Full wwPDB NMR Structure Validation Report (i)

Dec 10, 2022 – 09:20 PM EST

PDB ID	:	1FHO
Title	:	Solution Structure of the PH Domain from the C. Elegans Muscle Protein UNC-89
Authors	:	Blomberg, N.; Baraldi, E.; Sattler, M.; Saraste, M.; Nilges, M.
Deposited on	:	2000-08-02

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:

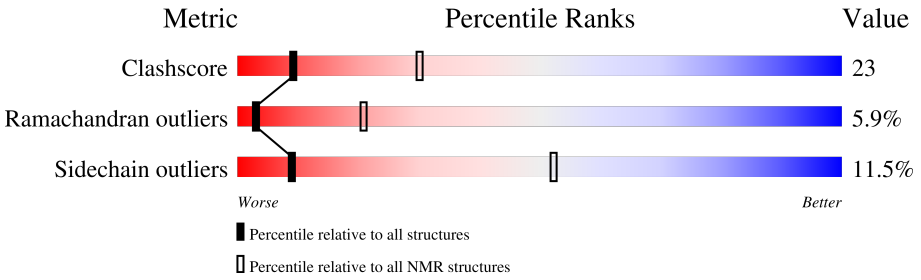
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.31.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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	119	37% 39% • 21%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 17 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:9-A:44, A:54-A:111 (94)	0.96	17

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 and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1961 atoms, of which 965 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called UNC-89.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	119	1961	630	965	173	191	2	0

There is a discrepancy between the modelled and reference sequences:

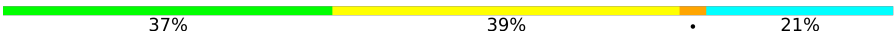
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O01761

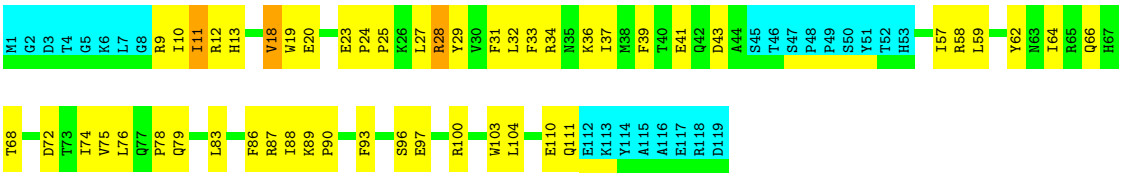
4 Residue-property plots (i)

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: UNC-89

Chain A: 



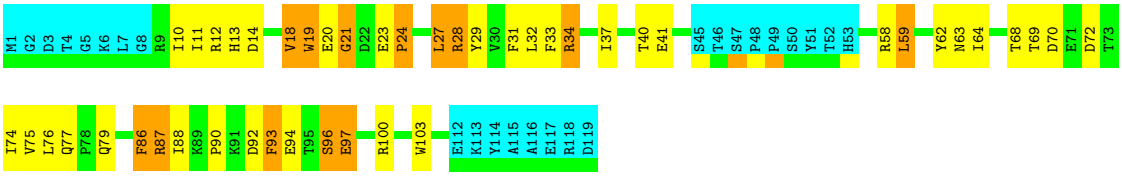
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

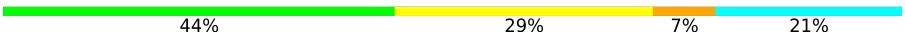
• Molecule 1: UNC-89

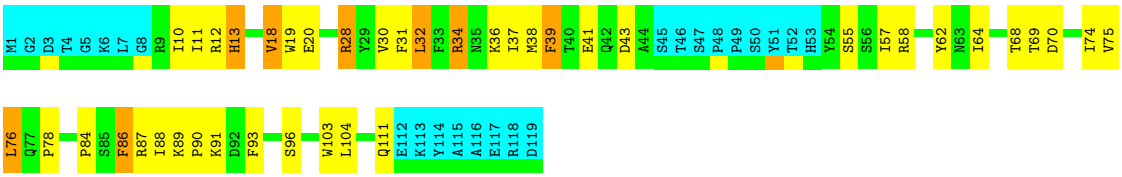
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: UNC-89

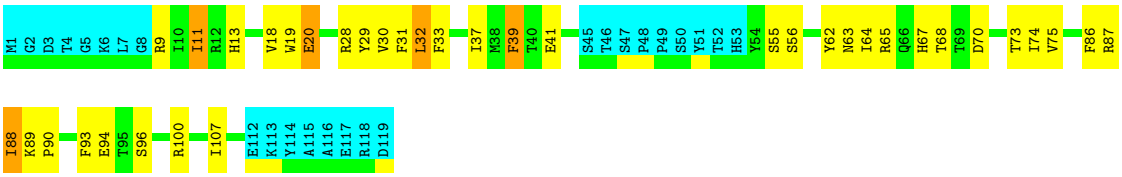
Chain A: 



4.2.3 Score per residue for model 3

- Molecule 1: UNC-89

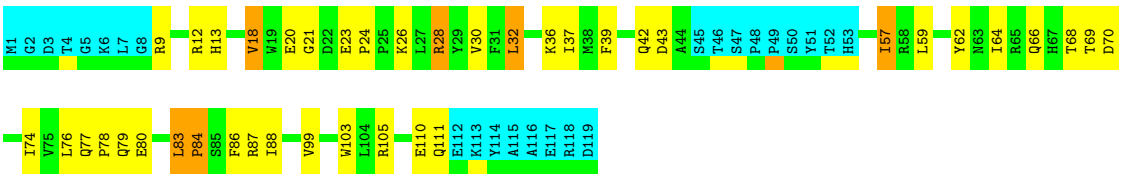
Chain A: 48% 27% • 21%



4.2.4 Score per residue for model 4

- Molecule 1: UNC-89

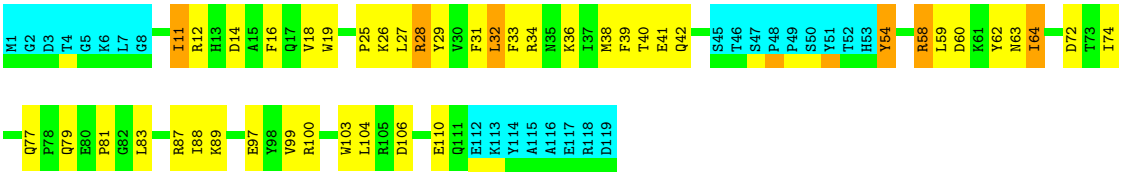
Chain A: 45% 29% 5% 21%



4.2.5 Score per residue for model 5

- Molecule 1: UNC-89

Chain A: 42% 32% 5% 21%



4.2.6 Score per residue for model 6

- Molecule 1: UNC-89

Chain A: 39% 35% 5% 21%

M1 G2 D3 T4 G5 K6 L7 G8 R9 I10 I11 R12 H13 D14 A15 F16 Q17 V18 W19 E20 G21 D22 E23 P24 P25 K26 L27 R28 Y29 V30 F31 L32 F33 R34 I37 M38 F39 D43 A44 S45 T46 S47 P48 P49 S50 Y51 T52 H53 R58 L59 Y62 N63 I64 D70

I74 V75 L76 Q77 P78 Q79 E80 L83 P84 S85 F86 R87 I88 K89 P90 K91 D92 F93 E94 T95 S96 W103 E110 Q111 E112 K113 Y114 A115 A116 E117 R118 D119

4.2.7 Score per residue for model 7

- Molecule 1: UNC-89

Chain A: 39% 28% 11% • 21%

M1 G2 D3 T4 G5 K6 L7 G8 R9 I10 I11 R12 F16 Q17 V18 W19 E20 E23 P24 P25 V30 F31 L32 K36 I37 M38 F39 T40 E41 Q42 D43 A44 S45 T46 S47 P48 P49 S50 Y51 T52 H53 Y54 I57 R58 L59 Y62 N63 I64 T68 T69 D70 E71 D72

T73 I74 V75 L76 L83 F86 R87 I88 K89 P90 K91 D92 F93 S96 E97 Y98 V99 R100 W103 L104 E110 Q111 E112 K113 Y114 A115 A116 E117 R118 D119

4.2.8 Score per residue for model 8

- Molecule 1: UNC-89

Chain A: 35% 36% 8% 21%

M1 G2 D3 T4 G5 K6 L7 G8 R9 I10 I11 R12 H13 F16 Q17 V18 W19 D22 E23 P24 P25 R28 F31 L32 F33 R34 N35 K36 I37 M38 F39 T40 E41 Q42 D43 A44 S45 T46 S47 P48 P49 S50 Y51 T52 H53 Y54 I57 R58 Y62 N63 I64 T68

D72 V75 L76 Q77 P78 Q79 E80 P81 G82 L83 P84 S85 F86 R87 I88 K89 P90 K91 T95 S96 V99 R100 W103 L104 R105 D106 I107 E110 Q111 E112 K113 Y114 A115 A116 E117 R118 D119

4.2.9 Score per residue for model 9

- Molecule 1: UNC-89

Chain A: 34% 34% 11% 21%

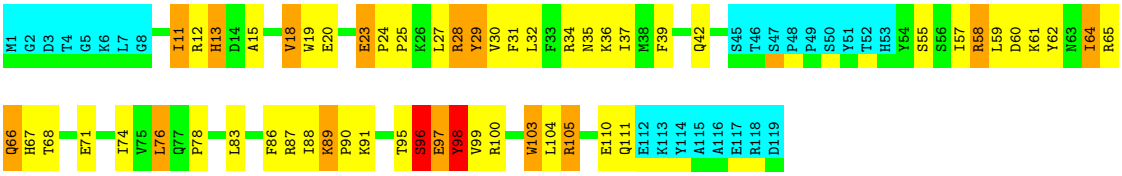
M1 G2 D3 T4 G5 K6 L7 G8 R9 I10 I11 R12 H13 D14 Q17 V18 W19 E20 G21 D22 E23 P24 P25 K26 L27 R28 F31 L32 F33 R34 N35 K36 I37 M38 F39 T40 E41 Q42 D43 A44 S45 T46 S47 P48 P49 S50 Y51 T52 H53 I57 R58 L59 D60 K61 Y62 N63 I64

R65 Q66 D72 T73 I74 V75 L76 Q77 P78 Q79 L83 P84 S85 F86 R87 I88 K89 P90 K91 D92 R100 W103 L104 E109 E110 Q111 E112 K113 Y114 A115 A116 E117 R118 D119

4.2.10 Score per residue for model 10

- Molecule 1: UNC-89

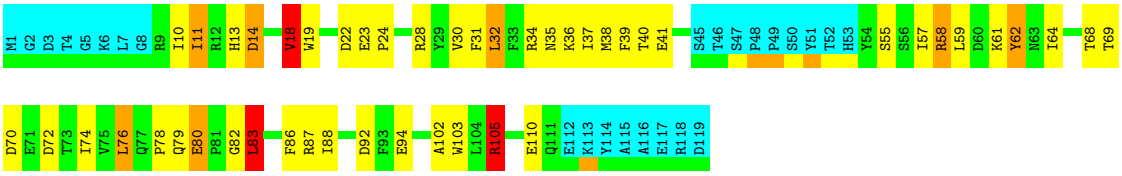
Chain A: 32% 34% 12% • 21%



4.2.11 Score per residue for model 11

- Molecule 1: UNC-89

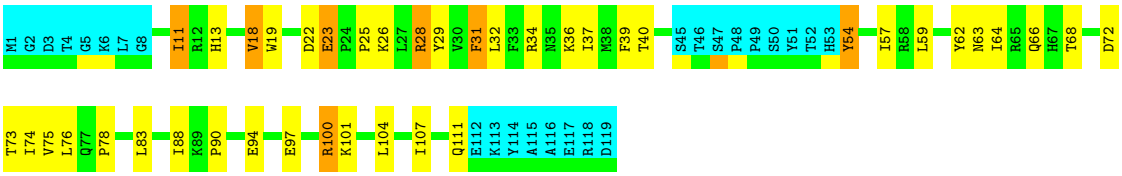
Chain A: 39% 32% 6% • 21%



4.2.12 Score per residue for model 12

- Molecule 1: UNC-89

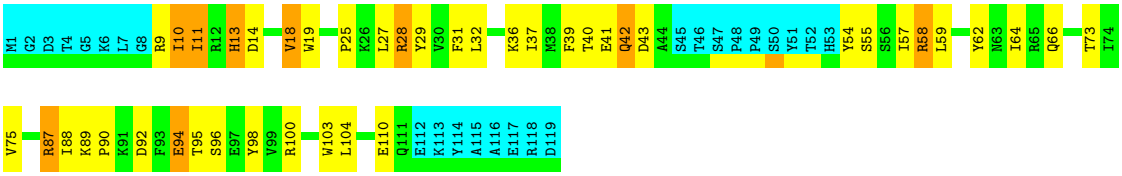
Chain A: 45% 29% 6% 21%



4.2.13 Score per residue for model 13

- Molecule 1: UNC-89

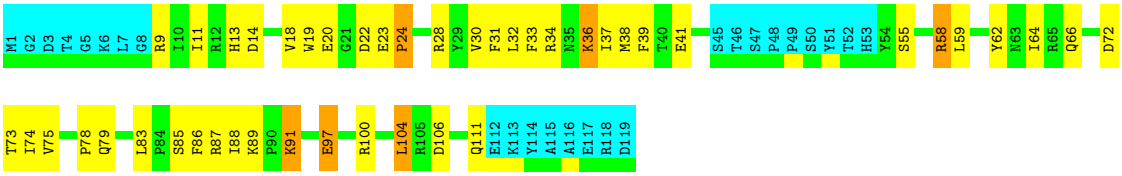
Chain A: 43% 29% 8% 21%



4.2.14 Score per residue for model 14

- Molecule 1: UNC-89

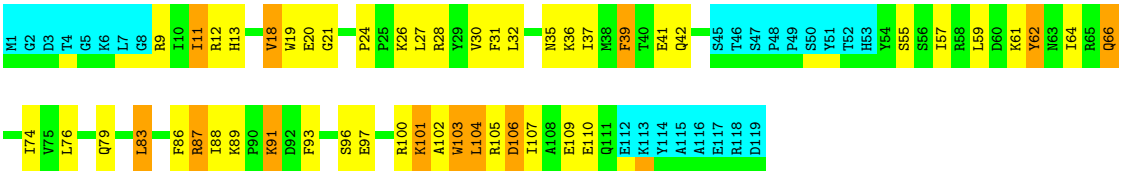
Chain A: 41% 33% 5% 21%



4.2.15 Score per residue for model 15

- Molecule 1: UNC-89

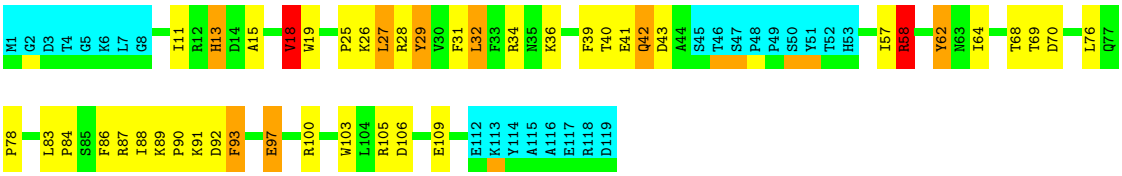
Chain A: 37% 32% 10% 21%



4.2.16 Score per residue for model 16

- Molecule 1: UNC-89

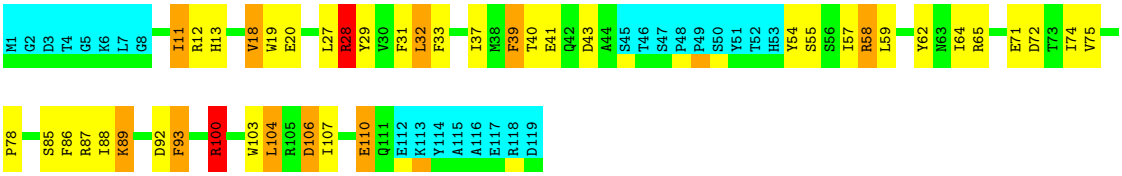
Chain A: 42% 29% 7% • 21%



4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: UNC-89

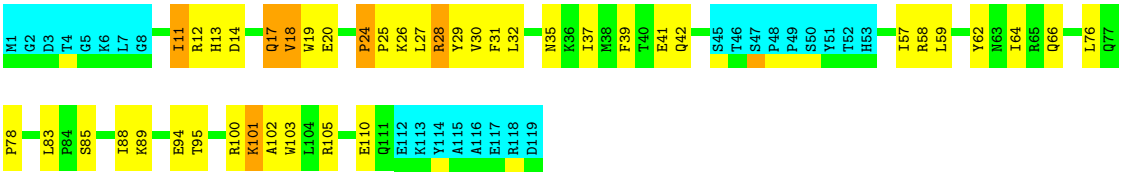
Chain A: 43% 26% 8% • 21%



4.2.18 Score per residue for model 18

- Molecule 1: UNC-89

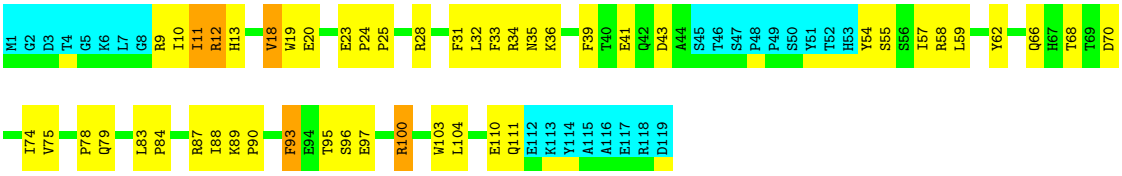
Chain A: 44% 30% 5% 21%



4.2.19 Score per residue for model 19

- Molecule 1: UNC-89

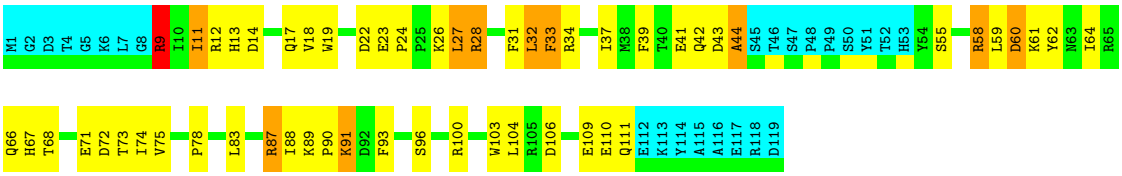
Chain A: 38% 37% • 21%



4.2.20 Score per residue for model 20

- Molecule 1: UNC-89

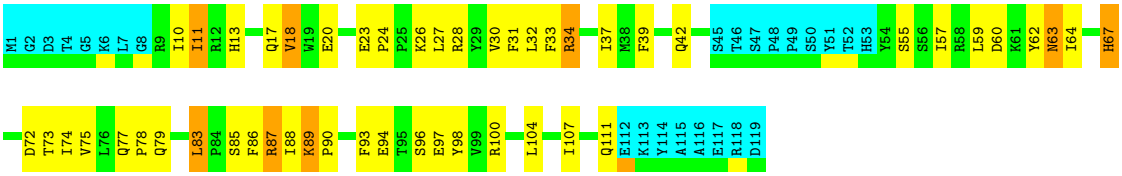
Chain A: 33% 37% 8% • 21%



4.2.21 Score per residue for model 21

- Molecule 1: UNC-89

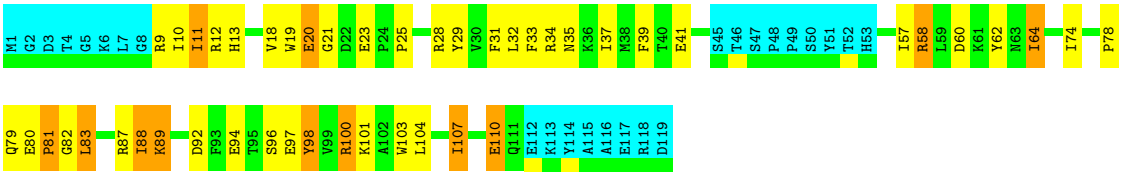
Chain A: 37% 35% 7% 21%



4.2.22 Score per residue for model 22

- Molecule 1: UNC-89

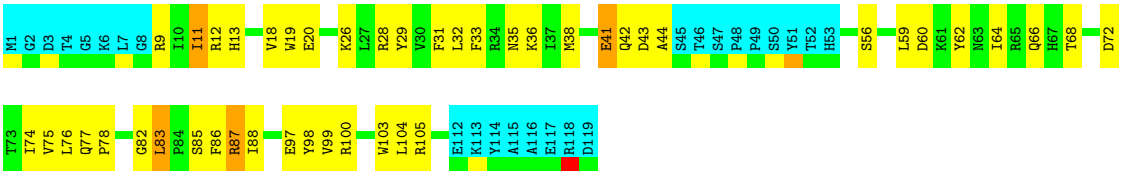
Chain A: 39% 29% 10% 21%



4.2.23 Score per residue for model 23

- Molecule 1: UNC-89

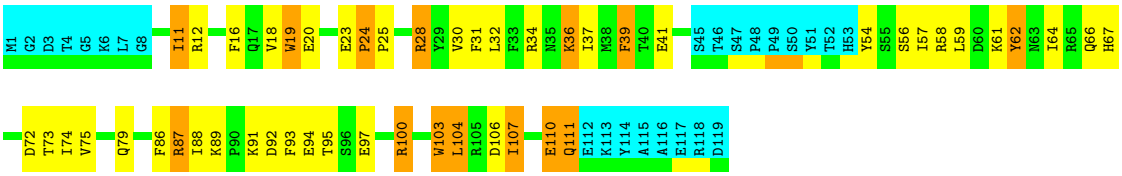
Chain A: 40% 35% • 21%



4.2.24 Score per residue for model 24

- Molecule 1: UNC-89

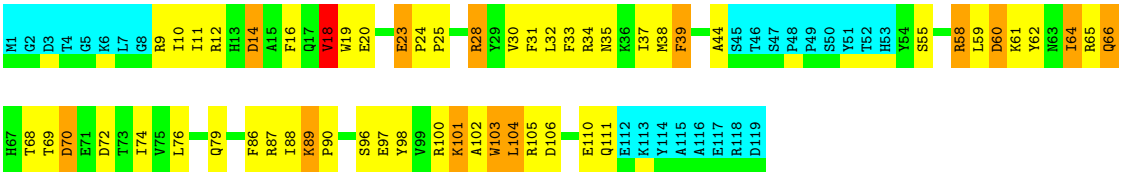
Chain A: 37% 30% 12% 21%



4.2.25 Score per residue for model 25

- Molecule 1: UNC-89

Chain A: 32% 35% 11% • 21%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Automated NOE assignment,Torsion angle dynamics, Cartesian simulated annealing.*.

Of the 50 calculated structures, 25 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
ARIA	structure solution	0.5
CNS	structure solution	0.5
CNS	refinement	0.5

No chemical shift data was provided.

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	A	0.39±0.04	0±0/829 (0.0± 0.0%)	0.61±0.04	0±0/1122 (0.0± 0.0%)
All	All	0.39	0/20725 (0.0%)	0.61	2/28050 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.8±0.7
All	All	0	19

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	100	ARG	NE-CZ-NH1	-6.30	117.15	120.30	17	1
1	A	100	ARG	NE-CZ-NH2	-6.04	117.28	120.30	23	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	100	ARG	Sidechain	4
1	A	28	ARG	Sidechain	4
1	A	58	ARG	Sidechain	3
1	A	105	ARG	Sidechain	3
1	A	34	ARG	Sidechain	2
1	A	9	ARG	Sidechain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	12	ARG	Sidechain	1

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	807	789	787	36±8
All	All	20175	19725	19675	908

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 23.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:VAL:HG21	1:A:88:ILE:HA	1.10	1.21	25	14
1:A:79:GLN:HB2	1:A:83:LEU:HD23	1.04	1.24	4	1
1:A:18:VAL:HG11	1:A:88:ILE:HA	1.01	1.15	6	11
1:A:90:PRO:HG2	1:A:100:ARG:HG3	0.95	1.37	13	3
1:A:77:GLN:HB3	1:A:78:PRO:HD3	0.94	1.37	9	1
1:A:37:ILE:HG13	1:A:59:LEU:HD11	0.92	1.41	24	1
1:A:20:GLU:HA	1:A:86:PHE:HB2	0.92	1.41	1	10
1:A:75:VAL:HG22	1:A:87:ARG:HG3	0.88	1.41	1	1
1:A:97:GLU:HA	1:A:100:ARG:HH12	0.87	1.27	1	1
1:A:23:GLU:HB3	1:A:24:PRO:HD3	0.87	1.44	6	3
1:A:78:PRO:HB3	1:A:83:LEU:HD22	0.85	1.46	22	1
1:A:18:VAL:HG13	1:A:89:LYS:HG2	0.85	1.47	25	3
1:A:59:LEU:HG	1:A:62:TYR:HE2	0.84	1.31	24	1
1:A:74:ILE:HB	1:A:88:ILE:HG13	0.82	1.49	10	12
1:A:62:TYR:CE2	1:A:64:ILE:HB	0.81	2.11	22	13
1:A:32:LEU:HD22	1:A:37:ILE:HG12	0.80	1.52	22	12
1:A:18:VAL:CG1	1:A:88:ILE:HA	0.80	2.05	6	6
1:A:27:LEU:HB2	1:A:43:ASP:HB2	0.80	1.53	16	1
1:A:12:ARG:HG3	1:A:103:TRP:HB2	0.80	1.54	7	1
1:A:18:VAL:HG22	1:A:19:TRP:H	0.80	1.36	22	2
1:A:80:GLU:HB2	1:A:83:LEU:HB2	0.79	1.53	4	1
1:A:13:HIS:HB2	1:A:31:PHE:HD1	0.78	1.38	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:LYS:HE3	1:A:91:LYS:HG2	0.78	1.55	14	1
1:A:20:GLU:HB3	1:A:23:GLU:HB2	0.77	1.55	22	1
1:A:78:PRO:HD3	1:A:85:SER:HB3	0.77	1.57	17	6
1:A:26:LYS:HB2	1:A:28:ARG:HH21	0.76	1.41	5	1
1:A:59:LEU:HG	1:A:62:TYR:CE2	0.76	2.16	24	1
1:A:26:LYS:HG3	1:A:43:ASP:HB2	0.76	1.57	23	1
1:A:23:GLU:HB3	1:A:24:PRO:HD2	0.75	1.55	19	2
1:A:37:ILE:HB	1:A:57:ILE:HG22	0.74	1.59	24	2
1:A:28:ARG:HH12	1:A:55:SER:HB2	0.74	1.39	3	1
1:A:75:VAL:HG22	1:A:87:ARG:HB3	0.74	1.60	24	2
1:A:32:LEU:HB3	1:A:37:ILE:HG12	0.74	1.60	20	1
1:A:17:GLN:HG2	1:A:27:LEU:HB2	0.74	1.57	18	1
1:A:30:VAL:HA	1:A:39:PHE:CB	0.73	2.13	15	2
1:A:18:VAL:HG12	1:A:19:TRP:CE3	0.72	2.20	25	4
1:A:15:ALA:HA	1:A:29:TYR:HA	0.72	1.62	10	3
1:A:90:PRO:HB3	1:A:100:ARG:HD2	0.72	1.62	25	1
1:A:64:ILE:HD11	1:A:74:ILE:HG23	0.71	1.62	5	4
1:A:28:ARG:HG2	1:A:41:GLU:HA	0.71	1.62	14	3
1:A:28:ARG:HB3	1:A:41:GLU:HG2	0.71	1.61	8	3
1:A:22:ASP:O	1:A:24:PRO:HD2	0.71	1.85	8	1
1:A:76:LEU:HD11	1:A:86:PHE:HD2	0.71	1.45	11	2
1:A:23:GLU:HG3	1:A:24:PRO:HD2	0.71	1.62	7	2
1:A:99:VAL:HG13	1:A:103:TRP:CD1	0.71	2.20	8	1
1:A:81:PRO:HD2	1:A:83:LEU:HB3	0.70	1.63	5	1
1:A:19:TRP:CD1	1:A:25:PRO:HD3	0.70	2.21	7	1
1:A:20:GLU:HB2	1:A:28:ARG:HH22	0.70	1.46	2	2
1:A:18:VAL:HG23	1:A:19:TRP:CE3	0.70	2.21	14	7
1:A:18:VAL:HG21	1:A:88:ILE:CA	0.69	2.12	25	5
1:A:19:TRP:HA	1:A:24:PRO:O	0.69	1.88	20	2
1:A:12:ARG:HB3	1:A:103:TRP:CZ2	0.69	2.22	19	6
1:A:28:ARG:HG2	1:A:41:GLU:HB3	0.69	1.65	23	1
1:A:9:ARG:HG3	1:A:33:PHE:HE1	0.69	1.47	19	1
1:A:31:PHE:HB3	1:A:33:PHE:HE1	0.68	1.47	5	3
1:A:28:ARG:HG2	1:A:28:ARG:HH11	0.68	1.46	18	1
1:A:14:ASP:HB2	1:A:103:TRP:CZ2	0.68	2.24	11	5
1:A:62:TYR:HA	1:A:79:GLN:HA	0.68	1.63	4	1
1:A:59:LEU:HA	1:A:62:TYR:HB2	0.68	1.66	15	1
1:A:59:LEU:HA	1:A:62:TYR:CE1	0.68	2.23	1	4
1:A:18:VAL:HG11	1:A:89:LYS:HB2	0.67	1.64	13	2
1:A:74:ILE:HB	1:A:88:ILE:HD11	0.67	1.66	1	1
1:A:20:GLU:HB3	1:A:28:ARG:HH11	0.66	1.50	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:VAL:HG22	1:A:39:PHE:HE1	0.66	1.51	3	3
1:A:62:TYR:CE1	1:A:64:ILE:HB	0.66	2.25	25	8
1:A:66:GLN:HA	1:A:73:THR:O	0.66	1.91	12	5
1:A:32:LEU:HG	1:A:103:TRP:HZ3	0.66	1.51	24	4
1:A:76:LEU:HD11	1:A:86:PHE:CD2	0.66	2.25	10	2
1:A:65:ARG:HB2	1:A:75:VAL:HB	0.66	1.66	3	1
1:A:90:PRO:CB	1:A:100:ARG:HA	0.65	2.21	8	1
1:A:30:VAL:HG22	1:A:39:PHE:CE1	0.65	2.27	3	6
1:A:63:ASN:HB3	1:A:77:GLN:HB2	0.65	1.69	5	2
1:A:14:ASP:HB3	1:A:16:PHE:CE1	0.65	2.27	5	2
1:A:82:GLY:O	1:A:83:LEU:HB2	0.65	1.92	22	3
1:A:75:VAL:HG12	1:A:87:ARG:HG2	0.64	1.69	19	2
1:A:104:LEU:O	1:A:107:ILE:HG22	0.64	1.93	8	1
1:A:18:VAL:CG2	1:A:88:ILE:HA	0.64	2.13	25	11
1:A:18:VAL:HG21	1:A:89:LYS:H	0.64	1.52	15	5
1:A:74:ILE:HG13	1:A:100:ARG:HH22	0.64	1.52	9	1
1:A:77:GLN:CB	1:A:78:PRO:HD3	0.64	2.18	9	1
1:A:77:GLN:HB3	1:A:78:PRO:CD	0.64	2.21	9	1
1:A:86:PHE:HE1	1:A:88:ILE:HG23	0.63	1.52	2	2
1:A:97:GLU:HA	1:A:100:ARG:NH1	0.63	2.07	1	1
1:A:86:PHE:CE1	1:A:88:ILE:HG23	0.63	2.29	2	5
1:A:19:TRP:HD1	1:A:25:PRO:HD3	0.63	1.52	7	1
1:A:90:PRO:HB3	1:A:100:ARG:NH1	0.63	2.09	1	1
1:A:18:VAL:HG11	1:A:88:ILE:CA	0.63	2.08	6	5
1:A:57:ILE:HG12	1:A:83:LEU:HD11	0.63	1.71	7	1
1:A:78:PRO:HB3	1:A:83:LEU:HB2	0.63	1.71	20	2
1:A:23:GLU:N	1:A:24:PRO:HD3	0.62	2.09	24	4
1:A:30:VAL:HA	1:A:39:PHE:HB3	0.62	1.70	15	2
1:A:90:PRO:HB2	1:A:100:ARG:HA	0.62	1.71	8	1
1:A:62:TYR:HA	1:A:78:PRO:O	0.62	1.95	9	1
1:A:11:ILE:HB	1:A:32:LEU:O	0.62	1.94	5	6
1:A:62:TYR:HE1	1:A:64:ILE:HB	0.62	1.54	23	6
1:A:12:ARG:HB2	1:A:103:TRP:CE3	0.62	2.30	7	1
1:A:32:LEU:HB3	1:A:103:TRP:CH2	0.62	2.29	23	2
1:A:78:PRO:HB3	1:A:83:LEU:O	0.62	1.94	19	3
1:A:28:ARG:HG3	1:A:41:GLU:HB3	0.62	1.72	13	1
1:A:101:LYS:HE3	1:A:101:LYS:HA	0.62	1.72	18	1
1:A:12:ARG:HB2	1:A:103:TRP:HE3	0.61	1.55	7	1
1:A:31:PHE:HB2	1:A:38:MET:HB2	0.61	1.71	25	1
1:A:78:PRO:HB2	1:A:80:GLU:HB3	0.61	1.70	11	1
1:A:93:PHE:CE2	1:A:97:GLU:HG2	0.61	2.30	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ILE:HG22	1:A:32:LEU:HD13	0.61	1.71	5	1
1:A:62:TYR:HE2	1:A:64:ILE:HB	0.61	1.53	8	2
1:A:89:LYS:HD2	1:A:91:LYS:HB2	0.61	1.71	16	2
1:A:36:LYS:HD3	1:A:56:SER:HB3	0.61	1.70	24	1
1:A:20:GLU:HA	1:A:86:PHE:CB	0.61	2.25	15	3
1:A:11:ILE:O	1:A:12:ARG:HD2	0.61	1.96	10	4
1:A:61:LYS:HB3	1:A:79:GLN:HB2	0.61	1.73	11	1
1:A:94:GLU:HA	1:A:97:GLU:HG3	0.61	1.73	24	1
1:A:11:ILE:CG2	1:A:32:LEU:HD13	0.60	2.26	5	1
1:A:13:HIS:HB2	1:A:31:PHE:CD1	0.60	2.28	8	13
1:A:39:PHE:HB2	1:A:56:SER:HA	0.60	1.72	3	1
1:A:36:LYS:HB2	1:A:57:ILE:O	0.60	1.96	8	4
1:A:29:TYR:HB3	1:A:31:PHE:CE1	0.60	2.32	23	4
1:A:24:PRO:HB2	1:A:25:PRO:HD3	0.60	1.72	18	1
1:A:10:ILE:HG23	1:A:11:ILE:HG13	0.60	1.74	11	4
1:A:29:TYR:O	1:A:39:PHE:HA	0.60	1.97	13	5
1:A:97:GLU:HG2	1:A:100:ARG:NH2	0.60	2.10	14	1
1:A:32:LEU:HB3	1:A:103:TRP:HH2	0.60	1.57	23	2
1:A:90:PRO:HB3	1:A:100:ARG:HB2	0.59	1.73	9	1
1:A:27:LEU:O	1:A:42:GLN:HB3	0.59	1.97	21	2
1:A:27:LEU:HD22	1:A:41:GLU:OE1	0.59	1.96	16	1
1:A:30:VAL:HA	1:A:39:PHE:HB2	0.59	1.75	10	2
1:A:24:PRO:CB	1:A:25:PRO:HD3	0.59	2.27	18	1
1:A:18:VAL:HB	1:A:19:TRP:CE3	0.59	2.33	24	1
1:A:36:LYS:HE3	1:A:38:MET:HB2	0.59	1.74	14	1
1:A:24:PRO:HB2	1:A:25:PRO:CD	0.59	2.28	18	1
1:A:12:ARG:NE	1:A:31:PHE:HB3	0.59	2.13	20	1
1:A:16:PHE:CD2	1:A:18:VAL:HG22	0.59	2.33	24	1
1:A:96:SER:O	1:A:97:GLU:HB3	0.59	1.97	1	1
1:A:80:GLU:HG2	1:A:81:PRO:HD2	0.59	1.73	8	1
1:A:18:VAL:HG11	1:A:89:LYS:H	0.58	1.58	14	4
1:A:97:GLU:O	1:A:100:ARG:HB3	0.58	1.99	16	3
1:A:100:ARG:HA	1:A:103:TRP:CD1	0.58	2.33	24	3
1:A:76:LEU:HD22	1:A:86:PHE:CD2	0.58	2.33	4	1
1:A:28:ARG:CZ	1:A:28:ARG:HB3	0.57	2.29	5	2
1:A:21:GLY:H	1:A:86:PHE:HB3	0.57	1.59	15	1
1:A:14:ASP:HB3	1:A:16:PHE:HE1	0.57	1.58	25	1
1:A:34:ARG:O	1:A:35:ASN:HB3	0.57	1.97	11	2
1:A:80:GLU:N	1:A:81:PRO:HD3	0.57	2.13	22	1
1:A:28:ARG:HA	1:A:41:GLU:HA	0.57	1.76	9	2
1:A:12:ARG:O	1:A:31:PHE:HA	0.57	1.99	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:LEU:HD12	1:A:84:PRO:HD2	0.57	1.76	9	4
1:A:106:ASP:O	1:A:110:GLU:HA	0.57	1.98	17	2
1:A:18:VAL:HG13	1:A:28:ARG:HH22	0.57	1.59	6	1
1:A:68:THR:HG22	1:A:69:THR:H	0.57	1.59	11	3
1:A:59:LEU:HA	1:A:62:TYR:CE2	0.57	2.35	6	1
1:A:94:GLU:HG2	1:A:95:THR:H	0.57	1.58	18	1
1:A:39:PHE:O	1:A:55:SER:HB2	0.57	2.00	10	3
1:A:9:ARG:HA	1:A:33:PHE:CD1	0.57	2.34	25	2
1:A:20:GLU:N	1:A:24:PRO:HD2	0.56	2.14	24	2
1:A:32:LEU:HD21	1:A:103:TRP:HZ3	0.56	1.59	1	6
1:A:31:PHE:HB3	1:A:33:PHE:CE1	0.56	2.34	5	4
1:A:69:THR:O	1:A:70:ASP:HB2	0.56	1.99	25	2
1:A:97:GLU:HA	1:A:100:ARG:HD2	0.56	1.75	19	1
1:A:106:ASP:HA	1:A:110:GLU:CB	0.56	2.29	20	1
1:A:19:TRP:CH2	1:A:89:LYS:HE2	0.56	2.34	2	1
1:A:59:LEU:HD12	1:A:62:TYR:CE2	0.56	2.36	4	2
1:A:90:PRO:HA	1:A:100:ARG:HG3	0.56	1.76	9	1
1:A:10:ILE:HG13	1:A:11:ILE:HG13	0.56	1.77	21	2
1:A:32:LEU:HG	1:A:103:TRP:CZ3	0.56	2.35	24	4
1:A:89:LYS:HD2	1:A:90:PRO:HD2	0.56	1.77	20	1
1:A:62:TYR:CE2	1:A:76:LEU:HB3	0.56	2.36	15	1
1:A:12:ARG:HB2	1:A:32:LEU:N	0.56	2.16	20	1
1:A:23:GLU:O	1:A:25:PRO:HD3	0.56	2.00	24	1
1:A:74:ILE:HD11	1:A:104:LEU:HG	0.56	1.76	22	7
1:A:12:ARG:CG	1:A:103:TRP:HB2	0.56	2.30	7	1
1:A:63:ASN:HB2	1:A:78:PRO:HD2	0.56	1.77	9	1
1:A:18:VAL:O	1:A:25:PRO:HA	0.55	2.01	19	4
1:A:12:ARG:HD2	1:A:33:PHE:CE1	0.55	2.36	20	1
1:A:93:PHE:HB3	1:A:100:ARG:HD3	0.55	1.76	19	1
1:A:24:PRO:HB3	1:A:25:PRO:HD2	0.55	1.78	7	1
1:A:22:ASP:C	1:A:24:PRO:HD3	0.55	2.22	20	2
1:A:76:LEU:HD22	1:A:86:PHE:CE2	0.55	2.35	15	1
1:A:27:LEU:HB3	1:A:42:GLN:O	0.55	2.02	18	1
1:A:9:ARG:HB3	1:A:12:ARG:HG2	0.55	1.77	20	1
1:A:89:LYS:CE	1:A:91:LYS:HG2	0.55	2.29	14	1
1:A:14:ASP:HB2	1:A:103:TRP:NE1	0.55	2.17	20	1
1:A:18:VAL:HG11	1:A:89:LYS:HG2	0.55	1.78	24	2
1:A:97:GLU:C	1:A:99:VAL:H	0.55	2.06	23	1
1:A:59:LEU:HA	1:A:62:TYR:CD2	0.54	2.37	24	2
1:A:39:PHE:CE1	1:A:57:ILE:HG12	0.54	2.37	13	3
1:A:11:ILE:HD11	1:A:111:GLN:HA	0.54	1.79	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:PRO:HB3	1:A:83:LEU:HB3	0.54	1.77	16	4
1:A:13:HIS:HB2	1:A:31:PHE:HD2	0.54	1.61	12	2
1:A:79:GLN:HG3	1:A:83:LEU:HD22	0.54	1.79	9	1
1:A:105:ARG:NE	1:A:105:ARG:HA	0.54	2.17	10	1
1:A:100:ARG:NH1	1:A:100:ARG:HB3	0.54	2.18	1	1
1:A:18:VAL:HG13	1:A:28:ARG:NH2	0.54	2.18	6	1
1:A:75:VAL:HG22	1:A:87:ARG:CG	0.54	2.25	1	1
1:A:11:ILE:HG22	1:A:32:LEU:HD12	0.54	1.80	20	1
1:A:13:HIS:HB2	1:A:31:PHE:CD2	0.53	2.38	22	2
1:A:96:SER:O	1:A:100:ARG:HD3	0.53	2.03	15	1
1:A:19:TRP:HB3	1:A:23:GLU:HA	0.53	1.79	20	1
1:A:64:ILE:HD13	1:A:65:ARG:N	0.53	2.18	25	1
1:A:39:PHE:HB3	1:A:55:SER:HB3	0.53	1.78	2	1
1:A:74:ILE:HD11	1:A:104:LEU:HD13	0.53	1.79	23	2
1:A:76:LEU:HD21	1:A:86:PHE:CE1	0.53	2.39	8	1
1:A:75:VAL:HB	1:A:77:GLN:HE22	0.53	1.64	23	1
1:A:27:LEU:HD21	1:A:29:TYR:CE1	0.53	2.37	18	1
1:A:16:PHE:HD2	1:A:18:VAL:HG22	0.53	1.62	24	1
1:A:16:PHE:CE1	1:A:30:VAL:HG23	0.53	2.39	24	1
1:A:18:VAL:CG1	1:A:89:LYS:H	0.53	2.16	10	1
1:A:59:LEU:HD23	1:A:110:GLU:HG3	0.53	1.80	19	1
1:A:64:ILE:HD11	1:A:74:ILE:CG2	0.53	2.34	24	4
1:A:20:GLU:HB3	1:A:28:ARG:NE	0.53	2.19	6	1
1:A:11:ILE:HG23	1:A:106:ASP:HB3	0.53	1.81	15	1
1:A:12:ARG:HB3	1:A:33:PHE:CD1	0.53	2.38	20	1
1:A:110:GLU:HA	1:A:110:GLU:OE1	0.53	2.03	24	1
1:A:89:LYS:HG3	1:A:89:LYS:O	0.53	2.04	7	2
1:A:87:ARG:HH11	1:A:87:ARG:HG2	0.53	1.64	20	1
1:A:19:TRP:HZ3	1:A:89:LYS:HD3	0.52	1.63	5	1
1:A:67:HIS:HB2	1:A:73:THR:HB	0.52	1.81	21	2
1:A:18:VAL:CG2	1:A:19:TRP:H	0.52	2.15	22	1
1:A:28:ARG:HD3	1:A:41:GLU:H	0.52	1.63	16	1
1:A:62:TYR:HE2	1:A:76:LEU:HD23	0.52	1.65	15	1
1:A:90:PRO:HG3	1:A:100:ARG:HG3	0.52	1.82	12	1
1:A:58:ARG:HG2	1:A:58:ARG:O	0.52	2.05	13	3
1:A:32:LEU:HD12	1:A:107:ILE:HD11	0.52	1.80	15	1
1:A:18:VAL:HG11	1:A:89:LYS:N	0.52	2.19	2	2
1:A:32:LEU:HD11	1:A:103:TRP:CH2	0.52	2.39	5	1
1:A:18:VAL:HB	1:A:89:LYS:H	0.52	1.64	20	2
1:A:74:ILE:HB	1:A:88:ILE:CG1	0.52	2.35	6	3
1:A:36:LYS:CB	1:A:58:ARG:HA	0.52	2.34	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LEU:O	1:A:62:TYR:HD1	0.52	1.88	20	1
1:A:89:LYS:HD2	1:A:92:ASP:HB2	0.52	1.79	22	1
1:A:110:GLU:O	1:A:111:GLN:HG3	0.52	2.05	7	1
1:A:60:ASP:OD2	1:A:61:LYS:HD3	0.52	2.05	20	1
1:A:59:LEU:HD13	1:A:62:TYR:HE1	0.51	1.65	7	2
1:A:12:ARG:CB	1:A:103:TRP:HB2	0.51	2.35	15	1
1:A:16:PHE:CD1	1:A:18:VAL:HG12	0.51	2.40	7	1
1:A:59:LEU:HD13	1:A:62:TYR:CE1	0.51	2.41	20	1
1:A:18:VAL:HG13	1:A:89:LYS:CG	0.51	2.31	25	1
1:A:27:LEU:O	1:A:42:GLN:HB2	0.51	2.04	20	2
1:A:20:GLU:HB3	1:A:24:PRO:HG2	0.51	1.82	24	1
1:A:91:LYS:HA	1:A:100:ARG:NH1	0.51	2.20	24	1
1:A:20:GLU:CA	1:A:86:PHE:HB2	0.51	2.35	6	1
1:A:66:GLN:HB3	1:A:74:ILE:HD13	0.51	1.82	25	4
1:A:14:ASP:HB2	1:A:103:TRP:CE2	0.51	2.41	11	1
1:A:20:GLU:HB2	1:A:28:ARG:NH2	0.51	2.20	24	3
1:A:26:LYS:HB2	1:A:28:ARG:HH12	0.51	1.66	12	1
1:A:32:LEU:HD12	1:A:33:PHE:N	0.51	2.21	23	2
1:A:19:TRP:HH2	1:A:89:LYS:HE2	0.51	1.65	2	1
1:A:18:VAL:HG11	1:A:89:LYS:CG	0.51	2.36	24	1
1:A:18:VAL:HG22	1:A:19:TRP:N	0.51	2.13	22	3
1:A:59:LEU:HA	1:A:62:TYR:CD1	0.51	2.40	19	3
1:A:16:PHE:CD2	1:A:88:ILE:HB	0.51	2.40	25	2
1:A:23:GLU:HB2	1:A:24:PRO:HD3	0.51	1.81	10	1
1:A:97:GLU:HG2	1:A:100:ARG:HH22	0.51	1.64	14	1
1:A:62:TYR:CE1	1:A:83:LEU:HD13	0.51	2.41	15	1
1:A:11:ILE:CG2	1:A:32:LEU:HD12	0.51	2.36	20	1
1:A:58:ARG:HG3	1:A:58:ARG:HH11	0.51	1.66	17	2
1:A:61:LYS:O	1:A:79:GLN:HG2	0.51	2.06	15	2
1:A:32:LEU:CD2	1:A:37:ILE:HG23	0.51	2.35	10	3
1:A:75:VAL:HG12	1:A:87:ARG:HB3	0.51	1.81	23	2
1:A:73:THR:HG23	1:A:89:LYS:HG2	0.51	1.82	20	1
1:A:100:ARG:O	1:A:104:LEU:HB3	0.51	2.06	15	1
1:A:29:TYR:HB3	1:A:31:PHE:CZ	0.50	2.41	3	1
1:A:28:ARG:HD2	1:A:39:PHE:CD2	0.50	2.42	6	1
1:A:19:TRP:HZ3	1:A:89:LYS:HE2	0.50	1.66	8	1
1:A:95:THR:O	1:A:96:SER:HB2	0.50	2.05	10	1
1:A:28:ARG:HG2	1:A:41:GLU:CA	0.50	2.35	14	1
1:A:103:TRP:HA	1:A:106:ASP:HB2	0.50	1.84	24	1
1:A:60:ASP:OD1	1:A:61:LYS:HG3	0.50	2.06	10	1
1:A:89:LYS:CD	1:A:91:LYS:HB2	0.50	2.37	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:TRP:HZ3	1:A:89:LYS:HG3	0.50	1.66	3	1
1:A:12:ARG:HE	1:A:31:PHE:HB3	0.50	1.64	20	1
1:A:89:LYS:HD2	1:A:92:ASP:CB	0.50	2.37	22	1
1:A:37:ILE:HB	1:A:57:ILE:HB	0.49	1.82	15	10
1:A:19:TRP:HA	1:A:25:PRO:HA	0.49	1.82	8	6
1:A:37:ILE:HG13	1:A:59:LEU:HD21	0.49	1.84	10	1
1:A:64:ILE:HD12	1:A:76:LEU:HG	0.49	1.84	15	1
1:A:66:GLN:HG2	1:A:104:LEU:HD11	0.49	1.84	15	1
1:A:31:PHE:HB2	1:A:38:MET:HB3	0.49	1.84	2	1
1:A:24:PRO:CB	1:A:25:PRO:HD2	0.49	2.37	7	1
1:A:92:ASP:HB3	1:A:96:SER:OG	0.49	2.06	13	1
1:A:32:LEU:HD23	1:A:37:ILE:HG23	0.49	1.84	3	5
1:A:72:ASP:HB3	1:A:104:LEU:HD13	0.49	1.82	5	1
1:A:37:ILE:HD11	1:A:62:TYR:CZ	0.49	2.43	7	1
1:A:78:PRO:CB	1:A:83:LEU:HB3	0.49	2.38	10	1
1:A:62:TYR:HE1	1:A:83:LEU:HD13	0.49	1.66	15	1
1:A:94:GLU:HA	1:A:101:LYS:HD2	0.49	1.84	22	1
1:A:9:ARG:HH11	1:A:9:ARG:HG2	0.49	1.67	13	1
1:A:58:ARG:HB3	1:A:83:LEU:HD11	0.49	1.83	18	1
1:A:28:ARG:HG2	1:A:39:PHE:HD2	0.49	1.67	20	1
1:A:90:PRO:HB2	1:A:93:PHE:O	0.49	2.06	3	1
1:A:65:ARG:HB2	1:A:75:VAL:HG22	0.49	1.84	9	1
1:A:36:LYS:HA	1:A:59:LEU:HD13	0.49	1.84	24	1
1:A:72:ASP:HB2	1:A:104:LEU:HD23	0.49	1.85	24	1
1:A:28:ARG:HG2	1:A:42:GLN:H	0.49	1.68	10	1
1:A:39:PHE:CE1	1:A:55:SER:HB2	0.49	2.42	11	1
1:A:24:PRO:CB	1:A:25:PRO:CD	0.49	2.91	18	1
1:A:95:THR:HA	1:A:98:TYR:HD2	0.48	1.68	13	1
1:A:26:LYS:HA	1:A:43:ASP:HB3	0.48	1.85	16	1
1:A:17:GLN:HG3	1:A:26:LYS:O	0.48	2.08	21	1
1:A:97:GLU:O	1:A:98:TYR:HB3	0.48	2.07	10	1
1:A:22:ASP:C	1:A:24:PRO:HD2	0.48	2.27	8	1
1:A:59:LEU:HD12	1:A:62:TYR:CE1	0.48	2.43	18	1
1:A:17:GLN:HA	1:A:27:LEU:HA	0.48	1.84	20	3
1:A:67:HIS:HB3	1:A:71:GLU:HB2	0.48	1.84	10	1
1:A:96:SER:HB2	1:A:100:ARG:HD3	0.48	1.84	3	1
1:A:99:VAL:HG12	1:A:103:TRP:CD1	0.48	2.43	5	1
1:A:104:LEU:HD22	1:A:104:LEU:O	0.48	2.09	15	1
1:A:104:LEU:O	1:A:107:ILE:HB	0.48	2.08	24	3
1:A:19:TRP:CZ3	1:A:89:LYS:HG3	0.48	2.44	3	1
1:A:79:GLN:NE2	1:A:80:GLU:HG3	0.48	2.24	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ARG:HH21	1:A:102:ALA:HB1	0.48	1.69	18	1
1:A:18:VAL:HG23	1:A:89:LYS:HG2	0.48	1.85	19	1
1:A:36:LYS:HB2	1:A:58:ARG:HA	0.48	1.84	8	2
1:A:40:THR:HG22	1:A:54:TYR:HA	0.48	1.84	13	1
1:A:75:VAL:HG12	1:A:87:ARG:CG	0.48	2.39	13	1
1:A:27:LEU:HD12	1:A:29:TYR:HE1	0.48	1.68	1	1
1:A:11:ILE:CD1	1:A:111:GLN:HA	0.48	2.39	19	1
1:A:11:ILE:HG22	1:A:12:ARG:N	0.47	2.24	23	2
1:A:79:GLN:HG3	1:A:81:PRO:HG3	0.47	1.85	22	1
1:A:23:GLU:CB	1:A:24:PRO:HD3	0.47	2.28	6	1
1:A:66:GLN:HG2	1:A:104:LEU:HD21	0.47	1.85	15	1
1:A:78:PRO:HB3	1:A:83:LEU:HD23	0.47	1.85	23	1
1:A:72:ASP:HB2	1:A:100:ARG:NE	0.47	2.24	1	1
1:A:78:PRO:HG3	1:A:84:PRO:O	0.47	2.09	2	1
1:A:92:ASP:O	1:A:93:PHE:HB2	0.47	2.09	17	3
1:A:23:GLU:CG	1:A:24:PRO:HD2	0.47	2.38	1	1
1:A:26:LYS:HE3	1:A:43:ASP:HB2	0.47	1.85	6	1
1:A:72:ASP:HB3	1:A:104:LEU:CD2	0.47	2.39	9	1
1:A:105:ARG:O	1:A:109:GLU:HG2	0.47	2.09	15	2
1:A:106:ASP:O	1:A:110:GLU:HG2	0.47	2.09	24	1
1:A:10:ILE:HG23	1:A:11:ILE:H	0.47	1.69	6	1
1:A:28:ARG:HA	1:A:40:THR:O	0.47	2.09	1	1
1:A:58:ARG:HB3	1:A:79:GLN:NE2	0.47	2.25	9	1
1:A:9:ARG:HD3	1:A:33:PHE:HE1	0.47	1.69	14	1
1:A:20:GLU:H	1:A:24:PRO:HD2	0.47	1.68	24	2
1:A:72:ASP:CB	1:A:104:LEU:HD22	0.47	2.39	17	1
1:A:100:ARG:NE	1:A:100:ARG:HA	0.47	2.25	25	1
1:A:74:ILE:HD12	1:A:107:ILE:HG21	0.47	1.87	17	2
1:A:59:LEU:HD12	1:A:62:TYR:HE2	0.47	1.68	4	3
1:A:58:ARG:HG3	1:A:60:ASP:HB2	0.47	1.85	5	1
1:A:18:VAL:CG2	1:A:89:LYS:H	0.47	2.23	8	1
1:A:28:ARG:HG3	1:A:39:PHE:CE2	0.46	2.45	2	1
1:A:18:VAL:HB	1:A:87:ARG:O	0.46	2.10	8	1
1:A:97:GLU:CB	1:A:100:ARG:HG3	0.46	2.40	22	1
1:A:18:VAL:CG2	1:A:19:TRP:N	0.46	2.78	3	1
1:A:74:ILE:HD11	1:A:104:LEU:HD12	0.46	1.87	5	1
1:A:20:GLU:HG2	1:A:21:GLY:H	0.46	1.71	1	1
1:A:28:ARG:HB3	1:A:41:GLU:HA	0.46	1.88	1	1
1:A:28:ARG:HH12	1:A:41:GLU:HA	0.46	1.71	5	1
1:A:22:ASP:O	1:A:23:GLU:HB2	0.46	2.10	6	1
1:A:16:PHE:CD1	1:A:16:PHE:C	0.46	2.88	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:PRO:O	1:A:26:LYS:HG3	0.46	2.10	15	1
1:A:68:THR:HA	1:A:72:ASP:HA	0.46	1.87	8	3
1:A:19:TRP:HB2	1:A:87:ARG:HE	0.46	1.70	15	1
1:A:72:ASP:HB2	1:A:104:LEU:HD21	0.46	1.87	20	1
1:A:62:TYR:HB2	1:A:79:GLN:CG	0.46	2.40	4	1
1:A:28:ARG:NH1	1:A:55:SER:HB2	0.46	2.18	3	1
1:A:20:GLU:HG2	1:A:28:ARG:NH1	0.46	2.25	4	1
1:A:86:PHE:CE2	1:A:88:ILE:HG23	0.46	2.45	14	2
1:A:106:ASP:HA	1:A:110:GLU:HB2	0.46	1.86	20	1
1:A:32:LEU:CD2	1:A:103:TRP:HZ3	0.46	2.23	20	1
1:A:16:PHE:CE2	1:A:30:VAL:CG2	0.46	2.99	7	1
1:A:79:GLN:HG3	1:A:83:LEU:CD2	0.46	2.41	9	1
1:A:58:ARG:HD3	1:A:79:GLN:HE22	0.46	1.69	19	1
1:A:65:ARG:HB2	1:A:75:VAL:CG2	0.46	2.41	9	2
1:A:15:ALA:HB2	1:A:29:TYR:HB3	0.46	1.88	10	1
1:A:63:ASN:HD22	1:A:77:GLN:HB3	0.45	1.70	1	1
1:A:74:ILE:HD11	1:A:104:LEU:HB3	0.45	1.87	12	1
1:A:102:ALA:O	1:A:105:ARG:HB2	0.45	2.11	11	2
1:A:28:ARG:HD2	1:A:39:PHE:HD2	0.45	1.71	14	1
1:A:62:TYR:CE2	1:A:76:LEU:HD23	0.45	2.47	15	1
1:A:76:LEU:HD13	1:A:86:PHE:CD2	0.45	2.47	16	1
1:A:11:ILE:HB	1:A:32:LEU:HB2	0.45	1.87	18	1
1:A:78:PRO:HB3	1:A:83:LEU:CB	0.45	2.41	20	1
1:A:13:HIS:HA	1:A:30:VAL:O	0.45	2.12	18	4
1:A:26:LYS:HB3	1:A:42:GLN:O	0.45	2.12	4	1
1:A:79:GLN:CB	1:A:83:LEU:HD23	0.45	2.17	4	1
1:A:23:GLU:HB3	1:A:24:PRO:CD	0.45	2.30	6	1
1:A:16:PHE:HA	1:A:92:ASP:OD1	0.45	2.11	7	1
1:A:10:ILE:HD13	1:A:34:ARG:HB2	0.45	1.86	8	1
1:A:76:LEU:O	1:A:85:SER:HA	0.45	2.11	9	1
1:A:77:GLN:CB	1:A:78:PRO:CD	0.45	2.91	9	1
1:A:36:LYS:HA	1:A:59:LEU:HB2	0.45	1.88	12	3
1:A:28:ARG:CD	1:A:40:THR:HA	0.45	2.41	16	1
1:A:62:TYR:HA	1:A:79:GLN:HB3	0.45	1.88	19	1
1:A:90:PRO:HB3	1:A:100:ARG:HB3	0.45	1.89	19	1
1:A:75:VAL:HG22	1:A:87:ARG:HG2	0.45	1.89	6	1
1:A:79:GLN:O	1:A:80:GLU:HG3	0.45	2.12	11	1
1:A:41:GLU:HG2	1:A:42:GLN:H	0.45	1.72	16	1
1:A:76:LEU:HD13	1:A:86:PHE:CZ	0.45	2.47	25	1
1:A:75:VAL:HG13	1:A:87:ARG:HG3	0.45	1.89	21	1
1:A:18:VAL:HG21	1:A:88:ILE:HG22	0.45	1.88	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:HIS:C	1:A:103:TRP:HZ2	0.45	2.15	20	1
1:A:26:LYS:HE3	1:A:43:ASP:OD2	0.45	2.11	20	1
1:A:41:GLU:HG2	1:A:42:GLN:N	0.45	2.27	16	1
1:A:60:ASP:CG	1:A:61:LYS:HD3	0.45	2.33	20	1
1:A:106:ASP:O	1:A:111:GLN:HG2	0.45	2.11	20	1
1:A:30:VAL:HG22	1:A:39:PHE:HB3	0.45	1.88	7	1
1:A:104:LEU:HD23	1:A:105:ARG:N	0.45	2.26	25	1
1:A:11:ILE:HG13	1:A:34:ARG:H	0.44	1.72	5	1
1:A:93:PHE:HD2	1:A:96:SER:HA	0.44	1.72	7	2
1:A:19:TRP:CZ3	1:A:89:LYS:HG2	0.44	2.47	10	1
1:A:103:TRP:C	1:A:105:ARG:H	0.44	2.16	16	1
1:A:68:THR:HB	1:A:71:GLU:O	0.44	2.12	20	1
1:A:72:ASP:HB2	1:A:100:ARG:HG2	0.44	1.88	21	1
1:A:11:ILE:HG21	1:A:32:LEU:HG	0.44	1.88	23	1
1:A:22:ASP:O	1:A:23:GLU:CB	0.44	2.65	12	2
1:A:39:PHE:O	1:A:55:SER:HB3	0.44	2.12	13	1
1:A:9:ARG:HA	1:A:33:PHE:CE2	0.44	2.47	6	1
1:A:61:LYS:O	1:A:79:GLN:HA	0.44	2.12	9	1
1:A:90:PRO:HB3	1:A:100:ARG:NE	0.44	2.27	10	1
1:A:58:ARG:H	1:A:58:ARG:HD2	0.44	1.72	25	2
1:A:59:LEU:HD13	1:A:110:GLU:HB3	0.44	1.89	6	1
1:A:59:LEU:HD23	1:A:62:TYR:CE2	0.44	2.47	6	1
1:A:16:PHE:CE2	1:A:30:VAL:HG23	0.44	2.47	7	1
1:A:9:ARG:HG2	1:A:33:PHE:CE1	0.44	2.48	9	1
1:A:39:PHE:CZ	1:A:86:PHE:CZ	0.44	3.05	25	1
1:A:26:LYS:CB	1:A:28:ARG:HH21	0.44	2.21	5	1
1:A:36:LYS:HE3	1:A:38:MET:SD	0.44	2.52	5	1
1:A:10:ILE:HG21	1:A:34:ARG:HB2	0.44	1.90	9	1
1:A:59:LEU:HA	1:A:62:TYR:HE1	0.44	1.67	19	1
1:A:78:PRO:HB3	1:A:83:LEU:CD2	0.44	2.32	22	1
1:A:64:ILE:HG13	1:A:75:VAL:O	0.44	2.13	12	1
1:A:101:LYS:O	1:A:105:ARG:HG3	0.44	2.13	15	1
1:A:101:LYS:H	1:A:101:LYS:HD2	0.43	1.73	25	1
1:A:26:LYS:HE2	1:A:43:ASP:OD1	0.43	2.12	4	1
1:A:90:PRO:CA	1:A:100:ARG:HG3	0.43	2.42	9	1
1:A:32:LEU:HD11	1:A:103:TRP:CZ3	0.43	2.48	16	1
1:A:67:HIS:HD2	1:A:75:VAL:HG11	0.43	1.74	20	1
1:A:74:ILE:CG1	1:A:100:ARG:HH22	0.43	2.24	9	1
1:A:64:ILE:HG23	1:A:107:ILE:HG23	0.43	1.90	12	1
1:A:18:VAL:HG21	1:A:89:LYS:N	0.43	2.26	15	1
1:A:90:PRO:HG3	1:A:100:ARG:NE	0.43	2.28	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:GLU:HG3	1:A:28:ARG:NH2	0.43	2.28	23	1
1:A:31:PHE:HB2	1:A:38:MET:O	0.43	2.14	23	1
1:A:32:LEU:HD21	1:A:103:TRP:CZ3	0.43	2.46	1	1
1:A:86:PHE:HE2	1:A:88:ILE:HG23	0.43	1.73	21	1
1:A:12:ARG:O	1:A:32:LEU:HD12	0.43	2.14	5	1
1:A:58:ARG:HD2	1:A:60:ASP:HB2	0.43	1.89	10	1
1:A:29:TYR:HB2	1:A:31:PHE:CE1	0.43	2.49	16	1
1:A:39:PHE:CE1	1:A:55:SER:HB3	0.43	2.48	17	1
1:A:19:TRP:CZ3	1:A:89:LYS:HE2	0.43	2.48	8	1
1:A:99:VAL:O	1:A:103:TRP:HD1	0.43	1.95	4	2
1:A:37:ILE:HG22	1:A:38:MET:N	0.43	2.29	11	1
1:A:89:LYS:HD2	1:A:91:LYS:CB	0.43	2.42	16	1
1:A:60:ASP:O	1:A:61:LYS:HD2	0.43	2.13	25	1
1:A:72:ASP:HB2	1:A:100:ARG:HD2	0.43	1.89	14	1
1:A:12:ARG:HB3	1:A:103:TRP:CE3	0.43	2.48	25	1
1:A:90:PRO:HG3	1:A:100:ARG:HG2	0.43	1.90	3	1
1:A:16:PHE:HE2	1:A:30:VAL:CG2	0.43	2.26	7	1
1:A:96:SER:C	1:A:98:TYR:H	0.43	2.17	21	2
1:A:80:GLU:C	1:A:82:GLY:H	0.43	2.17	11	1
1:A:63:ASN:ND2	1:A:65:ARG:HD3	0.43	2.28	3	1
1:A:90:PRO:HG2	1:A:94:GLU:HA	0.43	1.90	3	1
1:A:34:ARG:O	1:A:34:ARG:HD3	0.43	2.14	9	1
1:A:62:TYR:HB3	1:A:79:GLN:CD	0.43	2.34	9	1
1:A:100:ARG:HG2	1:A:100:ARG:HH11	0.43	1.74	10	1
1:A:107:ILE:O	1:A:110:GLU:HG3	0.43	2.14	22	1
1:A:68:THR:O	1:A:70:ASP:N	0.42	2.50	2	1
1:A:17:GLN:O	1:A:17:GLN:HG3	0.42	2.14	6	1
1:A:96:SER:O	1:A:98:TYR:N	0.42	2.52	25	2
1:A:26:LYS:HD2	1:A:41:GLU:HB3	0.42	1.90	18	1
1:A:28:ARG:O	1:A:28:ARG:HG3	0.42	2.14	18	1
1:A:39:PHE:CZ	1:A:55:SER:HB3	0.42	2.50	20	1
1:A:10:ILE:HG23	1:A:11:ILE:N	0.42	2.28	6	1
1:A:29:TYR:CD1	1:A:41:GLU:HB2	0.42	2.49	16	1
1:A:81:PRO:HD2	1:A:83:LEU:CB	0.42	2.40	5	1
1:A:28:ARG:CB	1:A:41:GLU:HG2	0.42	2.39	8	1
1:A:20:GLU:O	1:A:20:GLU:HG2	0.42	2.14	9	1
1:A:94:GLU:C	1:A:96:SER:H	0.42	2.18	13	1
1:A:18:VAL:CG2	1:A:89:LYS:HG2	0.42	2.43	19	1
1:A:58:ARG:H	1:A:58:ARG:HD3	0.42	1.74	20	1
1:A:20:GLU:CB	1:A:28:ARG:HG3	0.42	2.44	21	1
1:A:22:ASP:O	1:A:23:GLU:HB3	0.42	2.15	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:THR:O	1:A:96:SER:HB3	0.42	2.14	19	1
1:A:36:LYS:HD2	1:A:56:SER:HB2	0.42	1.92	23	1
1:A:17:GLN:H	1:A:92:ASP:HB2	0.42	1.75	6	1
1:A:59:LEU:HD12	1:A:62:TYR:HE1	0.42	1.73	21	1
1:A:9:ARG:HA	1:A:33:PHE:CE1	0.42	2.50	3	1
1:A:58:ARG:HD3	1:A:79:GLN:CD	0.42	2.34	5	1
1:A:23:GLU:HB2	1:A:24:PRO:CD	0.42	2.44	10	1
1:A:27:LEU:O	1:A:28:ARG:HD3	0.42	2.15	20	1
1:A:101:LYS:HD2	1:A:101:LYS:N	0.42	2.29	25	1
1:A:39:PHE:O	1:A:55:SER:HA	0.42	2.14	19	1
1:A:90:PRO:HA	1:A:93:PHE:CE1	0.42	2.50	2	1
1:A:27:LEU:HB3	1:A:43:ASP:HB2	0.42	1.91	13	1
1:A:19:TRP:CD1	1:A:25:PRO:HG3	0.42	2.49	16	1
1:A:28:ARG:HD2	1:A:40:THR:HA	0.42	1.92	16	1
1:A:89:LYS:HA	1:A:90:PRO:HD3	0.42	1.77	16	1
1:A:29:TYR:HB2	1:A:40:THR:OG1	0.42	2.15	17	1
1:A:86:PHE:CD1	1:A:88:ILE:HG23	0.42	2.50	24	1
1:A:101:LYS:HA	1:A:101:LYS:CE	0.41	2.44	18	1
1:A:58:ARG:HD3	1:A:59:LEU:N	0.41	2.31	14	1
1:A:41:GLU:HG3	1:A:54:TYR:CD2	0.41	2.50	19	1
1:A:16:PHE:O	1:A:18:VAL:HG23	0.41	2.14	25	1
1:A:59:LEU:HD23	1:A:62:TYR:HE2	0.41	1.75	6	1
1:A:30:VAL:HG22	1:A:39:PHE:CB	0.41	2.45	7	1
1:A:89:LYS:HD3	1:A:91:LYS:HD2	0.41	1.92	8	1
1:A:62:TYR:HA	1:A:79:GLN:OE1	0.41	2.15	14	1
1:A:28:ARG:HG2	1:A:39:PHE:CE2	0.41	2.50	25	1
1:A:78:PRO:CD	1:A:85:SER:HB3	0.41	2.43	14	1
1:A:106:ASP:HA	1:A:110:GLU:HB3	0.41	1.92	20	1
1:A:100:ARG:HH21	1:A:103:TRP:HB3	0.41	1.75	9	1
1:A:97:GLU:O	1:A:98:TYR:CB	0.41	2.69	10	1
1:A:62:TYR:CB	1:A:79:GLN:HB3	0.41	2.45	4	1
1:A:96:SER:O	1:A:97:GLU:HB2	0.41	2.16	10	1
1:A:10:ILE:HG21	1:A:34:ARG:N	0.41	2.30	11	1
1:A:23:GLU:N	1:A:24:PRO:CD	0.41	2.83	11	1
1:A:9:ARG:O	1:A:10:ILE:HG22	0.41	2.16	8	1
1:A:19:TRP:HB2	1:A:87:ARG:NE	0.41	2.31	8	1
1:A:19:TRP:CH2	1:A:89:LYS:HD3	0.41	2.50	17	1
1:A:29:TYR:HB3	1:A:31:PHE:CE2	0.41	2.51	3	2
1:A:19:TRP:CZ3	1:A:89:LYS:HD3	0.41	2.50	17	1
1:A:31:PHE:HB3	1:A:33:PHE:CZ	0.41	2.50	1	1
1:A:69:THR:O	1:A:70:ASP:HB3	0.41	2.14	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ASP:HB2	1:A:100:ARG:HE	0.41	1.75	1	1
1:A:28:ARG:HD3	1:A:39:PHE:CD2	0.41	2.51	8	1
1:A:12:ARG:HB2	1:A:103:TRP:CB	0.41	2.46	10	1
1:A:12:ARG:HD2	1:A:33:PHE:CZ	0.41	2.51	20	1
1:A:76:LEU:O	1:A:78:PRO:HD3	0.41	2.15	23	1
1:A:98:TYR:O	1:A:102:ALA:HB3	0.40	2.15	25	1
1:A:31:PHE:O	1:A:38:MET:N	0.40	2.50	2	1
1:A:64:ILE:HD11	1:A:74:ILE:HG22	0.40	1.92	4	1
1:A:76:LEU:N	1:A:76:LEU:HD12	0.40	2.31	7	1
1:A:12:ARG:HB3	1:A:103:TRP:HB2	0.40	1.93	15	1
1:A:58:ARG:O	1:A:62:TYR:HD1	0.40	1.99	19	1
1:A:33:PHE:HB3	1:A:34:ARG:H	0.40	1.53	20	1
1:A:79:GLN:H	1:A:79:GLN:CD	0.40	2.20	14	1
1:A:67:HIS:O	1:A:72:ASP:HA	0.40	2.16	24	1
1:A:28:ARG:NH1	1:A:41:GLU:HA	0.40	2.32	5	1
1:A:110:GLU:HG3	1:A:110:GLU:O	0.40	2.16	15	1
1:A:27:LEU:HD23	1:A:28:ARG:N	0.40	2.31	17	1
1:A:58:ARG:HD3	1:A:60:ASP:HB3	0.40	1.93	22	1
1:A:97:GLU:C	1:A:99:VAL:N	0.40	2.74	23	1
1:A:76:LEU:HD21	1:A:86:PHE:CE2	0.40	2.51	2	1
1:A:101:LYS:O	1:A:104:LEU:HG	0.40	2.17	12	1
1:A:97:GLU:HB2	1:A:100:ARG:HG3	0.40	1.93	22	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	94/119 (79%)	72±4 (76±4%)	17±4 (18±4%)	6±2 (6±3%)	3	21
All	All	2350/2975 (79%)	1793 (76%)	419 (18%)	138 (6%)	3	21

All 38 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	11	ILE	21
1	A	111	GLN	9
1	A	24	PRO	7
1	A	23	GLU	7
1	A	35	ASN	7
1	A	96	SER	6
1	A	83	LEU	6
1	A	70	ASP	6
1	A	34	ARG	5
1	A	93	PHE	5
1	A	94	GLU	5
1	A	97	GLU	4
1	A	18	VAL	4
1	A	60	ASP	4
1	A	21	GLY	3
1	A	92	ASP	3
1	A	91	LYS	3
1	A	10	ILE	3
1	A	68	THR	3
1	A	69	THR	2
1	A	78	PRO	2
1	A	84	PRO	2
1	A	72	ASP	2
1	A	98	TYR	2
1	A	110	GLU	2
1	A	54	TYR	2
1	A	44	ALA	2
1	A	59	LEU	1
1	A	9	ARG	1
1	A	95	THR	1
1	A	104	LEU	1
1	A	77	GLN	1
1	A	80	GLU	1
1	A	42	GLN	1
1	A	36	LYS	1
1	A	109	GLU	1
1	A	67	HIS	1
1	A	81	PRO	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	88/108 (81%)	78±3 (88±4%)	10±3 (12±4%)	9 52
All	All	2200/2700 (81%)	1946 (88%)	254 (12%)	9 52

All 63 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	87	ARG	17
1	A	58	ARG	15
1	A	18	VAL	14
1	A	32	LEU	13
1	A	28	ARG	10
1	A	76	LEU	9
1	A	110	GLU	9
1	A	104	LEU	9
1	A	39	PHE	7
1	A	13	HIS	6
1	A	68	THR	6
1	A	66	GLN	6
1	A	103	TRP	6
1	A	89	LYS	6
1	A	106	ASP	6
1	A	12	ARG	5
1	A	27	LEU	5
1	A	79	GLN	5
1	A	34	ARG	5
1	A	36	LYS	5
1	A	64	ILE	5
1	A	14	ASP	4
1	A	100	ARG	4
1	A	91	LYS	4
1	A	62	TYR	4
1	A	20	GLU	3
1	A	105	ARG	3
1	A	83	LEU	3
1	A	97	GLU	3
1	A	98	TYR	3
1	A	101	LYS	3
1	A	107	ILE	3
1	A	19	TRP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	86	PHE	2
1	A	93	PHE	2
1	A	10	ILE	2
1	A	70	ASP	2
1	A	88	ILE	2
1	A	54	TYR	2
1	A	96	SER	2
1	A	40	THR	2
1	A	43	ASP	2
1	A	59	LEU	2
1	A	29	TYR	2
1	A	31	PHE	2
1	A	63	ASN	2
1	A	55	SER	2
1	A	41	GLU	2
1	A	72	ASP	2
1	A	57	ILE	1
1	A	77	GLN	1
1	A	65	ARG	1
1	A	99	VAL	1
1	A	22	ASP	1
1	A	42	GLN	1
1	A	71	GLU	1
1	A	17	GLN	1
1	A	9	ARG	1
1	A	33	PHE	1
1	A	94	GLU	1
1	A	85	SER	1
1	A	95	THR	1
1	A	111	GLN	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)

No chemical shift data were provided