



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 08:12 PM UTC

PDB ID : 2LS0 / pdb_00002ls0
BMRB ID : 18404
Title : Solution Structure of the Target Recognition Domain of Zoocin A
Authors : Timkovich, R.; Chen, Y.; Simmonds, R.S.
Deposited on : 2012-04-17

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

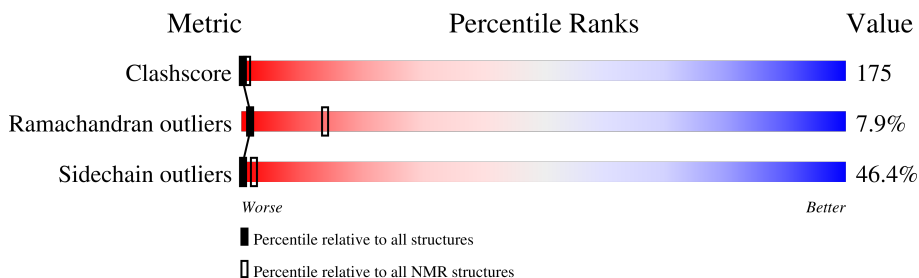
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

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	1	128	

2 Ensemble composition and analysis

This entry contains 10 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: *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	1:22-1:65, 1:76-1:128 (97)	0.16	10

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

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

NmrClust was unable to cluster the ensemble.

Error message: NMCparsrange - Unexpected character.

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1964 atoms, of which 970 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zoocin A endopeptidase.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	1	128	1964	621	970	179	192	2	0

There are 12 discrepancies between the modelled and reference sequences:

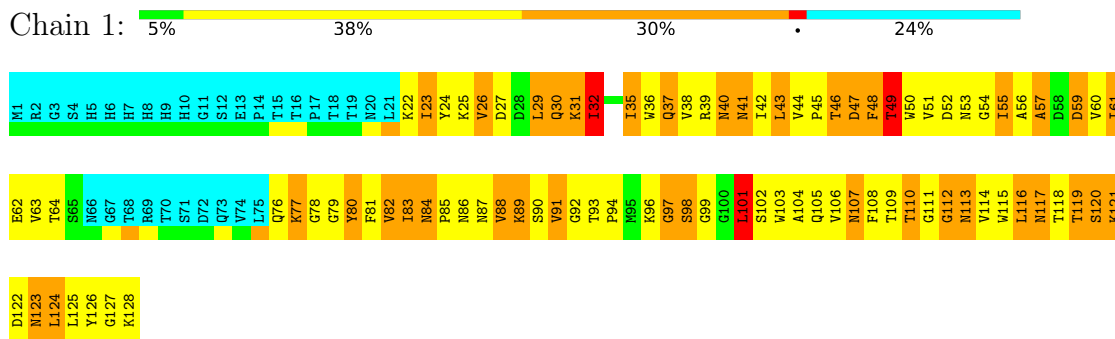
Chain	Residue	Modelled	Actual	Comment	Reference
1	1	MET	-	expression tag	UNP O54308
1	2	ARG	-	expression tag	UNP O54308
1	3	GLY	-	expression tag	UNP O54308
1	4	SER	-	expression tag	UNP O54308
1	5	HIS	-	expression tag	UNP O54308
1	6	HIS	-	expression tag	UNP O54308
1	7	HIS	-	expression tag	UNP O54308
1	8	HIS	-	expression tag	UNP O54308
1	9	HIS	-	expression tag	UNP O54308
1	10	HIS	-	expression tag	UNP O54308
1	11	GLY	-	expression tag	UNP O54308
1	12	SER	-	expression tag	UNP O54308

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: Zoocin A endopeptidase

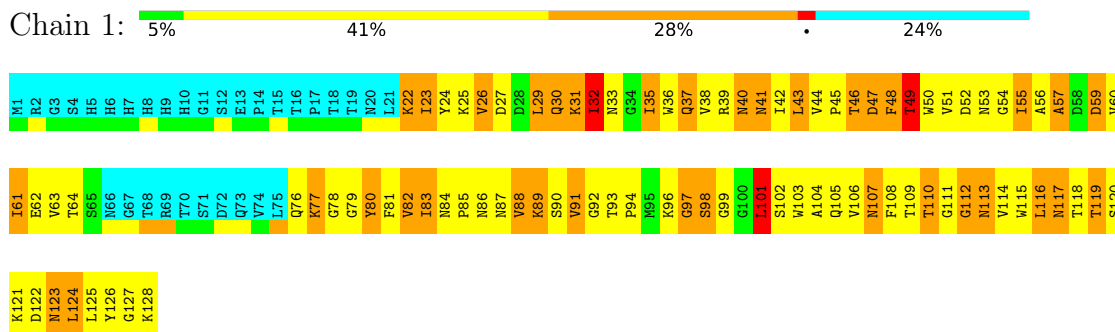


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

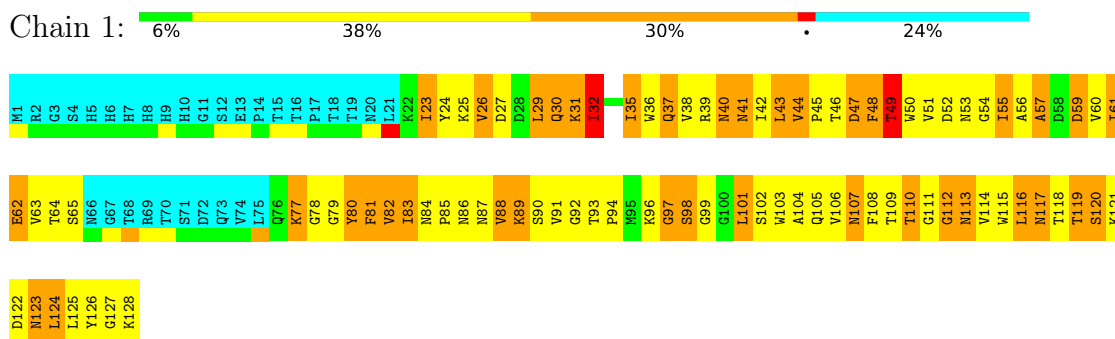
4.2.1 Score per residue for model 1

- Molecule 1: Zoocin A endopeptidase



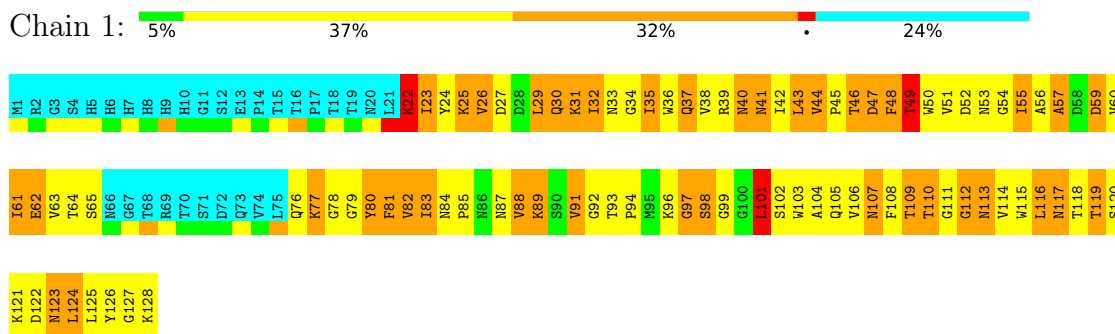
4.2.2 Score per residue for model 2

- Molecule 1: Zoocin A endopeptidase



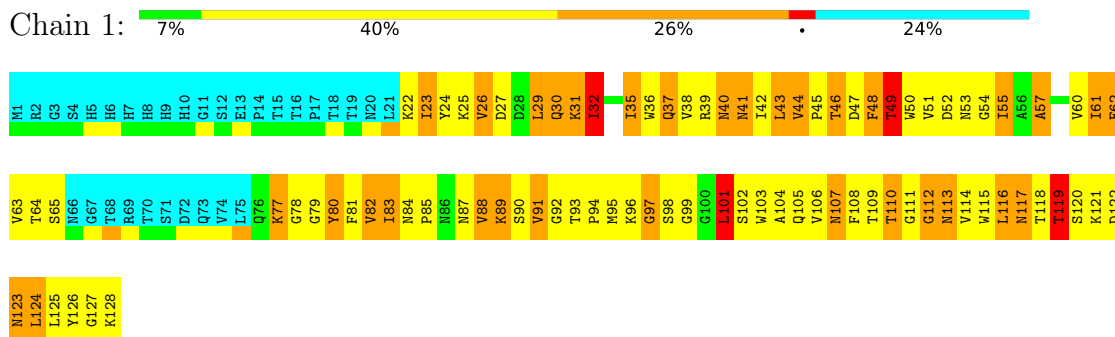
4.2.3 Score per residue for model 3

- Molecule 1: Zoocin A endopeptidase



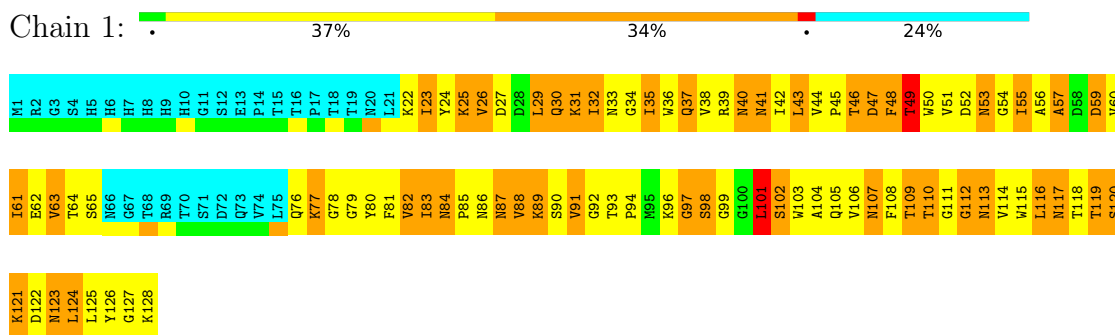
4.2.4 Score per residue for model 4

- Molecule 1: Zoocin A endopeptidase



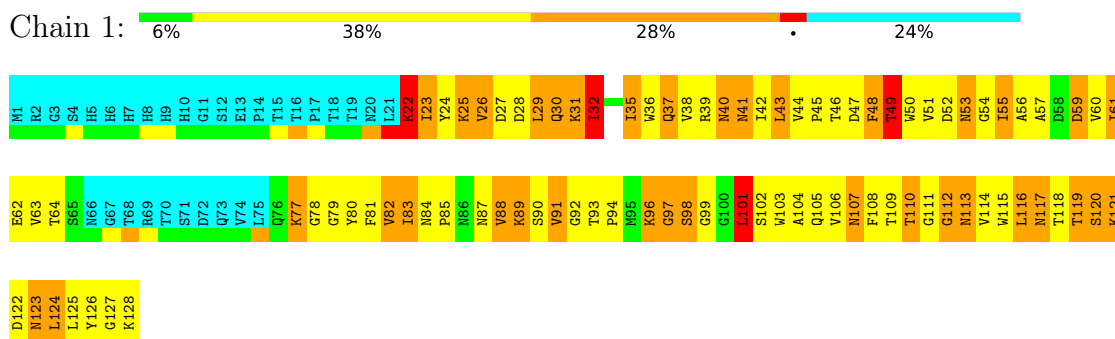
4.2.5 Score per residue for model 5

- Molecule 1: Zoocin A endopeptidase



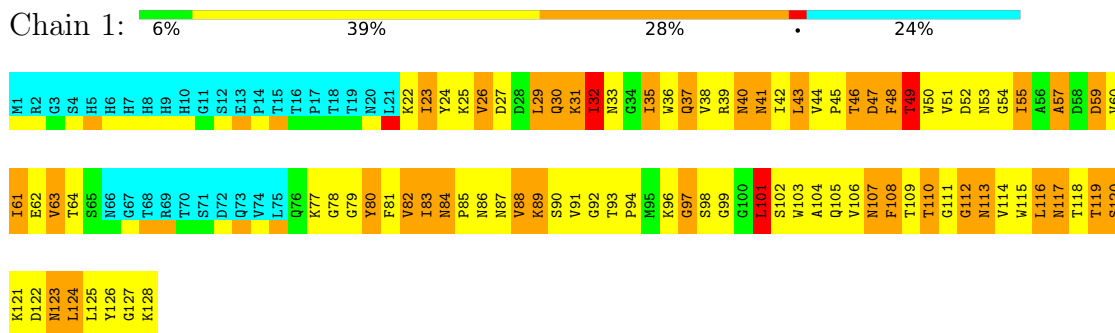
4.2.6 Score per residue for model 6

- Molecule 1: Zoocin A endopeptidase



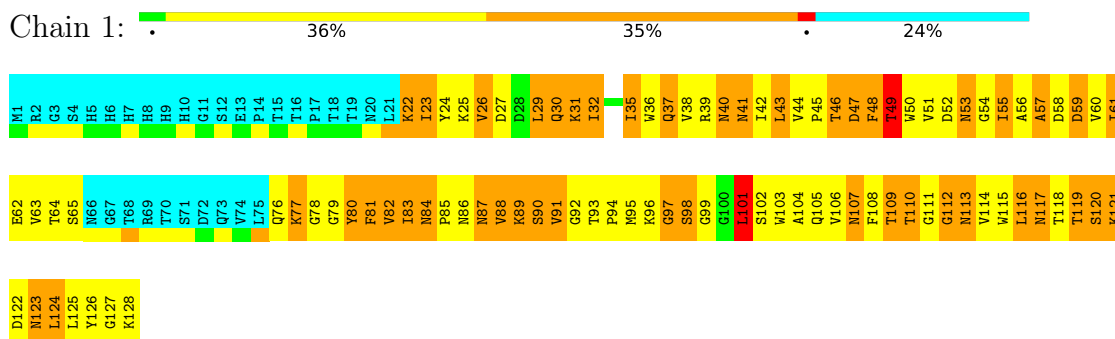
4.2.7 Score per residue for model 7

- Molecule 1: Zoocin A endopeptidase



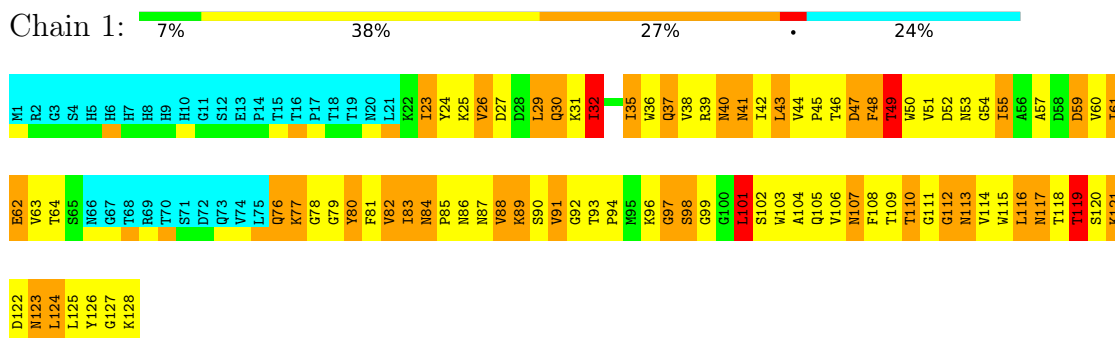
4.2.8 Score per residue for model 8

- Molecule 1: Zoocin A endopeptidase



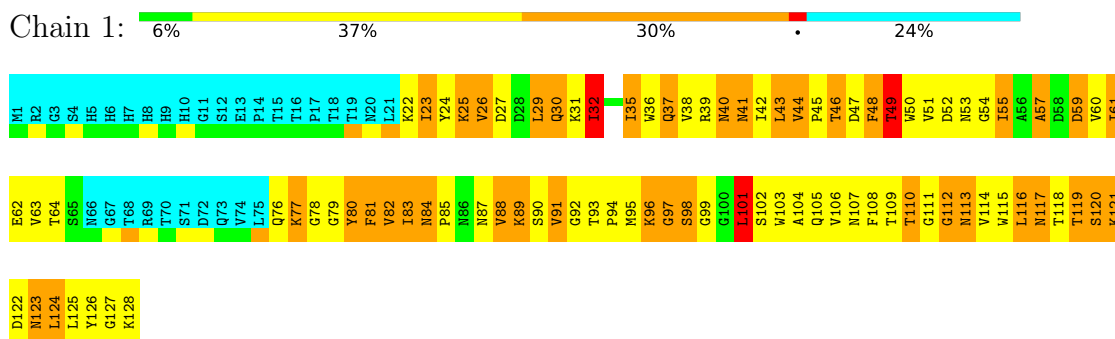
4.2.9 Score per residue for model 9

- Molecule 1: Zoocin A endopeptidase



4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Zoocin A endopeptidase



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 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
CNSSOLVE	structure solution	1.2
CNSSOLVE	refinement	1.2
ARIA	structure solution	2.0

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	1406
Number of shifts mapped to atoms	1406
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

6 Model quality i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	1	0.93±0.01	1±0/769 (0.1± 0.0%)	1.04±0.01	1±0/1046 (0.1± 0.0%)
All	All	0.93	10/7690 (0.1%)	1.04	9/10460 (0.1%)

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	1	88	VAL	N-CA	-5.57	1.39	1.46	7	10

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	1	32	ILE	N-CA-CB	-5.74	104.18	111.64	7	7
1	1	87	ASN	N-CA-C	-5.06	107.08	113.20	8	2

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	1	753	744	744	262±8
All	All	7530	7440	7440	2624

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 175.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:53:ASN:HA	1:1:115:TRP:HB2	1.05	1.28	2	10
1:1:124:LEU:HD22	1:1:124:LEU:H	1.00	1.17	6	10
1:1:29:LEU:O	1:1:30:GLN:NE2	0.98	1.97	3	10
1:1:120:SER:O	1:1:123:ASN:HB3	0.95	1.61	9	10
1:1:94:PRO:HB3	1:1:118:THR:HG21	0.94	1.36	5	10
1:1:32:ILE:HD13	1:1:50:TRP:CD2	0.91	1.99	1	10
1:1:32:ILE:HD13	1:1:50:TRP:CG	0.90	2.01	7	9
1:1:55:ILE:HD11	1:1:60:VAL:HG13	0.89	1.41	8	10
1:1:37:GLN:OE1	1:1:54:GLY:HA3	0.89	1.66	6	10
1:1:24:TYR:OH	1:1:124:LEU:HA	0.89	1.66	3	10
1:1:91:VAL:HG12	1:1:106:VAL:HG22	0.84	1.49	10	8
1:1:91:VAL:HG12	1:1:106:VAL:CG2	0.83	2.02	10	8
1:1:55:ILE:HA	1:1:114:VAL:CG1	0.83	2.03	9	10
1:1:98:SER:HB2	1:1:103:TRP:CD2	0.82	2.09	4	10
1:1:32:ILE:HD12	1:1:37:GLN:NE2	0.81	1.90	6	9
1:1:61:ILE:HG13	1:1:82:VAL:O	0.81	1.75	6	10
1:1:32:ILE:HD12	1:1:50:TRP:CD1	0.80	2.12	8	2
1:1:109:THR:HG23	1:1:110:THR:H	0.79	1.35	6	7
1:1:61:ILE:HD11	1:1:84:ASN:HA	0.79	1.53	3	10
1:1:56:ALA:HB3	1:1:59:ASP:OD2	0.79	1.76	5	6
1:1:40:ASN:O	1:1:44:VAL:N	0.78	2.16	5	10
1:1:88:VAL:C	1:1:89:LYS:HE2	0.78	2.03	5	4
1:1:89:LYS:HD2	1:1:107:ASN:O	0.78	1.77	7	10
1:1:49:THR:HG22	1:1:51:VAL:HG12	0.77	1.56	4	10
1:1:94:PRO:CB	1:1:118:THR:HG21	0.77	2.09	5	10
1:1:46:THR:HG23	1:1:47:ASP:OD2	0.77	1.80	1	5
1:1:84:ASN:HB3	1:1:87:ASN:HB2	0.77	1.57	7	10
1:1:30:GLN:O	1:1:32:ILE:HG13	0.77	1.79	10	9
1:1:37:GLN:HA	1:1:55:ILE:O	0.77	1.78	3	10
1:1:39:ARG:HG2	1:1:48:PHE:HB2	0.77	1.56	1	10
1:1:32:ILE:HG23	1:1:50:TRP:HB3	0.77	1.56	6	10
1:1:38:VAL:HG11	1:1:81:PHE:CZ	0.77	2.15	1	10
1:1:61:ILE:HD12	1:1:82:VAL:HG12	0.77	1.57	3	6
1:1:34:GLY:O	1:1:35:ILE:HD13	0.76	1.80	5	2
1:1:44:VAL:HG21	1:1:48:PHE:CE2	0.76	2.16	6	10
1:1:95:MET:HE2	1:1:115:TRP:CH2	0.76	2.14	4	2
1:1:26:VAL:HG23	1:1:80:TYR:N	0.76	1.96	2	10
1:1:55:ILE:HD11	1:1:60:VAL:CG1	0.76	2.11	8	10
1:1:122:ASP:HB2	1:1:128:LYS:HD2	0.76	1.58	7	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:89:LYS:N	1:1:89:LYS:CE	0.75	2.50	2	9
1:1:117:ASN:OD1	1:1:119:THR:HG22	0.74	1.83	8	8
1:1:38:VAL:CG2	1:1:57:ALA:HB2	0.73	2.13	8	10
1:1:38:VAL:O	1:1:55:ILE:CG2	0.73	2.36	8	10
1:1:124:LEU:HD22	1:1:124:LEU:N	0.73	1.95	7	10
1:1:89:LYS:HB2	1:1:107:ASN:HB3	0.72	1.60	9	10
1:1:29:LEU:HB3	1:1:77:LYS:HB3	0.72	1.61	9	10
1:1:32:ILE:HG13	1:1:37:GLN:HB3	0.72	1.61	5	5
1:1:84:ASN:O	1:1:88:VAL:HG23	0.71	1.84	6	10
1:1:24:TYR:HB3	1:1:81:PHE:CE1	0.71	2.19	8	10
1:1:24:TYR:HB2	1:1:81:PHE:O	0.71	1.85	7	10
1:1:108:PHE:CE1	1:1:114:VAL:HB	0.71	2.20	7	8
1:1:26:VAL:HG23	1:1:79:GLY:C	0.70	2.10	8	10
1:1:123:ASN:O	1:1:127:GLY:N	0.70	2.24	1	10
1:1:38:VAL:O	1:1:55:ILE:HG23	0.69	1.87	6	10
1:1:51:VAL:HG13	1:1:52:ASP:N	0.69	2.03	4	10
1:1:44:VAL:HG21	1:1:48:PHE:CD2	0.69	2.22	10	10
1:1:123:ASN:O	1:1:127:GLY:HA2	0.69	1.88	1	10
1:1:87:ASN:CG	1:1:109:THR:HG21	0.69	2.13	2	7
1:1:120:SER:O	1:1:123:ASN:CB	0.68	2.41	2	10
1:1:49:THR:CG2	1:1:51:VAL:HG12	0.68	2.18	4	10
1:1:37:GLN:HG3	1:1:54:GLY:CA	0.68	2.19	5	10
1:1:53:ASN:CA	1:1:115:TRP:HB2	0.67	2.16	5	10
1:1:38:VAL:HG23	1:1:57:ALA:HB2	0.67	1.66	4	10
1:1:123:ASN:HA	1:1:128:LYS:N	0.67	2.03	6	10
1:1:61:ILE:HG12	1:1:84:ASN:HB2	0.67	1.65	3	10
1:1:34:GLY:C	1:1:35:ILE:HD13	0.67	2.15	3	2
1:1:24:TYR:CE1	1:1:83:ILE:HD13	0.67	2.25	6	10
1:1:123:ASN:O	1:1:127:GLY:CA	0.67	2.43	1	10
1:1:61:ILE:HD11	1:1:84:ASN:CA	0.67	2.20	3	8
1:1:89:LYS:HD3	1:1:108:PHE:C	0.67	2.14	8	10
1:1:27:ASP:HB2	1:1:40:ASN:HA	0.66	1.68	4	10
1:1:109:THR:HG23	1:1:110:THR:N	0.65	2.05	6	7
1:1:87:ASN:O	1:1:89:LYS:HE3	0.65	1.90	4	8
1:1:91:VAL:HG13	1:1:106:VAL:HG22	0.65	1.66	7	2
1:1:24:TYR:HH	1:1:124:LEU:HA	0.65	1.51	10	1
1:1:88:VAL:C	1:1:89:LYS:HE3	0.65	2.16	6	6
1:1:109:THR:CG2	1:1:110:THR:N	0.65	2.59	5	8
1:1:101:LEU:HD22	1:1:117:ASN:ND2	0.65	2.06	2	10
1:1:105:GLN:HB2	1:1:115:TRP:CZ2	0.65	2.27	3	10
1:1:29:LEU:HD11	1:1:36:TRP:HB3	0.65	1.69	5	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:30:GLN:HB2	1:1:32:ILE:HD11	0.64	1.67	4	10
1:1:88:VAL:C	1:1:89:LYS:CE	0.64	2.70	6	9
1:1:51:VAL:CG1	1:1:52:ASP:N	0.64	2.61	3	10
1:1:87:ASN:C	1:1:89:LYS:HE3	0.64	2.17	6	6
1:1:44:VAL:HG11	1:1:48:PHE:HB2	0.64	1.69	10	10
1:1:25:LYS:O	1:1:40:ASN:CB	0.64	2.46	9	10
1:1:39:ARG:HG2	1:1:44:VAL:HG11	0.64	1.70	9	10
1:1:89:LYS:N	1:1:89:LYS:CD	0.64	2.61	6	6
1:1:91:VAL:CG1	1:1:106:VAL:HG22	0.63	2.22	3	8
1:1:122:ASP:O	1:1:126:TYR:N	0.63	2.30	3	10
1:1:37:GLN:HG3	1:1:54:GLY:C	0.63	2.18	5	10
1:1:29:LEU:CB	1:1:37:GLN:O	0.63	2.46	9	10
1:1:37:GLN:CD	1:1:54:GLY:HA3	0.63	2.18	6	10
1:1:118:THR:C	1:1:120:SER:H	0.62	2.02	6	10
1:1:61:ILE:HG12	1:1:84:ASN:CB	0.62	2.24	7	10
1:1:83:ILE:HG23	1:1:108:PHE:CE2	0.62	2.30	6	9
1:1:123:ASN:C	1:1:123:ASN:ND2	0.62	2.56	8	10
1:1:88:VAL:CA	1:1:89:LYS:HE2	0.61	2.25	3	4
1:1:87:ASN:O	1:1:89:LYS:CE	0.61	2.48	7	10
1:1:63:VAL:HG21	1:1:82:VAL:HG23	0.61	1.72	1	3
1:1:103:TRP:CD1	1:1:103:TRP:N	0.61	2.69	7	10
1:1:101:LEU:HD12	1:1:101:LEU:H	0.61	1.55	1	10
1:1:55:ILE:HA	1:1:114:VAL:HG13	0.61	1.73	2	9
1:1:121:LYS:O	1:1:124:LEU:CD2	0.61	2.48	8	10
1:1:109:THR:HG22	1:1:110:THR:N	0.61	2.11	5	3
1:1:41:ASN:HD22	1:1:41:ASN:N	0.61	1.91	5	1
1:1:25:LYS:O	1:1:40:ASN:HB3	0.61	1.94	7	10
1:1:55:ILE:O	1:1:55:ILE:HG13	0.61	1.94	6	10
1:1:108:PHE:CD1	1:1:114:VAL:HB	0.61	2.30	6	10
1:1:48:PHE:CE1	1:1:53:ASN:O	0.60	2.54	1	10
1:1:29:LEU:HB2	1:1:37:GLN:O	0.60	1.97	9	10
1:1:55:ILE:CD1	1:1:60:VAL:HG13	0.60	2.25	3	10
1:1:39:ARG:HG2	1:1:48:PHE:CB	0.60	2.25	10	10
1:1:37:GLN:OE1	1:1:54:GLY:CA	0.60	2.47	1	10
1:1:32:ILE:CG2	1:1:50:TRP:HB3	0.60	2.26	5	9
1:1:85:PRO:O	1:1:88:VAL:HB	0.60	1.96	3	10
1:1:89:LYS:CD	1:1:89:LYS:N	0.60	2.64	5	4
1:1:103:TRP:CE2	1:1:117:ASN:HB2	0.59	2.32	7	10
1:1:26:VAL:HG22	1:1:81:PHE:CD1	0.59	2.33	3	10
1:1:37:GLN:HG3	1:1:54:GLY:HA3	0.59	1.73	5	10
1:1:101:LEU:HD13	1:1:103:TRP:CZ2	0.58	2.32	2	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:41:ASN:N	1:1:41:ASN:ND2	0.58	2.50	5	10
1:1:38:VAL:CG1	1:1:81:PHE:CZ	0.58	2.87	1	10
1:1:98:SER:CB	1:1:103:TRP:CD2	0.58	2.85	5	10
1:1:116:LEU:HD23	1:1:123:ASN:OD1	0.58	1.98	5	8
1:1:32:ILE:HG23	1:1:50:TRP:CB	0.57	2.26	7	10
1:1:122:ASP:CB	1:1:128:LYS:HD2	0.57	2.28	7	7
1:1:32:ILE:CD1	1:1:50:TRP:CD1	0.57	2.88	8	10
1:1:105:GLN:HG3	1:1:115:TRP:NE1	0.57	2.14	7	10
1:1:32:ILE:HD12	1:1:50:TRP:CG	0.57	2.34	8	1
1:1:122:ASP:O	1:1:127:GLY:N	0.57	2.38	3	10
1:1:39:ARG:HG2	1:1:48:PHE:CD2	0.57	2.34	9	9
1:1:87:ASN:O	1:1:89:LYS:HE2	0.57	2.00	7	1
1:1:53:ASN:HA	1:1:115:TRP:CB	0.56	2.21	5	6
1:1:37:GLN:CG	1:1:54:GLY:HA3	0.56	2.30	6	10
1:1:32:ILE:HD13	1:1:50:TRP:CD1	0.56	2.35	7	4
1:1:30:GLN:CB	1:1:32:ILE:HD11	0.56	2.29	8	4
1:1:23:ILE:HD11	1:1:64:THR:O	0.56	1.99	8	9
1:1:38:VAL:HB	1:1:55:ILE:CG2	0.56	2.31	2	10
1:1:43:LEU:O	1:1:103:TRP:CH2	0.56	2.59	2	10
1:1:55:ILE:CD1	1:1:60:VAL:CG1	0.56	2.84	8	10
1:1:26:VAL:HG22	1:1:81:PHE:HD1	0.56	1.59	5	10
1:1:41:ASN:N	1:1:41:ASN:HD22	0.56	1.99	1	7
1:1:88:VAL:CA	1:1:89:LYS:HE3	0.56	2.31	6	6
1:1:111:GLY:O	1:1:113:ASN:N	0.56	2.39	5	10
1:1:24:TYR:CD2	1:1:81:PHE:CZ	0.55	2.94	1	10
1:1:32:ILE:CD1	1:1:50:TRP:CG	0.55	2.89	8	8
1:1:38:VAL:HG11	1:1:81:PHE:CE1	0.55	2.36	1	8
1:1:32:ILE:HD12	1:1:37:GLN:CD	0.55	2.25	7	7
1:1:92:GLY:HA3	1:1:105:GLN:O	0.55	2.01	7	10
1:1:121:LYS:O	1:1:124:LEU:HD22	0.55	2.01	3	10
1:1:124:LEU:H	1:1:124:LEU:CD2	0.55	1.94	4	10
1:1:102:SER:O	1:1:118:THR:N	0.55	2.39	7	10
1:1:105:GLN:HB2	1:1:115:TRP:CH2	0.55	2.37	1	10
1:1:48:PHE:O	1:1:50:TRP:N	0.55	2.39	3	10
1:1:91:VAL:HA	1:1:106:VAL:HG22	0.55	1.78	5	10
1:1:89:LYS:HD3	1:1:109:THR:N	0.55	2.17	3	3
1:1:29:LEU:HA	1:1:37:GLN:O	0.55	2.01	6	10
1:1:30:GLN:HE21	1:1:30:GLN:HA	0.55	1.62	8	10
1:1:83:ILE:CD1	1:1:83:ILE:N	0.55	2.70	7	10
1:1:26:VAL:CG1	1:1:77:LYS:HA	0.54	2.31	3	9
1:1:89:LYS:CE	1:1:89:LYS:N	0.54	2.69	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:48:PHE:HE2	1:1:55:ILE:HG22	0.54	1.63	3	10
1:1:41:ASN:ND2	1:1:42:ILE:HD12	0.54	2.18	1	9
1:1:30:GLN:O	1:1:32:ILE:CG1	0.54	2.56	5	8
1:1:94:PRO:HB3	1:1:118:THR:CG2	0.54	2.27	9	7
1:1:29:LEU:HD23	1:1:77:LYS:HD2	0.54	1.79	6	4
1:1:98:SER:O	1:1:103:TRP:CZ2	0.54	2.60	2	10
1:1:43:LEU:O	1:1:117:ASN:HB3	0.53	2.02	6	10
1:1:40:ASN:O	1:1:44:VAL:C	0.53	2.52	8	10
1:1:123:ASN:HA	1:1:128:LYS:H	0.53	1.62	6	10
1:1:63:VAL:HG13	1:1:82:VAL:HB	0.53	1.80	3	4
1:1:87:ASN:C	1:1:89:LYS:HE2	0.53	2.27	3	4
1:1:32:ILE:CD1	1:1:50:TRP:CD2	0.53	2.90	8	6
1:1:25:LYS:HB2	1:1:40:ASN:HB3	0.53	1.79	3	10
1:1:32:ILE:HD13	1:1:50:TRP:CE2	0.53	2.36	1	7
1:1:96:LYS:HA	1:1:101:LEU:O	0.53	2.03	6	10
1:1:89:LYS:HD2	1:1:89:LYS:N	0.53	2.19	5	3
1:1:32:ILE:CD1	1:1:50:TRP:CE2	0.52	2.91	8	10
1:1:45:PRO:O	1:1:46:THR:HB	0.52	2.03	7	10
1:1:118:THR:O	1:1:120:SER:N	0.52	2.43	6	10
1:1:29:LEU:CA	1:1:37:GLN:O	0.52	2.56	6	10
1:1:105:GLN:HG3	1:1:115:TRP:CE2	0.52	2.38	7	10
1:1:102:SER:C	1:1:103:TRP:CD1	0.52	2.87	9	10
1:1:32:ILE:CG1	1:1:37:GLN:HB3	0.52	2.32	5	7
1:1:81:PHE:CE2	1:1:83:ILE:HD11	0.52	2.39	2	10
1:1:29:LEU:C	1:1:30:GLN:NE2	0.52	2.67	1	10
1:1:52:ASP:O	1:1:115:TRP:HD1	0.52	1.87	6	8
1:1:60:VAL:CG1	1:1:83:ILE:HG13	0.52	2.35	2	10
1:1:98:SER:HB2	1:1:103:TRP:CE2	0.52	2.39	7	10
1:1:122:ASP:HB2	1:1:128:LYS:CD	0.52	2.34	3	8
1:1:59:ASP:HB3	1:1:108:PHE:HB3	0.52	1.82	9	6
1:1:97:GLY:O	1:1:99:GLY:N	0.52	2.42	5	10
1:1:89:LYS:CD	1:1:108:PHE:C	0.52	2.83	8	10
1:1:91:VAL:HG13	1:1:106:VAL:CG2	0.52	2.35	7	1
1:1:44:VAL:HA	1:1:103:TRP:CH2	0.52	2.40	5	10
1:1:87:ASN:O	1:1:109:THR:N	0.52	2.43	10	9
1:1:122:ASP:O	1:1:126:TYR:HB2	0.52	2.05	5	9
1:1:25:LYS:HD2	1:1:42:ILE:HD11	0.52	1.81	9	1
1:1:40:ASN:O	1:1:44:VAL:CA	0.51	2.58	6	10
1:1:98:SER:HB3	1:1:103:TRP:CH2	0.51	2.41	2	10
1:1:118:THR:C	1:1:120:SER:N	0.51	2.68	6	10
1:1:124:LEU:N	1:1:124:LEU:CD2	0.51	2.69	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:89:LYS:HE2	1:1:89:LYS:N	0.51	2.20	7	4
1:1:23:ILE:HG12	1:1:80:TYR:HB2	0.51	1.82	9	1
1:1:36:TRP:O	1:1:57:ALA:N	0.51	2.43	6	10
1:1:124:LEU:N	1:1:124:LEU:HD13	0.51	2.21	3	10
1:1:24:TYR:CD1	1:1:83:ILE:HD13	0.51	2.40	6	7
1:1:29:LEU:HB2	1:1:38:VAL:HA	0.51	1.83	9	7
1:1:98:SER:CB	1:1:103:TRP:CE2	0.51	2.94	7	10
1:1:48:PHE:CD1	1:1:103:TRP:HZ3	0.51	2.24	4	10
1:1:49:THR:HG1	1:1:53:ASN:CG	0.51	2.14	5	2
1:1:89:LYS:HD2	1:1:89:LYS:H	0.50	1.67	5	9
1:1:104:ALA:O	1:1:115:TRP:HA	0.50	2.07	7	10
1:1:23:ILE:HG13	1:1:63:VAL:CG2	0.50	2.36	9	6
1:1:24:TYR:O	1:1:80:TYR:HB3	0.50	2.07	1	8
1:1:62:GLU:O	1:1:62:GLU:HG3	0.50	2.07	2	1
1:1:83:ILE:HG23	1:1:108:PHE:HE2	0.50	1.66	5	4
1:1:101:LEU:CD1	1:1:103:TRP:HE1	0.50	2.20	4	10
1:1:30:GLN:NE2	1:1:30:GLN:HA	0.50	2.21	3	6
1:1:87:ASN:OD1	1:1:109:THR:HG22	0.50	2.06	3	3
1:1:26:VAL:O	1:1:78:GLY:N	0.50	2.43	8	8
1:1:39:ARG:CG	1:1:48:PHE:HB2	0.50	2.35	9	1
1:1:25:LYS:O	1:1:40:ASN:CG	0.50	2.55	8	10
1:1:32:ILE:O	1:1:35:ILE:O	0.50	2.29	9	10
1:1:49:THR:HG22	1:1:51:VAL:CG1	0.50	2.31	4	8
1:1:102:SER:C	1:1:118:THR:HG22	0.50	2.32	8	8
1:1:41:ASN:ND2	1:1:41:ASN:H	0.49	2.05	8	10
1:1:37:GLN:HG2	1:1:38:VAL:N	0.49	2.21	8	9
1:1:41:ASN:ND2	1:1:42:ILE:CD1	0.49	2.76	5	9
1:1:83:ILE:CG2	1:1:108:PHE:CE2	0.49	2.94	6	7
1:1:38:VAL:C	1:1:55:ILE:HG23	0.49	2.32	6	10
1:1:103:TRP:HA	1:1:117:ASN:HA	0.49	1.83	6	10
1:1:38:VAL:HB	1:1:55:ILE:HG23	0.49	1.83	8	10
1:1:104:ALA:HB2	1:1:118:THR:HG21	0.49	1.84	2	8
1:1:62:GLU:HG2	1:1:80:TYR:O	0.49	2.08	6	2
1:1:51:VAL:CG1	1:1:52:ASP:H	0.49	2.20	4	10
1:1:109:THR:HG22	1:1:110:THR:H	0.49	1.68	5	3
1:1:32:ILE:HB	1:1:37:GLN:CB	0.49	2.38	7	3
1:1:25:LYS:CB	1:1:40:ASN:HB3	0.49	2.37	4	4
1:1:49:THR:CB	1:1:53:ASN:HB2	0.49	2.37	7	9
1:1:98:SER:CB	1:1:103:TRP:CE3	0.49	2.96	1	10
1:1:48:PHE:CD1	1:1:103:TRP:CZ3	0.48	3.01	4	10
1:1:109:THR:CG2	1:1:110:THR:H	0.48	2.17	2	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:25:LYS:HG3	1:1:42:ILE:HD11	0.48	1.83	10	4
1:1:117:ASN:OD1	1:1:119:THR:OG1	0.48	2.32	4	2
1:1:37:GLN:CG	1:1:54:GLY:CA	0.48	2.92	4	10
1:1:53:ASN:N	1:1:53:ASN:HD22	0.48	2.07	8	5
1:1:38:VAL:CA	1:1:55:ILE:HG23	0.48	2.39	4	10
1:1:48:PHE:CE2	1:1:55:ILE:HG22	0.48	2.43	2	10
1:1:101:LEU:HD13	1:1:103:TRP:NE1	0.48	2.23	9	10
1:1:108:PHE:CD1	1:1:114:VAL:CG2	0.48	2.96	6	8
1:1:91:VAL:HG12	1:1:92:GLY:N	0.48	2.24	2	2
1:1:32:ILE:CG2	1:1:50:TRP:CB	0.48	2.92	4	9
1:1:116:LEU:O	1:1:118:THR:N	0.48	2.47	10	10
1:1:125:LEU:HD12	1:1:125:LEU:H	0.48	1.68	3	10
1:1:105:GLN:CD	1:1:115:TRP:CZ2	0.48	2.92	5	10
1:1:38:VAL:O	1:1:48:PHE:CD2	0.47	2.67	1	9
1:1:98:SER:HB3	1:1:103:TRP:CZ2	0.47	2.44	2	10
1:1:44:VAL:HG11	1:1:48:PHE:CB	0.47	2.38	10	5
1:1:87:ASN:CG	1:1:109:THR:CG2	0.47	2.87	9	7
1:1:122:ASP:O	1:1:126:TYR:CB	0.47	2.62	2	9
1:1:116:LEU:HD22	1:1:124:LEU:HD12	0.47	1.87	5	2
1:1:122:ASP:CB	1:1:128:LYS:CD	0.47	2.92	3	4
1:1:32:ILE:HB	1:1:37:GLN:HB2	0.47	1.86	7	5
1:1:94:PRO:HA	1:1:104:ALA:HA	0.47	1.86	1	9
1:1:101:LEU:HD13	1:1:103:TRP:HE1	0.47	1.68	9	10
1:1:104:ALA:CB	1:1:118:THR:CB	0.47	2.93	2	10
1:1:89:LYS:H	1:1:89:LYS:HD2	0.47	1.69	6	1
1:1:24:TYR:HB3	1:1:81:PHE:CD1	0.47	2.45	7	10
1:1:43:LEU:CD2	1:1:123:ASN:HD21	0.47	2.23	8	10
1:1:57:ALA:O	1:1:60:VAL:HG22	0.47	2.10	8	7
1:1:43:LEU:N	1:1:43:LEU:HD13	0.47	2.24	4	3
1:1:89:LYS:N	1:1:89:LYS:HD2	0.47	2.25	6	3
1:1:49:THR:OG1	1:1:53:ASN:OD1	0.46	2.33	4	6
1:1:24:TYR:CZ	1:1:83:ILE:CD1	0.46	2.99	2	2
1:1:31:LYS:C	1:1:32:ILE:HG12	0.46	2.35	8	4
1:1:42:ILE:C	1:1:43:LEU:HD13	0.46	2.35	4	2
1:1:41:ASN:HD22	1:1:42:ILE:HD12	0.46	1.69	8	7
1:1:63:VAL:HG21	1:1:82:VAL:CG2	0.46	2.38	1	2
1:1:39:ARG:CG	1:1:48:PHE:CD2	0.46	2.99	2	10
1:1:92:GLY:CA	1:1:105:GLN:O	0.46	2.63	10	10
1:1:24:TYR:CZ	1:1:83:ILE:HG12	0.46	2.45	2	3
1:1:24:TYR:CE1	1:1:83:ILE:CD1	0.46	2.98	6	1
1:1:46:THR:HG23	1:1:47:ASP:CG	0.46	2.36	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:22:LYS:CB	1:1:126:TYR:O	0.45	2.63	1	6
1:1:104:ALA:CB	1:1:118:THR:HB	0.45	2.41	6	10
1:1:105:GLN:CG	1:1:115:TRP:CE2	0.45	2.99	4	10
1:1:62:GLU:HA	1:1:81:PHE:HA	0.45	1.88	4	3
1:1:121:LYS:O	1:1:125:LEU:HD13	0.45	2.11	6	6
1:1:23:ILE:HG23	1:1:24:TYR:O	0.45	2.11	2	6
1:1:27:ASP:OD1	1:1:41:ASN:OD1	0.45	2.35	2	1
1:1:87:ASN:C	1:1:89:LYS:CE	0.45	2.89	3	2
1:1:38:VAL:O	1:1:55:ILE:HG22	0.45	2.11	8	3
1:1:121:LYS:HG3	1:1:122:ASP:N	0.45	2.26	5	1
1:1:90:SER:O	1:1:106:VAL:HG13	0.45	2.11	9	5
1:1:101:LEU:HB2	1:1:103:TRP:HE1	0.45	1.71	1	10
1:1:30:GLN:NE2	1:1:30:GLN:CA	0.45	2.79	3	10
1:1:43:LEU:HD21	1:1:123:ASN:ND2	0.45	2.27	10	3
1:1:101:LEU:HB2	1:1:117:ASN:HD22	0.45	1.71	5	9
1:1:121:LYS:C	1:1:123:ASN:N	0.45	2.75	3	7
1:1:108:PHE:N	1:1:112:GLY:O	0.45	2.49	4	9
1:1:61:ILE:CD1	1:1:82:VAL:HG12	0.45	2.38	8	2
1:1:81:PHE:CD1	1:1:81:PHE:N	0.44	2.85	2	10
1:1:44:VAL:HA	1:1:103:TRP:HH2	0.44	1.69	5	7
1:1:44:VAL:CG2	1:1:48:PHE:CE2	0.44	2.96	6	5
1:1:28:ASP:O	1:1:39:ARG:HD3	0.44	2.12	6	1
1:1:30:GLN:C	1:1:32:ILE:HG12	0.44	2.37	8	1
1:1:107:ASN:HA	1:1:112:GLY:O	0.44	2.12	9	5
1:1:108:PHE:CG	1:1:114:VAL:HG21	0.44	2.47	8	2
1:1:89:LYS:N	1:1:89:LYS:HE2	0.44	2.27	2	6
1:1:106:VAL:CG1	1:1:108:PHE:CE1	0.44	3.01	10	7
1:1:125:LEU:HD12	1:1:125:LEU:N	0.44	2.27	8	8
1:1:59:ASP:OD1	1:1:59:ASP:N	0.44	2.51	9	3
1:1:106:VAL:HG12	1:1:108:PHE:CE1	0.44	2.48	9	3
1:1:89:LYS:CD	1:1:109:THR:N	0.44	2.81	3	2
1:1:122:ASP:O	1:1:126:TYR:CA	0.43	2.66	2	7
1:1:59:ASP:CB	1:1:108:PHE:CD2	0.43	3.01	3	1
1:1:80:TYR:N	1:1:80:TYR:CD1	0.43	2.84	3	1
1:1:52:ASP:OD1	1:1:113:ASN:ND2	0.43	2.51	4	4
1:1:26:VAL:HB	1:1:78:GLY:H	0.43	1.73	9	4
1:1:24:TYR:CE2	1:1:116:LEU:HD21	0.43	2.47	6	4
1:1:101:LEU:H	1:1:101:LEU:CD1	0.43	2.25	9	6
1:1:25:LYS:HB2	1:1:42:ILE:CD1	0.43	2.44	5	2
1:1:60:VAL:HG12	1:1:83:ILE:HG23	0.43	1.90	9	1
1:1:32:ILE:HG22	1:1:50:TRP:O	0.43	2.13	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:37:GLN:NE2	1:1:39:ARG:HD2	0.43	2.29	6	1
1:1:31:LYS:HD3	1:1:36:TRP:CD2	0.43	2.48	1	6
1:1:105:GLN:CB	1:1:115:TRP:CZ2	0.43	3.01	4	9
1:1:24:TYR:OH	1:1:83:ILE:HG12	0.43	2.14	2	1
1:1:39:ARG:CG	1:1:48:PHE:HD2	0.43	2.27	2	5
1:1:43:LEU:O	1:1:103:TRP:CZ3	0.43	2.72	8	5
1:1:32:ILE:O	1:1:33:ASN:CG	0.43	2.61	5	1
1:1:63:VAL:CG2	1:1:82:VAL:HG23	0.43	2.42	1	1
1:1:49:THR:O	1:1:53:ASN:N	0.43	2.51	4	3
1:1:26:VAL:HG11	1:1:77:LYS:HA	0.43	1.90	3	1
1:1:38:VAL:CG2	1:1:57:ALA:CB	0.43	2.94	8	1
1:1:101:LEU:HD13	1:1:103:TRP:CE2	0.42	2.49	4	10
1:1:27:ASP:OD2	1:1:41:ASN:ND2	0.42	2.52	2	4
1:1:29:LEU:O	1:1:77:LYS:HD2	0.42	2.13	5	2
1:1:87:ASN:OD1	1:1:109:THR:CG2	0.42	2.68	3	2
1:1:30:GLN:C	1:1:32:ILE:HG13	0.42	2.37	7	2
1:1:43:LEU:HD13	1:1:43:LEU:N	0.42	2.28	9	1
1:1:43:LEU:HD21	1:1:123:ASN:HD21	0.42	1.75	8	1
1:1:104:ALA:C	1:1:115:TRP:CE3	0.42	2.98	7	5
1:1:59:ASP:OD2	1:1:111:GLY:HA3	0.42	2.14	8	1
1:1:32:ILE:O	1:1:33:ASN:ND2	0.42	2.53	3	1
1:1:43:LEU:HG	1:1:116:LEU:HD23	0.42	1.91	4	2
1:1:49:THR:CG2	1:1:51:VAL:CG1	0.42	2.95	4	1
1:1:116:LEU:HD22	1:1:124:LEU:CD1	0.42	2.44	5	1
1:1:24:TYR:O	1:1:80:TYR:HA	0.42	2.15	4	9
1:1:43:LEU:HG	1:1:123:ASN:OD1	0.42	2.14	6	4
1:1:44:VAL:HG11	1:1:48:PHE:CG	0.42	2.50	6	3
1:1:43:LEU:CG	1:1:123:ASN:ND2	0.42	2.83	2	2
1:1:62:GLU:HA	1:1:81:PHE:CB	0.42	2.45	4	1
1:1:60:VAL:CG1	1:1:83:ILE:CG1	0.42	2.98	1	4
1:1:43:LEU:HG	1:1:123:ASN:ND2	0.42	2.29	4	1
1:1:60:VAL:HG11	1:1:83:ILE:CD1	0.41	2.45	1	5
1:1:27:ASP:CG	1:1:41:ASN:H	0.41	2.22	8	1
1:1:62:GLU:O	1:1:62:GLU:CD	0.41	2.63	3	1
1:1:88:VAL:N	1:1:89:LYS:HE2	0.41	2.29	3	2
1:1:48:PHE:CZ	1:1:53:ASN:O	0.41	2.73	8	2
1:1:38:VAL:N	1:1:55:ILE:O	0.41	2.53	3	2
1:1:40:ASN:HB2	1:1:42:ILE:HD12	0.41	1.92	9	1
1:1:122:ASP:HB3	1:1:128:LYS:HG3	0.41	1.93	2	2
1:1:91:VAL:HG12	1:1:106:VAL:HG21	0.41	1.85	10	2
1:1:32:ILE:HG22	1:1:33:ASN:OD1	0.41	2.15	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:38:VAL:O	1:1:48:PHE:CE2	0.41	2.74	6	1
1:1:26:VAL:CG2	1:1:80:TYR:N	0.41	2.80	8	3
1:1:42:ILE:HG22	1:1:43:LEU:HD13	0.41	1.92	4	2
1:1:89:LYS:HE3	1:1:109:THR:CB	0.41	2.45	3	1
1:1:89:LYS:O	1:1:90:SER:HB3	0.41	2.16	5	1
1:1:61:ILE:HG21	1:1:84:ASN:OD1	0.41	2.16	8	1
1:1:26:VAL:HG13	1:1:38:VAL:HG13	0.41	1.92	1	1
1:1:42:ILE:HD12	1:1:42:ILE:H	0.41	1.76	10	2
1:1:89:LYS:HE2	1:1:89:LYS:CA	0.41	2.46	4	1
1:1:48:PHE:CE1	1:1:103:TRP:CE3	0.41	3.08	7	3
1:1:49:THR:OG1	1:1:53:ASN:CG	0.41	2.62	5	2
1:1:106:VAL:HB	1:1:108:PHE:HE1	0.41	1.76	7	1
1:1:46:THR:C	1:1:47:ASP:CG	0.41	2.89	8	2
1:1:33:ASN:ND2	1:1:51:VAL:O	0.40	2.54	1	1
1:1:48:PHE:CD2	1:1:54:GLY:HA2	0.40	2.51	3	1
1:1:48:PHE:CE1	1:1:103:TRP:CZ3	0.40	3.09	5	1
1:1:61:ILE:CD1	1:1:84:ASN:CG	0.40	2.95	9	1
1:1:91:VAL:CG1	1:1:106:VAL:CG2	0.40	2.93	3	1
1:1:108:PHE:O	1:1:112:GLY:HA2	0.40	2.17	5	1
1:1:108:PHE:CD1	1:1:114:VAL:CB	0.40	3.02	6	1
1:1:61:ILE:CG1	1:1:82:VAL:O	0.40	2.63	8	1
1:1:24:TYR:CD2	1:1:81:PHE:CE2	0.40	3.09	2	1
1:1:122:ASP:HB3	1:1:126:TYR:HB2	0.40	1.93	5	1
1:1:22:LYS:HB2	1:1:126:TYR:CD2	0.40	2.52	10	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	1	96/128 (75%)	70±1 (73±1%)	18±1 (19±1%)	8±1 (8±1%)	1	14
All	All	960/1280 (75%)	699 (73%)	185 (19%)	76 (8%)	1	14

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	1	49	THR	10
1	1	97	GLY	10
1	1	112	GLY	10
1	1	119	THR	10
1	1	101	LEU	9
1	1	57	ALA	8
1	1	98	SER	8
1	1	46	THR	7
1	1	22	LYS	3
1	1	65	SER	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	1	83/111 (75%)	44±2 (54±3%)	38±2 (46±3%)	0 2
All	All	830/1110 (75%)	445 (54%)	385 (46%)	0 2

All 54 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	1	23	ILE	10
1	1	26	VAL	10
1	1	29	LEU	10
1	1	30	GLN	10
1	1	31	LYS	10
1	1	32	ILE	10
1	1	35	ILE	10
1	1	37	GLN	10
1	1	40	ASN	10
1	1	41	ASN	10
1	1	43	LEU	10
1	1	47	ASP	10
1	1	48	PHE	10
1	1	49	THR	10
1	1	55	ILE	10
1	1	61	ILE	10

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Mol	Chain	Res	Type	Models (Total)
1	1	82	VAL	10
1	1	83	ILE	10
1	1	89	LYS	10
1	1	93	THR	10
1	1	101	LEU	10
1	1	110	THR	10
1	1	113	ASN	10
1	1	116	LEU	10
1	1	117	ASN	10
1	1	123	ASN	10
1	1	124	LEU	10
1	1	59	ASP	9
1	1	77	LYS	9
1	1	107	ASN	9
1	1	80	TYR	8
1	1	91	VAL	8
1	1	62	GLU	7
1	1	86	ASN	6
1	1	120	SER	6
1	1	90	SER	5
1	1	84	ASN	5
1	1	121	LYS	5
1	1	22	LYS	4
1	1	44	VAL	4
1	1	65	SER	4
1	1	81	PHE	4
1	1	25	LYS	4
1	1	109	THR	3
1	1	53	ASN	3
1	1	119	THR	2
1	1	63	VAL	2
1	1	96	LYS	2
1	1	102	SER	1
1	1	33	ASN	1
1	1	108	PHE	1
1	1	58	ASP	1
1	1	76	GLN	1
1	1	95	MET	1

6.3.3 RNA

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 [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 88% for the well-defined parts and 83% 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	1406
Number of shifts mapped to atoms	1406
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	15

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	127	-0.10 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	114	-0.02 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	119	0.26 ± 0.12	None needed (< 0.5 ppm)
^{15}N	119	-0.12 ± 0.68	None needed (< 0.5 ppm)

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 88%, i.e. 1132 atoms were assigned a chemical shift out of a possible 1290. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	484/490 (99%)	198/202 (98%)	193/194 (99%)	93/94 (99%)
Sidechain	611/695 (88%)	388/451 (86%)	207/218 (95%)	16/26 (62%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	37/105 (35%)	33/51 (65%)	0/50 (0%)	4/4 (100%)
Overall	1132/1290 (88%)	619/704 (88%)	400/462 (87%)	113/124 (91%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1406 atoms were assigned a chemical shift out of a possible 1690. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	622/644 (97%)	257/265 (97%)	246/256 (96%)	119/123 (97%)
Sidechain	747/893 (84%)	473/579 (82%)	255/279 (91%)	19/35 (54%)
Aromatic	37/153 (24%)	33/75 (44%)	0/62 (0%)	4/16 (25%)
Overall	1406/1690 (83%)	763/919 (83%)	501/597 (84%)	142/174 (82%)

7.1.4 Statistically unusual chemical shifts [i](#)

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	1	2	ARG	NE	127.34	76.53 – 92.65	26.5
1	1	31	LYS	HB2	-0.99	0.58 – 2.97	-11.6
1	1	23	ILE	CG2	28.14	10.93 – 24.12	8.1
1	1	39	ARG	HD3	1.08	1.81 – 4.39	-7.8
1	1	31	LYS	HG2	-0.45	0.13 – 2.61	-7.3
1	1	30	GLN	HB2	0.31	0.80 – 3.29	-7.0
1	1	105	GLN	HG2	0.67	1.01 – 3.62	-6.3
1	1	8	HIS	CB	43.24	19.76 – 40.75	6.2
1	1	39	ARG	HG2	-0.01	0.26 – 2.87	-6.0
1	1	105	GLN	HB2	0.56	0.80 – 3.29	-6.0
1	1	24	TYR	HB3	0.58	0.93 – 4.76	-5.9
1	1	31	LYS	HB3	0.26	0.46 – 3.04	-5.8
1	1	40	ASN	HD21	9.98	4.94 – 9.72	5.5
1	1	117	ASN	HB2	1.13	1.27 – 4.34	-5.5
1	1	8	HIS	HB2	1.28	1.36 – 4.85	-5.2

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 1:

