:A:17:ARG:NH1	1:A:154:PRO:O	0.53	2.41	8	1
1:A:27:ASP:CB	1:A:54:LYS:NZ	0.53	2.71	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:PHE:CD2	1:A:7:ASN:ND2	0.53	2.77	2	2
1:A:13:ILE:HB	1:A:18:LEU:HD21	0.53	1.81	2	8
1:A:76:GLU:O	1:A:79:TYR:CD1	0.53	2.62	15	8
1:A:52:THR:HG22	1:A:71:ILE:HD13	0.53	1.80	12	6
1:A:101:GLU:CD	1:A:102:THR:N	0.53	2.62	16	2
1:A:76:GLU:H	1:A:76:GLU:CD	0.52	2.07	15	3
1:A:83:TYR:CZ	1:A:100:TYR:CD1	0.52	2.96	20	1
1:A:69:HIS:ND1	1:A:69:HIS:C	0.52	2.63	8	1
1:A:69:HIS:NE2	1:A:83:TYR:CG	0.52	2.77	17	2
1:A:130:GLU:O	1:A:134:VAL:HG12	0.52	2.05	2	1
1:A:157:TYR:CD1	1:A:157:TYR:O	0.52	2.62	16	2
1:A:33:ILE:HD13	1:A:149:TYR:HB2	0.52	1.80	5	11
1:A:68:LYS:HB3	1:A:86:ILE:HD11	0.52	1.81	12	6
1:A:21:ALA:HB1	1:A:146:ILE:HG23	0.52	1.81	12	5
1:A:91:LEU:HD22	1:A:98:ILE:HD11	0.52	1.80	18	3
1:A:143:PHE:CD1	1:A:143:PHE:O	0.52	2.62	14	1
1:A:69:HIS:CE1	1:A:85:LEU:HD21	0.52	2.39	6	2
1:A:130:GLU:O	1:A:134:VAL:HG22	0.52	2.05	18	8
1:A:4:THR:OG1	1:A:118:HIS:CD2	0.52	2.63	14	3
1:A:44:LEU:CD1	1:A:44:LEU:N	0.52	2.73	17	6
1:A:26:ALA:O	1:A:30:ILE:CD1	0.52	2.58	11	1
1:A:84:THR:HG23	1:A:98:ILE:O	0.51	2.06	3	5
1:A:100:TYR:CD2	1:A:116:ILE:O	0.51	2.63	6	2
1:A:76:GLU:O	1:A:79:TYR:CE1	0.51	2.64	3	8
1:A:96:GLU:CG	1:A:97:LYS:N	0.51	2.73	16	7
1:A:130:GLU:OE2	1:A:131:HIS:CE1	0.51	2.63	16	1
1:A:129:GLU:CD	1:A:129:GLU:H	0.51	2.07	1	2
1:A:143:PHE:O	1:A:143:PHE:CD2	0.51	2.64	8	1
1:A:83:TYR:CD1	1:A:83:TYR:N	0.51	2.79	13	1
1:A:96:GLU:OE1	1:A:120:HIS:CE1	0.51	2.64	1	1
1:A:134:VAL:HG23	1:A:135:GLY:N	0.51	2.20	10	14
1:A:156:ALA:O	1:A:158:ASN:ND2	0.51	2.44	7	1
1:A:88:GLY:C	1:A:90:ALA:N	0.51	2.64	11	20
1:A:47:ASN:HD22	1:A:47:ASN:N	0.51	2.03	2	13
1:A:69:HIS:C	1:A:69:HIS:CD2	0.51	2.84	17	3
1:A:155:ASP:C	1:A:158:ASN:ND2	0.51	2.64	7	3
1:A:47:ASN:HD22	1:A:47:ASN:H	0.51	1.47	3	5
1:A:157:TYR:O	1:A:157:TYR:CD2	0.51	2.63	10	3
1:A:25:ASP:CG	1:A:157:TYR:CE2	0.51	2.84	7	2
1:A:76:GLU:O	1:A:79:TYR:CE2	0.51	2.64	12	6
1:A:152:ASP:OD1	1:A:153:HIS:CE1	0.51	2.64	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ALA:HB2	1:A:145:LEU:HD21	0.51	1.83	16	1
1:A:92:THR:CG2	1:A:131:HIS:CE1	0.51	2.94	1	1
1:A:22:PHE:CE2	1:A:143:PHE:CE1	0.51	2.98	2	1
1:A:24:LEU:HD22	1:A:157:TYR:CD1	0.51	2.40	2	2
1:A:27:ASP:O	1:A:28:ASN:ND2	0.51	2.44	7	4
1:A:22:PHE:CZ	1:A:143:PHE:CE2	0.51	2.99	6	1
1:A:157:TYR:CD2	1:A:157:TYR:O	0.51	2.64	17	3
1:A:100:TYR:CZ	1:A:117:SER:OG	0.50	2.63	9	3
1:A:130:GLU:CD	1:A:131:HIS:N	0.50	2.65	16	1
1:A:25:ASP:O	1:A:29:LEU:HD23	0.50	2.06	20	1
1:A:63:GLN:N	1:A:63:GLN:NE2	0.50	2.59	6	1
1:A:155:ASP:OD1	1:A:155:ASP:N	0.50	2.42	12	1
1:A:95:ILE:CG2	1:A:96:GLU:N	0.50	2.74	7	18
1:A:99:SER:C	1:A:118:HIS:HD1	0.50	2.09	9	5
1:A:60:GLU:H	1:A:60:GLU:CD	0.50	2.10	8	5
1:A:156:ALA:C	1:A:157:TYR:CG	0.50	2.84	7	2
1:A:153:HIS:CE1	1:A:155:ASP:OD1	0.50	2.64	12	1
1:A:33:ILE:HB	1:A:145:LEU:HD12	0.50	1.83	10	2
1:A:124:ASN:ND2	1:A:124:ASN:N	0.50	2.60	10	3
1:A:7:ASN:N	1:A:7:ASN:HD22	0.50	2.05	1	2
1:A:19:PHE:O	1:A:23:VAL:CG2	0.50	2.59	1	2
1:A:63:GLN:H	1:A:63:GLN:CD	0.50	2.10	19	3
1:A:37:ALA:C	1:A:38:ILE:HD12	0.50	2.26	17	2
1:A:33:ILE:CD1	1:A:145:LEU:O	0.50	2.60	20	4
1:A:155:ASP:C	1:A:158:ASN:HD21	0.50	2.10	1	2
1:A:80:SER:C	1:A:81:TYR:CD2	0.50	2.85	9	1
1:A:139:ALA:HA	1:A:142:LEU:HG	0.50	1.84	15	4
1:A:28:ASN:ND2	1:A:28:ASN:C	0.50	2.64	17	1
1:A:81:TYR:CD1	1:A:81:TYR:O	0.50	2.65	17	2
1:A:47:ASN:N	1:A:47:ASN:ND2	0.50	2.59	2	8
1:A:27:ASP:CB	1:A:54:LYS:HZ1	0.50	2.19	14	1
1:A:34:ALA:CB	1:A:145:LEU:HD11	0.50	2.36	16	3
1:A:87:GLU:CD	1:A:88:GLY:N	0.50	2.65	7	3
1:A:30:ILE:HG23	1:A:31:PRO:CD	0.50	2.35	13	1
1:A:54:LYS:O	1:A:69:HIS:CE1	0.49	2.65	11	1
1:A:125:ILE:CG2	1:A:126:GLU:N	0.49	2.75	2	12
1:A:69:HIS:CD2	1:A:83:TYR:CD1	0.49	3.00	17	1
1:A:25:ASP:N	1:A:25:ASP:OD1	0.49	2.43	1	1
1:A:37:ALA:O	1:A:138:LYS:NZ	0.49	2.45	8	2
1:A:158:ASN:ND2	1:A:158:ASN:OXT	0.49	2.45	13	2
1:A:15:PRO:HG3	1:A:106:ALA:HB2	0.49	1.84	11	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:TYR:CE2	1:A:102:THR:OG1	0.49	2.63	5	1
1:A:150:LEU:H	1:A:150:LEU:CD2	0.49	2.19	20	8
1:A:87:GLU:CD	1:A:88:GLY:H	0.49	2.09	2	2
1:A:124:ASN:HD22	1:A:124:ASN:N	0.49	1.98	16	3
1:A:143:PHE:N	1:A:143:PHE:CD2	0.49	2.77	9	1
1:A:131:HIS:HD1	1:A:131:HIS:C	0.49	2.10	20	1
1:A:122:LYS:CB	1:A:122:LYS:NZ	0.49	2.76	4	1
1:A:8:GLU:N	1:A:8:GLU:CD	0.49	2.66	8	1
1:A:87:GLU:CG	1:A:88:GLY:N	0.49	2.76	11	4
1:A:22:PHE:CE2	1:A:104:LEU:HD11	0.49	2.43	11	1
1:A:17:ARG:NE	1:A:17:ARG:CA	0.49	2.75	15	2
1:A:20:LYS:CD	1:A:156:ALA:O	0.49	2.61	5	5
1:A:22:PHE:CE1	1:A:143:PHE:CZ	0.49	3.00	12	1
1:A:54:LYS:O	1:A:69:HIS:ND1	0.49	2.46	11	1
1:A:85:LEU:HD22	1:A:90:ALA:HB1	0.49	1.85	13	1
1:A:68:LYS:CB	1:A:86:ILE:HD11	0.49	2.37	1	4
1:A:25:ASP:O	1:A:28:ASN:N	0.48	2.46	7	3
1:A:25:ASP:O	1:A:29:LEU:N	0.48	2.46	6	8
1:A:95:ILE:HG22	1:A:96:GLU:N	0.48	2.23	16	17
1:A:155:ASP:CA	1:A:158:ASN:HD21	0.48	2.20	20	2
1:A:44:LEU:HD12	1:A:44:LEU:H	0.48	1.68	14	4
1:A:22:PHE:HA	1:A:26:ALA:HB2	0.48	1.84	6	3
1:A:34:ALA:CB	1:A:145:LEU:HG	0.48	2.36	17	4
1:A:118:HIS:ND1	1:A:118:HIS:C	0.48	2.66	1	1
1:A:76:GLU:O	1:A:79:TYR:CD2	0.48	2.66	12	5
1:A:5:PHE:CZ	1:A:7:ASN:CG	0.48	2.87	19	1
1:A:69:HIS:HE2	1:A:83:TYR:CB	0.48	2.21	2	1
1:A:4:THR:HG1	1:A:118:HIS:CD2	0.48	2.27	4	2
1:A:87:GLU:OE1	1:A:88:GLY:N	0.48	2.46	4	1
1:A:44:LEU:N	1:A:44:LEU:HD12	0.48	2.23	17	4
1:A:134:VAL:CG1	1:A:135:GLY:N	0.48	2.76	2	1
1:A:15:PRO:HA	1:A:18:LEU:HD12	0.48	1.86	11	1
1:A:86:ILE:CG1	1:A:87:GLU:N	0.48	2.77	6	6
1:A:139:ALA:O	1:A:142:LEU:N	0.48	2.46	16	3
1:A:87:GLU:OE2	1:A:88:GLY:N	0.48	2.47	16	1
1:A:33:ILE:HD13	1:A:145:LEU:HB3	0.48	1.84	11	1
1:A:24:LEU:CD2	1:A:157:TYR:CD2	0.48	2.97	20	1
1:A:100:TYR:CD1	1:A:116:ILE:O	0.48	2.66	2	1
1:A:69:HIS:CD2	1:A:69:HIS:C	0.48	2.86	19	3
1:A:83:TYR:CD2	1:A:83:TYR:N	0.47	2.81	8	3
1:A:17:ARG:NE	1:A:154:PRO:O	0.47	2.47	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ALA:CA	1:A:145:LEU:HG	0.47	2.38	11	1
1:A:121:THR:CG2	1:A:125:ILE:O	0.47	2.61	17	3
1:A:21:ALA:CB	1:A:150:LEU:HD21	0.47	2.38	11	5
1:A:9:PHE:CE1	1:A:10:THR:O	0.47	2.67	16	1
1:A:29:LEU:O	1:A:33:ILE:HG12	0.47	2.09	19	3
1:A:82:SER:CB	1:A:101:GLU:OE1	0.47	2.63	18	1
1:A:124:ASN:O	1:A:124:ASN:ND2	0.47	2.47	19	1
1:A:83:TYR:CE2	1:A:100:TYR:CE1	0.47	3.03	20	1
1:A:52:THR:CG2	1:A:71:ILE:HD13	0.47	2.40	17	6
1:A:9:PHE:CE2	1:A:10:THR:O	0.47	2.67	9	1
1:A:42:GLU:CA	1:A:54:LYS:NZ	0.47	2.76	11	1
1:A:150:LEU:O	1:A:154:PRO:N	0.47	2.48	2	2
1:A:36:GLN:C	1:A:36:GLN:NE2	0.47	2.67	17	1
1:A:16:SER:O	1:A:20:LYS:CG	0.47	2.62	7	5
1:A:138:LYS:O	1:A:142:LEU:CD2	0.47	2.63	11	4
1:A:60:GLU:CD	1:A:61:GLY:N	0.47	2.68	3	1
1:A:37:ALA:HB1	1:A:142:LEU:CD2	0.47	2.39	5	3
1:A:124:ASN:N	1:A:124:ASN:HD22	0.47	2.07	10	1
1:A:130:GLU:N	1:A:130:GLU:OE2	0.47	2.47	10	1
1:A:42:GLU:OE1	1:A:43:ILE:N	0.47	2.47	12	1
1:A:152:ASP:OD2	1:A:153:HIS:CE1	0.47	2.68	19	1
1:A:6:GLU:C	1:A:7:ASN:ND2	0.47	2.68	7	8
1:A:22:PHE:CE2	1:A:81:TYR:OH	0.47	2.67	3	1
1:A:68:LYS:O	1:A:86:ILE:CD1	0.47	2.63	20	1
1:A:155:ASP:O	1:A:158:ASN:OD1	0.47	2.33	1	2
1:A:150:LEU:O	1:A:154:PRO:CD	0.47	2.62	6	4
1:A:155:ASP:OD1	1:A:158:ASN:ND2	0.47	2.48	6	1
1:A:96:GLU:OE2	1:A:120:HIS:CD2	0.47	2.68	7	1
1:A:60:GLU:CG	1:A:61:GLY:N	0.47	2.78	11	1
1:A:101:GLU:OE2	1:A:102:THR:N	0.47	2.47	16	1
1:A:99:SER:O	1:A:118:HIS:ND1	0.47	2.45	20	2
1:A:92:THR:CG2	1:A:131:HIS:NE2	0.47	2.78	1	3
1:A:26:ALA:O	1:A:30:ILE:HG12	0.47	2.10	11	1
1:A:95:ILE:HG21	1:A:98:ILE:HD11	0.46	1.87	11	2
1:A:104:LEU:CD2	1:A:104:LEU:N	0.46	2.77	8	4
1:A:34:ALA:CB	1:A:145:LEU:HD13	0.46	2.40	6	1
1:A:58:PHE:CD1	1:A:59:GLY:N	0.46	2.83	12	2
1:A:54:LYS:HD2	1:A:55:LYS:N	0.46	2.25	9	1
1:A:96:GLU:CD	1:A:120:HIS:CE1	0.46	2.88	9	1
1:A:142:LEU:N	1:A:142:LEU:CD2	0.46	2.73	18	13
1:A:29:LEU:HD21	1:A:149:TYR:CE2	0.46	2.46	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ILE:HD11	1:A:38:ILE:HB	0.46	1.86	13	1
1:A:29:LEU:HD11	1:A:149:TYR:CD2	0.46	2.45	1	1
1:A:81:TYR:O	1:A:81:TYR:CG	0.46	2.69	16	2
1:A:78:SER:OG	1:A:103:LYS:NZ	0.46	2.49	8	1
1:A:33:ILE:O	1:A:145:LEU:CD1	0.46	2.64	11	1
1:A:25:ASP:OD2	1:A:25:ASP:N	0.46	2.48	20	1
1:A:33:ILE:C	1:A:35:PRO:HD3	0.46	2.30	10	13
1:A:53:ILE:HD12	1:A:53:ILE:N	0.46	2.26	16	4
1:A:16:SER:O	1:A:20:LYS:HG2	0.46	2.11	5	1
1:A:6:GLU:O	1:A:7:ASN:ND2	0.46	2.48	19	1
1:A:96:GLU:O	1:A:97:LYS:CG	0.46	2.63	16	2
1:A:90:ALA:HB3	1:A:91:LEU:HD22	0.46	1.88	8	17
1:A:149:TYR:OH	1:A:153:HIS:CD2	0.46	2.69	8	1
1:A:130:GLU:N	1:A:130:GLU:CD	0.46	2.70	5	3
1:A:24:LEU:CD2	1:A:157:TYR:CD1	0.46	2.98	16	2
1:A:44:LEU:HD11	1:A:55:LYS:N	0.46	2.25	14	1
1:A:15:PRO:HG2	1:A:106:ALA:HB2	0.46	1.87	16	1
1:A:131:HIS:C	1:A:131:HIS:ND1	0.46	2.69	20	1
1:A:25:ASP:CB	1:A:157:TYR:CE2	0.45	2.99	7	1
1:A:130:GLU:OE2	1:A:131:HIS:ND1	0.45	2.49	16	1
1:A:152:ASP:O	1:A:153:HIS:ND1	0.45	2.49	2	3
1:A:125:ILE:N	1:A:125:ILE:CD1	0.45	2.79	5	3
1:A:16:SER:OG	1:A:17:ARG:NH1	0.45	2.49	6	1
1:A:63:GLN:CD	1:A:63:GLN:N	0.45	2.70	19	1
1:A:81:TYR:CD1	1:A:82:SER:N	0.45	2.85	2	1
1:A:85:LEU:HD13	1:A:86:ILE:N	0.45	2.26	20	1
1:A:107:CYS:SG	1:A:111:SER:N	0.45	2.89	6	4
1:A:130:GLU:O	1:A:134:VAL:CG2	0.45	2.65	8	3
1:A:44:LEU:HD13	1:A:53:ILE:HG22	0.45	1.87	14	1
1:A:60:GLU:CD	1:A:60:GLU:N	0.45	2.70	19	2
1:A:7:ASN:N	1:A:7:ASN:ND2	0.45	2.64	1	2
1:A:33:ILE:O	1:A:35:PRO:CD	0.45	2.65	10	9
1:A:38:ILE:HD13	1:A:142:LEU:CD2	0.45	2.42	1	1
1:A:113:ILE:HD13	1:A:143:PHE:CE1	0.45	2.46	1	1
1:A:130:GLU:OE2	1:A:131:HIS:CG	0.45	2.70	16	1
1:A:117:SER:OG	1:A:119:TYR:CE1	0.45	2.70	18	1
1:A:72:ASP:OD2	1:A:82:SER:C	0.45	2.55	4	1
1:A:45:GLU:O	1:A:52:THR:CG2	0.45	2.56	11	4
1:A:98:ILE:CG2	1:A:119:TYR:CD2	0.45	3.00	20	2
1:A:20:LYS:HB3	1:A:24:LEU:HD22	0.44	1.89	3	4
1:A:130:GLU:O	1:A:134:VAL:HG13	0.44	2.11	18	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:SER:O	1:A:103:LYS:NZ	0.44	2.51	15	1
1:A:83:TYR:CD1	1:A:83:TYR:C	0.44	2.90	17	2
1:A:85:LEU:HD12	1:A:90:ALA:CB	0.44	2.42	8	2
1:A:30:ILE:O	1:A:34:ALA:C	0.44	2.55	11	2
1:A:33:ILE:CD1	1:A:145:LEU:C	0.44	2.85	17	1
1:A:134:VAL:HG13	1:A:135:GLY:H	0.44	1.73	2	1
1:A:97:LYS:CB	1:A:97:LYS:NZ	0.44	2.80	5	1
1:A:121:THR:OG1	1:A:125:ILE:CG2	0.44	2.66	15	3
1:A:24:LEU:CD2	1:A:157:TYR:CG	0.44	3.00	16	2
1:A:64:TYR:CD1	1:A:89:ASP:OD2	0.44	2.71	19	1
1:A:30:ILE:CG1	1:A:146:ILE:HD11	0.44	2.42	15	4
1:A:55:LYS:HE3	1:A:68:LYS:HZ3	0.44	1.72	6	1
1:A:37:ALA:C	1:A:138:LYS:HZ1	0.44	2.16	7	1
1:A:43:ILE:HG23	1:A:54:LYS:CB	0.44	2.43	9	1
1:A:66:TYR:CD2	1:A:66:TYR:N	0.44	2.85	20	1
1:A:132:VAL:O	1:A:136:LYS:CB	0.44	2.66	2	7
1:A:63:GLN:N	1:A:63:GLN:CD	0.44	2.71	13	1
1:A:17:ARG:N	1:A:17:ARG:HD3	0.44	2.26	17	1
1:A:5:PHE:CD1	1:A:5:PHE:O	0.44	2.70	19	1
1:A:122:LYS:O	1:A:123:GLY:C	0.44	2.56	8	3
1:A:140:HIS:O	1:A:140:HIS:ND1	0.44	2.50	10	2
1:A:48:GLY:O	1:A:74:ILE:HD12	0.44	2.13	14	5
1:A:4:THR:OG1	1:A:118:HIS:NE2	0.44	2.47	4	1
1:A:34:ALA:CB	1:A:145:LEU:CD1	0.44	2.96	6	2
1:A:37:ALA:C	1:A:138:LYS:NZ	0.44	2.72	7	1
1:A:26:ALA:O	1:A:30:ILE:CG1	0.44	2.66	20	2
1:A:149:TYR:CZ	1:A:153:HIS:ND1	0.43	2.86	3	1
1:A:71:ILE:H	1:A:71:ILE:HD12	0.43	1.71	8	2
1:A:29:LEU:HD13	1:A:149:TYR:CG	0.43	2.48	14	1
1:A:29:LEU:HB3	1:A:146:ILE:HG12	0.43	1.90	20	1
1:A:85:LEU:HD12	1:A:90:ALA:HB3	0.43	1.90	8	3
1:A:29:LEU:O	1:A:33:ILE:CD1	0.43	2.66	11	1
1:A:92:THR:OG1	1:A:93:ASP:N	0.43	2.50	20	2
1:A:69:HIS:NE2	1:A:83:TYR:CD1	0.43	2.86	2	1
1:A:34:ALA:N	1:A:145:LEU:CD1	0.43	2.79	20	2
1:A:25:ASP:O	1:A:29:LEU:CB	0.43	2.65	19	3
1:A:127:ILE:N	1:A:127:ILE:HD13	0.43	2.29	7	1
1:A:71:ILE:HD12	1:A:71:ILE:N	0.43	2.27	8	1
1:A:20:LYS:HB2	1:A:24:LEU:HD21	0.43	1.89	12	2
1:A:69:HIS:CE1	1:A:83:TYR:CG	0.43	3.07	18	1
1:A:117:SER:OG	1:A:119:TYR:CZ	0.43	2.71	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ALA:C	1:A:26:ALA:HB2	0.43	2.34	17	2
1:A:40:GLN:CG	1:A:41:ALA:N	0.43	2.81	11	7
1:A:145:LEU:O	1:A:148:SER:OG	0.43	2.33	4	1
1:A:114:LYS:CB	1:A:114:LYS:NZ	0.43	2.82	5	1
1:A:68:LYS:O	1:A:86:ILE:HG13	0.43	2.13	11	1
1:A:130:GLU:OE1	1:A:131:HIS:N	0.43	2.52	16	1
1:A:18:LEU:O	1:A:22:PHE:HB2	0.43	2.14	2	3
1:A:93:ASP:OD1	1:A:93:ASP:N	0.43	2.51	2	1
1:A:152:ASP:C	1:A:153:HIS:ND1	0.43	2.72	2	1
1:A:81:TYR:CE1	1:A:104:LEU:HD21	0.43	2.49	9	1
1:A:59:GLY:O	1:A:62:SER:OG	0.43	2.36	10	1
1:A:152:ASP:O	1:A:153:HIS:CD2	0.43	2.71	20	1
1:A:24:LEU:HD22	1:A:157:TYR:CD2	0.43	2.49	18	3
1:A:43:ILE:CG2	1:A:54:LYS:CB	0.43	2.96	9	1
1:A:96:GLU:CD	1:A:120:HIS:ND1	0.43	2.72	9	1
1:A:144:LYS:NZ	1:A:144:LYS:C	0.43	2.73	11	1
1:A:67:VAL:CG2	1:A:68:LYS:N	0.43	2.81	13	1
1:A:81:TYR:CD1	1:A:81:TYR:C	0.43	2.92	17	1
1:A:121:THR:HG21	1:A:126:GLU:CA	0.42	2.43	5	1
1:A:13:ILE:CD1	1:A:147:GLU:O	0.42	2.67	6	1
1:A:22:PHE:CZ	1:A:143:PHE:CD2	0.42	3.07	7	1
1:A:69:HIS:ND1	1:A:85:LEU:CD2	0.42	2.82	12	1
1:A:134:VAL:CG2	1:A:135:GLY:N	0.42	2.82	10	2
1:A:41:ALA:CB	1:A:54:LYS:NZ	0.42	2.81	10	1
1:A:91:LEU:HD22	1:A:98:ILE:CG1	0.42	2.44	18	2
1:A:60:GLU:CD	1:A:60:GLU:H	0.42	2.17	19	1
1:A:22:PHE:CE2	1:A:143:PHE:CD2	0.42	3.07	7	1
1:A:125:ILE:N	1:A:125:ILE:HD12	0.42	2.27	5	1
1:A:81:TYR:OH	1:A:104:LEU:HD11	0.42	2.14	9	1
1:A:143:PHE:CD1	1:A:143:PHE:C	0.42	2.93	14	1
1:A:6:GLU:CG	1:A:116:ILE:HD12	0.42	2.44	19	1
1:A:149:TYR:O	1:A:152:ASP:OD1	0.42	2.38	16	3
1:A:30:ILE:HG13	1:A:34:ALA:HB3	0.42	1.90	13	1
1:A:33:ILE:CD1	1:A:145:LEU:HB3	0.42	2.44	13	4
1:A:23:VAL:CG2	1:A:24:LEU:N	0.42	2.83	5	2
1:A:17:ARG:CZ	1:A:154:PRO:O	0.42	2.68	8	1
1:A:86:ILE:HD12	1:A:87:GLU:N	0.42	2.30	11	1
1:A:36:GLN:NE2	1:A:37:ALA:N	0.42	2.68	17	1
1:A:101:GLU:O	1:A:116:ILE:HG12	0.42	2.14	19	1
1:A:124:ASN:C	1:A:124:ASN:HD22	0.42	2.17	20	1
1:A:33:ILE:HD12	1:A:146:ILE:N	0.42	2.30	5	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:LEU:O	1:A:92:THR:C	0.42	2.58	11	2
1:A:156:ALA:O	1:A:158:ASN:N	0.42	2.53	14	2
1:A:47:ASN:N	1:A:47:ASN:HD22	0.42	2.12	10	1
1:A:30:ILE:O	1:A:34:ALA:N	0.42	2.52	17	5
1:A:86:ILE:HD12	1:A:87:GLU:CB	0.42	2.45	11	1
1:A:27:ASP:HB2	1:A:54:LYS:HZ1	0.42	1.75	14	1
1:A:97:LYS:O	1:A:120:HIS:CB	0.42	2.68	15	1
1:A:24:LEU:HD23	1:A:157:TYR:CB	0.42	2.44	19	1
1:A:34:ALA:CB	1:A:145:LEU:HD23	0.42	2.44	1	1
1:A:85:LEU:CD1	1:A:90:ALA:CB	0.42	2.98	8	2
1:A:140:HIS:HD1	1:A:140:HIS:C	0.42	2.18	13	1
1:A:65:GLY:O	1:A:66:TYR:CD1	0.42	2.73	14	1
1:A:84:THR:HG23	1:A:98:ILE:C	0.42	2.35	17	1
1:A:99:SER:O	1:A:100:TYR:CD1	0.42	2.73	17	1
1:A:75:ASP:N	1:A:75:ASP:OD1	0.42	2.52	19	1
1:A:69:HIS:CD2	1:A:69:HIS:N	0.41	2.88	7	2
1:A:81:TYR:OH	1:A:104:LEU:CD1	0.41	2.68	9	1
1:A:40:GLN:CD	1:A:41:ALA:H	0.41	2.17	15	3
1:A:65:GLY:O	1:A:66:TYR:CD2	0.41	2.73	10	1
1:A:38:ILE:N	1:A:38:ILE:CD1	0.41	2.82	14	2
1:A:47:ASN:ND2	1:A:47:ASN:C	0.41	2.73	17	1
1:A:96:GLU:HG2	1:A:97:LYS:N	0.41	2.30	18	1
1:A:21:ALA:O	1:A:26:ALA:CB	0.41	2.67	2	2
1:A:21:ALA:HB1	1:A:150:LEU:HD21	0.41	1.91	11	1
1:A:105:VAL:O	1:A:112:THR:N	0.41	2.53	17	9
1:A:48:GLY:O	1:A:74:ILE:CD1	0.41	2.69	1	3
1:A:17:ARG:NH1	1:A:20:LYS:CE	0.41	2.83	6	1
1:A:18:LEU:O	1:A:22:PHE:N	0.41	2.53	6	2
1:A:149:TYR:CE2	1:A:153:HIS:ND1	0.41	2.88	12	1
1:A:38:ILE:HD13	1:A:58:PHE:CZ	0.41	2.50	15	1
1:A:36:GLN:HE21	1:A:36:GLN:C	0.41	2.18	17	1
1:A:78:SER:C	1:A:79:TYR:CG	0.41	2.93	15	1
1:A:34:ALA:HB2	1:A:145:LEU:HD13	0.41	1.92	6	1
1:A:16:SER:CB	1:A:17:ARG:HH11	0.41	2.28	11	1
1:A:36:GLN:OE1	1:A:37:ALA:HB2	0.41	2.16	1	1
1:A:149:TYR:OH	1:A:153:HIS:ND1	0.41	2.54	3	1
1:A:13:ILE:O	1:A:111:SER:OG	0.41	2.33	6	1
1:A:131:HIS:CD2	1:A:131:HIS:C	0.41	2.93	7	1
1:A:25:ASP:O	1:A:29:LEU:CG	0.41	2.68	20	2
1:A:36:GLN:CG	1:A:37:ALA:N	0.41	2.83	3	1
1:A:96:GLU:HG2	1:A:120:HIS:O	0.41	2.16	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:GLY:O	1:A:52:THR:HB	0.41	2.15	6	1
1:A:94:THR:O	1:A:125:ILE:HG21	0.41	2.16	5	1
1:A:103:LYS:NZ	1:A:105:VAL:HG12	0.41	2.31	16	1
1:A:29:LEU:CD1	1:A:146:ILE:HG23	0.41	2.46	2	1
1:A:72:ASP:OD1	1:A:84:THR:OG1	0.41	2.39	7	1
1:A:66:TYR:CD1	1:A:66:TYR:N	0.41	2.88	11	1
1:A:33:ILE:CG1	1:A:145:LEU:HD12	0.41	2.45	16	1
1:A:4:THR:CG2	1:A:118:HIS:CE1	0.40	3.04	6	1
1:A:157:TYR:CD2	1:A:157:TYR:N	0.40	2.86	6	1
1:A:81:TYR:CD2	1:A:81:TYR:N	0.40	2.87	9	1
1:A:72:ASP:O	1:A:73:SER:OG	0.40	2.38	10	2
1:A:138:LYS:O	1:A:141:GLY:N	0.40	2.54	10	1
1:A:62:SER:OG	1:A:63:GLN:N	0.40	2.55	11	1
1:A:133:LYS:O	1:A:137:GLU:CB	0.40	2.69	11	1
1:A:22:PHE:CA	1:A:26:ALA:HB2	0.40	2.46	13	1
1:A:30:ILE:HD11	1:A:38:ILE:CB	0.40	2.47	13	1
1:A:64:TYR:OH	1:A:138:LYS:NZ	0.40	2.49	15	1
1:A:55:LYS:C	1:A:56:ILE:HD12	0.40	2.36	6	1
1:A:91:LEU:HD22	1:A:98:ILE:CD1	0.40	2.46	18	1
1:A:152:ASP:OD2	1:A:153:HIS:ND1	0.40	2.53	19	1
1:A:148:SER:O	1:A:152:ASP:OD2	0.40	2.38	3	1
1:A:25:ASP:OD1	1:A:157:TYR:CE2	0.40	2.74	6	1
1:A:33:ILE:O	1:A:35:PRO:HD2	0.40	2.16	10	1
1:A:41:ALA:C	1:A:54:LYS:HZ3	0.40	2.20	10	1
1:A:43:ILE:N	1:A:54:LYS:HZ1	0.40	2.14	11	1
1:A:42:GLU:CD	1:A:43:ILE:O	0.40	2.59	12	1
1:A:136:LYS:CB	1:A:136:LYS:NZ	0.40	2.84	2	1
1:A:81:TYR:CZ	1:A:102:THR:OG1	0.40	2.72	5	1
1:A:124:ASN:ND2	1:A:124:ASN:H	0.40	2.15	9	1
1:A:104:LEU:HD23	1:A:104:LEU:N	0.40	2.31	14	1
1:A:25:ASP:OD2	1:A:157:TYR:N	0.40	2.54	19	1
1:A:22:PHE:CE2	1:A:23:VAL:HG13	0.40	2.52	1	1
1:A:87:GLU:CG	1:A:88:GLY:H	0.40	2.29	11	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	156/158 (99%)	143±2 (92±1%)	12±2 (8±1%)	1±1 (1±1%)	24 71
All	All	3120/3160 (99%)	2859 (92%)	235 (8%)	26 (1%)	24 71

All 5 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	125	ILE	13
1	A	157	TYR	4
1	A	123	GLY	3
1	A	34	ALA	3
1	A	37	ALA	3

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	134/134 (100%)	101±3 (76±2%)	33±3 (24±2%)	2 26
All	All	2680/2680 (100%)	2028 (76%)	652 (24%)	2 26

All 93 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	20	LYS	20
1	A	43	ILE	20
1	A	47	ASN	20
1	A	91	LEU	20
1	A	98	ILE	20
1	A	116	ILE	20
1	A	142	LEU	20
1	A	151	LYS	20
1	A	102	THR	19
1	A	29	LEU	18
1	A	54	LYS	17
1	A	124	ASN	17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	158	ASN	17
1	A	96	GLU	16
1	A	99	SER	16
1	A	105	VAL	16
1	A	104	LEU	15
1	A	145	LEU	13
1	A	10	THR	12
1	A	33	ILE	12
1	A	40	GLN	12
1	A	94	THR	11
1	A	7	ASN	10
1	A	64	TYR	10
1	A	25	ASP	9
1	A	118	HIS	9
1	A	86	ILE	9
1	A	3	TYR	8
1	A	69	HIS	8
1	A	119	TYR	8
1	A	5	PHE	7
1	A	30	ILE	7
1	A	100	TYR	7
1	A	8	GLU	7
1	A	17	ARG	7
1	A	66	TYR	7
1	A	78	SER	7
1	A	122	LYS	6
1	A	97	LYS	6
1	A	22	PHE	5
1	A	76	GLU	5
1	A	85	LEU	5
1	A	114	LYS	5
1	A	152	ASP	5
1	A	140	HIS	5
1	A	144	LYS	5
1	A	111	SER	5
1	A	155	ASP	5
1	A	58	PHE	5
1	A	9	PHE	4
1	A	89	ASP	4
1	A	121	THR	4
1	A	143	PHE	4
1	A	134	VAL	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	157	TYR	4
1	A	120	HIS	4
1	A	36	GLN	3
1	A	32	LYS	3
1	A	117	SER	3
1	A	60	GLU	3
1	A	63	GLN	3
1	A	68	LYS	3
1	A	6	GLU	3
1	A	27	ASP	3
1	A	39	LYS	3
1	A	82	SER	3
1	A	75	ASP	2
1	A	67	VAL	2
1	A	87	GLU	2
1	A	149	TYR	2
1	A	73	SER	2
1	A	84	THR	2
1	A	153	HIS	2
1	A	38	ILE	2
1	A	130	GLU	2
1	A	115	SER	2
1	A	72	ASP	2
1	A	136	LYS	2
1	A	24	LEU	2
1	A	138	LYS	2
1	A	80	SER	1
1	A	107	CYS	1
1	A	128	LYS	1
1	A	70	ARG	1
1	A	55	LYS	1
1	A	81	TYR	1
1	A	62	SER	1
1	A	56	ILE	1
1	A	42	GLU	1
1	A	129	GLU	1
1	A	101	GLU	1
1	A	28	ASN	1
1	A	11	SER	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

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 (i)

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 80% 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 (i)

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	1680
Number of shifts mapped to atoms	1680
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	155	-0.44 ± 0.18	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	140	-0.16 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	144	0.01 ± 0.06	None needed (< 0.5 ppm)
^{15}N	144	0.55 ± 0.39	None needed (imprecise)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 1676 atoms were assigned a chemical shift out of a possible 2097. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	749/786 (95%)	308/321 (96%)	297/314 (95%)	144/151 (95%)
Sidechain	927/1119 (83%)	604/727 (83%)	315/362 (87%)	8/30 (27%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/192 (0%)	0/94 (0%)	0/92 (0%)	0/6 (0%)
Overall	1676/2097 (80%)	912/1142 (80%)	612/768 (80%)	152/187 (81%)

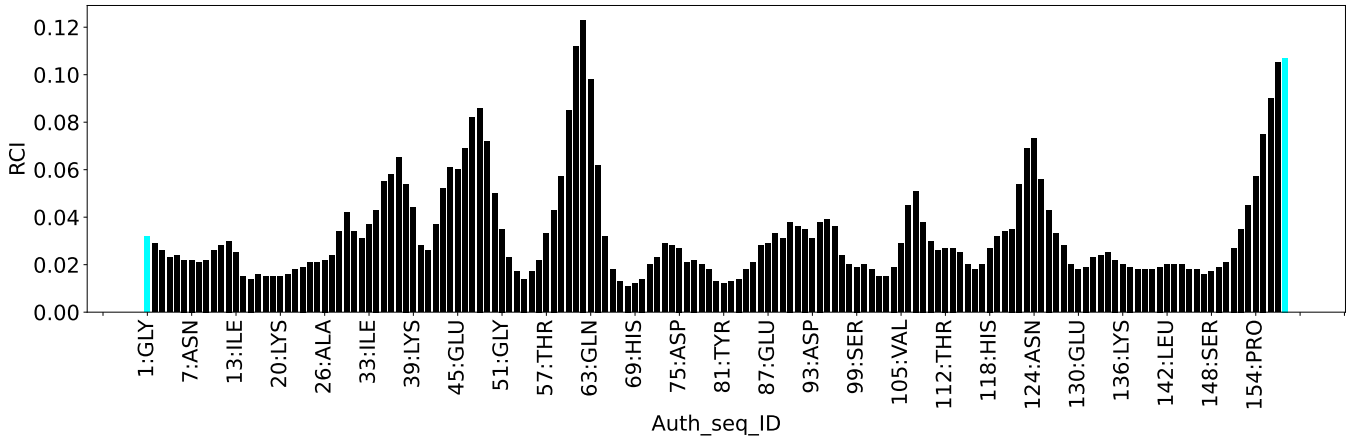
The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1680 atoms were assigned a chemical shift out of a possible 2103. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	753/792 (95%)	310/324 (96%)	299/316 (95%)	144/152 (95%)
Sidechain	927/1119 (83%)	604/727 (83%)	315/362 (87%)	8/30 (27%)
Aromatic	0/192 (0%)	0/94 (0%)	0/92 (0%)	0/6 (0%)
Overall	1680/2103 (80%)	914/1145 (80%)	614/770 (80%)	152/188 (81%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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: