



Full wwPDB NMR Structure Validation Report ⓘ

Nov 1, 2021 – 07:09 PM EDT

PDB ID : 2KWC
Title : The NMR structure of the autophagy-related protein Atg8
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Adachi, W.; Fujioka, Y.; Noda, N.N.; Ohsumi, Y.; Inagaki, F.
Deposited on : 2010-04-05

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

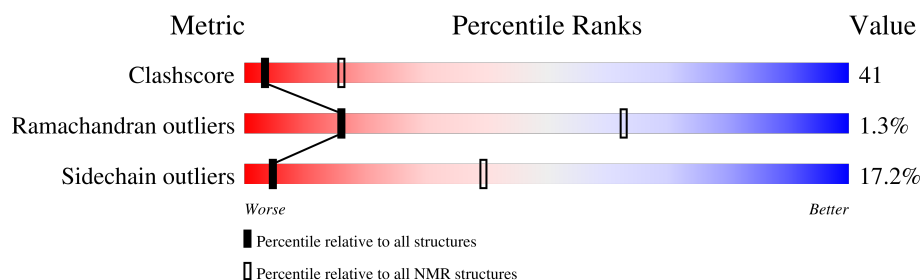
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	116	<div> <div>41%</div> <div>39%</div> <div>8%</div> <div>13%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:14-A:114 (101)	0.34	3

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

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

3 Entry composition

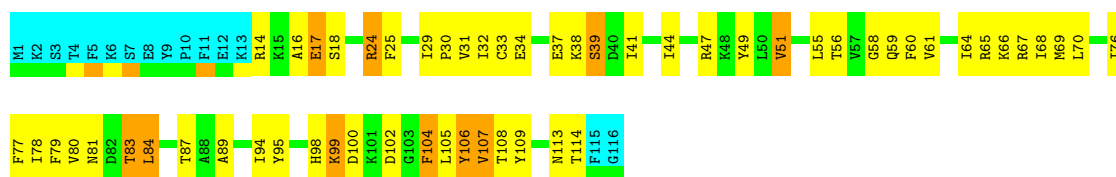
There is only 1 type of molecule in this entry. The entry contains 1905 atoms, of which 958 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Autophagy-related protein 8.

Mol	Chain	Residues	Atoms						Trace
1	A	116	Total	C	H	N	O	S	0
			1905	614	958	156	173	4	

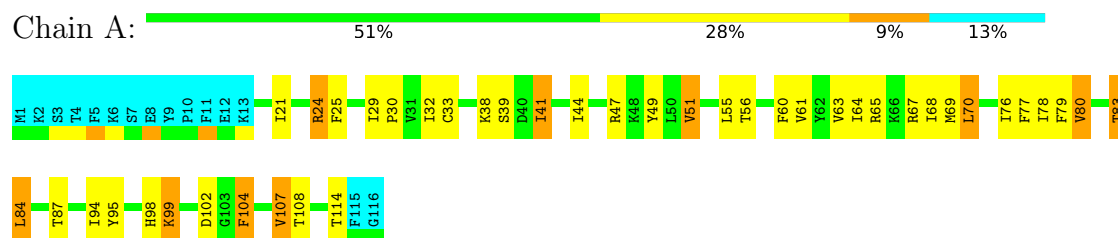
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	PRO	LYS	engineered mutation	UNP P38182



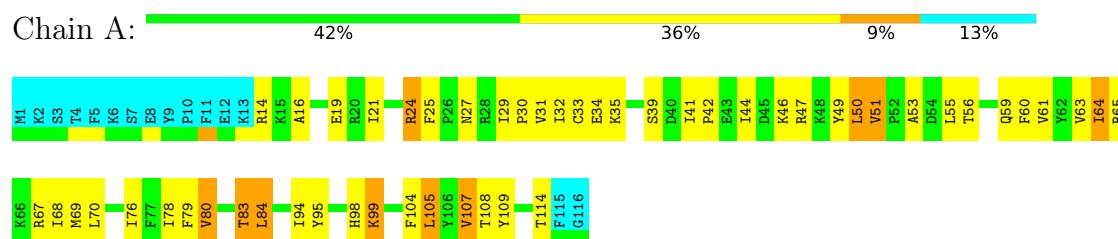
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Autophagy-related protein 8



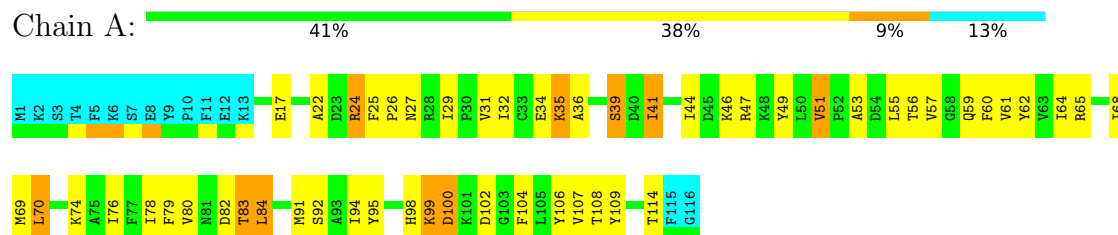
4.2.4 Score per residue for model 4

- Molecule 1: Autophagy-related protein 8



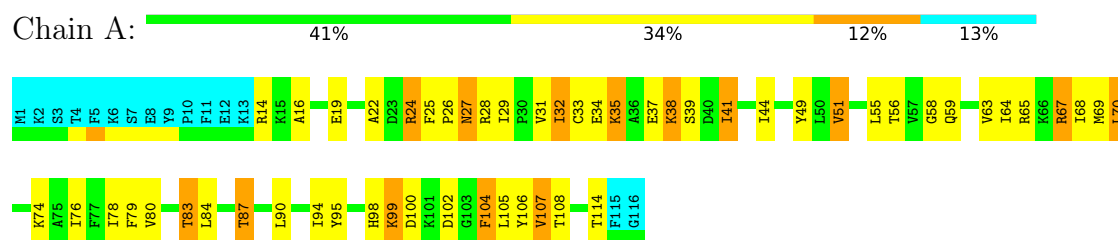
4.2.5 Score per residue for model 5

- Molecule 1: Autophagy-related protein 8



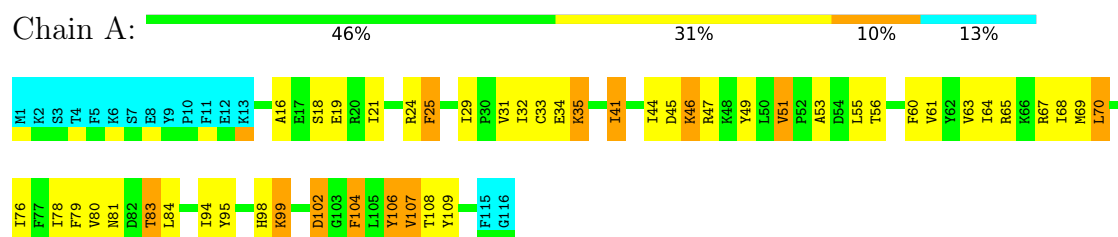
4.2.6 Score per residue for model 6

- Molecule 1: Autophagy-related protein 8



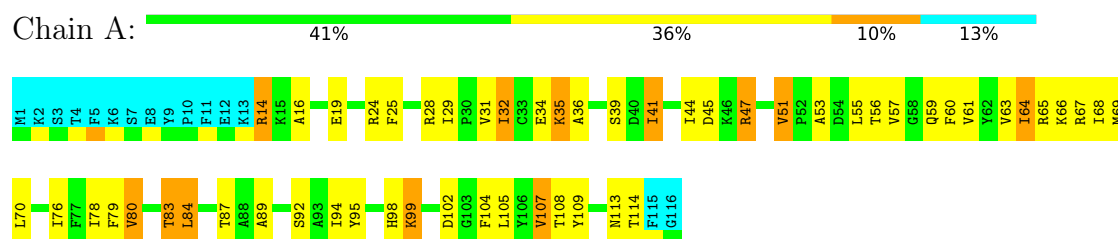
4.2.7 Score per residue for model 7

- Molecule 1: Autophagy-related protein 8



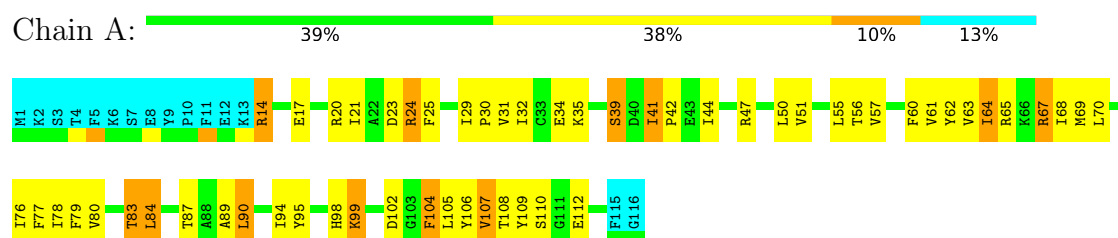
4.2.8 Score per residue for model 8

- Molecule 1: Autophagy-related protein 8



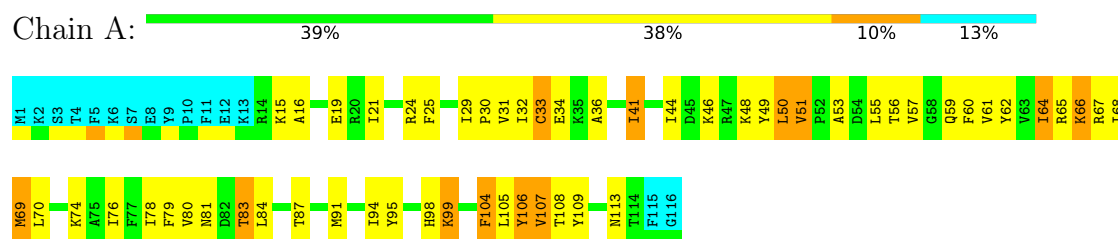
4.2.9 Score per residue for model 9

- Molecule 1: Autophagy-related protein 8



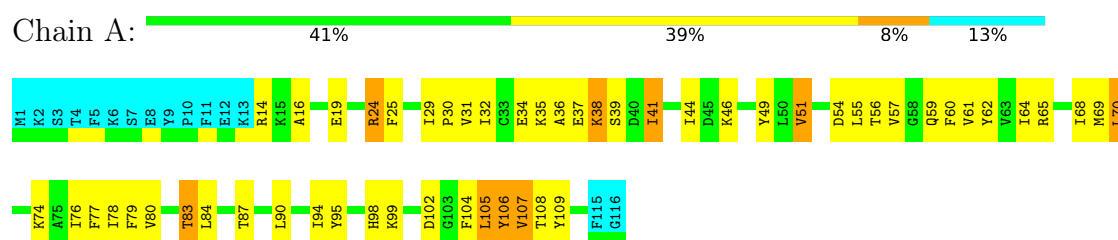
4.2.10 Score per residue for model 10

- Molecule 1: Autophagy-related protein 8



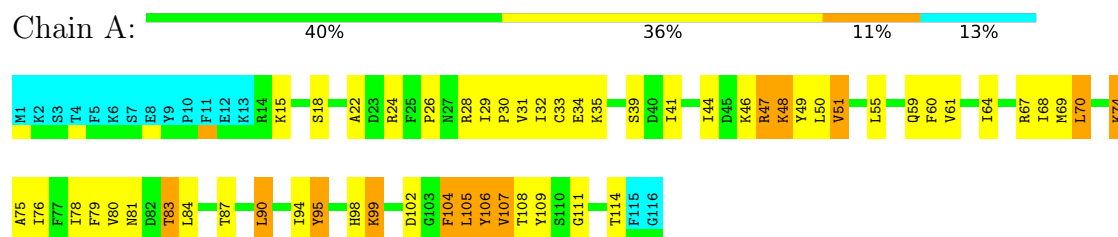
4.2.11 Score per residue for model 11

- Molecule 1: Autophagy-related protein 8



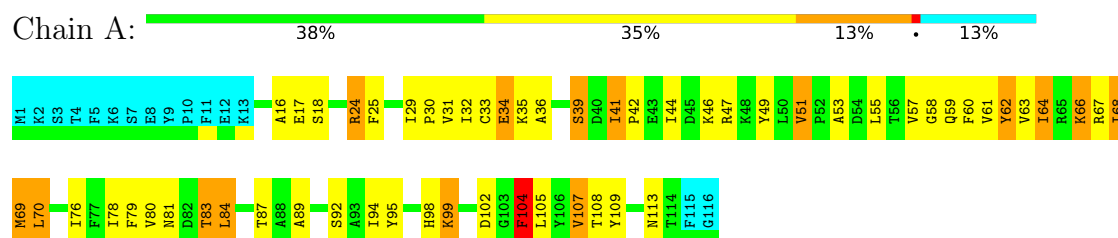
4.2.12 Score per residue for model 12

- Molecule 1: Autophagy-related protein 8



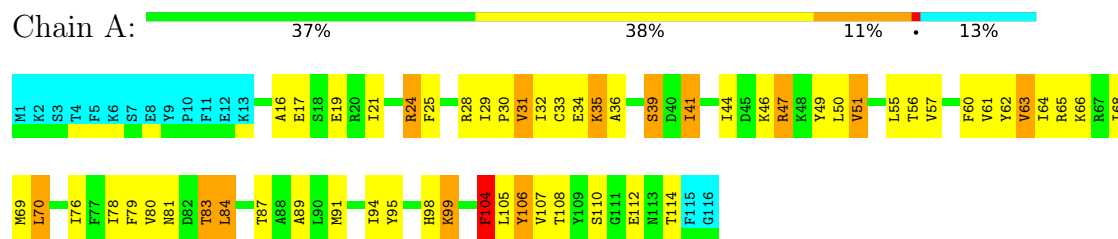
4.2.13 Score per residue for model 13

- Molecule 1: Autophagy-related protein 8



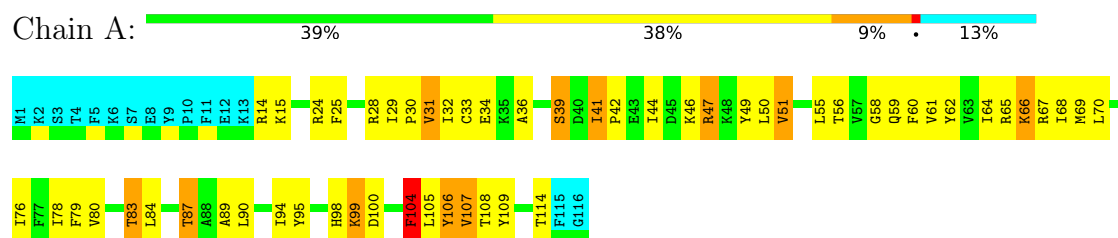
4.2.14 Score per residue for model 14

- Molecule 1: Autophagy-related protein 8



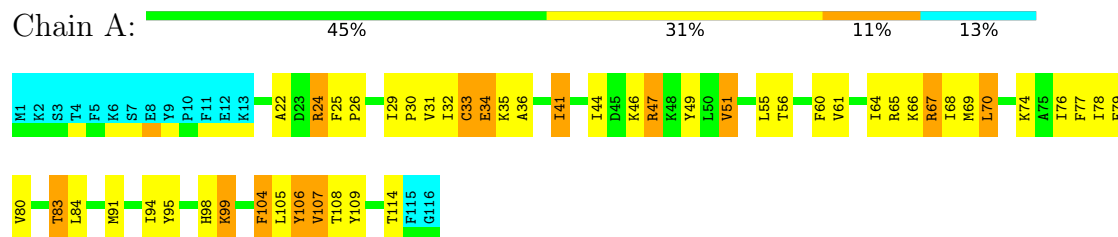
4.2.15 Score per residue for model 15

- Molecule 1: Autophagy-related protein 8



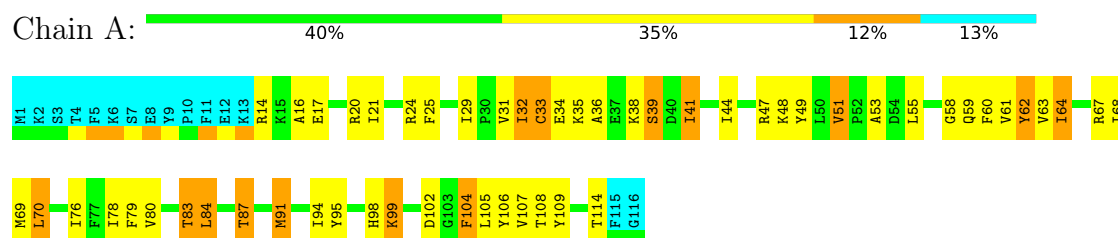
4.2.16 Score per residue for model 16

- Molecule 1: Autophagy-related protein 8



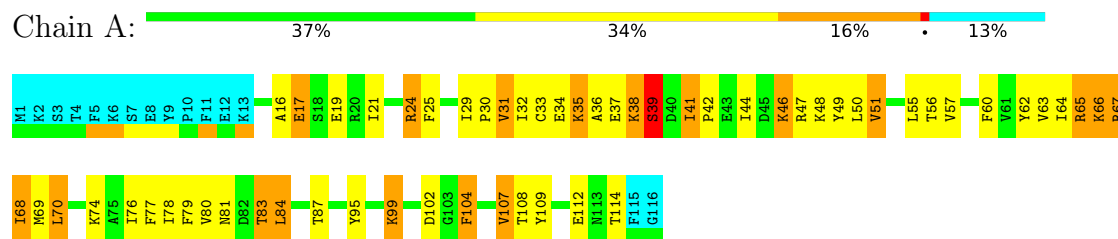
4.2.17 Score per residue for model 17

- Molecule 1: Autophagy-related protein 8



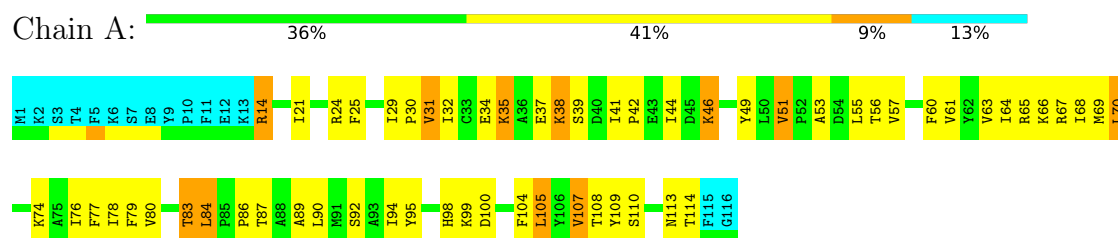
4.2.18 Score per residue for model 18

- Molecule 1: Autophagy-related protein 8



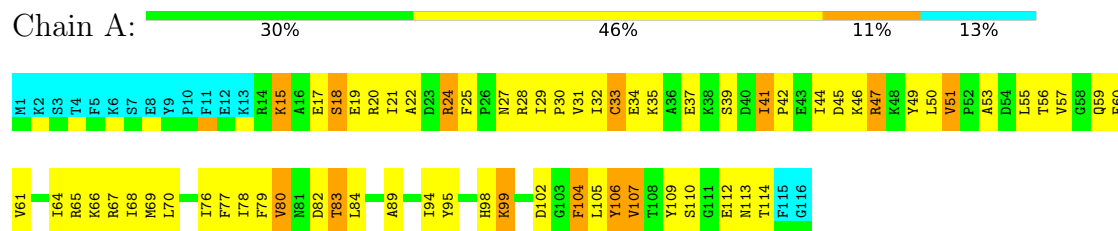
4.2.19 Score per residue for model 19

- Molecule 1: Autophagy-related protein 8



4.2.20 Score per residue for model 20

- Molecule 1: Autophagy-related protein 8



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

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	1497
Number of shifts mapped to atoms	1497
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

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	819	836	837	67±8
All	All	16380	16720	16740	1342

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 41.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:ILE:HD12	1:A:70:LEU:HD22	1.07	1.25	18	13
1:A:79:PHE:CE2	1:A:84:LEU:HD12	0.99	1.93	1	5
1:A:34:GLU:O	1:A:108:THR:HG23	0.92	1.64	5	17
1:A:51:VAL:HG13	1:A:55:LEU:HD22	0.90	1.41	9	1
1:A:36:ALA:HB2	1:A:108:THR:HG22	0.86	1.45	8	6
1:A:17:GLU:O	1:A:21:ILE:HD12	0.86	1.70	17	1
1:A:41:ILE:HD11	1:A:109:TYR:CE1	0.85	2.05	16	9
1:A:65:ARG:HH21	1:A:76:ILE:HG22	0.84	1.33	19	1
1:A:68:ILE:HD12	1:A:70:LEU:HD12	0.82	1.49	20	7
1:A:94:ILE:HG23	1:A:98:HIS:CD2	0.81	2.10	1	16
1:A:61:VAL:HG22	1:A:78:ILE:HG13	0.81	1.52	20	8
1:A:61:VAL:HG22	1:A:78:ILE:HG12	0.80	1.54	16	8
1:A:51:VAL:HG12	1:A:55:LEU:HD13	0.80	1.50	17	15
1:A:32:ILE:CG2	1:A:47:ARG:HH21	0.79	1.90	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:VAL:CG1	1:A:55:LEU:HD22	0.78	2.08	9	1
1:A:36:ALA:HB2	1:A:108:THR:CG2	0.78	2.08	8	5
1:A:29:ILE:HG23	1:A:95:TYR:CD2	0.78	2.14	13	8
1:A:95:TYR:CD2	1:A:105:LEU:HD23	0.77	2.15	11	4
1:A:79:PHE:CE1	1:A:84:LEU:HD13	0.76	2.16	16	2
1:A:31:VAL:HG22	1:A:105:LEU:CB	0.75	2.11	12	7
1:A:79:PHE:CE2	1:A:84:LEU:HD13	0.74	2.17	9	8
1:A:57:VAL:O	1:A:61:VAL:HG23	0.72	1.84	20	5
1:A:63:VAL:HG12	1:A:64:ILE:HD12	0.72	1.59	14	1
1:A:44:ILE:CG2	1:A:68:ILE:HG23	0.72	2.15	18	11
1:A:31:VAL:HG22	1:A:105:LEU:HB3	0.72	1.59	13	6
1:A:31:VAL:HG22	1:A:105:LEU:HB2	0.72	1.60	12	2
1:A:31:VAL:CG2	1:A:105:LEU:HD13	0.72	2.14	17	1
1:A:41:ILE:HD12	1:A:68:ILE:HD13	0.70	1.63	5	1
1:A:79:PHE:CE2	1:A:84:LEU:CD1	0.69	2.75	8	5
1:A:49:TYR:CE1	1:A:63:VAL:CG1	0.69	2.75	19	1
1:A:78:ILE:N	1:A:78:ILE:HD13	0.69	2.02	16	1
1:A:80:VAL:O	1:A:83:THR:HG22	0.69	1.88	13	19
1:A:78:ILE:O	1:A:84:LEU:HD12	0.69	1.88	16	8
1:A:95:TYR:CD2	1:A:105:LEU:CD2	0.69	2.76	11	4
1:A:98:HIS:O	1:A:105:LEU:HD23	0.69	1.87	17	1
1:A:28:ARG:HG3	1:A:50:LEU:HD11	0.68	1.65	15	2
1:A:49:TYR:CE1	1:A:63:VAL:HG12	0.68	2.23	19	1
1:A:68:ILE:HD11	1:A:76:ILE:CD1	0.67	2.19	5	13
1:A:49:TYR:CD1	1:A:63:VAL:CG1	0.67	2.78	19	2
1:A:61:VAL:HG22	1:A:78:ILE:CG1	0.67	2.18	16	15
1:A:68:ILE:CD1	1:A:76:ILE:HD12	0.67	2.19	18	12
1:A:49:TYR:CD2	1:A:60:PHE:CE1	0.67	2.82	12	1
1:A:68:ILE:HD12	1:A:70:LEU:CD1	0.67	2.20	9	7
1:A:29:ILE:CG2	1:A:95:TYR:CD2	0.66	2.77	13	6
1:A:36:ALA:HB3	1:A:39:SER:HB3	0.66	1.66	15	2
1:A:35:LYS:HG2	1:A:41:ILE:HD11	0.66	1.66	18	2
1:A:31:VAL:HG11	1:A:60:PHE:CZ	0.66	2.26	18	9
1:A:76:ILE:HD11	1:A:109:TYR:CD1	0.66	2.25	20	1
1:A:106:TYR:CD1	1:A:106:TYR:N	0.65	2.64	14	10
1:A:33:CYS:HB2	1:A:107:VAL:HG13	0.65	1.66	15	4
1:A:32:ILE:HD13	1:A:47:ARG:O	0.65	1.90	20	4
1:A:79:PHE:CD2	1:A:84:LEU:HD12	0.65	2.27	8	2
1:A:112:GLU:HG3	1:A:114:THR:HG23	0.65	1.68	20	1
1:A:60:PHE:CE1	1:A:64:ILE:HD11	0.64	2.26	3	6
1:A:80:VAL:CG2	1:A:98:HIS:CE1	0.64	2.80	1	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:PHE:CE2	1:A:64:ILE:HD11	0.64	2.28	20	5
1:A:83:THR:HG23	1:A:84:LEU:N	0.64	2.07	11	17
1:A:95:TYR:CD2	1:A:105:LEU:HD13	0.64	2.27	16	1
1:A:44:ILE:HG23	1:A:68:ILE:HG23	0.64	1.68	4	14
1:A:68:ILE:HD11	1:A:76:ILE:HD13	0.63	1.68	5	6
1:A:31:VAL:HG22	1:A:105:LEU:CG	0.63	2.24	4	1
1:A:41:ILE:HD12	1:A:68:ILE:CD1	0.63	2.23	5	1
1:A:32:ILE:CG1	1:A:104:PHE:CD1	0.63	2.82	11	10
1:A:42:PRO:O	1:A:68:ILE:HG22	0.63	1.93	13	6
1:A:68:ILE:CD1	1:A:70:LEU:HD22	0.63	2.21	10	5
1:A:89:ALA:HB1	1:A:94:ILE:HD11	0.62	1.71	9	7
1:A:31:VAL:HG11	1:A:60:PHE:CE2	0.62	2.29	17	2
1:A:41:ILE:HD11	1:A:109:TYR:HE1	0.62	1.54	11	7
1:A:95:TYR:HB2	1:A:105:LEU:HD11	0.62	1.69	17	1
1:A:80:VAL:HG23	1:A:98:HIS:CE1	0.62	2.30	17	10
1:A:24:ARG:CG	1:A:25:PHE:CE1	0.62	2.82	7	1
1:A:31:VAL:CG1	1:A:60:PHE:CZ	0.61	2.83	17	3
1:A:51:VAL:CG1	1:A:55:LEU:HD13	0.61	2.25	19	15
1:A:79:PHE:CZ	1:A:84:LEU:HD12	0.61	2.30	15	2
1:A:21:ILE:HG21	1:A:30:PRO:HG3	0.60	1.73	14	7
1:A:77:PHE:C	1:A:78:ILE:HD13	0.60	2.15	16	2
1:A:31:VAL:HG22	1:A:105:LEU:HG	0.60	1.74	4	1
1:A:30:PRO:O	1:A:104:PHE:CD2	0.60	2.55	12	2
1:A:63:VAL:CG1	1:A:64:ILE:HD12	0.60	2.27	14	1
1:A:95:TYR:CD2	1:A:105:LEU:CD1	0.60	2.85	16	1
1:A:68:ILE:CD1	1:A:76:ILE:CD1	0.60	2.80	5	15
1:A:33:CYS:SG	1:A:109:TYR:CD2	0.60	2.95	12	6
1:A:56:THR:HG22	1:A:90:LEU:CD1	0.60	2.27	6	5
1:A:79:PHE:CE2	1:A:114:THR:O	0.59	2.55	1	9
1:A:79:PHE:CZ	1:A:114:THR:O	0.59	2.55	18	9
1:A:78:ILE:CG2	1:A:107:VAL:CG2	0.59	2.80	11	9
1:A:98:HIS:O	1:A:106:TYR:CE1	0.59	2.55	10	8
1:A:109:TYR:CD1	1:A:109:TYR:O	0.59	2.56	11	7
1:A:33:CYS:SG	1:A:109:TYR:CE2	0.59	2.95	2	1
1:A:24:ARG:CG	1:A:25:PHE:CE2	0.59	2.86	17	3
1:A:30:PRO:O	1:A:104:PHE:CD1	0.59	2.56	2	4
1:A:31:VAL:HG23	1:A:105:LEU:HD13	0.59	1.73	17	1
1:A:49:TYR:CD2	1:A:60:PHE:CZ	0.58	2.91	12	1
1:A:78:ILE:C	1:A:79:PHE:CD1	0.58	2.77	15	5
1:A:33:CYS:SG	1:A:107:VAL:HG23	0.58	2.38	13	1
1:A:35:LYS:HZ2	1:A:42:PRO:C	0.58	2.02	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ILE:HG22	1:A:32:ILE:O	0.58	1.98	6	14
1:A:31:VAL:HG12	1:A:49:TYR:HB2	0.58	1.75	18	4
1:A:79:PHE:CE1	1:A:114:THR:O	0.58	2.57	19	5
1:A:79:PHE:CD2	1:A:84:LEU:CD1	0.57	2.87	4	3
1:A:44:ILE:HG21	1:A:67:ARG:HB3	0.57	1.76	15	5
1:A:68:ILE:HD12	1:A:70:LEU:CD2	0.57	2.24	10	4
1:A:77:PHE:CE2	1:A:113:ASN:ND2	0.57	2.72	20	2
1:A:76:ILE:HD11	1:A:109:TYR:HD1	0.57	1.58	20	1
1:A:55:LEU:HD11	1:A:59:GLN:CB	0.57	2.30	8	9
1:A:33:CYS:SG	1:A:107:VAL:HG13	0.57	2.40	18	1
1:A:35:LYS:CG	1:A:41:ILE:HD11	0.56	2.30	18	3
1:A:68:ILE:HB	1:A:70:LEU:HD13	0.56	1.77	12	9
1:A:51:VAL:HG21	1:A:60:PHE:CE1	0.56	2.36	9	1
1:A:24:ARG:CG	1:A:25:PHE:CZ	0.56	2.89	7	6
1:A:95:TYR:CD1	1:A:95:TYR:O	0.56	2.59	19	10
1:A:94:ILE:CG2	1:A:98:HIS:CD2	0.56	2.88	13	7
1:A:95:TYR:CB	1:A:105:LEU:HD11	0.56	2.31	17	1
1:A:31:VAL:HG11	1:A:60:PHE:CE1	0.55	2.36	11	3
1:A:60:PHE:O	1:A:64:ILE:HD12	0.55	2.00	12	3
1:A:55:LEU:HD11	1:A:59:GLN:HB2	0.55	1.79	1	8
1:A:33:CYS:CB	1:A:49:TYR:CE1	0.55	2.90	20	1
1:A:28:ARG:CD	1:A:28:ARG:N	0.55	2.70	6	4
1:A:79:PHE:CD1	1:A:79:PHE:N	0.55	2.74	4	5
1:A:34:GLU:CG	1:A:47:ARG:NH2	0.55	2.70	15	1
1:A:80:VAL:HG22	1:A:98:HIS:ND1	0.55	2.17	9	3
1:A:68:ILE:HD11	1:A:76:ILE:HD12	0.55	1.79	20	4
1:A:35:LYS:NZ	1:A:41:ILE:CG1	0.54	2.70	14	1
1:A:44:ILE:HG22	1:A:67:ARG:O	0.54	2.02	18	1
1:A:61:VAL:HG12	1:A:65:ARG:HH21	0.54	1.62	4	1
1:A:57:VAL:HG22	1:A:91:MET:SD	0.54	2.43	10	3
1:A:49:TYR:CE2	1:A:64:ILE:CD1	0.54	2.91	1	3
1:A:44:ILE:HD12	1:A:46:LYS:O	0.54	2.02	7	3
1:A:32:ILE:HG13	1:A:104:PHE:CD1	0.54	2.38	1	7
1:A:32:ILE:HG12	1:A:104:PHE:CD1	0.54	2.38	1	7
1:A:49:TYR:CD1	1:A:63:VAL:HG11	0.54	2.38	19	1
1:A:32:ILE:HD13	1:A:104:PHE:CD1	0.53	2.39	6	1
1:A:95:TYR:C	1:A:95:TYR:CD1	0.53	2.81	4	14
1:A:32:ILE:CG2	1:A:32:ILE:O	0.53	2.56	17	1
1:A:81:ASN:N	1:A:81:ASN:HD22	0.53	2.02	14	5
1:A:49:TYR:CB	1:A:60:PHE:CE1	0.53	2.91	10	2
1:A:33:CYS:HB2	1:A:49:TYR:CE1	0.53	2.39	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:ILE:HG21	1:A:109:TYR:CD2	0.53	2.39	2	1
1:A:56:THR:HG22	1:A:90:LEU:HD12	0.53	1.81	6	4
1:A:79:PHE:CZ	1:A:84:LEU:HD13	0.52	2.38	12	5
1:A:80:VAL:HG22	1:A:98:HIS:CE1	0.52	2.39	13	3
1:A:32:ILE:HG13	1:A:104:PHE:CE1	0.52	2.40	4	1
1:A:109:TYR:CD1	1:A:109:TYR:C	0.52	2.82	5	5
1:A:80:VAL:CG2	1:A:98:HIS:ND1	0.52	2.72	13	3
1:A:24:ARG:HG2	1:A:25:PHE:CE2	0.52	2.39	17	3
1:A:32:ILE:CG1	1:A:104:PHE:CE1	0.52	2.93	4	3
1:A:64:ILE:HG22	1:A:68:ILE:HD11	0.52	1.80	6	3
1:A:98:HIS:CB	1:A:105:LEU:HD11	0.52	2.34	2	5
1:A:86:PRO:HG2	1:A:89:ALA:HB2	0.52	1.81	19	1
1:A:80:VAL:HG22	1:A:83:THR:HG22	0.52	1.81	10	9
1:A:79:PHE:CD2	1:A:108:THR:O	0.52	2.63	19	2
1:A:24:ARG:HG3	1:A:25:PHE:CZ	0.51	2.40	15	4
1:A:33:CYS:HB2	1:A:49:TYR:CE2	0.51	2.41	10	1
1:A:29:ILE:HD12	1:A:91:MET:CB	0.51	2.35	17	1
1:A:60:PHE:CE1	1:A:64:ILE:CD1	0.51	2.93	5	1
1:A:95:TYR:HA	1:A:105:LEU:HD21	0.51	1.83	17	2
1:A:32:ILE:HG12	1:A:104:PHE:CE1	0.51	2.41	14	3
1:A:32:ILE:HG23	1:A:47:ARG:CD	0.51	2.36	9	1
1:A:100:ASP:CG	1:A:106:TYR:CE1	0.51	2.84	15	1
1:A:104:PHE:O	1:A:106:TYR:CE2	0.51	2.64	17	1
1:A:78:ILE:HG22	1:A:107:VAL:CG2	0.51	2.36	19	8
1:A:32:ILE:HG23	1:A:47:ARG:HD2	0.51	1.83	9	1
1:A:20:ARG:CG	1:A:21:ILE:N	0.51	2.74	20	2
1:A:49:TYR:CD1	1:A:63:VAL:HG12	0.51	2.41	18	1
1:A:95:TYR:CD1	1:A:95:TYR:C	0.51	2.85	11	3
1:A:41:ILE:HD11	1:A:109:TYR:CD1	0.50	2.42	16	3
1:A:41:ILE:HD12	1:A:76:ILE:HD11	0.50	1.81	3	3
1:A:14:ARG:HG3	1:A:104:PHE:CE2	0.50	2.41	8	1
1:A:80:VAL:O	1:A:83:THR:CG2	0.50	2.60	3	10
1:A:24:ARG:HD2	1:A:25:PHE:CE1	0.50	2.41	9	11
1:A:77:PHE:O	1:A:78:ILE:HD13	0.50	2.05	20	1
1:A:83:THR:CG2	1:A:84:LEU:N	0.50	2.74	7	7
1:A:68:ILE:C	1:A:69:MET:CG	0.50	2.80	13	2
1:A:55:LEU:CD2	1:A:56:THR:O	0.50	2.60	10	14
1:A:22:ALA:O	1:A:26:PRO:CD	0.50	2.60	6	4
1:A:24:ARG:HG2	1:A:25:PHE:CZ	0.50	2.41	7	3
1:A:109:TYR:C	1:A:109:TYR:CD1	0.50	2.85	8	1
1:A:58:GLY:CA	1:A:87:THR:OG1	0.50	2.60	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:ILE:O	1:A:69:MET:CG	0.50	2.60	17	17
1:A:18:SER:HB2	1:A:104:PHE:CE1	0.50	2.42	20	1
1:A:95:TYR:O	1:A:99:LYS:CB	0.50	2.60	9	17
1:A:107:VAL:CG2	1:A:108:THR:N	0.50	2.74	15	14
1:A:77:PHE:CD1	1:A:112:GLU:O	0.50	2.64	18	2
1:A:35:LYS:H	1:A:47:ARG:NH2	0.49	2.05	8	1
1:A:89:ALA:HB1	1:A:94:ILE:CG1	0.49	2.36	15	1
1:A:32:ILE:CG2	1:A:47:ARG:NH2	0.49	2.70	18	1
1:A:78:ILE:O	1:A:84:LEU:CD1	0.49	2.60	2	5
1:A:32:ILE:CD1	1:A:47:ARG:O	0.49	2.60	4	6
1:A:22:ALA:O	1:A:26:PRO:CG	0.49	2.60	6	2
1:A:29:ILE:HG22	1:A:105:LEU:CD1	0.49	2.38	17	1
1:A:49:TYR:CE2	1:A:64:ILE:HG13	0.49	2.42	1	3
1:A:60:PHE:CD1	1:A:64:ILE:CD1	0.49	2.95	3	1
1:A:51:VAL:CG2	1:A:60:PHE:CE1	0.48	2.96	9	1
1:A:49:TYR:CE1	1:A:64:ILE:HG13	0.48	2.42	13	4
1:A:53:ALA:HB1	1:A:92:SER:HB3	0.48	1.85	13	4
1:A:33:CYS:CB	1:A:107:VAL:HG13	0.48	2.36	15	2
1:A:33:CYS:HB3	1:A:49:TYR:CE1	0.48	2.44	6	5
1:A:49:TYR:HB3	1:A:60:PHE:CE1	0.48	2.43	10	2
1:A:84:LEU:HD13	1:A:113:ASN:ND2	0.48	2.22	10	1
1:A:32:ILE:CG1	1:A:104:PHE:CD2	0.48	2.97	20	1
1:A:63:VAL:HG23	1:A:64:ILE:N	0.48	2.24	8	2
1:A:60:PHE:CZ	1:A:64:ILE:HD11	0.48	2.42	14	2
1:A:29:ILE:HD13	1:A:91:MET:O	0.48	2.08	16	2
1:A:28:ARG:CG	1:A:50:LEU:HD11	0.48	2.38	15	1
1:A:32:ILE:HG23	1:A:47:ARG:HG3	0.48	1.84	20	2
1:A:33:CYS:SG	1:A:107:VAL:CG1	0.48	3.02	18	1
1:A:31:VAL:CG1	1:A:107:VAL:CG1	0.48	2.91	6	3
1:A:35:LYS:HA	1:A:109:TYR:CE1	0.48	2.44	13	3
1:A:79:PHE:CE1	1:A:84:LEU:HD12	0.48	2.44	20	1
1:A:24:ARG:HG3	1:A:25:PHE:CE1	0.48	2.44	8	4
1:A:112:GLU:HG2	1:A:114:THR:HG23	0.48	1.85	14	1
1:A:80:VAL:HG21	1:A:98:HIS:CE1	0.47	2.43	1	3
1:A:60:PHE:O	1:A:64:ILE:CD1	0.47	2.62	4	5
1:A:44:ILE:HD13	1:A:109:TYR:OH	0.47	2.09	13	1
1:A:24:ARG:HB3	1:A:25:PHE:CD2	0.47	2.44	15	5
1:A:41:ILE:CD1	1:A:68:ILE:HD13	0.47	2.37	5	1
1:A:64:ILE:HD12	1:A:64:ILE:N	0.47	2.24	7	4
1:A:81:ASN:ND2	1:A:98:HIS:ND1	0.47	2.61	13	1
1:A:37:GLU:CG	1:A:38:LYS:N	0.47	2.78	18	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:GLU:O	1:A:108:THR:CG2	0.47	2.60	10	2
1:A:60:PHE:O	1:A:63:VAL:CG2	0.47	2.63	17	1
1:A:18:SER:O	1:A:22:ALA:HB2	0.47	2.09	20	1
1:A:22:ALA:O	1:A:26:PRO:CB	0.47	2.62	6	4
1:A:95:TYR:HB2	1:A:105:LEU:HD22	0.47	1.84	8	3
1:A:80:VAL:HG13	1:A:98:HIS:CE1	0.47	2.44	16	2
1:A:77:PHE:CE2	1:A:113:ASN:HB2	0.47	2.45	2	1
1:A:98:HIS:HB3	1:A:105:LEU:HD11	0.47	1.85	2	3
1:A:36:ALA:HB3	1:A:39:SER:OG	0.47	2.09	14	2
1:A:95:TYR:CE1	1:A:99:LYS:HB2	0.47	2.44	17	1
1:A:18:SER:HB2	1:A:104:PHE:CE2	0.47	2.45	13	1
1:A:35:LYS:CD	1:A:36:ALA:N	0.47	2.78	8	2
1:A:78:ILE:HD13	1:A:109:TYR:HB3	0.47	1.87	9	2
1:A:59:GLN:O	1:A:62:TYR:CB	0.46	2.63	17	3
1:A:100:ASP:CG	1:A:106:TYR:CD1	0.46	2.88	5	1
1:A:49:TYR:N	1:A:49:TYR:CD1	0.46	2.82	16	1
1:A:29:ILE:HD11	1:A:53:ALA:HA	0.46	1.87	10	5
1:A:53:ALA:HB1	1:A:92:SER:CB	0.46	2.39	13	3
1:A:78:ILE:CG2	1:A:107:VAL:HG21	0.46	2.40	11	11
1:A:81:ASN:ND2	1:A:106:TYR:CE2	0.46	2.84	2	1
1:A:60:PHE:CD2	1:A:64:ILE:HD13	0.46	2.46	13	3
1:A:41:ILE:CD1	1:A:76:ILE:HD11	0.46	2.41	5	3
1:A:33:CYS:HB3	1:A:49:TYR:CE2	0.46	2.46	7	2
1:A:31:VAL:HG13	1:A:107:VAL:CG1	0.46	2.41	17	2
1:A:24:ARG:HB3	1:A:25:PHE:CE2	0.46	2.46	1	2
1:A:24:ARG:HD2	1:A:25:PHE:CD1	0.46	2.46	5	9
1:A:34:GLU:HA	1:A:47:ARG:HH21	0.46	1.71	8	1
1:A:33:CYS:SG	1:A:107:VAL:CG2	0.46	3.04	13	1
1:A:64:ILE:O	1:A:67:ARG:N	0.46	2.49	13	13
1:A:33:CYS:CB	1:A:49:TYR:CE2	0.46	2.99	17	2
1:A:32:ILE:O	1:A:32:ILE:HG23	0.46	2.11	17	1
1:A:30:PRO:HB2	1:A:104:PHE:CE1	0.46	2.46	14	8
1:A:65:ARG:O	1:A:69:MET:N	0.46	2.49	16	15
1:A:107:VAL:HG22	1:A:108:THR:N	0.46	2.26	17	2
1:A:29:ILE:N	1:A:51:VAL:O	0.45	2.49	14	19
1:A:79:PHE:CD2	1:A:84:LEU:HD13	0.45	2.46	7	1
1:A:33:CYS:O	1:A:47:ARG:CB	0.45	2.64	14	2
1:A:94:ILE:O	1:A:98:HIS:N	0.45	2.50	12	15
1:A:60:PHE:CD2	1:A:64:ILE:CD1	0.45	2.99	13	4
1:A:29:ILE:CD1	1:A:91:MET:O	0.45	2.64	16	1
1:A:64:ILE:HG12	1:A:109:TYR:CE2	0.45	2.46	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:PHE:O	1:A:109:TYR:CB	0.45	2.65	9	2
1:A:76:ILE:CG1	1:A:110:SER:O	0.45	2.65	19	1
1:A:79:PHE:N	1:A:108:THR:O	0.45	2.49	17	2
1:A:49:TYR:CB	1:A:60:PHE:CZ	0.45	3.00	10	1
1:A:36:ALA:HB3	1:A:39:SER:HG	0.45	1.72	14	1
1:A:18:SER:HB2	1:A:104:PHE:CD2	0.45	2.46	13	1
1:A:62:TYR:CE2	1:A:66:LYS:HE3	0.45	2.46	15	1
1:A:95:TYR:CE2	1:A:105:LEU:HB2	0.45	2.47	15	1
1:A:15:LYS:O	1:A:19:GLU:N	0.45	2.50	20	1
1:A:95:TYR:O	1:A:99:LYS:N	0.45	2.50	20	11
1:A:60:PHE:CD1	1:A:64:ILE:HD11	0.45	2.47	3	2
1:A:57:VAL:O	1:A:60:PHE:N	0.45	2.50	14	4
1:A:14:ARG:NH1	1:A:106:TYR:OH	0.45	2.50	9	1
1:A:60:PHE:O	1:A:63:VAL:N	0.45	2.50	14	4
1:A:34:GLU:HG3	1:A:108:THR:HG23	0.45	1.87	13	1
1:A:14:ARG:CZ	1:A:106:TYR:OH	0.45	2.64	9	1
1:A:34:GLU:N	1:A:107:VAL:O	0.45	2.50	20	2
1:A:76:ILE:C	1:A:77:PHE:CD1	0.45	2.90	11	2
1:A:95:TYR:O	1:A:95:TYR:CD1	0.45	2.70	13	1
1:A:32:ILE:HG22	1:A:105:LEU:O	0.45	2.12	17	1
1:A:80:VAL:O	1:A:83:THR:N	0.45	2.50	18	4
1:A:49:TYR:CE1	1:A:63:VAL:HG13	0.45	2.46	14	1
1:A:60:PHE:C	1:A:62:TYR:N	0.45	2.70	18	3
1:A:16:ALA:O	1:A:19:GLU:N	0.45	2.51	10	8
1:A:14:ARG:NH2	1:A:106:TYR:OH	0.44	2.50	9	1
1:A:34:GLU:OE1	1:A:47:ARG:NE	0.44	2.50	9	1
1:A:62:TYR:CE2	1:A:66:LYS:HE2	0.44	2.48	13	1
1:A:14:ARG:CG	1:A:15:LYS:N	0.44	2.80	15	1
1:A:41:ILE:CD1	1:A:109:TYR:CE1	0.44	3.00	20	1
1:A:64:ILE:HG12	1:A:109:TYR:CD2	0.44	2.47	12	3
1:A:24:ARG:CD	1:A:25:PHE:CE1	0.44	3.00	20	1
1:A:51:VAL:HG11	1:A:55:LEU:HD13	0.44	1.88	11	1
1:A:14:ARG:HB3	1:A:104:PHE:CD2	0.44	2.47	17	1
1:A:55:LEU:HD23	1:A:56:THR:O	0.44	2.12	9	2
1:A:64:ILE:O	1:A:66:LYS:N	0.44	2.50	18	3
1:A:36:ALA:O	1:A:39:SER:N	0.44	2.50	17	2
1:A:24:ARG:CD	1:A:24:ARG:C	0.44	2.86	3	2
1:A:55:LEU:O	1:A:90:LEU:CD1	0.44	2.66	9	2
1:A:31:VAL:O	1:A:32:ILE:HD12	0.44	2.13	8	1
1:A:28:ARG:NH2	1:A:50:LEU:O	0.44	2.50	14	1
1:A:16:ALA:C	1:A:18:SER:N	0.44	2.71	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:VAL:O	1:A:67:ARG:NE	0.44	2.50	6	1
1:A:34:GLU:CD	1:A:47:ARG:NH2	0.44	2.70	15	1
1:A:100:ASP:OD1	1:A:106:TYR:CE1	0.44	2.71	15	1
1:A:98:HIS:O	1:A:105:LEU:CD2	0.44	2.64	17	1
1:A:14:ARG:HB2	1:A:104:PHE:CD2	0.44	2.47	19	1
1:A:31:VAL:HG13	1:A:105:LEU:HB3	0.44	1.90	20	1
1:A:39:SER:OG	1:A:41:ILE:HG23	0.43	2.13	5	2
1:A:100:ASP:OD2	1:A:106:TYR:CD1	0.43	2.71	5	1
1:A:48:LYS:CD	1:A:48:LYS:C	0.43	2.87	10	2
1:A:41:ILE:HD11	1:A:109:TYR:CE2	0.43	2.48	17	1
1:A:32:ILE:HG22	1:A:34:GLU:OE2	0.43	2.12	20	1
1:A:16:ALA:O	1:A:18:SER:N	0.43	2.51	2	1
1:A:57:VAL:O	1:A:60:PHE:CB	0.43	2.67	13	3
1:A:95:TYR:CE2	1:A:105:LEU:HD23	0.43	2.48	11	1
1:A:98:HIS:C	1:A:105:LEU:HD11	0.43	2.34	14	1
1:A:32:ILE:HD11	1:A:47:ARG:O	0.43	2.14	17	1
1:A:14:ARG:CG	1:A:104:PHE:CE2	0.43	3.02	8	1
1:A:35:LYS:HB2	1:A:109:TYR:CE1	0.43	2.48	19	1
1:A:63:VAL:HG23	1:A:64:ILE:HD12	0.43	1.90	4	2
1:A:14:ARG:O	1:A:17:GLU:N	0.43	2.51	17	1
1:A:44:ILE:HG22	1:A:67:ARG:HB3	0.43	1.90	20	1
1:A:42:PRO:O	1:A:68:ILE:CG2	0.43	2.66	13	1
1:A:64:ILE:C	1:A:66:LYS:N	0.43	2.72	10	4
1:A:60:PHE:O	1:A:64:ILE:HD13	0.43	2.14	13	2
1:A:60:PHE:CE2	1:A:78:ILE:HG21	0.43	2.48	14	1
1:A:31:VAL:HG22	1:A:105:LEU:HD13	0.43	1.89	17	1
1:A:60:PHE:O	1:A:62:TYR:N	0.42	2.53	14	2
1:A:63:VAL:CG1	1:A:64:ILE:N	0.42	2.81	14	1
1:A:31:VAL:CG1	1:A:107:VAL:HG11	0.42	2.44	4	2
1:A:30:PRO:HB3	1:A:50:LEU:HD21	0.42	1.91	18	2
1:A:14:ARG:C	1:A:16:ALA:N	0.42	2.72	8	1
1:A:34:GLU:CA	1:A:47:ARG:HH21	0.42	2.28	8	1
1:A:18:SER:O	1:A:21:ILE:N	0.42	2.53	7	1
1:A:49:TYR:CG	1:A:60:PHE:CZ	0.42	3.08	10	1
1:A:58:GLY:O	1:A:61:VAL:N	0.42	2.53	13	1
1:A:14:ARG:HB3	1:A:104:PHE:CE2	0.42	2.50	17	1
1:A:49:TYR:CE1	1:A:64:ILE:CD1	0.42	3.03	10	3
1:A:21:ILE:HD13	1:A:50:LEU:HD21	0.42	1.92	9	1
1:A:78:ILE:HG22	1:A:107:VAL:HG23	0.42	1.92	11	1
1:A:55:LEU:CD1	1:A:59:GLN:HB2	0.42	2.45	2	3
1:A:102:ASP:OD1	1:A:104:PHE:N	0.42	2.52	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:VAL:O	1:A:83:THR:CB	0.42	2.68	18	1
1:A:27:ASN:HD22	1:A:27:ASN:N	0.42	2.13	20	1
1:A:77:PHE:CZ	1:A:113:ASN:HB2	0.42	2.50	1	1
1:A:35:LYS:N	1:A:47:ARG:NH2	0.42	2.67	8	1
1:A:49:TYR:CZ	1:A:64:ILE:HG13	0.42	2.50	20	1
1:A:80:VAL:CG1	1:A:98:HIS:CE1	0.41	3.03	16	2
1:A:30:PRO:HB3	1:A:50:LEU:HD23	0.41	1.90	10	2
1:A:60:PHE:CD2	1:A:64:ILE:HD11	0.41	2.50	12	1
1:A:33:CYS:SG	1:A:107:VAL:HG22	0.41	2.55	18	1
1:A:110:SER:C	1:A:112:GLU:N	0.41	2.73	9	1
1:A:44:ILE:CD1	1:A:109:TYR:OH	0.41	2.67	13	1
1:A:60:PHE:O	1:A:63:VAL:HG22	0.41	2.15	17	1
1:A:17:GLU:CG	1:A:104:PHE:CE1	0.41	3.03	20	1
1:A:80:VAL:HG12	1:A:83:THR:HG22	0.41	1.93	11	5
1:A:78:ILE:HD12	1:A:109:TYR:HB3	0.41	1.91	19	1
1:A:32:ILE:HG12	1:A:104:PHE:CD2	0.41	2.50	20	1
1:A:64:ILE:O	1:A:68:ILE:CG1	0.41	2.68	6	1
1:A:20:ARG:O	1:A:23:ASP:N	0.41	2.53	9	1
1:A:60:PHE:CE2	1:A:64:ILE:CD1	0.41	3.04	11	1
1:A:33:CYS:HB3	1:A:49:TYR:CZ	0.41	2.50	16	1
1:A:32:ILE:CG2	1:A:47:ARG:NH1	0.41	2.84	3	1
1:A:55:LEU:HD23	1:A:56:THR:N	0.41	2.31	19	1
1:A:24:ARG:C	1:A:24:ARG:CD	0.41	2.89	18	3
1:A:27:ASN:N	1:A:27:ASN:ND2	0.41	2.67	6	1
1:A:32:ILE:CD1	1:A:104:PHE:CE1	0.41	3.04	6	1
1:A:22:ALA:O	1:A:26:PRO:N	0.41	2.54	16	1
1:A:14:ARG:CD	1:A:106:TYR:OH	0.41	2.69	6	1
1:A:32:ILE:CG2	1:A:47:ARG:HD2	0.41	2.46	9	1
1:A:15:LYS:O	1:A:18:SER:N	0.41	2.53	12	1
1:A:31:VAL:HG23	1:A:105:LEU:CD1	0.41	2.45	17	1
1:A:79:PHE:CE2	1:A:110:SER:HB2	0.41	2.51	20	1
1:A:33:CYS:SG	1:A:34:GLU:N	0.41	2.94	12	1
1:A:55:LEU:O	1:A:90:LEU:HD13	0.41	2.16	12	1
1:A:24:ARG:O	1:A:24:ARG:CD	0.41	2.69	16	1
1:A:81:ASN:N	1:A:81:ASN:ND2	0.40	2.68	12	2
1:A:98:HIS:O	1:A:99:LYS:C	0.40	2.60	9	2
1:A:24:ARG:HG3	1:A:25:PHE:CD1	0.40	2.51	7	1
1:A:64:ILE:HG22	1:A:65:ARG:N	0.40	2.31	10	1
1:A:98:HIS:O	1:A:106:TYR:CZ	0.40	2.73	10	1
1:A:59:GLN:O	1:A:62:TYR:N	0.40	2.55	17	1
1:A:35:LYS:HB2	1:A:109:TYR:CZ	0.40	2.51	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:HIS:O	1:A:105:LEU:CD1	0.40	2.70	8	1
1:A:110:SER:O	1:A:112:GLU:N	0.40	2.55	9	1
1:A:48:LYS:C	1:A:49:TYR:CD1	0.40	2.94	12	1
1:A:80:VAL:O	1:A:81:ASN:C	0.40	2.60	18	1
1:A:56:THR:O	1:A:57:VAL:C	0.40	2.60	11	1
1:A:80:VAL:O	1:A:80:VAL:CG2	0.40	2.69	20	1
1:A:75:ALA:O	1:A:111:GLY:O	0.40	2.40	12	1
1:A:39:SER:OG	1:A:110:SER:OG	0.40	2.40	14	1
1:A:29:ILE:HG22	1:A:105:LEU:HD12	0.40	1.92	17	1
1:A:38:LYS:O	1:A:39:SER:C	0.40	2.60	17	1
1:A:37:GLU:O	1:A:39:SER:O	0.40	2.40	20	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	101/116 (87%)	89±3 (88±3%)	11±2 (11±2%)	1±1 (1±1%)	16	63
All	All	2020/2320 (87%)	1771 (88%)	223 (11%)	26 (1%)	16	63

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	104	PHE	15
1	A	39	SER	8
1	A	17	GLU	1
1	A	74	LYS	1
1	A	65	ARG	1

6.3.2 Protein sidechains [i](#)

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

was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	90/104 (87%)	75±3 (83±3%)	15±3 (17±3%)	5	39
All	All	1800/2080 (87%)	1491 (83%)	309 (17%)	5	39

All 47 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	41	ILE	20
1	A	83	THR	20
1	A	99	LYS	20
1	A	51	VAL	19
1	A	107	VAL	18
1	A	87	THR	14
1	A	24	ARG	13
1	A	46	LYS	13
1	A	70	LEU	12
1	A	35	LYS	12
1	A	84	LEU	11
1	A	106	TYR	10
1	A	39	SER	9
1	A	47	ARG	9
1	A	66	LYS	9
1	A	74	LYS	8
1	A	17	GLU	6
1	A	64	ILE	6
1	A	38	LYS	5
1	A	102	ASP	5
1	A	67	ARG	5
1	A	100	ASP	4
1	A	80	VAL	4
1	A	105	LEU	4
1	A	62	TYR	4
1	A	33	CYS	4
1	A	104	PHE	4
1	A	31	VAL	4
1	A	27	ASN	3
1	A	50	LEU	3
1	A	32	ILE	3
1	A	45	ASP	3
1	A	14	ARG	3
1	A	48	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	82	ASP	2
1	A	90	LEU	2
1	A	15	LYS	2
1	A	69	MET	2
1	A	34	GLU	2
1	A	68	ILE	2
1	A	25	PHE	1
1	A	54	ASP	1
1	A	95	TYR	1
1	A	113	ASN	1
1	A	63	VAL	1
1	A	91	MET	1
1	A	18	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

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 91% 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	1497
Number of shifts mapped to atoms	1497
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	116	-0.08 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	111	0.07 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	100	0.03 ± 0.12	None needed (< 0.5 ppm)
^{15}N	107	0.28 ± 0.44	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 91%, i.e. 1192 atoms were assigned a chemical shift out of a possible 1307. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	481/489 (98%)	194/194 (100%)	194/202 (96%)	93/93 (100%)
Sidechain	622/726 (86%)	383/428 (89%)	233/263 (89%)	6/35 (17%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	89/92 (97%)	47/49 (96%)	42/42 (100%)	0/1 (0%)
Overall	1192/1307 (91%)	624/671 (93%)	469/507 (93%)	99/129 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1372 atoms were assigned a chemical shift out of a possible 1507. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	546/562 (97%)	223/223 (100%)	216/232 (93%)	107/107 (100%)
Sidechain	707/818 (86%)	439/485 (91%)	262/295 (89%)	6/38 (16%)
Aromatic	119/127 (94%)	63/68 (93%)	56/58 (97%)	0/1 (0%)
Overall	1372/1507 (91%)	725/776 (93%)	534/585 (91%)	113/146 (77%)

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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	24	ARG	NE	117.58	92.63 – 76.73	20.7
1	A	32	ILE	HD11	-0.86	2.13 – -0.77	-5.3
1	A	32	ILE	HD12	-0.86	2.13 – -0.77	-5.3
1	A	32	ILE	HD13	-0.86	2.13 – -0.77	-5.3

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.

Random coil index (RCI) for chain A:

