



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 01:32 am GMT

PDB ID : 2N0T
Title : Structural ensemble of the enzyme cyclophilin reveals an orchestrated mode of action at atomic resolution
Authors : Chi, C.N.; Voegeli, B.; Bibow, S.; Strotz, D.; Orts, J.; Guntert, P.; Riek, R.
Deposited on : 2015-03-13

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

<http://wwpdb.org/validation/2016/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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

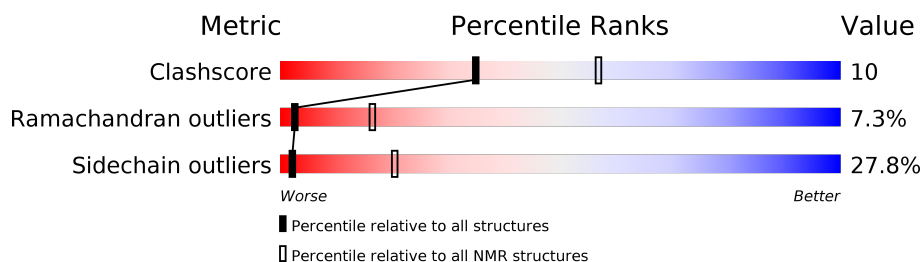
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	165	<p>47% 47% 7%</p>

2 Ensemble composition and analysis ⓘ

This entry contains 40 models. Model 13 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:1-A:64, A:76-A:165 (154)	0.69	13

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 7 clusters and 1 single-model cluster was found.

Cluster number	Models
1	6, 10, 11, 13, 18, 19, 23, 27, 29, 30, 35, 36
2	4, 5, 14, 15, 16, 17, 28
3	2, 3, 25, 39, 40
4	1, 8, 12, 37, 38
5	21, 22, 33, 34
6	7, 20, 26
7	9, 31, 32
Single-model clusters	24

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2500 atoms, of which 1235 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase A.

Mol	Chain	Residues	Atoms						Trace
1	A	165	Total	C	H	N	O	S	0
			2500	802	1235	218	236	9	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Peptidyl-prolyl cis-trans isomerase A

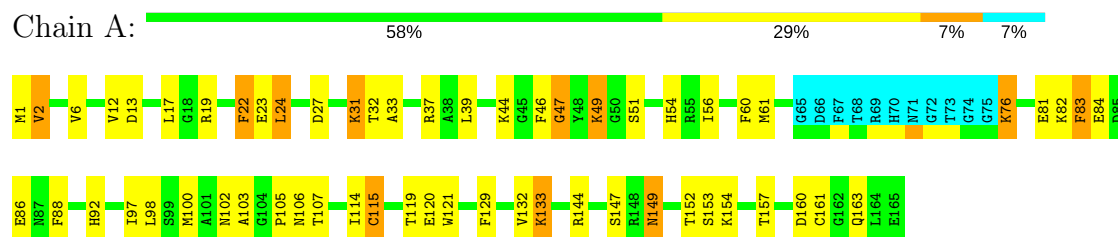


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

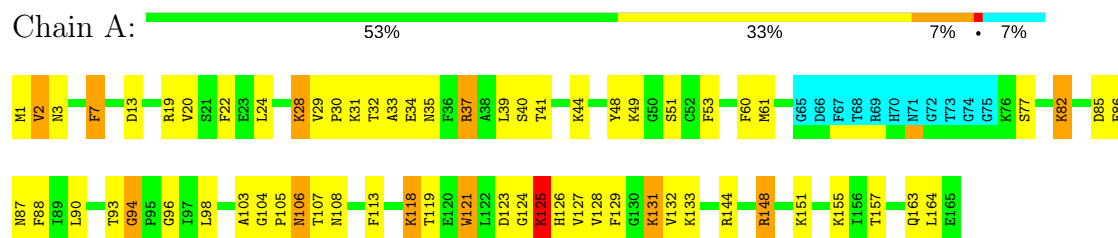
4.2.1 Score per residue for model 1

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



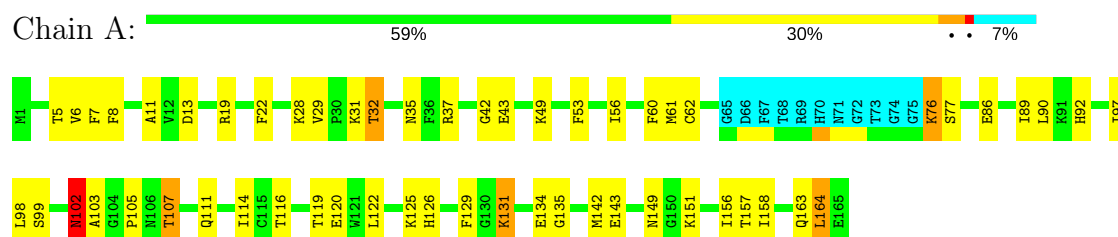
4.2.2 Score per residue for model 2

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



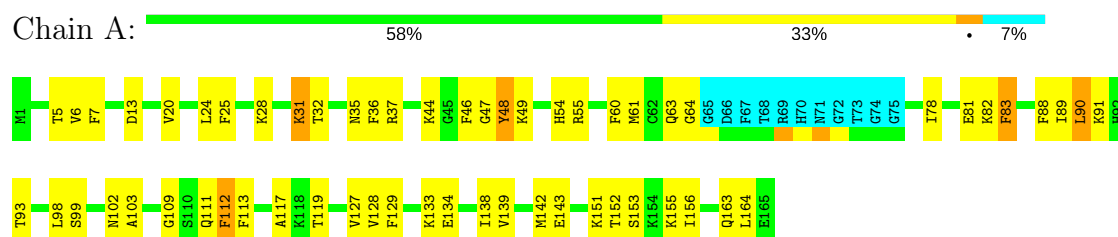
4.2.3 Score per residue for model 3

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



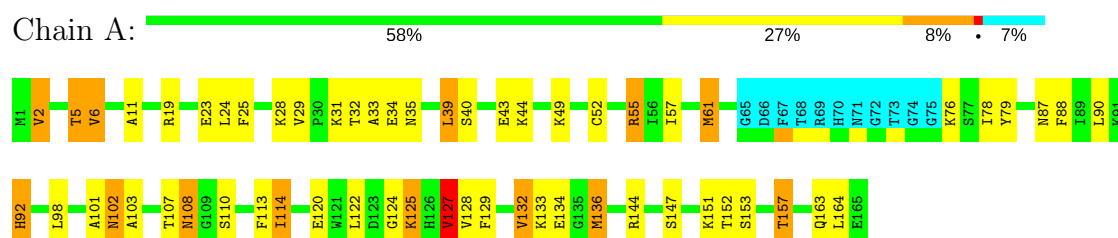
4.2.4 Score per residue for model 4

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



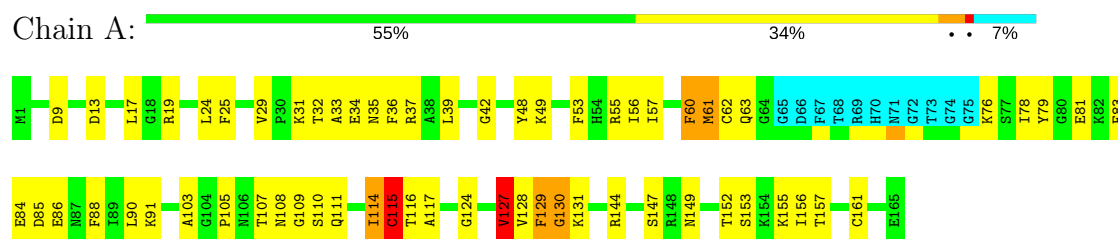
4.2.5 Score per residue for model 5

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



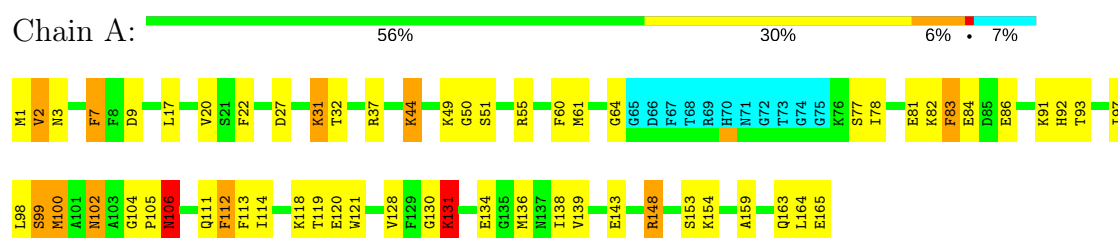
4.2.6 Score per residue for model 6

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



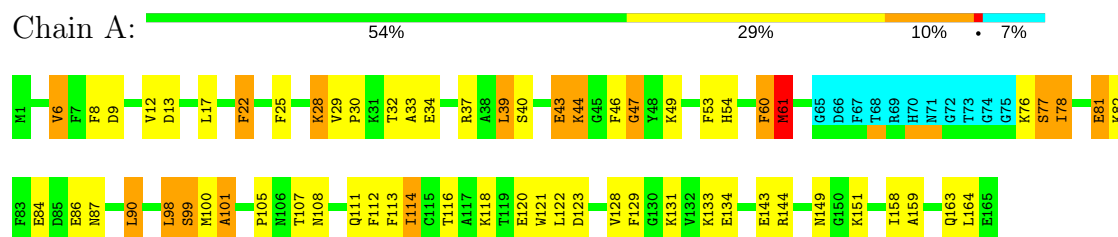
4.2.7 Score per residue for model 7

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



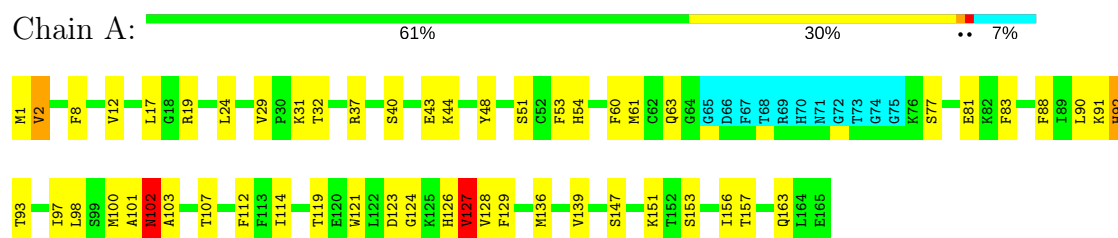
4.2.8 Score per residue for model 8

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



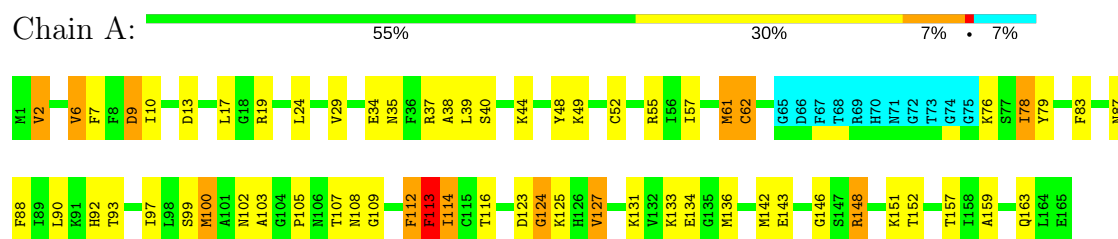
4.2.9 Score per residue for model 9

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



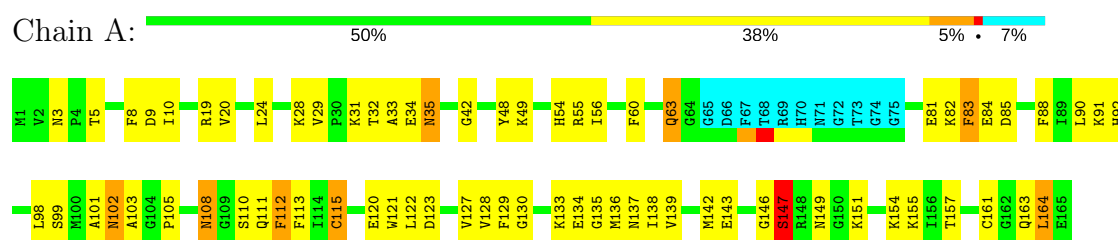
4.2.10 Score per residue for model 10

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



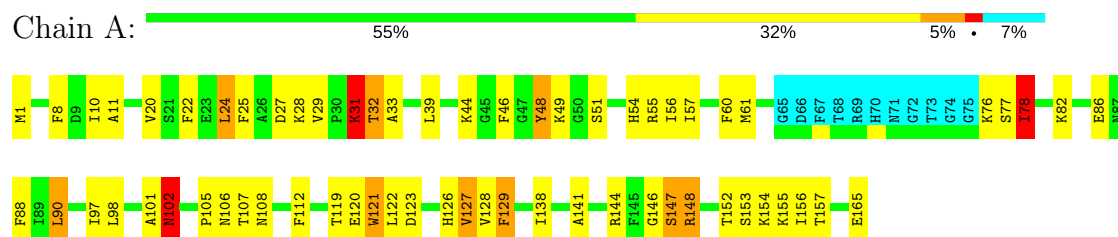
4.2.11 Score per residue for model 11

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



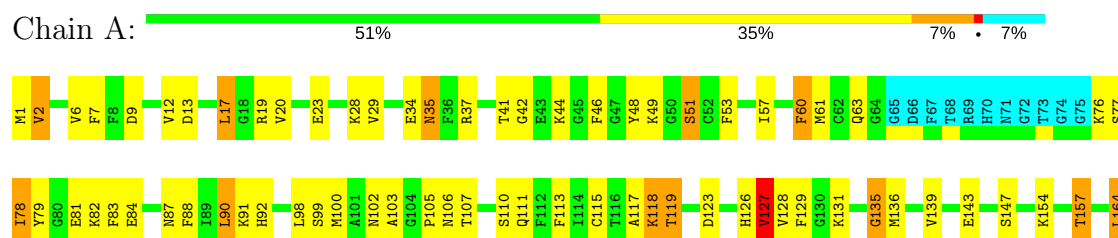
4.2.12 Score per residue for model 12

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



4.2.13 Score per residue for model 13 (medoid)

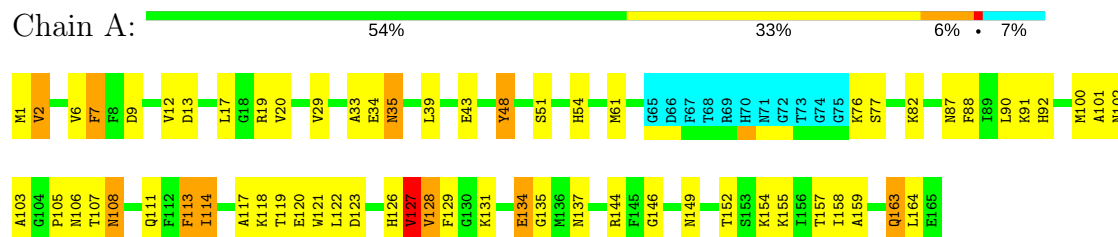
- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



E165

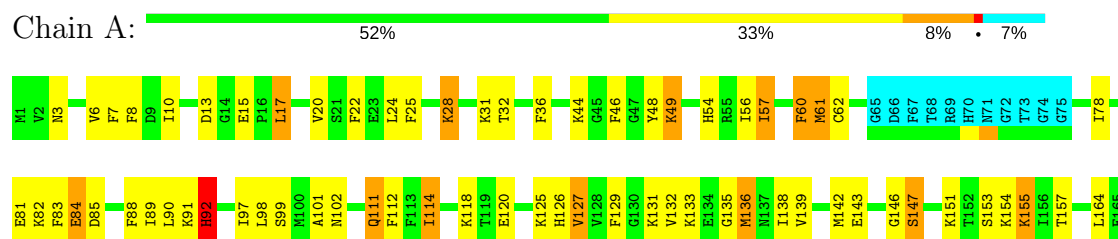
4.2.14 Score per residue for model 14

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



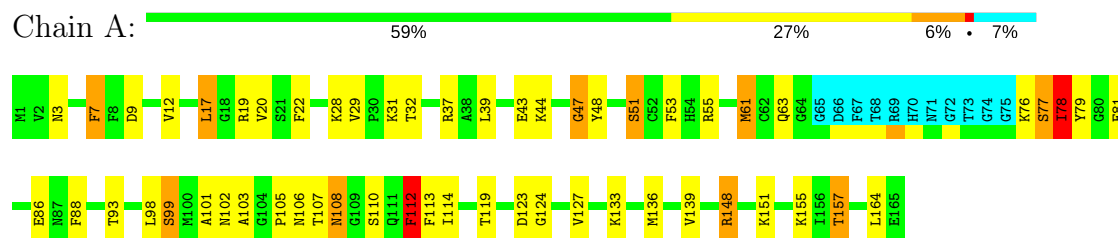
4.2.15 Score per residue for model 15

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



4.2.16 Score per residue for model 16

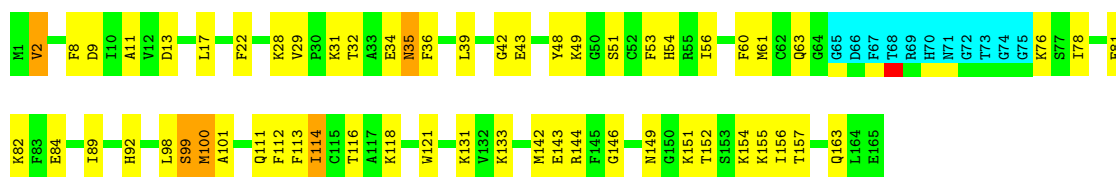
- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



4.2.17 Score per residue for model 17

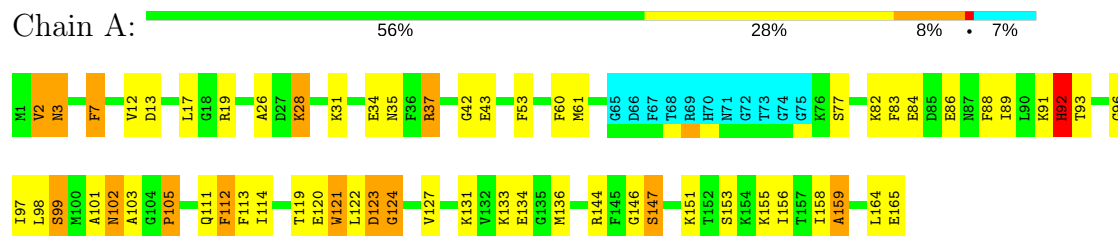
- Molecule 1: Peptidyl-prolyl cis-trans isomerase A





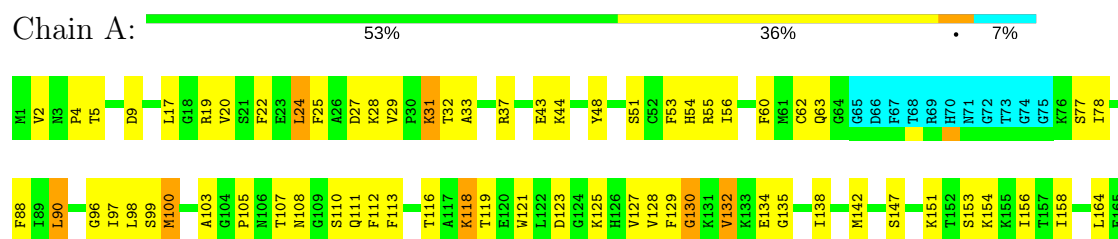
4.2.18 Score per residue for model 18

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



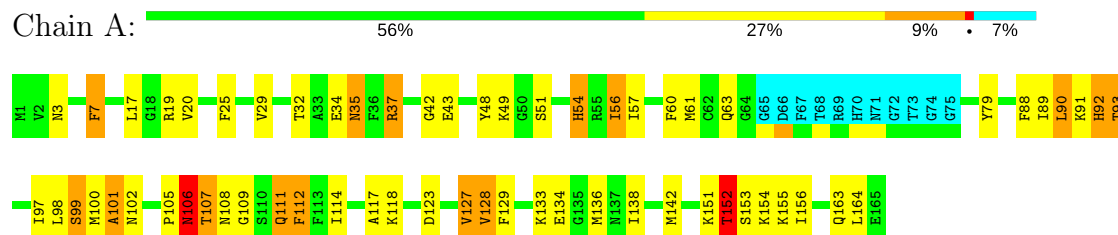
4.2.19 Score per residue for model 19

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



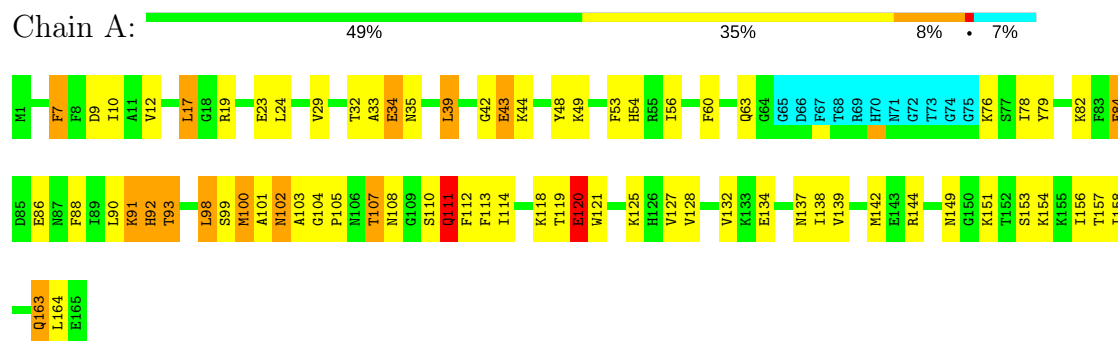
4.2.20 Score per residue for model 20

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



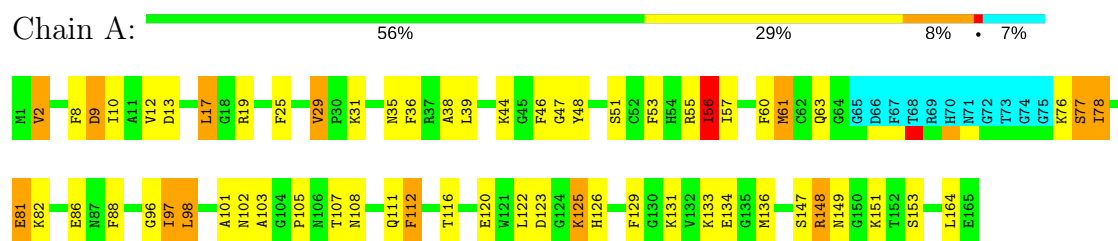
4.2.21 Score per residue for model 21

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



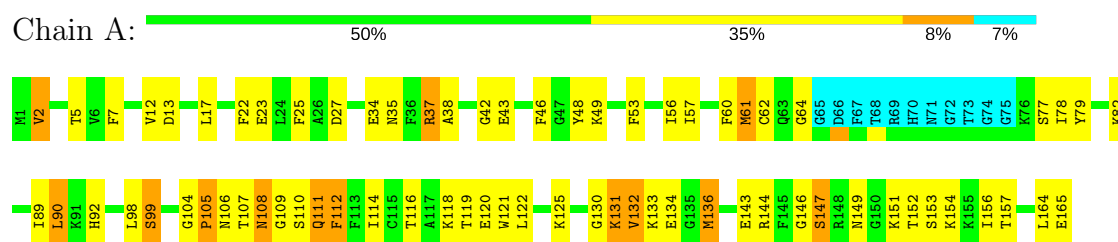
4.2.22 Score per residue for model 22

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



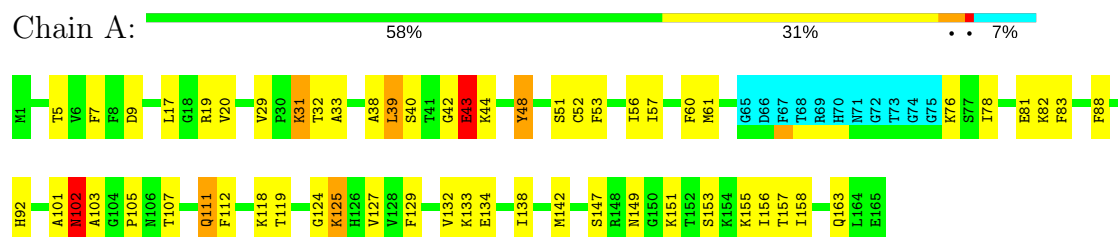
4.2.23 Score per residue for model 23

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



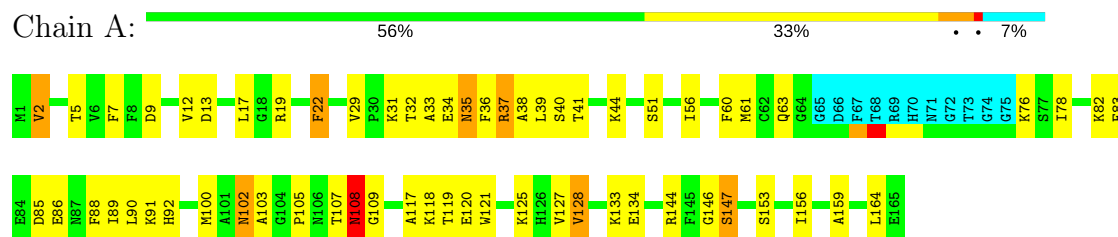
4.2.24 Score per residue for model 24

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



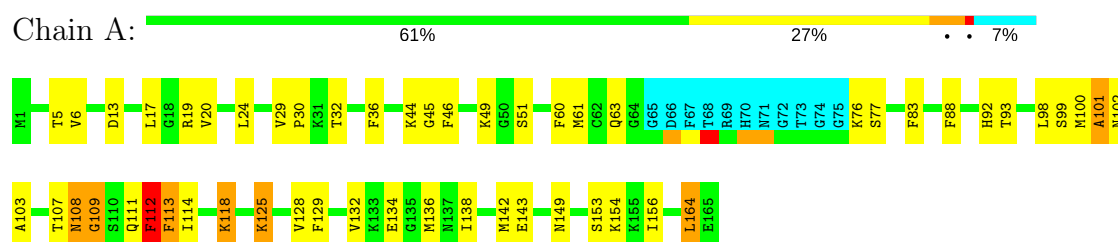
4.2.25 Score per residue for model 25

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



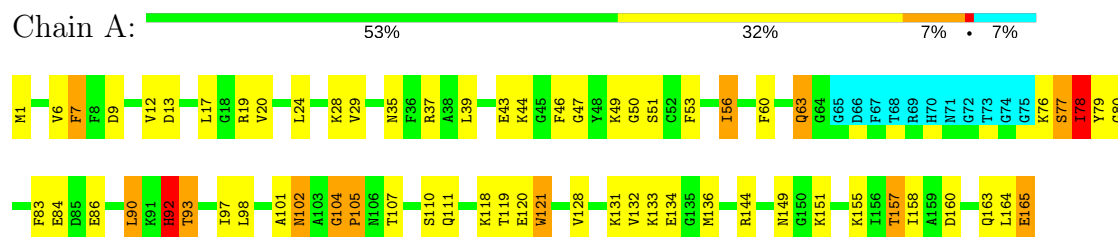
4.2.26 Score per residue for model 26

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



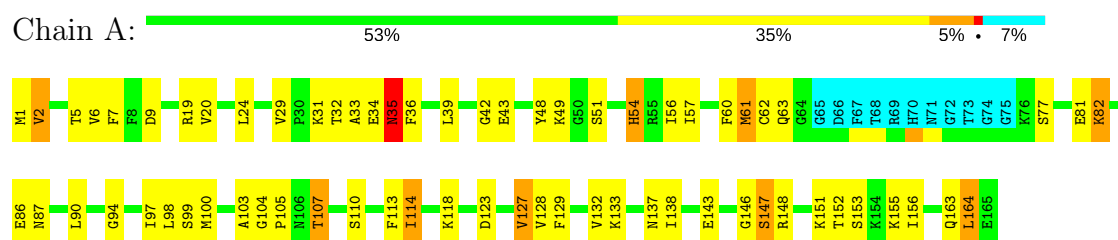
4.2.27 Score per residue for model 27

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



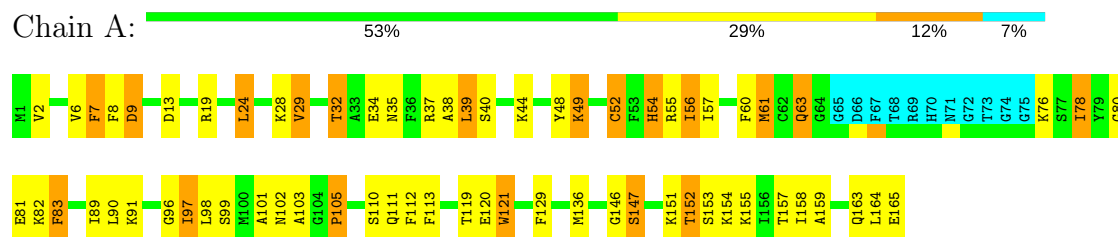
4.2.28 Score per residue for model 28

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A

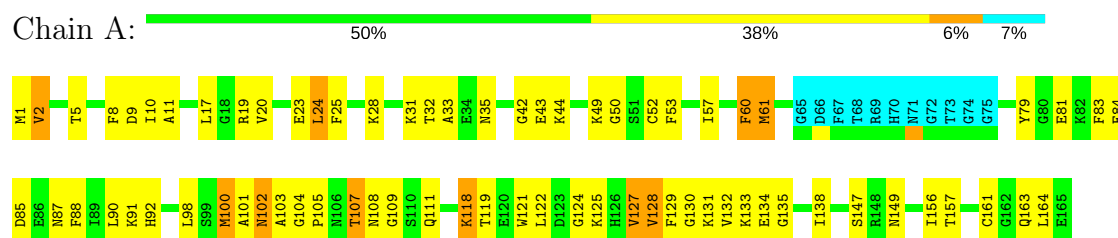


4.2.29 Score per residue for model 29

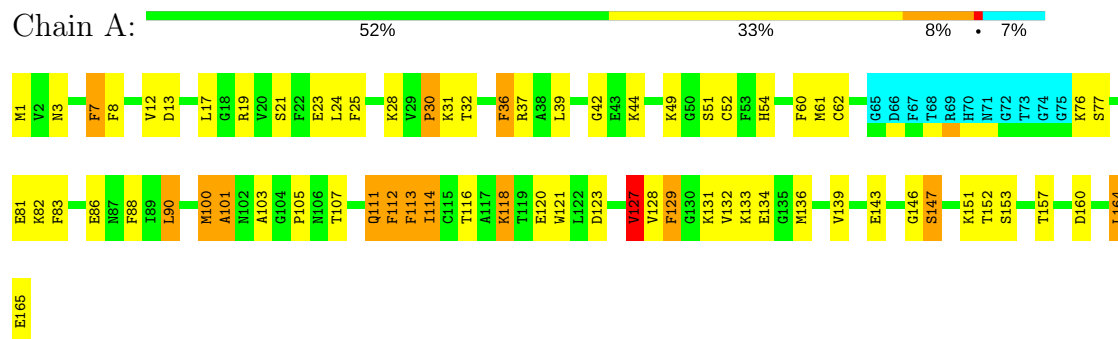
- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



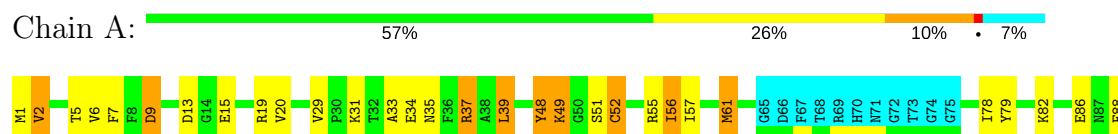
- Molecule 1: Peptidyl-prolyl cis-trans isomerase A

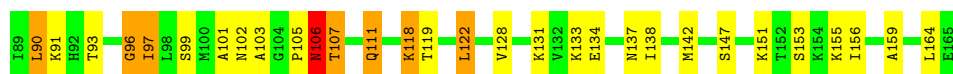


- Molecule 1: Peptidyl-prolyl cis-trans isomerase A



- Molecule 1: Peptidyl-prolyl cis-trans isomerase A

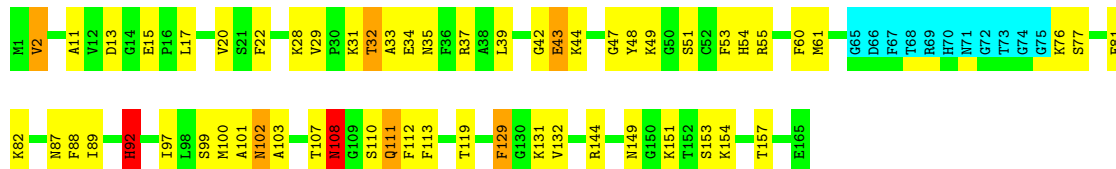




4.2.33 Score per residue for model 33

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A

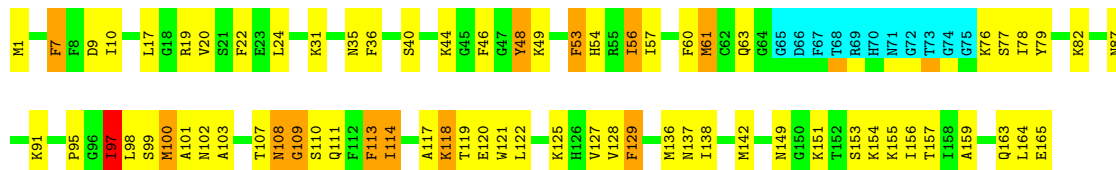
Chain A: 58% 30% 7%



4.2.34 Score per residue for model 34

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A

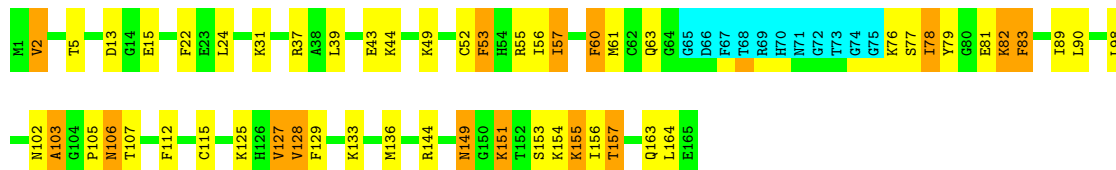
Chain A: 50% 35% 7% 7%



4.2.35 Score per residue for model 35

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A

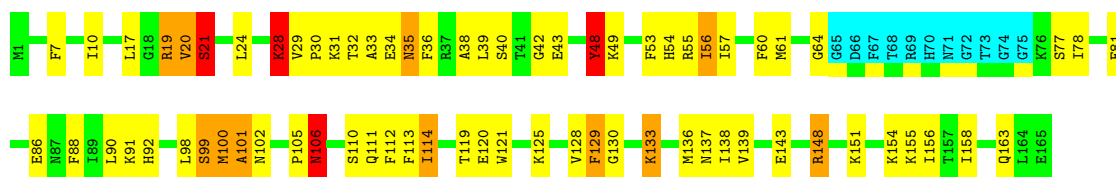
Chain A: 61% 23% 9% 7%



4.2.36 Score per residue for model 36

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A

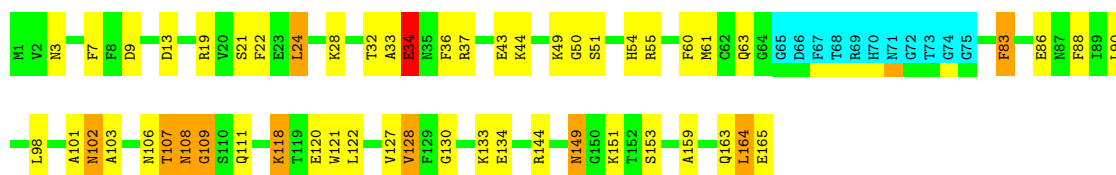
Chain A: 50% 34% 7% 7%



4.2.37 Score per residue for model 37

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A

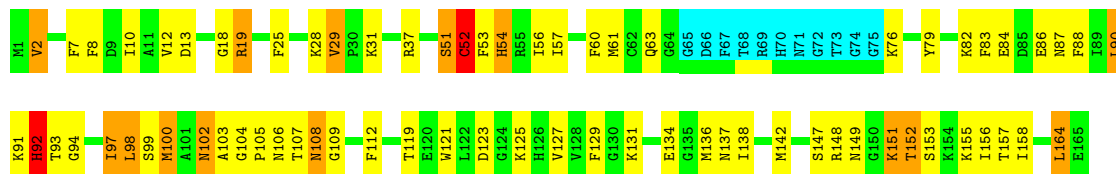
Chain A:



4.2.38 Score per residue for model 38

- Molecule 1: Peptidyl-prolyl cis-trans isomerase A

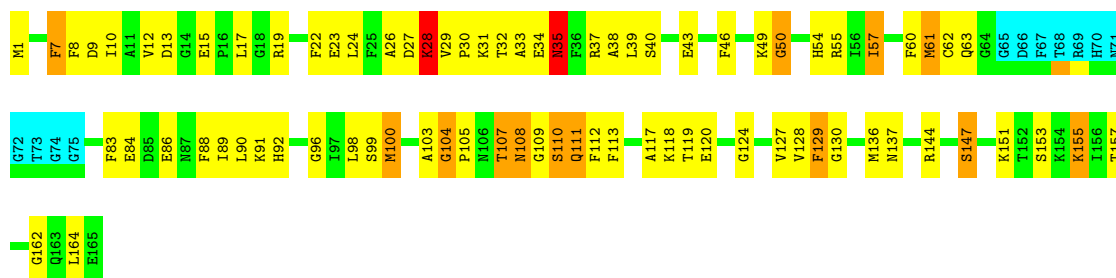
Chain A:



4.2.39 Score per residue for model 39

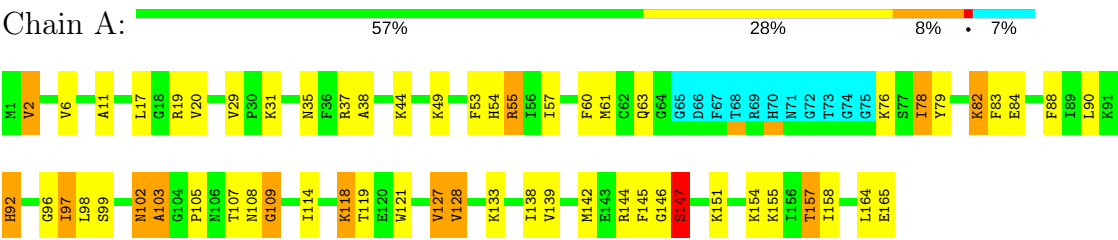
- Molecule 1: Peptidyl-prolyl cis-trans isomerase A

Chain A:



4.2.40 Score per residue for model 40

• Molecule 1: Peptidyl-prolyl cis-trans isomerase A



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 40 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
CYANA	structure solution	
CYANA	refinement	

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

Chemical shift file(s)	2n0t_cs.str
Number of chemical shift lists	1
Total number of shifts	1786
Number of shifts mapped to atoms	1786
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

No validations of the models with respect to experimental NMR restraints is performed at this time.

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	1187	1170	1172	24±6
All	All	47480	46800	46880	946

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:ALA:HB3	1:A:107:THR:HG21	1.02	1.31	1	8
1:A:12:VAL:HG22	1:A:156:ILE:HG22	0.90	1.38	38	2
1:A:101:ALA:O	1:A:102:ASN:HB2	0.85	1.71	11	1
1:A:104:GLY:N	1:A:105:PRO:HD2	0.85	1.86	28	6
1:A:99:SER:O	1:A:100:MET:O	0.82	1.96	17	2
1:A:103:ALA:HB3	1:A:107:THR:OG1	0.80	1.76	40	13
1:A:104:GLY:N	1:A:105:PRO:CD	0.78	2.46	28	3
1:A:101:ALA:O	1:A:102:ASN:CB	0.78	2.31	11	9
1:A:20:VAL:HG22	1:A:138:ILE:HG21	0.74	1.58	32	3
1:A:119:THR:HG22	1:A:121:TRP:CZ2	0.74	2.17	9	15
1:A:127:VAL:O	1:A:128:VAL:HB	0.74	1.82	20	2
1:A:103:ALA:HB3	1:A:107:THR:CB	0.73	2.13	35	9
1:A:151:LYS:O	1:A:152:THR:HG22	0.73	1.84	20	1
1:A:33:ALA:HB2	1:A:129:PHE:CD1	0.72	2.19	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:VAL:HG23	1:A:33:ALA:HB2	0.72	1.60	2	3
1:A:38:ALA:HB3	1:A:78:ILE:HG21	0.72	1.59	40	3
1:A:152:THR:HG23	1:A:153:SER:N	0.72	1.98	20	1
1:A:29:VAL:O	1:A:33:ALA:HB2	0.71	1.85	14	8
1:A:39:LEU:HD13	1:A:39:LEU:O	0.71	1.85	39	2
1:A:127:VAL:HG13	1:A:128:VAL:N	0.71	1.99	30	1
1:A:7:PHE:CD1	1:A:164:LEU:HD21	0.70	2.21	16	10
1:A:158:ILE:O	1:A:159:ALA:HB3	0.70	1.86	18	1
1:A:98:LEU:HD22	1:A:129:PHE:O	0.70	1.86	5	2
1:A:5:THR:HG22	1:A:164:LEU:HD21	0.70	1.64	4	6
1:A:103:ALA:HB3	1:A:107:THR:HB	0.69	1.63	39	4
1:A:116:THR:HG21	1:A:143:GLU:OE2	0.69	1.86	23	3
1:A:127:VAL:O	1:A:128:VAL:CB	0.69	2.40	20	2
1:A:92:HIS:HB3	1:A:97:ILE:HG21	0.68	1.64	7	7
1:A:107:THR:O	1:A:108:ASN:C	0.68	2.32	38	7
1:A:92:HIS:CB	1:A:97:ILE:HG21	0.68	2.18	7	3
1:A:29:VAL:HG21	1:A:129:PHE:CB	0.68	2.19	28	8
1:A:62:CYS:HB2	1:A:114:ILE:HG23	0.67	1.65	28	2
1:A:39:LEU:HD12	1:A:78:ILE:HG22	0.67	1.65	21	1
1:A:24:LEU:CD1	1:A:33:ALA:HB1	0.67	2.18	12	1
1:A:99:SER:O	1:A:100:MET:C	0.66	2.33	19	2
1:A:33:ALA:HB2	1:A:129:PHE:CD2	0.66	2.24	1	3
1:A:77:SER:O	1:A:78:ILE:CG1	0.66	2.43	12	1
1:A:91:LYS:O	1:A:93:THR:HG23	0.66	1.90	9	2
1:A:38:ALA:HB3	1:A:78:ILE:HD13	0.66	1.64	10	4
1:A:25:PHE:CD2	1:A:90:LEU:HD11	0.65	2.26	15	2
1:A:24:LEU:HD22	1:A:129:PHE:CE2	0.65	2.26	11	5
1:A:24:LEU:HD13	1:A:33:ALA:O	0.65	1.92	6	2
1:A:24:LEU:HD22	1:A:129:PHE:CZ	0.65	2.27	39	1
1:A:20:VAL:CG2	1:A:138:ILE:HG21	0.64	2.22	32	5
1:A:57:ILE:HD12	1:A:61:MET:CE	0.64	2.22	10	4
1:A:99:SER:OG	1:A:128:VAL:HG22	0.64	1.93	8	1
1:A:129:PHE:O	1:A:130:GLY:O	0.64	2.15	19	2
1:A:29:VAL:HG21	1:A:129:PHE:HB2	0.64	1.69	14	6
1:A:117:ALA:O	1:A:119:THR:HG23	0.64	1.92	34	5
1:A:20:VAL:HG21	1:A:22:PHE:CZ	0.64	2.28	34	2
1:A:105:PRO:O	1:A:107:THR:HG23	0.64	1.93	38	9
1:A:10:ILE:HD12	1:A:138:ILE:CG2	0.64	2.22	30	3
1:A:12:VAL:HG22	1:A:156:ILE:HG13	0.64	1.69	9	1
1:A:98:LEU:HD22	1:A:112:PHE:CE1	0.63	2.28	12	1
1:A:90:LEU:O	1:A:128:VAL:HG11	0.63	1.93	14	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:PHE:CE2	1:A:56:ILE:HD12	0.63	2.29	34	1
1:A:22:PHE:CE1	1:A:114:ILE:HD11	0.63	2.29	15	1
1:A:158:ILE:O	1:A:159:ALA:CB	0.63	2.47	18	1
1:A:9:ASP:O	1:A:10:ILE:HD13	0.63	1.93	22	2
1:A:29:VAL:O	1:A:29:VAL:HG23	0.63	1.94	11	3
1:A:39:LEU:O	1:A:39:LEU:HD13	0.63	1.93	5	4
1:A:56:ILE:HD11	1:A:156:ILE:CD1	0.62	2.24	21	2
1:A:119:THR:HG22	1:A:121:TRP:CH2	0.62	2.28	14	2
1:A:101:ALA:HB3	1:A:111:GLN:CG	0.62	2.24	26	2
1:A:54:HIS:CE1	1:A:152:THR:HG21	0.62	2.29	20	1
1:A:123:ASP:O	1:A:124:GLY:C	0.62	2.38	10	3
1:A:114:ILE:HG21	1:A:139:VAL:CG1	0.62	2.25	9	1
1:A:129:PHE:O	1:A:129:PHE:CG	0.61	2.53	26	8
1:A:4:PRO:O	1:A:24:LEU:HD12	0.61	1.94	19	1
1:A:25:PHE:CE2	1:A:90:LEU:HD22	0.61	2.29	19	2
1:A:101:ALA:HB3	1:A:111:GLN:O	0.61	1.96	22	2
1:A:44:LYS:HD2	1:A:78:ILE:HG23	0.61	1.71	22	1
1:A:28:LYS:HG3	1:A:90:LEU:HD21	0.61	1.71	5	1
1:A:25:PHE:CG	1:A:90:LEU:HD11	0.61	2.31	15	1
1:A:92:HIS:CD2	1:A:97:ILE:HG21	0.61	2.31	10	1
1:A:103:ALA:C	1:A:105:PRO:HD2	0.60	2.15	21	14
1:A:146:GLY:HA2	1:A:152:THR:HG22	0.60	1.73	14	6
1:A:44:LYS:HD2	1:A:78:ILE:HD12	0.60	1.72	4	3
1:A:56:ILE:HD12	1:A:156:ILE:CD1	0.60	2.26	28	1
1:A:146:GLY:O	1:A:147:SER:C	0.60	2.39	40	10
1:A:98:LEU:HD23	1:A:99:SER:N	0.60	2.11	13	6
1:A:127:VAL:HG12	1:A:128:VAL:H	0.60	1.54	37	7
1:A:101:ALA:HB3	1:A:111:GLN:HB3	0.60	1.74	21	3
1:A:98:LEU:HD23	1:A:112:PHE:HB2	0.60	1.73	39	2
1:A:57:ILE:HD12	1:A:61:MET:HE2	0.60	1.74	10	1
1:A:20:VAL:HG12	1:A:135:GLY:O	0.59	1.97	15	2
1:A:29:VAL:HG21	1:A:129:PHE:CD2	0.59	2.32	36	1
1:A:5:THR:O	1:A:164:LEU:HD23	0.59	1.97	11	1
1:A:39:LEU:HD13	1:A:78:ILE:HD11	0.59	1.73	8	1
1:A:53:PHE:CE2	1:A:156:ILE:HD12	0.59	2.32	35	1
1:A:116:THR:HG21	1:A:143:GLU:CD	0.59	2.18	10	2
1:A:7:PHE:HB3	1:A:164:LEU:HD22	0.59	1.73	4	5
1:A:51:SER:O	1:A:157:THR:HG22	0.59	1.98	13	1
1:A:101:ALA:HB2	1:A:112:PHE:O	0.59	1.96	16	1
1:A:57:ILE:HD11	1:A:61:MET:CE	0.59	2.28	30	1
1:A:39:LEU:CD1	1:A:78:ILE:HD11	0.59	2.27	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:SER:C	1:A:78:ILE:HG23	0.59	2.17	12	1
1:A:10:ILE:HD11	1:A:20:VAL:HB	0.59	1.75	12	1
1:A:53:PHE:CE1	1:A:158:ILE:HD11	0.59	2.33	40	3
1:A:79:TYR:CG	1:A:79:TYR:O	0.59	2.56	13	1
1:A:82:LYS:HG3	1:A:107:THR:HG22	0.59	1.75	2	4
1:A:20:VAL:HG21	1:A:138:ILE:HG21	0.58	1.74	11	2
1:A:12:VAL:CG2	1:A:17:LEU:HD13	0.58	2.28	18	6
1:A:93:THR:O	1:A:93:THR:HG23	0.58	1.97	27	1
1:A:142:MET:SD	1:A:156:ILE:HD13	0.58	2.38	26	7
1:A:101:ALA:HB3	1:A:111:GLN:HG2	0.58	1.74	32	2
1:A:99:SER:HB3	1:A:128:VAL:HG22	0.58	1.74	36	1
1:A:29:VAL:HB	1:A:32:THR:HG22	0.58	1.75	21	1
1:A:56:ILE:O	1:A:57:ILE:HD13	0.58	1.97	20	1
1:A:10:ILE:HD12	1:A:138:ILE:HG21	0.58	1.75	11	2
1:A:98:LEU:HD13	1:A:99:SER:N	0.58	2.13	16	1
1:A:98:LEU:HD22	1:A:112:PHE:CD1	0.58	2.34	19	1
1:A:25:PHE:CZ	1:A:90:LEU:HD21	0.58	2.33	4	1
1:A:98:LEU:HD12	1:A:130:GLY:CA	0.58	2.28	36	1
1:A:101:ALA:HB3	1:A:111:GLN:HG3	0.58	1.75	11	1
1:A:108:ASN:O	1:A:109:GLY:C	0.58	2.41	26	4
1:A:25:PHE:CE2	1:A:90:LEU:HD11	0.58	2.34	23	5
1:A:113:PHE:O	1:A:114:ILE:C	0.58	2.42	34	5
1:A:151:LYS:O	1:A:152:THR:CG2	0.57	2.52	20	1
1:A:5:THR:HG23	1:A:22:PHE:O	0.57	1.98	19	5
1:A:48:TYR:CE1	1:A:158:ILE:HD13	0.57	2.33	36	1
1:A:122:LEU:HD13	1:A:126:HIS:CD2	0.57	2.34	22	2
1:A:12:VAL:HG22	1:A:17:LEU:HD23	0.57	1.75	22	1
1:A:39:LEU:HD11	1:A:48:TYR:HB2	0.57	1.77	32	1
1:A:90:LEU:HB2	1:A:128:VAL:HG13	0.57	1.74	28	7
1:A:39:LEU:HB2	1:A:78:ILE:HG21	0.57	1.76	5	1
1:A:77:SER:O	1:A:78:ILE:HB	0.57	1.99	22	2
1:A:105:PRO:O	1:A:106:ASN:C	0.56	2.43	35	12
1:A:139:VAL:HG12	1:A:143:GLU:OE1	0.56	2.00	15	1
1:A:163:GLN:O	1:A:164:LEU:HB2	0.56	1.99	7	8
1:A:36:PHE:HA	1:A:39:LEU:HD12	0.56	1.75	36	5
1:A:24:LEU:HD22	1:A:129:PHE:CD2	0.56	2.35	5	2
1:A:78:ILE:HD12	1:A:79:TYR:CD2	0.56	2.34	40	1
1:A:98:LEU:O	1:A:128:VAL:HG13	0.56	2.01	40	6
1:A:35:ASN:ND2	1:A:78:ILE:HG23	0.56	2.16	4	2
1:A:152:THR:CG2	1:A:153:SER:N	0.56	2.69	20	1
1:A:92:HIS:HB3	1:A:128:VAL:HG21	0.56	1.76	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:LEU:HD12	1:A:130:GLY:HA3	0.56	1.77	30	2
1:A:126:HIS:C	1:A:127:VAL:HG23	0.56	2.21	13	3
1:A:116:THR:HG21	1:A:143:GLU:OE1	0.55	2.01	10	2
1:A:11:ALA:O	1:A:156:ILE:HG23	0.55	2.02	17	2
1:A:92:HIS:NE2	1:A:128:VAL:HG21	0.55	2.16	40	1
1:A:127:VAL:HG22	1:A:128:VAL:H	0.55	1.61	30	1
1:A:39:LEU:HD11	1:A:48:TYR:CB	0.55	2.31	32	1
1:A:39:LEU:HB2	1:A:78:ILE:HD12	0.55	1.77	16	2
1:A:90:LEU:HD12	1:A:128:VAL:CG1	0.55	2.31	32	2
1:A:100:MET:O	1:A:101:ALA:HB2	0.55	2.01	36	2
1:A:6:VAL:HG12	1:A:163:GLN:HG3	0.55	1.78	3	2
1:A:28:LYS:HG2	1:A:89:ILE:HG21	0.55	1.77	3	2
1:A:11:ALA:HB3	1:A:157:THR:O	0.55	2.02	5	4
1:A:57:ILE:HG23	1:A:148:ARG:O	0.55	2.02	12	1
1:A:56:ILE:HD12	1:A:156:ILE:HD13	0.55	1.78	28	1
1:A:90:LEU:HD12	1:A:128:VAL:HG12	0.55	1.79	32	1
1:A:34:GLU:O	1:A:35:ASN:C	0.55	2.45	39	17
1:A:37:ARG:O	1:A:41:THR:HG23	0.55	2.01	2	1
1:A:138:ILE:O	1:A:142:MET:HB2	0.55	2.02	34	7
1:A:20:VAL:HG13	1:A:138:ILE:HG21	0.55	1.79	20	4
1:A:85:ASP:OD1	1:A:127:VAL:HG21	0.55	2.01	25	1
1:A:101:ALA:HB2	1:A:113:PHE:HB3	0.55	1.77	34	1
1:A:20:VAL:CG1	1:A:132:VAL:HG13	0.54	2.32	27	2
1:A:12:VAL:HG22	1:A:17:LEU:HD13	0.54	1.78	14	7
1:A:55:ARG:NH2	1:A:57:ILE:HD11	0.54	2.16	12	1
1:A:53:PHE:CE2	1:A:156:ILE:HG21	0.54	2.37	18	1
1:A:9:ASP:CB	1:A:159:ALA:HB3	0.54	2.33	37	4
1:A:26:ALA:HA	1:A:33:ALA:HB1	0.54	1.79	39	1
1:A:87:ASN:O	1:A:127:VAL:HG22	0.54	2.01	28	1
1:A:97:ILE:HD12	1:A:128:VAL:HG11	0.53	1.80	20	2
1:A:89:ILE:C	1:A:90:LEU:HD22	0.53	2.23	25	1
1:A:57:ILE:HD12	1:A:60:PHE:HB3	0.53	1.79	35	5
1:A:52:CYS:HB3	1:A:157:THR:HG22	0.53	1.80	24	1
1:A:98:LEU:HD23	1:A:112:PHE:CD2	0.53	2.38	4	1
1:A:9:ASP:HB2	1:A:159:ALA:HB3	0.53	1.79	25	2
1:A:132:VAL:HG11	1:A:136:MET:HG2	0.53	1.80	5	2
1:A:17:LEU:HD12	1:A:17:LEU:O	0.53	2.03	10	4
1:A:97:ILE:HD13	1:A:131:LYS:HB3	0.53	1.79	3	1
1:A:151:LYS:O	1:A:152:THR:CB	0.53	2.57	20	2
1:A:56:ILE:HD11	1:A:156:ILE:HD11	0.53	1.79	21	1
1:A:33:ALA:HB2	1:A:129:PHE:CE2	0.53	2.38	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:VAL:HG11	1:A:128:VAL:O	0.53	2.03	6	1
1:A:3:ASN:OD1	1:A:26:ALA:HB3	0.53	2.04	18	1
1:A:6:VAL:HG11	1:A:24:LEU:HD11	0.53	1.80	15	2
1:A:55:ARG:O	1:A:57:ILE:HD12	0.53	2.04	40	1
1:A:48:TYR:CE2	1:A:158:ILE:HD11	0.53	2.39	14	1
1:A:77:SER:O	1:A:78:ILE:CB	0.52	2.56	22	4
1:A:17:LEU:O	1:A:17:LEU:HD12	0.52	2.03	31	3
1:A:44:LYS:HG2	1:A:78:ILE:HG21	0.52	1.80	8	1
1:A:90:LEU:HD12	1:A:128:VAL:HG11	0.52	1.81	27	1
1:A:107:THR:O	1:A:109:GLY:N	0.52	2.42	20	8
1:A:90:LEU:O	1:A:128:VAL:HG21	0.52	2.04	19	1
1:A:98:LEU:HD13	1:A:130:GLY:C	0.52	2.25	39	1
1:A:87:ASN:O	1:A:127:VAL:HG23	0.52	2.04	30	1
1:A:32:THR:HG21	1:A:108:ASN:ND2	0.52	2.19	11	1
1:A:112:PHE:CZ	1:A:114:ILE:HD11	0.52	2.40	7	2
1:A:34:GLU:O	1:A:37:ARG:N	0.51	2.43	29	11
1:A:48:TYR:O	1:A:49:LYS:C	0.51	2.47	32	1
1:A:108:ASN:O	1:A:109:GLY:O	0.51	2.29	26	2
1:A:112:PHE:CE2	1:A:114:ILE:HD11	0.51	2.39	8	4
1:A:32:THR:HG22	1:A:32:THR:O	0.51	2.06	5	1
1:A:99:SER:CB	1:A:128:VAL:HG22	0.51	2.35	36	1
1:A:113:PHE:O	1:A:113:PHE:CG	0.51	2.61	34	3
1:A:83:PHE:N	1:A:83:PHE:CD1	0.51	2.78	35	5
1:A:92:HIS:HB2	1:A:97:ILE:HG21	0.51	1.82	38	1
1:A:9:ASP:O	1:A:158:ILE:HD13	0.51	2.06	27	1
1:A:56:ILE:CD1	1:A:156:ILE:HD13	0.51	2.35	36	2
1:A:96:GLY:CA	1:A:132:VAL:HG23	0.51	2.36	2	1
1:A:38:ALA:HB1	1:A:43:GLU:CD	0.51	2.26	39	1
1:A:32:THR:HG21	1:A:127:VAL:HG11	0.51	1.81	21	2
1:A:129:PHE:CG	1:A:129:PHE:O	0.51	2.64	31	2
1:A:77:SER:O	1:A:78:ILE:HG13	0.51	2.06	12	1
1:A:38:ALA:CB	1:A:78:ILE:HD13	0.51	2.36	10	1
1:A:46:PHE:O	1:A:47:GLY:C	0.50	2.49	8	3
1:A:89:ILE:O	1:A:90:LEU:HD23	0.50	2.06	39	2
1:A:56:ILE:HD11	1:A:156:ILE:HD12	0.50	1.81	6	1
1:A:6:VAL:CG2	1:A:24:LEU:HD11	0.50	2.36	29	1
1:A:155:LYS:HD2	1:A:157:THR:HG23	0.50	1.82	15	2
1:A:102:ASN:CG	1:A:107:THR:HG22	0.50	2.27	12	1
1:A:18:GLY:O	1:A:19:ARG:HB3	0.50	2.07	38	1
1:A:113:PHE:CG	1:A:113:PHE:O	0.50	2.64	39	1
1:A:114:ILE:HG21	1:A:139:VAL:HG11	0.50	1.84	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:ASN:O	1:A:127:VAL:HG13	0.50	2.07	10	1
1:A:5:THR:CG2	1:A:164:LEU:HD21	0.50	2.37	4	1
1:A:92:HIS:O	1:A:93:THR:HG22	0.49	2.07	27	1
1:A:113:PHE:CD1	1:A:113:PHE:C	0.49	2.86	7	2
1:A:101:ALA:HB3	1:A:111:GLN:CB	0.49	2.37	21	2
1:A:47:GLY:O	1:A:48:TYR:CB	0.49	2.60	4	1
1:A:42:GLY:O	1:A:43:GLU:C	0.49	2.51	33	3
1:A:31:LYS:HG2	1:A:32:THR:N	0.49	2.23	12	1
1:A:112:PHE:CZ	1:A:114:ILE:HD12	0.49	2.42	21	1
1:A:5:THR:HG21	1:A:164:LEU:HD22	0.49	1.85	30	1
1:A:6:VAL:HG11	1:A:40:SER:OG	0.49	2.07	10	3
1:A:114:ILE:O	1:A:115:CYS:CB	0.49	2.60	6	2
1:A:25:PHE:CD2	1:A:90:LEU:HD21	0.49	2.42	23	2
1:A:53:PHE:CD2	1:A:156:ILE:HD12	0.49	2.43	35	1
1:A:102:ASN:HB2	1:A:107:THR:HG23	0.49	1.85	32	1
1:A:7:PHE:CE1	1:A:164:LEU:HD21	0.49	2.42	18	2
1:A:99:SER:HA	1:A:128:VAL:HG22	0.49	1.85	40	1
1:A:96:GLY:HA2	1:A:114:ILE:HD11	0.49	1.84	18	1
1:A:56:ILE:HD11	1:A:156:ILE:HD13	0.49	1.84	25	2
1:A:119:THR:O	1:A:120:GLU:CB	0.49	2.61	21	1
1:A:98:LEU:HD22	1:A:112:PHE:CD2	0.49	2.42	26	1
1:A:28:LYS:HG2	1:A:90:LEU:HD21	0.49	1.85	36	2
1:A:8:PHE:CE2	1:A:158:ILE:HD13	0.49	2.42	29	1
1:A:57:ILE:HD11	1:A:61:MET:CG	0.48	2.37	15	2
1:A:130:GLY:O	1:A:131:LYS:CB	0.48	2.61	23	2
1:A:28:LYS:HB2	1:A:90:LEU:HD11	0.48	1.84	13	1
1:A:56:ILE:HD12	1:A:152:THR:HG21	0.48	1.84	1	1
1:A:20:VAL:CG1	1:A:138:ILE:HG21	0.48	2.39	34	4
1:A:25:PHE:O	1:A:29:VAL:HG23	0.48	2.08	22	1
1:A:96:GLY:O	1:A:132:VAL:HG23	0.48	2.07	19	1
1:A:90:LEU:HD22	1:A:129:PHE:HA	0.48	1.86	4	1
1:A:6:VAL:CG1	1:A:24:LEU:HD12	0.48	2.38	27	1
1:A:96:GLY:O	1:A:98:LEU:HD12	0.48	2.08	39	1
1:A:57:ILE:HG23	1:A:61:MET:O	0.48	2.08	32	2
1:A:9:ASP:HB3	1:A:159:ALA:HB3	0.48	1.86	10	4
1:A:51:SER:N	1:A:157:THR:HG22	0.48	2.23	16	1
1:A:28:LYS:HG3	1:A:89:ILE:HG21	0.48	1.85	18	1
1:A:24:LEU:HD12	1:A:33:ALA:HB1	0.48	1.84	37	1
1:A:98:LEU:O	1:A:128:VAL:HG22	0.47	2.09	20	2
1:A:29:VAL:HG21	1:A:129:PHE:CG	0.47	2.44	24	2
1:A:32:THR:OG1	1:A:127:VAL:HG11	0.47	2.09	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LEU:CB	1:A:128:VAL:HG13	0.47	2.39	25	1
1:A:55:ARG:HD3	1:A:57:ILE:HD11	0.47	1.86	36	1
1:A:98:LEU:O	1:A:128:VAL:HG23	0.47	2.08	11	2
1:A:77:SER:O	1:A:78:ILE:HD12	0.47	2.10	8	1
1:A:50:GLY:O	1:A:157:THR:HG22	0.47	2.09	27	1
1:A:6:VAL:CG1	1:A:24:LEU:HD11	0.47	2.39	15	3
1:A:101:ALA:HB2	1:A:111:GLN:OE1	0.47	2.09	20	1
1:A:98:LEU:O	1:A:128:VAL:HA	0.47	2.10	40	1
1:A:89:ILE:HG22	1:A:89:ILE:O	0.47	2.09	20	1
1:A:94:GLY:O	1:A:97:ILE:HG23	0.47	2.09	38	1
1:A:98:LEU:HD12	1:A:130:GLY:C	0.47	2.30	37	1
1:A:32:THR:OG1	1:A:127:VAL:HG21	0.47	2.09	19	1
1:A:25:PHE:CD2	1:A:90:LEU:HD13	0.47	2.44	31	3
1:A:24:LEU:HD21	1:A:36:PHE:CD2	0.47	2.45	31	1
1:A:44:LYS:CD	1:A:78:ILE:HD12	0.47	2.39	7	1
1:A:101:ALA:O	1:A:102:ASN:O	0.47	2.32	18	1
1:A:57:ILE:HD12	1:A:60:PHE:CB	0.47	2.40	30	1
1:A:56:ILE:CD1	1:A:156:ILE:HD12	0.47	2.40	6	1
1:A:127:VAL:O	1:A:127:VAL:HG23	0.47	2.09	39	1
1:A:98:LEU:HD13	1:A:112:PHE:CD1	0.47	2.44	19	1
1:A:92:HIS:CD2	1:A:119:THR:HG23	0.46	2.45	33	1
1:A:108:ASN:CG	1:A:127:VAL:HG21	0.46	2.31	37	1
1:A:48:TYR:HE1	1:A:158:ILE:HD13	0.46	1.70	36	1
1:A:10:ILE:HG21	1:A:142:MET:CE	0.46	2.40	38	1
1:A:90:LEU:HD12	1:A:128:VAL:O	0.46	2.10	11	2
1:A:91:LYS:O	1:A:92:HIS:C	0.46	2.53	21	1
1:A:93:THR:HG22	1:A:97:ILE:HD11	0.46	1.86	20	1
1:A:83:PHE:CD1	1:A:83:PHE:N	0.46	2.81	1	2
1:A:38:ALA:HB1	1:A:44:LYS:HE2	0.46	1.86	25	1
1:A:39:LEU:HD11	1:A:47:GLY:HA2	0.46	1.88	16	1
1:A:34:GLU:HG3	1:A:78:ILE:HD11	0.46	1.86	21	1
1:A:98:LEU:HD23	1:A:112:PHE:CB	0.46	2.41	22	1
1:A:48:TYR:OH	1:A:158:ILE:HD11	0.46	2.11	19	1
1:A:132:VAL:HG11	1:A:139:VAL:HG21	0.46	1.87	31	2
1:A:92:HIS:O	1:A:93:THR:CB	0.46	2.64	20	1
1:A:32:THR:HG23	1:A:100:MET:CE	0.46	2.40	7	1
1:A:164:LEU:HD22	1:A:164:LEU:N	0.46	2.26	13	1
1:A:164:LEU:N	1:A:164:LEU:HD22	0.46	2.25	34	1
1:A:105:PRO:O	1:A:107:THR:HG22	0.46	2.10	1	1
1:A:102:ASN:HB3	1:A:107:THR:O	0.46	2.11	9	2
1:A:7:PHE:CG	1:A:164:LEU:HD21	0.46	2.46	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:PHE:O	1:A:61:MET:HB3	0.46	2.10	8	1
1:A:32:THR:O	1:A:33:ALA:C	0.46	2.55	33	1
1:A:102:ASN:OD1	1:A:107:THR:HG22	0.46	2.11	3	1
1:A:29:VAL:HG23	1:A:29:VAL:O	0.46	2.11	13	2
1:A:96:GLY:O	1:A:97:ILE:HG12	0.46	2.10	32	2
1:A:98:LEU:HD23	1:A:113:PHE:O	0.45	2.12	11	2
1:A:29:VAL:O	1:A:29:VAL:CG2	0.45	2.63	17	2
1:A:61:MET:O	1:A:61:MET:HG2	0.45	2.11	8	1
1:A:32:THR:HG21	1:A:100:MET:HE1	0.45	1.87	33	1
1:A:132:VAL:HG11	1:A:136:MET:CG	0.45	2.40	5	1
1:A:57:ILE:HG22	1:A:147:SER:O	0.45	2.11	13	3
1:A:9:ASP:C	1:A:10:ILE:HD13	0.45	2.32	22	1
1:A:127:VAL:O	1:A:127:VAL:HG13	0.45	2.11	19	1
1:A:22:PHE:CG	1:A:22:PHE:O	0.45	2.68	39	1
1:A:119:THR:HB	1:A:122:LEU:HD22	0.45	1.88	32	1
1:A:57:ILE:HD11	1:A:61:MET:HE2	0.45	1.88	30	1
1:A:44:LYS:CD	1:A:78:ILE:HD13	0.45	2.41	25	1
1:A:10:ILE:HG21	1:A:142:MET:SD	0.45	2.52	15	1
1:A:39:LEU:HD12	1:A:78:ILE:HG13	0.45	1.87	16	1
1:A:126:HIS:O	1:A:127:VAL:CB	0.45	2.65	12	2
1:A:98:LEU:HD12	1:A:130:GLY:O	0.45	2.11	11	1
1:A:126:HIS:O	1:A:127:VAL:HB	0.45	2.12	12	2
1:A:119:THR:HG22	1:A:121:TRP:CZ3	0.45	2.47	30	1
1:A:57:ILE:HD11	1:A:61:MET:SD	0.45	2.52	5	1
1:A:77:SER:O	1:A:78:ILE:C	0.45	2.54	13	1
1:A:164:LEU:CD2	1:A:164:LEU:N	0.45	2.79	37	1
1:A:111:GLN:O	1:A:112:PHE:CB	0.45	2.64	23	1
1:A:45:GLY:C	1:A:46:PHE:CG	0.45	2.91	26	1
1:A:53:PHE:CE2	1:A:158:ILE:HD11	0.45	2.47	38	1
1:A:10:ILE:HD13	1:A:142:MET:SD	0.45	2.52	15	1
1:A:32:THR:O	1:A:32:THR:HG22	0.45	2.12	17	2
1:A:20:VAL:O	1:A:21:SER:CB	0.45	2.65	36	1
1:A:92:HIS:C	1:A:93:THR:HG22	0.44	2.33	20	1
1:A:10:ILE:CG2	1:A:156:ILE:HG23	0.44	2.41	30	1
1:A:56:ILE:HG22	1:A:146:GLY:HA3	0.44	1.88	29	1
1:A:97:ILE:HD13	1:A:97:ILE:N	0.44	2.27	38	1
1:A:104:GLY:H	1:A:105:PRO:HD2	0.44	1.72	39	2
1:A:17:LEU:HD13	1:A:138:ILE:HG23	0.44	1.89	36	1
1:A:112:PHE:CE1	1:A:114:ILE:HD11	0.44	2.47	20	1
1:A:114:ILE:O	1:A:114:ILE:HG23	0.44	2.13	31	2
1:A:89:ILE:O	1:A:89:ILE:HG22	0.44	2.12	25	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:ILE:C	1:A:98:LEU:HD23	0.44	2.33	28	2
1:A:57:ILE:N	1:A:57:ILE:HD13	0.44	2.27	39	1
1:A:77:SER:C	1:A:78:ILE:CG2	0.44	2.86	12	1
1:A:12:VAL:CG2	1:A:17:LEU:HD23	0.44	2.43	13	2
1:A:92:HIS:C	1:A:93:THR:HG23	0.44	2.33	26	2
1:A:97:ILE:O	1:A:97:ILE:HG22	0.44	2.12	34	2
1:A:93:THR:CG2	1:A:97:ILE:HD11	0.44	2.43	20	1
1:A:98:LEU:N	1:A:98:LEU:HD12	0.44	2.27	4	1
1:A:138:ILE:O	1:A:142:MET:HB3	0.44	2.12	21	4
1:A:8:PHE:CE1	1:A:158:ILE:HG23	0.44	2.48	8	1
1:A:10:ILE:HD13	1:A:142:MET:CE	0.44	2.43	15	1
1:A:32:THR:HG21	1:A:127:VAL:CG1	0.44	2.43	16	1
1:A:34:GLU:O	1:A:36:PHE:N	0.44	2.51	25	2
1:A:98:LEU:HD13	1:A:112:PHE:CE1	0.44	2.47	19	1
1:A:101:ALA:HB2	1:A:111:GLN:O	0.44	2.12	29	1
1:A:12:VAL:O	1:A:13:ASP:CB	0.43	2.66	38	2
1:A:20:VAL:HG13	1:A:134:GLU:O	0.43	2.13	14	1
1:A:98:LEU:HD22	1:A:129:PHE:CE1	0.43	2.48	15	1
1:A:100:MET:O	1:A:101:ALA:CB	0.43	2.66	36	1
1:A:124:GLY:O	1:A:125:LYS:CB	0.43	2.66	2	1
1:A:39:LEU:HD13	1:A:111:GLN:OE1	0.43	2.12	17	1
1:A:98:LEU:HD11	1:A:112:PHE:CD1	0.43	2.48	21	1
1:A:23:GLU:O	1:A:24:LEU:HB2	0.43	2.14	1	1
1:A:61:MET:CG	1:A:61:MET:O	0.43	2.66	8	1
1:A:62:CYS:HB3	1:A:114:ILE:HG23	0.43	1.90	3	1
1:A:12:VAL:HG21	1:A:17:LEU:HD13	0.43	1.89	1	2
1:A:29:VAL:HG12	1:A:32:THR:OG1	0.43	2.14	29	1
1:A:146:GLY:O	1:A:147:SER:O	0.43	2.36	15	2
1:A:100:MET:CG	1:A:127:VAL:HG12	0.43	2.43	30	1
1:A:57:ILE:HD12	1:A:148:ARG:O	0.43	2.13	38	1
1:A:93:THR:O	1:A:94:GLY:O	0.43	2.37	2	1
1:A:127:VAL:CG1	1:A:128:VAL:N	0.43	2.69	30	1
1:A:127:VAL:HG12	1:A:128:VAL:N	0.43	2.29	40	1
1:A:20:VAL:HG13	1:A:138:ILE:HG13	0.43	1.91	30	2
1:A:12:VAL:HG21	1:A:17:LEU:HD23	0.43	1.90	16	1
1:A:32:THR:HG22	1:A:129:PHE:CD1	0.43	2.49	20	1
1:A:102:ASN:O	1:A:103:ALA:HB3	0.43	2.13	14	1
1:A:55:ARG:O	1:A:56:ILE:O	0.43	2.36	32	1
1:A:29:VAL:HG21	1:A:129:PHE:HB3	0.43	1.89	5	2
1:A:94:GLY:HA3	1:A:97:ILE:HD11	0.43	1.91	28	1
1:A:152:THR:HG21	1:A:156:ILE:HD12	0.43	1.91	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ASN:HD22	1:A:78:ILE:HD12	0.42	1.74	22	1
1:A:12:VAL:HG23	1:A:15:GLU:HG2	0.42	1.90	39	1
1:A:7:PHE:CD1	1:A:7:PHE:C	0.42	2.89	34	1
1:A:36:PHE:CD1	1:A:39:LEU:HD12	0.42	2.48	31	1
1:A:7:PHE:CD1	1:A:164:LEU:CD2	0.42	3.02	21	2
1:A:103:ALA:HB3	1:A:107:THR:CG2	0.42	2.43	35	1
1:A:139:VAL:HG12	1:A:139:VAL:O	0.42	2.14	40	6
1:A:39:LEU:HD12	1:A:78:ILE:CG2	0.42	2.41	21	1
1:A:32:THR:HG22	1:A:129:PHE:CZ	0.42	2.50	3	2
1:A:91:LYS:O	1:A:92:HIS:O	0.42	2.37	20	1
1:A:132:VAL:HG11	1:A:136:MET:HB2	0.42	1.91	15	1
1:A:164:LEU:HD23	1:A:164:LEU:C	0.42	2.35	35	1
1:A:122:LEU:O	1:A:123:ASP:CB	0.42	2.67	11	1
1:A:104:GLY:N	1:A:107:THR:OG1	0.42	2.53	38	1
1:A:115:CYS:C	1:A:116:THR:HG23	0.42	2.35	6	1
1:A:139:VAL:O	1:A:139:VAL:HG12	0.42	2.13	9	3
1:A:10:ILE:HG21	1:A:142:MET:HE1	0.42	1.90	34	1
1:A:20:VAL:HG22	1:A:135:GLY:HA3	0.42	1.92	14	1
1:A:57:ILE:HD11	1:A:61:MET:HE3	0.42	1.90	30	1
1:A:151:LYS:O	1:A:152:THR:HB	0.42	2.15	38	1
1:A:116:THR:O	1:A:117:ALA:HB2	0.42	2.14	6	1
1:A:32:THR:HG22	1:A:129:PHE:CE1	0.42	2.49	20	1
1:A:92:HIS:O	1:A:93:THR:HB	0.42	2.15	20	1
1:A:132:VAL:HG13	1:A:132:VAL:O	0.42	2.15	26	1
1:A:61:MET:HG2	1:A:62:CYS:N	0.42	2.30	10	1
1:A:103:ALA:CB	1:A:107:THR:HG21	0.42	2.45	30	1
1:A:56:ILE:HG22	1:A:56:ILE:O	0.42	2.14	22	1
1:A:142:MET:SD	1:A:156:ILE:HG21	0.42	2.55	26	1
1:A:5:THR:C	1:A:6:VAL:HG22	0.41	2.35	5	1
1:A:132:VAL:HG23	1:A:132:VAL:O	0.41	2.15	24	1
1:A:98:LEU:C	1:A:98:LEU:HD23	0.41	2.36	3	1
1:A:92:HIS:HD2	1:A:128:VAL:HG11	0.41	1.74	40	1
1:A:98:LEU:HD23	1:A:114:ILE:HG12	0.41	1.91	16	1
1:A:99:SER:O	1:A:112:PHE:HB2	0.41	2.14	11	1
1:A:32:THR:HG22	1:A:129:PHE:CE2	0.41	2.50	15	1
1:A:24:LEU:HD11	1:A:33:ALA:HB1	0.41	1.90	12	1
1:A:109:GLY:O	1:A:110:SER:CB	0.41	2.69	39	2
1:A:23:GLU:O	1:A:24:LEU:CB	0.41	2.68	30	1
1:A:24:LEU:HD13	1:A:37:ARG:HG3	0.41	1.92	29	1
1:A:38:ALA:HB1	1:A:43:GLU:OE2	0.41	2.15	23	1
1:A:5:THR:HG22	1:A:164:LEU:HD23	0.41	1.92	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:VAL:O	1:A:128:VAL:CG2	0.41	2.69	20	1
1:A:32:THR:HG23	1:A:100:MET:HE3	0.41	1.91	30	1
1:A:25:PHE:O	1:A:29:VAL:HG22	0.41	2.16	5	1
1:A:35:ASN:O	1:A:78:ILE:HG21	0.41	2.14	6	1
1:A:163:GLN:C	1:A:165:GLU:H	0.41	2.18	27	1
1:A:35:ASN:C	1:A:35:ASN:OD1	0.41	2.58	34	1
1:A:6:VAL:HG23	1:A:22:PHE:CD2	0.41	2.50	8	1
1:A:115:CYS:SG	1:A:119:THR:HG23	0.41	2.55	13	1
1:A:12:VAL:HG23	1:A:12:VAL:O	0.41	2.16	39	2
1:A:77:SER:O	1:A:78:ILE:HG22	0.41	2.15	16	1
1:A:32:THR:HG22	1:A:129:PHE:CG	0.41	2.50	31	1
1:A:11:ALA:HB3	1:A:157:THR:OG1	0.41	2.15	33	1
1:A:57:ILE:O	1:A:57:ILE:HG22	0.41	2.15	36	1
1:A:22:PHE:N	1:A:22:PHE:CD1	0.41	2.89	1	1
1:A:39:LEU:C	1:A:39:LEU:HD13	0.41	2.36	25	1
1:A:100:MET:SD	1:A:127:VAL:HG23	0.41	2.56	39	1
1:A:51:SER:O	1:A:157:THR:HG23	0.41	2.16	38	1
1:A:51:SER:O	1:A:52:CYS:CB	0.41	2.69	38	1
1:A:113:PHE:O	1:A:113:PHE:CD2	0.41	2.74	5	1
1:A:25:PHE:CD2	1:A:90:LEU:HD22	0.41	2.50	6	1
1:A:90:LEU:HB2	1:A:128:VAL:HG11	0.41	1.92	6	1
1:A:162:GLY:O	1:A:164:LEU:HD23	0.41	2.16	39	1
1:A:10:ILE:HG22	1:A:17:LEU:HD12	0.41	1.93	36	1
1:A:10:ILE:HG21	1:A:142:MET:HE2	0.41	1.92	10	1
1:A:7:PHE:C	1:A:7:PHE:CD1	0.41	2.93	20	1
1:A:78:ILE:HG23	1:A:79:TYR:N	0.41	2.31	35	1
1:A:57:ILE:O	1:A:61:MET:O	0.41	2.39	29	1
1:A:6:VAL:HG13	1:A:40:SER:OG	0.41	2.15	29	1
1:A:101:ALA:HB2	1:A:113:PHE:CD2	0.41	2.51	14	1
1:A:99:SER:HB3	1:A:113:PHE:HB2	0.41	1.93	10	1
1:A:113:PHE:CD2	1:A:113:PHE:O	0.41	2.74	28	1
1:A:10:ILE:HD13	1:A:158:ILE:HD13	0.41	1.91	21	1
1:A:138:ILE:O	1:A:141:ALA:HB3	0.40	2.16	12	1
1:A:122:LEU:HD13	1:A:126:HIS:NE2	0.40	2.31	3	1
1:A:100:MET:HE2	1:A:129:PHE:CE1	0.40	2.51	9	1
1:A:28:LYS:CG	1:A:89:ILE:HG21	0.40	2.46	15	1
1:A:77:SER:O	1:A:78:ILE:HG23	0.40	2.16	12	1
1:A:127:VAL:C	1:A:128:VAL:HG23	0.40	2.37	40	1
1:A:158:ILE:N	1:A:158:ILE:HD12	0.40	2.31	36	1
1:A:155:LYS:HE2	1:A:157:THR:HG23	0.40	1.93	35	1
1:A:114:ILE:O	1:A:115:CYS:HB2	0.40	2.16	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LEU:HD22	1:A:90:LEU:N	0.40	2.32	36	1
1:A:123:ASP:O	1:A:125:LYS:N	0.40	2.55	10	1
1:A:112:PHE:C	1:A:112:PHE:CD1	0.40	2.95	17	1
1:A:97:ILE:HG23	1:A:128:VAL:HG11	0.40	1.92	12	1
1:A:57:ILE:O	1:A:57:ILE:HG23	0.40	2.16	32	1
1:A:91:LYS:O	1:A:97:ILE:HD11	0.40	2.16	32	1
1:A:137:ASN:O	1:A:138:ILE:C	0.40	2.60	38	1
1:A:49:LYS:O	1:A:50:GLY:C	0.40	2.58	39	1
1:A:112:PHE:HE2	1:A:114:ILE:HD11	0.40	1.76	10	1
1:A:30:PRO:O	1:A:31:LYS:C	0.40	2.60	31	1
1:A:102:ASN:OD1	1:A:102:ASN:C	0.40	2.59	4	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	152/165 (92%)	107±6 (70±4%)	34±5 (22±3%)	11±3 (7±2%)	2	16
All	All	6080/6600 (92%)	4271 (70%)	1366 (22%)	443 (7%)	2	16

All 77 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	2	VAL	22
1	A	102	ASN	20
1	A	127	VAL	20
1	A	118	LYS	16
1	A	108	ASN	16
1	A	92	HIS	15
1	A	42	GLY	12
1	A	81	GLU	12
1	A	147	SER	11
1	A	151	LYS	10
1	A	63	GLN	10

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Mol	Chain	Res	Type	Models (Total)
1	A	149	ASN	10
1	A	100	MET	9
1	A	51	SER	9
1	A	114	ILE	8
1	A	124	GLY	8
1	A	112	PHE	8
1	A	148	ARG	8
1	A	125	LYS	8
1	A	49	LYS	8
1	A	76	LYS	7
1	A	31	LYS	7
1	A	48	TYR	7
1	A	52	CYS	7
1	A	101	ALA	7
1	A	111	GLN	7
1	A	61	MET	6
1	A	30	PRO	6
1	A	105	PRO	6
1	A	35	ASN	6
1	A	132	VAL	5
1	A	47	GLY	5
1	A	78	ILE	5
1	A	135	GLY	5
1	A	128	VAL	5
1	A	109	GLY	5
1	A	54	HIS	5
1	A	106	ASN	5
1	A	43	GLU	5
1	A	123	ASP	4
1	A	113	PHE	4
1	A	28	LYS	4
1	A	131	LYS	4
1	A	129	PHE	4
1	A	103	ALA	4
1	A	56	ILE	4
1	A	50	GLY	4
1	A	133	LYS	3
1	A	104	GLY	3
1	A	24	LEU	3
1	A	96	GLY	3
1	A	97	ILE	3
1	A	64	GLY	3

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Mol	Chain	Res	Type	Models (Total)
1	A	152	THR	3
1	A	84	GLU	3
1	A	85	ASP	3
1	A	164	LEU	2
1	A	115	CYS	2
1	A	120	GLU	2
1	A	130	GLY	2
1	A	55	ARG	2
1	A	34	GLU	2
1	A	20	VAL	2
1	A	80	GLY	2
1	A	93	THR	2
1	A	117	ALA	2
1	A	99	SER	2
1	A	33	ALA	2
1	A	21	SER	1
1	A	91	LYS	1
1	A	53	PHE	1
1	A	95	PRO	1
1	A	44	LYS	1
1	A	19	ARG	1
1	A	159	ALA	1
1	A	126	HIS	1
1	A	94	GLY	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	126/133 (95%)	91±4 (72±3%)	35±4 (28±3%)	2	20
All	All	5040/5320 (95%)	3637 (72%)	1403 (28%)	2	20

All 110 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	60	PHE	35

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Mol	Chain	Res	Type	Models (Total)
1	A	61	MET	33
1	A	19	ARG	31
1	A	88	PHE	30
1	A	31	LYS	27
1	A	82	LYS	26
1	A	153	SER	26
1	A	49	LYS	25
1	A	133	LYS	24
1	A	134	GLU	23
1	A	13	ASP	23
1	A	83	PHE	22
1	A	155	LYS	22
1	A	44	LYS	22
1	A	136	MET	21
1	A	151	LYS	21
1	A	37	ARG	21
1	A	2	VAL	20
1	A	54	HIS	20
1	A	48	TYR	20
1	A	86	GLU	20
1	A	157	THR	20
1	A	120	GLU	20
1	A	7	PHE	20
1	A	154	LYS	19
1	A	77	SER	19
1	A	76	LYS	18
1	A	28	LYS	18
1	A	144	ARG	18
1	A	131	LYS	17
1	A	118	LYS	17
1	A	111	GLN	17
1	A	99	SER	16
1	A	53	PHE	16
1	A	43	GLU	16
1	A	17	LEU	16
1	A	29	VAL	15
1	A	63	GLN	15
1	A	163	GLN	15
1	A	112	PHE	14
1	A	102	ASN	14
1	A	9	ASP	14
1	A	91	LYS	14

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Mol	Chain	Res	Type	Models (Total)
1	A	55	ARG	14
1	A	90	LEU	14
1	A	56	ILE	14
1	A	1	MET	14
1	A	84	GLU	14
1	A	110	SER	14
1	A	32	THR	14
1	A	164	LEU	13
1	A	100	MET	13
1	A	125	LYS	13
1	A	51	SER	13
1	A	92	HIS	12
1	A	79	TYR	12
1	A	149	ASN	12
1	A	113	PHE	12
1	A	39	LEU	11
1	A	78	ILE	11
1	A	35	ASN	11
1	A	147	SER	11
1	A	121	TRP	11
1	A	8	PHE	11
1	A	107	THR	10
1	A	165	GLU	10
1	A	81	GLU	10
1	A	3	ASN	9
1	A	98	LEU	9
1	A	22	PHE	9
1	A	122	LEU	9
1	A	123	ASP	9
1	A	108	ASN	9
1	A	137	ASN	8
1	A	143	GLU	8
1	A	6	VAL	8
1	A	87	ASN	8
1	A	24	LEU	7
1	A	127	VAL	7
1	A	40	SER	7
1	A	93	THR	7
1	A	97	ILE	7
1	A	46	PHE	7
1	A	106	ASN	7
1	A	27	ASP	6

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Mol	Chain	Res	Type	Models (Total)
1	A	148	ARG	6
1	A	62	CYS	6
1	A	23	GLU	6
1	A	152	THR	5
1	A	114	ILE	5
1	A	36	PHE	5
1	A	115	CYS	4
1	A	119	THR	4
1	A	57	ILE	4
1	A	161	CYS	4
1	A	15	GLU	4
1	A	52	CYS	4
1	A	128	VAL	3
1	A	34	GLU	3
1	A	160	ASP	3
1	A	21	SER	3
1	A	116	THR	3
1	A	129	PHE	3
1	A	89	ILE	3
1	A	5	THR	3
1	A	41	THR	2
1	A	85	ASP	2
1	A	145	PHE	1
1	A	142	MET	1
1	A	132	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates 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 81% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: 2n0t_cs.str

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	1786
Number of shifts mapped to atoms	1786
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	81

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	164	0.11 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	138	0.46 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	156	1.10 ± 0.33	Should be applied

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 81%, i.e. 1495 atoms were assigned a chemical shift out of a possible 1850. 10 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	597/758 (79%)	299/302 (99%)	153/308 (50%)	145/148 (98%)
Sidechain	795/917 (87%)	511/541 (94%)	269/336 (80%)	15/40 (38%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	103/175 (59%)	78/96 (81%)	24/75 (32%)	1/4 (25%)
Overall	1495/1850 (81%)	888/939 (95%)	446/719 (62%)	161/192 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1574 atoms were assigned a chemical shift out of a possible 1964. 10 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	641/813 (79%)	321/324 (99%)	164/330 (50%)	156/159 (98%)
Sidechain	823/960 (86%)	529/566 (93%)	278/350 (79%)	16/44 (36%)
Aromatic	110/191 (58%)	84/105 (80%)	25/81 (31%)	1/5 (20%)
Overall	1574/1964 (80%)	934/995 (94%)	467/761 (61%)	173/208 (83%)

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	8	PHE	CD2	2.87	137.34 – 125.84	-111.9
1	A	22	PHE	CD2	8.19	137.34 – 125.84	-107.3
1	A	53	PHE	CE2	1.01	136.81 – 124.71	-107.2
1	A	46	PHE	CE2	1.27	136.81 – 124.71	-107.0
1	A	129	PHE	CE2	2.81	136.81 – 124.71	-105.7
1	A	8	PHE	CD1	2.87	137.63 – 125.43	-105.5
1	A	8	PHE	CE2	5.54	136.81 – 124.71	-103.5
1	A	22	PHE	CD1	8.19	137.63 – 125.43	-101.1
1	A	79	TYR	CE1	2.02	124.14 – 111.74	-93.5
1	A	53	PHE	CE1	1.01	137.92 – 123.42	-89.4
1	A	46	PHE	CE1	1.27	137.92 – 123.42	-89.2
1	A	8	PHE	CE1	5.54	137.92 – 123.42	-86.3
1	A	79	TYR	CE2	2.02	124.68 – 111.18	-85.9
1	A	25	PHE	CZ	2.71	137.04 – 121.44	-81.1
1	A	67	PHE	CZ	3.15	137.04 – 121.44	-80.8
1	A	88	PHE	CZ	8.01	137.04 – 121.44	-77.7
1	A	7	PHE	CD2	42.95	137.34 – 125.84	-77.1
1	A	8	PHE	CZ	9.27	137.04 – 121.44	-76.9
1	A	46	PHE	CD2	43.35	137.34 – 125.84	-76.7
1	A	22	PHE	CE2	41.07	136.81 – 124.71	-74.1
1	A	7	PHE	CD1	42.95	137.63 – 125.43	-72.6
1	A	46	PHE	CD1	43.35	137.63 – 125.43	-72.3

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	7	PHE	CE2	53.44	136.81 – 124.71	-63.9
1	A	22	PHE	CE1	41.07	137.92 – 123.42	-61.8
1	A	53	PHE	CZ	41.16	137.04 – 121.44	-56.5
1	A	92	HIS	CE1	5.32	149.70 – 125.30	-54.2
1	A	7	PHE	CE1	53.44	137.92 – 123.42	-53.3
1	A	70	HIS	CD2	2.17	137.40 – 103.40	-34.8
1	A	92	HIS	CD2	8.29	137.40 – 103.40	-33.0
1	A	54	HIS	CD2	8.73	137.40 – 103.40	-32.8
1	A	31	LYS	CG	59.57	30.67 – 19.17	30.1
1	A	68	THR	CG2	52.78	27.15 – 15.95	27.9
1	A	93	THR	CG2	52.57	27.15 – 15.95	27.7
1	A	95	PRO	CG	57.29	32.66 – 21.76	27.6
1	A	32	THR	CG2	52.17	27.15 – 15.95	27.3
1	A	5	THR	CG2	52.13	27.15 – 15.95	27.3
1	A	41	THR	CG2	52.06	27.15 – 15.95	27.2
1	A	31	LYS	CD	59.57	34.86 – 23.06	25.9
1	A	73	THR	CG2	50.55	27.15 – 15.95	25.9
1	A	76	LYS	CD	59.27	34.86 – 23.06	25.7
1	A	55	ARG	CG	58.00	33.23 – 21.23	25.6
1	A	16	PRO	CB	62.11	37.79 – 25.89	25.4
1	A	95	PRO	CB	61.95	37.79 – 25.89	25.3
1	A	100	MET	CG	61.92	38.33 – 25.73	23.7
1	A	56	ILE	CG2	47.56	24.63 – 10.43	21.2
1	A	11	ALA	CB	52.56	28.03 – 9.93	18.6
1	A	32	THR	CB	38.88	78.10 – 61.30	-18.3
1	A	56	ILE	CD1	44.28	21.91 – 5.01	18.2
1	A	107	THR	CB	39.20	78.10 – 61.30	-18.2
1	A	21	SER	CB	36.77	71.24 – 56.34	-18.1
1	A	78	ILE	CD1	44.02	21.91 – 5.01	18.1
1	A	73	THR	CB	40.76	78.10 – 61.30	-17.2
1	A	5	THR	CB	41.14	78.10 – 61.30	-17.0
1	A	69	ARG	CB	61.53	39.81 – 21.51	16.9
1	A	57	ILE	CG1	57.09	36.54 – 18.94	16.7
1	A	77	SER	CB	38.96	71.24 – 56.34	-16.7
1	A	10	ILE	CD1	41.27	21.91 – 5.01	16.5
1	A	34	GLU	CB	57.90	38.65 – 21.35	16.1
1	A	37	ARG	CG	45.21	33.23 – 21.23	15.0
1	A	29	VAL	CG1	40.20	28.40 – 14.60	13.6
1	A	70	HIS	CB	58.43	40.69 – 19.69	13.4
1	A	20	VAL	CG1	37.22	28.40 – 14.60	11.4
1	A	6	VAL	CG1	36.66	28.40 – 14.60	11.0
1	A	12	VAL	CG1	36.14	28.40 – 14.60	10.6

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	90	LEU	CD1	41.73	32.77 – 16.57	10.5
1	A	2	VAL	CG1	35.83	28.40 – 14.60	10.4
1	A	20	VAL	CG2	36.85	29.20 – 13.40	9.8
1	A	39	LEU	CD1	40.37	32.77 – 16.57	9.7
1	A	12	VAL	CG2	36.53	29.20 – 13.40	9.6
1	A	24	LEU	CD1	39.82	32.77 – 16.57	9.3
1	A	32	THR	CA	37.68	75.37 – 49.07	-9.3
1	A	98	LEU	CD1	39.58	32.77 – 16.57	9.2
1	A	98	LEU	CD2	39.53	32.60 – 15.60	9.1
1	A	6	VAL	CG2	35.60	29.20 – 13.40	9.0
1	A	29	VAL	CG2	35.55	29.20 – 13.40	9.0
1	A	17	LEU	CD2	39.12	32.60 – 15.60	8.8
1	A	90	LEU	CD2	37.46	32.60 – 15.60	7.9
1	A	76	LYS	HE3	1.51	3.86 – 1.96	-7.4
1	A	108	ASN	HB3	0.92	4.41 – 1.11	-5.6
1	A	31	LYS	HE3	1.86	3.86 – 1.96	-5.5
1	A	39	LEU	HB3	-0.33	3.34 – -0.26	-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.

Random coil index (RCI) for chain A:

