



Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 03:08 AM UTC

PDB ID : 1OT4 / pdb_00001ot4
Title : Solution structure of Cu(II)-CopC from Pseudomonas syringae
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Structural Proteomics in Europe (SPINE)
Deposited on : 2003-03-21

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

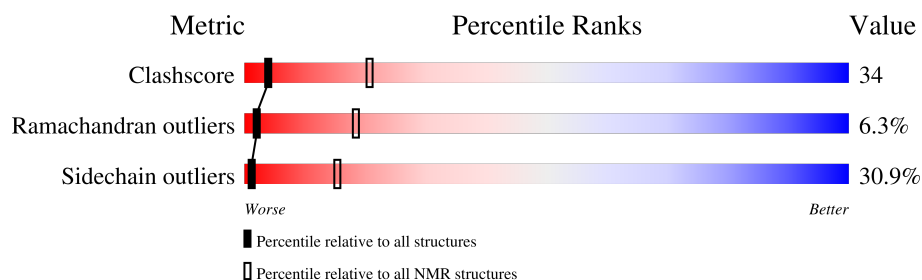
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	102	25% 36% 8% 30%

2 Ensemble composition and analysis

This entry contains 35 models. Model 7 is the overall representative, medoid model (most similar to other models).

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:4-A:26, A:35-A:42, A:51-A:59, A:64-A:84, A:93-A:102 (71)	0.42	7

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

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

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

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1486 atoms, of which 747 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Copper resistance protein C.

Mol	Chain	Residues	Atoms							Trace
1	A	102	Total	C	H	N	O	S		0
			1485	466	747	124	143	5		

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

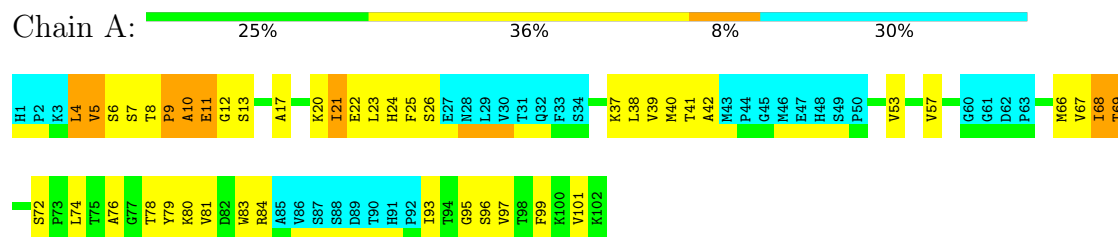
Mol	Chain	Residues	Atoms	
2	A	1	Total	Cu
			1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Copper resistance protein C

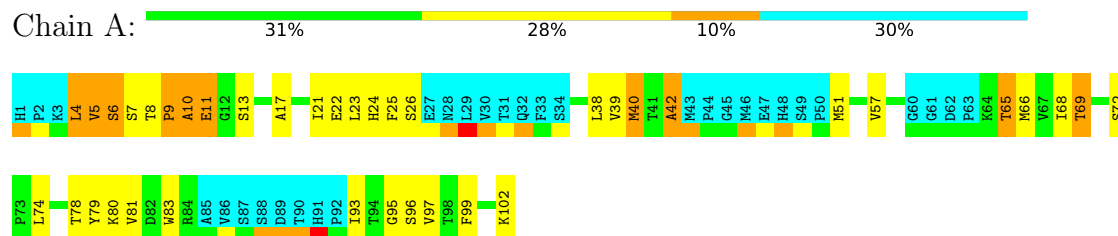


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

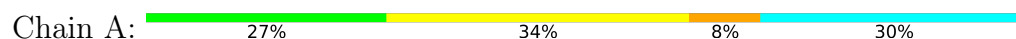
4.2.1 Score per residue for model 1

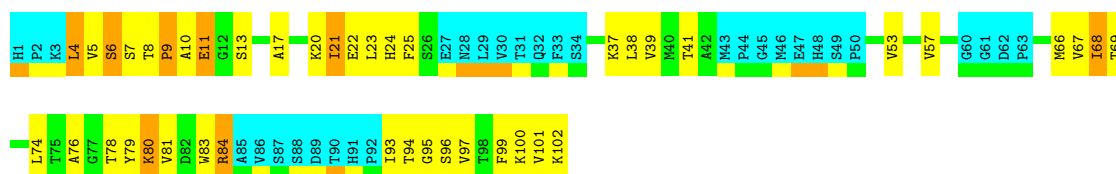
- Molecule 1: Copper resistance protein C



4.2.2 Score per residue for model 2

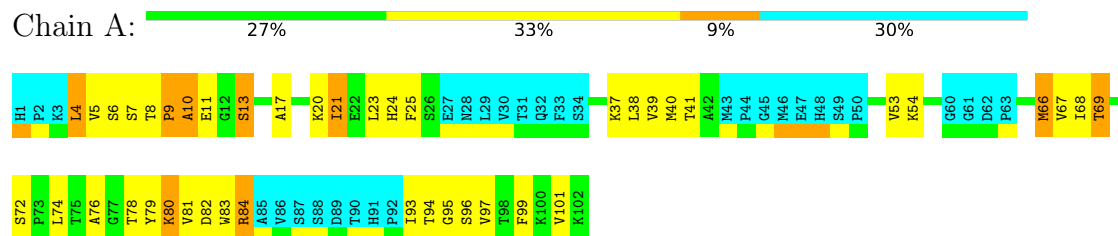
- Molecule 1: Copper resistance protein C





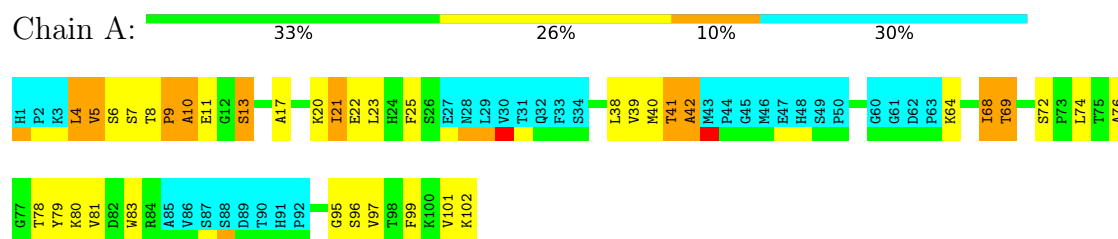
4.2.3 Score per residue for model 3

- Molecule 1: Copper resistance protein C



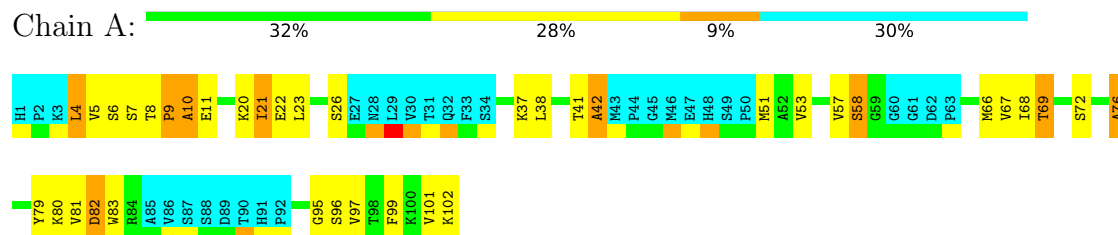
4.2.4 Score per residue for model 4

- Molecule 1: Copper resistance protein C



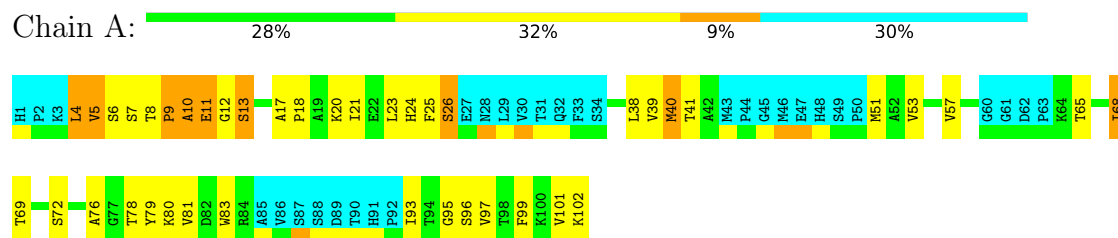
4.2.5 Score per residue for model 5

- Molecule 1: Copper resistance protein C



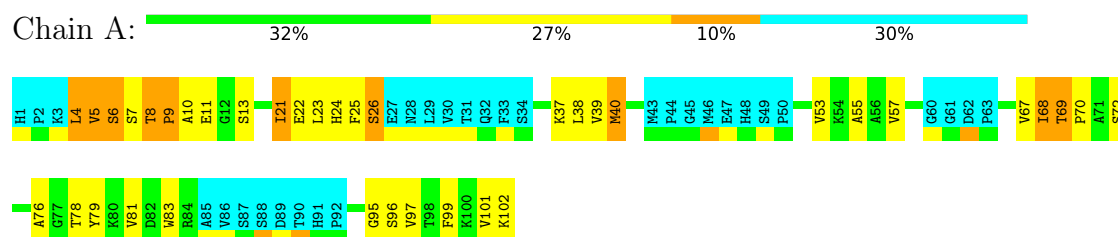
4.2.6 Score per residue for model 6

- Molecule 1: Copper resistance protein C



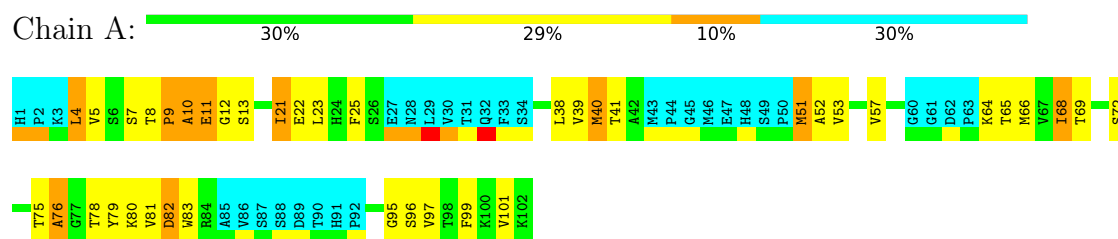
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Copper resistance protein C



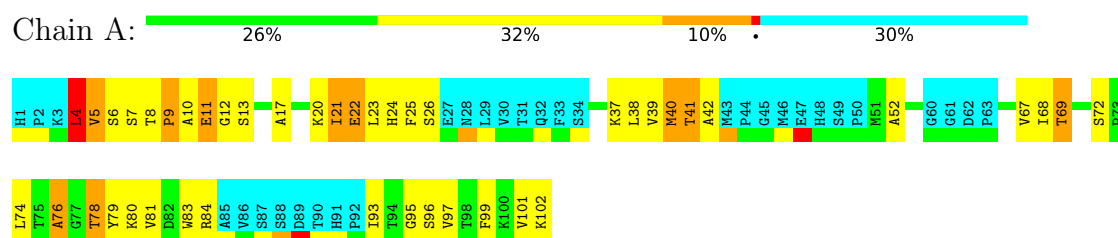
4.2.8 Score per residue for model 8

- Molecule 1: Copper resistance protein C



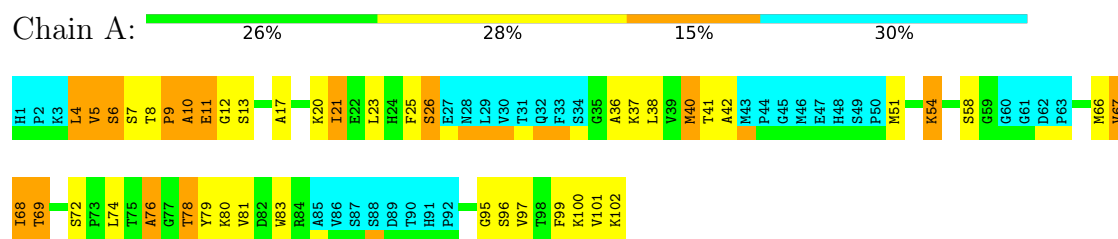
4.2.9 Score per residue for model 9

- Molecule 1: Copper resistance protein C



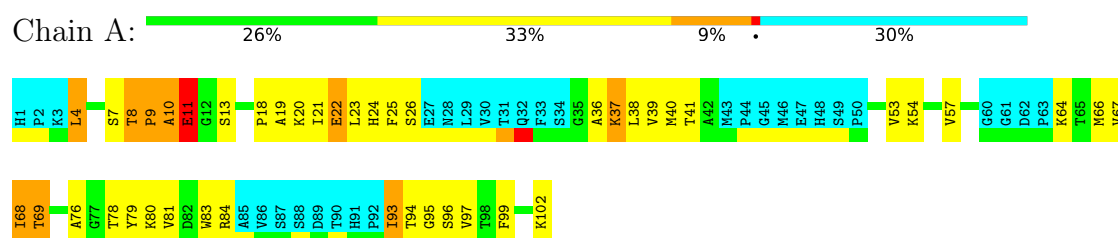
4.2.10 Score per residue for model 10

- Molecule 1: Copper resistance protein C



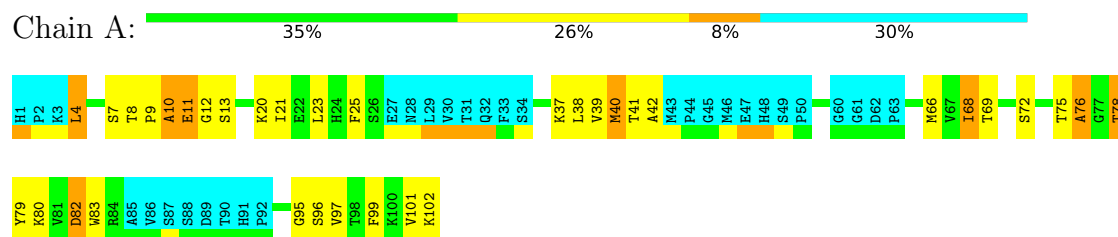
4.2.11 Score per residue for model 11

- Molecule 1: Copper resistance protein C



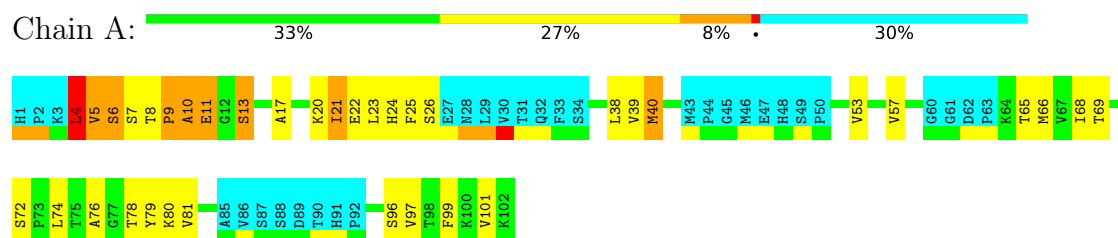
4.2.12 Score per residue for model 12

- Molecule 1: Copper resistance protein C



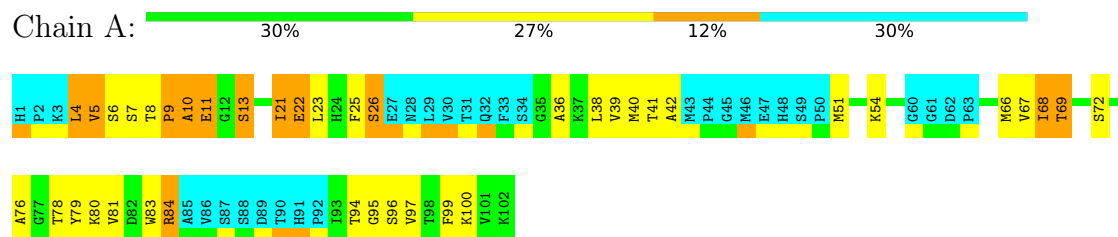
4.2.13 Score per residue for model 13

- Molecule 1: Copper resistance protein C



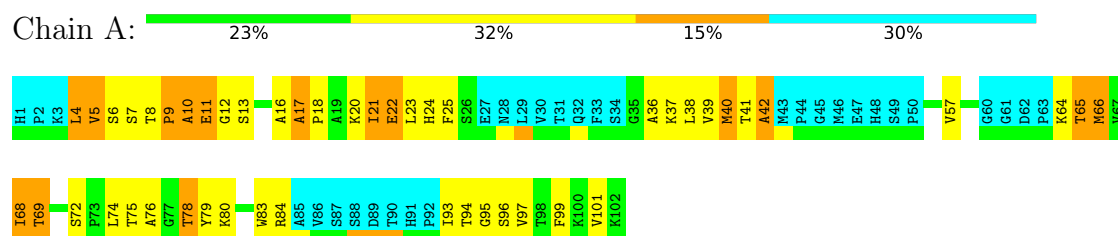
4.2.14 Score per residue for model 14

- Molecule 1: Copper resistance protein C



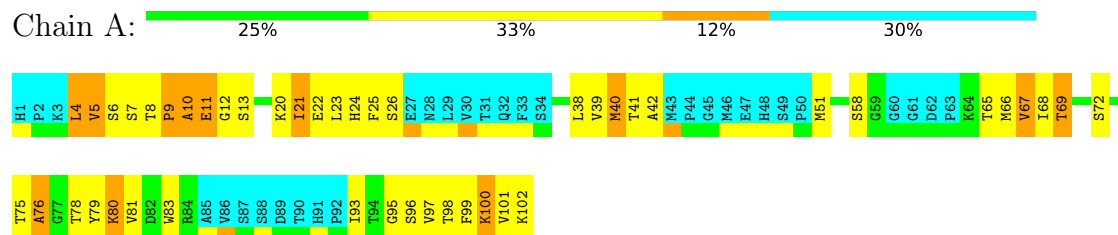
4.2.15 Score per residue for model 15

- Molecule 1: Copper resistance protein C



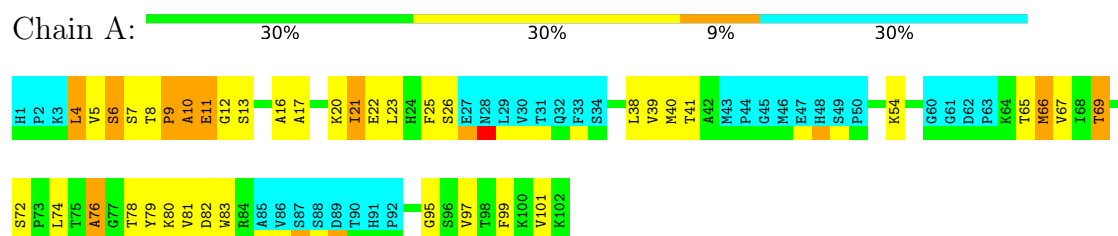
4.2.16 Score per residue for model 16

- Molecule 1: Copper resistance protein C



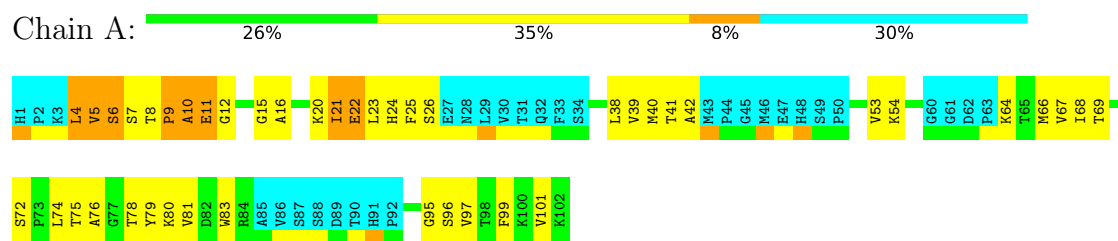
4.2.17 Score per residue for model 17

- Molecule 1: Copper resistance protein C



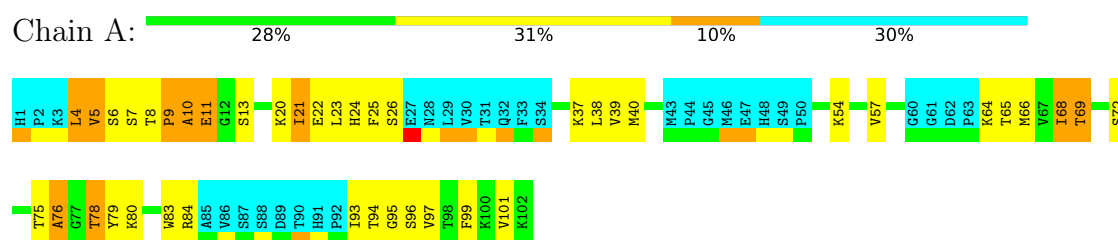
4.2.18 Score per residue for model 18

- Molecule 1: Copper resistance protein C



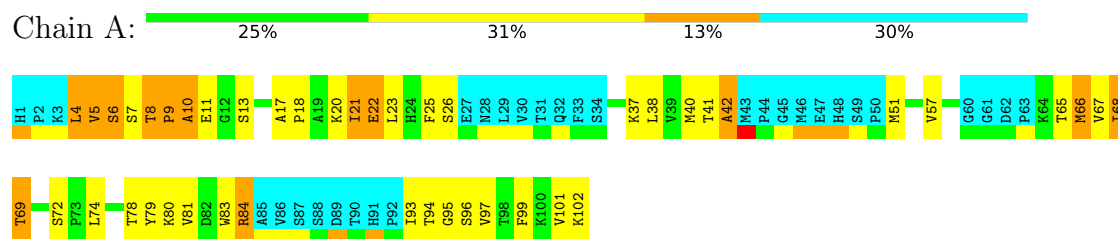
4.2.19 Score per residue for model 19

- Molecule 1: Copper resistance protein C



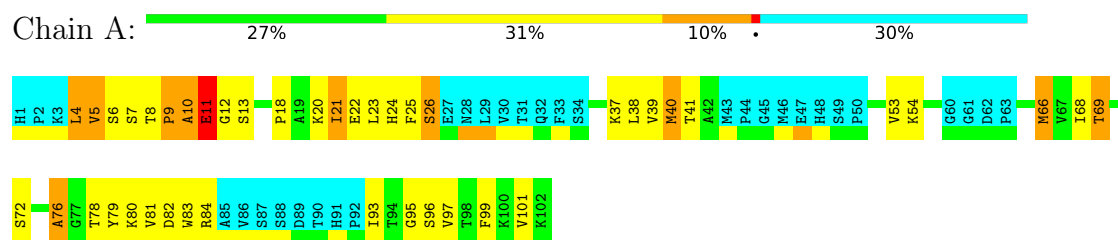
4.2.20 Score per residue for model 20

- Molecule 1: Copper resistance protein C



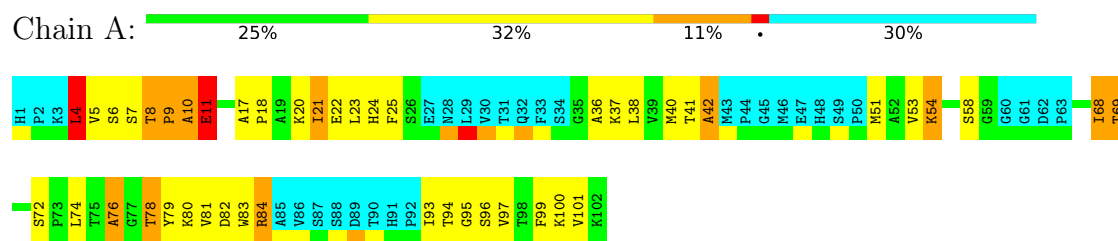
4.2.21 Score per residue for model 21

- Molecule 1: Copper resistance protein C



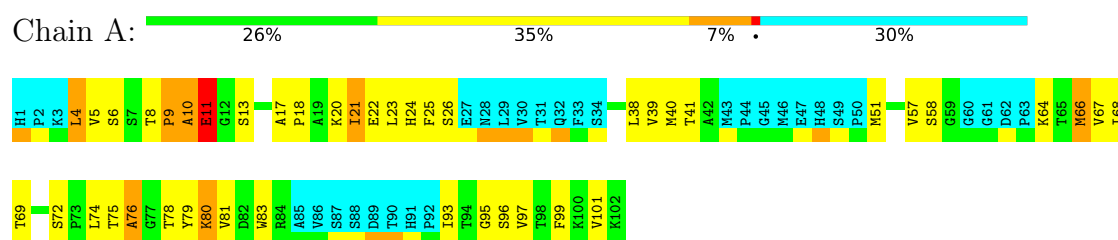
4.2.22 Score per residue for model 22

- Molecule 1: Copper resistance protein C



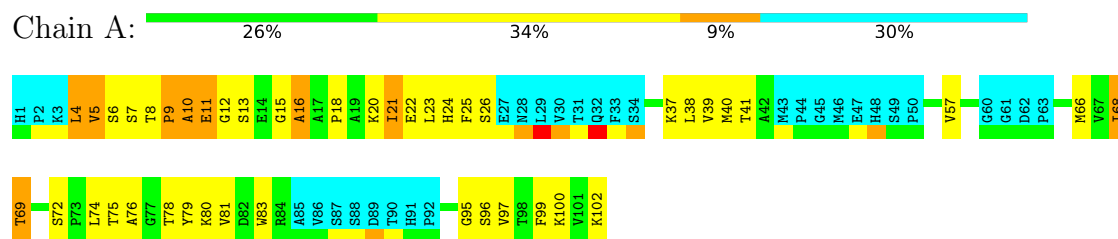
4.2.23 Score per residue for model 23

- Molecule 1: Copper resistance protein C



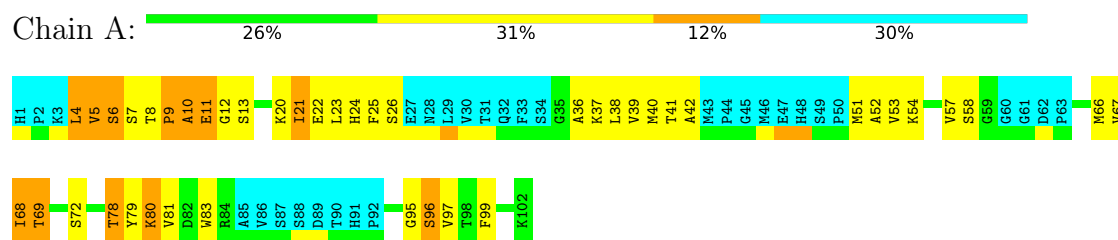
4.2.24 Score per residue for model 24

- Molecule 1: Copper resistance protein C



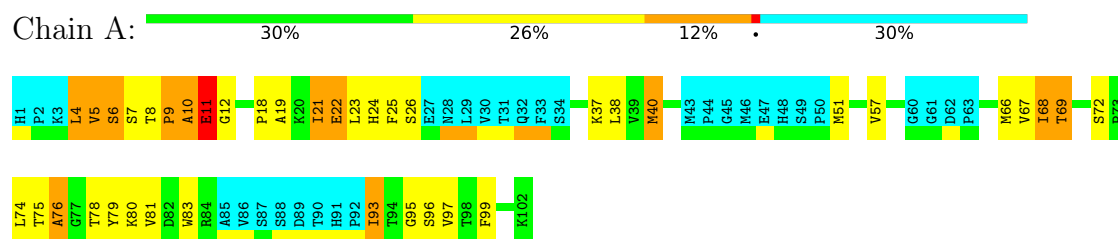
4.2.25 Score per residue for model 25

- Molecule 1: Copper resistance protein C



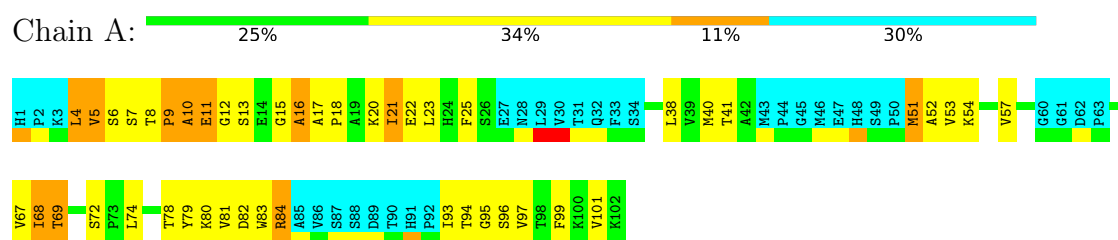
4.2.26 Score per residue for model 26

- Molecule 1: Copper resistance protein C



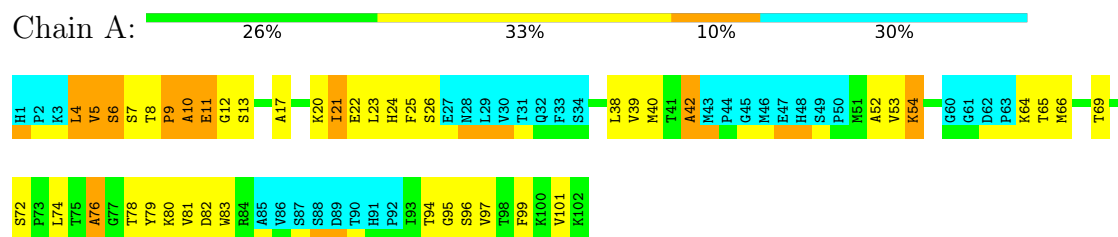
4.2.27 Score per residue for model 27

- Molecule 1: Copper resistance protein C



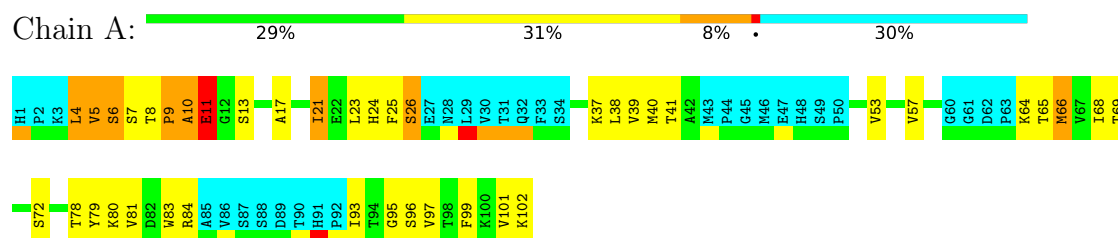
4.2.28 Score per residue for model 28

- Molecule 1: Copper resistance protein C



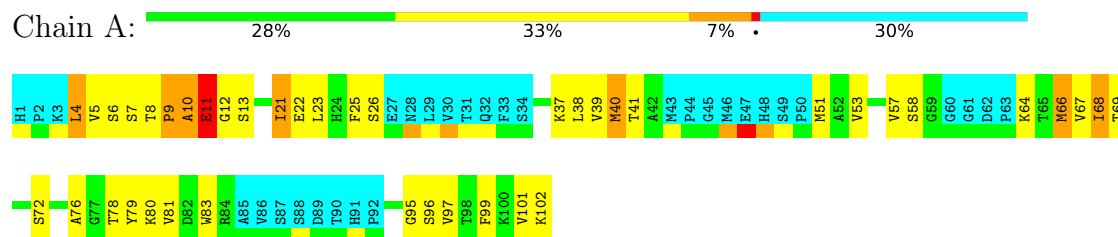
4.2.29 Score per residue for model 29

- Molecule 1: Copper resistance protein C



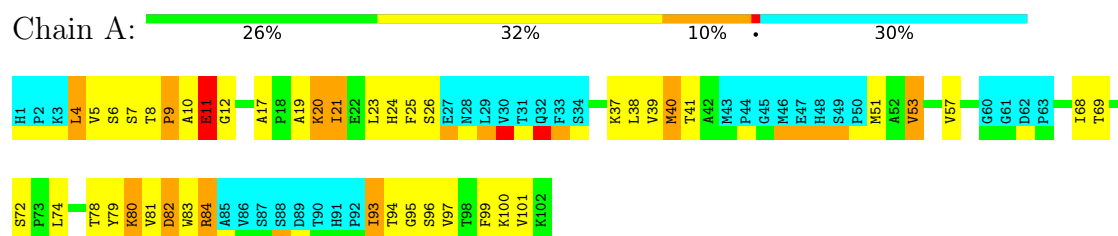
4.2.30 Score per residue for model 30

- Molecule 1: Copper resistance protein C



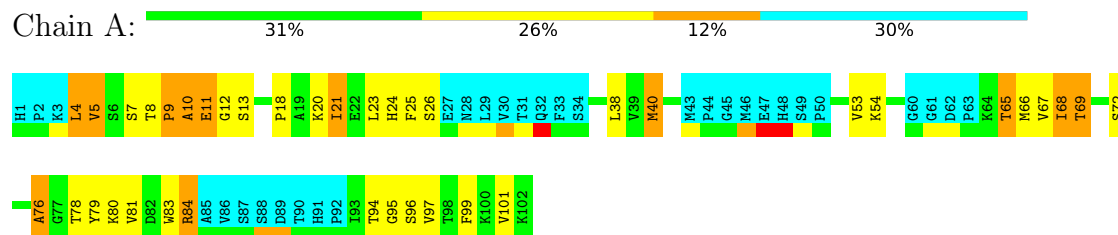
4.2.31 Score per residue for model 31

- Molecule 1: Copper resistance protein C



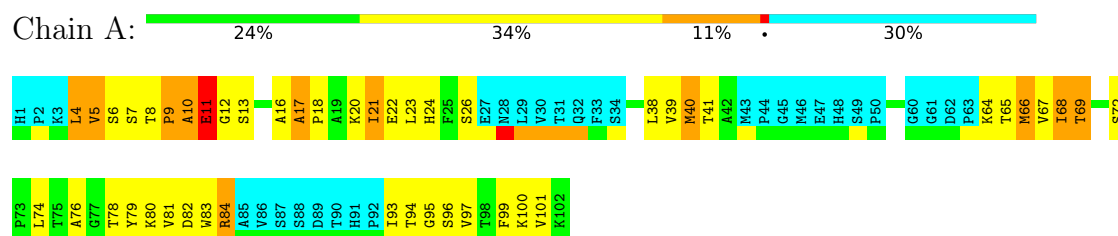
4.2.32 Score per residue for model 32

- Molecule 1: Copper resistance protein C



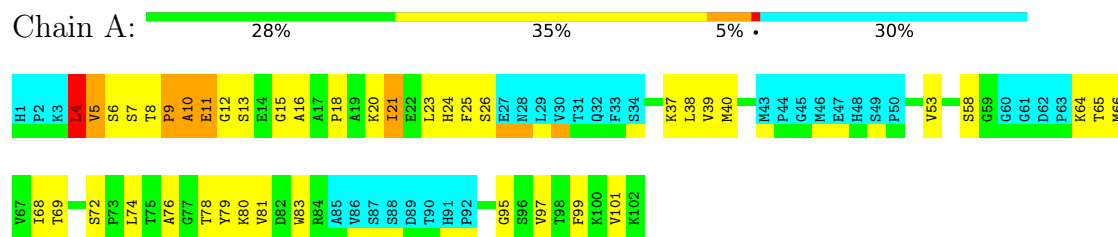
4.2.33 Score per residue for model 33

- Molecule 1: Copper resistance protein C



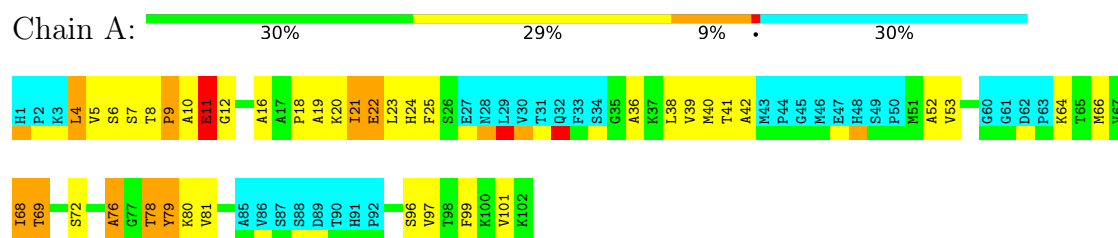
4.2.34 Score per residue for model 34

- Molecule 1: Copper resistance protein C



4.2.35 Score per residue for model 35

- Molecule 1: Copper resistance protein C



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 35 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
DYANA	structure solution	
DYANA	refinement	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
CU

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	509	538	538	35±4
All	All	17850	18830	18830	1235

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 34.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LEU:HD13	1:A:81:VAL:HG22	1.04	1.23	35	27
1:A:4:LEU:HD13	1:A:4:LEU:O	0.87	1.68	26	9
1:A:38:LEU:HD23	1:A:53:VAL:HG11	0.83	1.48	22	3
1:A:4:LEU:C	1:A:4:LEU:HD13	0.83	1.97	33	5
1:A:38:LEU:HD13	1:A:81:VAL:CG2	0.82	2.03	13	25
1:A:38:LEU:HD12	1:A:39:VAL:N	0.82	1.89	34	23
1:A:7:SER:HB2	1:A:23:LEU:HD23	0.81	1.52	5	34
1:A:38:LEU:CD1	1:A:81:VAL:HG22	0.80	2.06	35	6
1:A:57:VAL:HG12	1:A:68:ILE:HG13	0.76	1.56	7	10
1:A:9:PRO:HG2	1:A:97:VAL:HG11	0.75	1.59	11	35
1:A:38:LEU:HD21	1:A:74:LEU:HD21	0.74	1.58	3	6
1:A:84:ARG:CG	1:A:94:THR:HG22	0.73	2.13	22	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:PRO:CG	1:A:97:VAL:HG21	0.73	2.13	26	23
1:A:58:SER:HB2	1:A:67:VAL:HG23	0.72	1.60	10	1
1:A:7:SER:CB	1:A:23:LEU:HD23	0.72	2.15	27	34
1:A:38:LEU:HD12	1:A:39:VAL:H	0.72	1.45	4	17
1:A:38:LEU:HD11	1:A:79:TYR:HB3	0.72	1.62	34	19
1:A:18:PRO:HD2	1:A:74:LEU:HD12	0.72	1.61	24	5
1:A:38:LEU:HD13	1:A:81:VAL:HG23	0.71	1.60	10	2
1:A:84:ARG:HG2	1:A:94:THR:HG22	0.71	1.63	33	11
1:A:21:ILE:CD1	1:A:81:VAL:HG21	0.70	2.15	35	3
1:A:9:PRO:HG2	1:A:97:VAL:HG21	0.69	1.65	13	19
1:A:23:LEU:HD11	1:A:68:ILE:HD13	0.69	1.62	11	9
1:A:21:ILE:HD11	1:A:81:VAL:HG21	0.68	1.64	35	4
1:A:8:THR:O	1:A:8:THR:HG22	0.66	1.89	20	11
1:A:4:LEU:C	1:A:4:LEU:HD22	0.66	2.14	32	7
1:A:38:LEU:O	1:A:53:VAL:HG12	0.66	1.91	5	6
1:A:24:HIS:C	1:A:25:PHE:CD1	0.66	2.74	23	11
1:A:23:LEU:CD1	1:A:68:ILE:HD13	0.65	2.22	27	5
1:A:41:THR:O	1:A:41:THR:HG23	0.65	1.91	23	20
1:A:78:THR:C	1:A:79:TYR:CD1	0.65	2.74	26	34
1:A:4:LEU:HD13	1:A:4:LEU:C	0.65	2.17	4	4
1:A:57:VAL:HG12	1:A:68:ILE:CG1	0.64	2.22	7	4
1:A:4:LEU:HD23	1:A:24:HIS:O	0.64	1.92	23	12
1:A:9:PRO:O	1:A:10:ALA:HB2	0.64	1.92	33	17
1:A:39:VAL:HG22	1:A:80:LYS:O	0.64	1.93	23	4
1:A:4:LEU:C	1:A:4:LEU:CD1	0.63	2.72	33	3
1:A:18:PRO:O	1:A:19:ALA:HB3	0.63	1.92	35	1
1:A:17:ALA:N	1:A:101:VAL:HG13	0.63	2.09	13	5
1:A:4:LEU:HD21	1:A:6:SER:C	0.62	2.19	26	12
1:A:79:TYR:N	1:A:79:TYR:CD1	0.62	2.68	35	13
1:A:38:LEU:CD2	1:A:74:LEU:HD21	0.62	2.24	3	5
1:A:10:ALA:HB2	1:A:18:PRO:HG3	0.62	1.72	6	7
1:A:4:LEU:HD23	1:A:25:PHE:CE1	0.62	2.30	27	3
1:A:76:ALA:HA	1:A:101:VAL:HG12	0.61	1.73	12	20
1:A:17:ALA:HB1	1:A:74:LEU:HB2	0.61	1.71	13	11
1:A:65:THR:C	1:A:66:MET:HE3	0.60	2.21	33	3
1:A:38:LEU:HD21	1:A:74:LEU:CD2	0.60	2.26	3	6
1:A:69:THR:O	1:A:69:THR:HG22	0.59	1.98	9	23
1:A:4:LEU:CB	1:A:25:PHE:CZ	0.59	2.85	31	5
1:A:4:LEU:HD22	1:A:5:VAL:N	0.59	2.12	32	13
1:A:5:VAL:HG21	1:A:26:SER:H	0.58	1.58	25	16
1:A:10:ALA:HB1	1:A:13:SER:HB2	0.58	1.75	13	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:PHE:C	1:A:99:PHE:CD1	0.58	2.80	19	25
1:A:4:LEU:HD11	1:A:7:SER:OG	0.58	1.97	30	2
1:A:11:GLU:HA	1:A:97:VAL:HG13	0.58	1.76	27	4
1:A:57:VAL:HG22	1:A:68:ILE:HG13	0.58	1.75	27	2
1:A:24:HIS:O	1:A:25:PHE:CD1	0.57	2.57	21	12
1:A:74:LEU:HD13	1:A:99:PHE:CZ	0.57	2.35	18	2
1:A:79:TYR:CD1	1:A:79:TYR:N	0.57	2.72	24	20
1:A:4:LEU:CB	1:A:83:TRP:CH2	0.56	2.88	27	4
1:A:24:HIS:CE1	1:A:65:THR:OG1	0.56	2.57	1	5
1:A:17:ALA:HB2	1:A:101:VAL:HG21	0.56	1.77	6	2
1:A:39:VAL:HG12	1:A:52:ALA:HA	0.55	1.77	9	4
1:A:38:LEU:HB2	1:A:81:VAL:HG22	0.55	1.77	34	1
1:A:19:ALA:HB3	1:A:20:LYS:HE2	0.55	1.78	31	1
1:A:4:LEU:HD23	1:A:25:PHE:CZ	0.55	2.37	27	3
1:A:18:PRO:CD	1:A:74:LEU:HD12	0.54	2.31	24	2
1:A:93:ILE:HD12	1:A:93:ILE:N	0.54	2.18	1	2
1:A:17:ALA:HB2	1:A:74:LEU:O	0.54	2.03	33	1
1:A:4:LEU:HD22	1:A:6:SER:N	0.53	2.19	24	24
1:A:4:LEU:HB2	1:A:25:PHE:CZ	0.53	2.38	3	10
1:A:4:LEU:HB2	1:A:83:TRP:CH2	0.53	2.38	27	3
1:A:78:THR:HG23	1:A:100:LYS:HG2	0.53	1.80	14	1
1:A:36:ALA:HB3	1:A:68:ILE:HD11	0.53	1.80	35	6
1:A:40:MET:CG	1:A:79:TYR:CE2	0.52	2.92	22	6
1:A:22:GLU:OE1	1:A:24:HIS:CD2	0.52	2.62	18	3
1:A:84:ARG:HG3	1:A:94:THR:HG22	0.52	1.82	22	1
1:A:23:LEU:HD11	1:A:68:ILE:CD1	0.52	2.35	11	2
1:A:79:TYR:HB2	1:A:99:PHE:CZ	0.52	2.39	18	34
1:A:40:MET:HG3	1:A:79:TYR:CE2	0.52	2.40	22	29
1:A:79:TYR:HB2	1:A:99:PHE:CE1	0.52	2.40	29	4
1:A:23:LEU:HD12	1:A:66:MET:HB3	0.52	1.82	14	3
1:A:36:ALA:CB	1:A:68:ILE:HD11	0.51	2.36	25	1
1:A:4:LEU:CD2	1:A:24:HIS:O	0.51	2.58	33	1
1:A:9:PRO:HB3	1:A:21:ILE:HG23	0.51	1.82	17	14
1:A:4:LEU:N	1:A:4:LEU:CD1	0.51	2.74	10	18
1:A:54:LYS:CG	1:A:54:LYS:O	0.51	2.59	18	3
1:A:9:PRO:O	1:A:10:ALA:CB	0.50	2.59	18	13
1:A:40:MET:HB2	1:A:79:TYR:CD2	0.50	2.41	25	5
1:A:4:LEU:HB2	1:A:25:PHE:CE2	0.50	2.41	7	12
1:A:41:THR:HG21	1:A:80:LYS:NZ	0.50	2.22	10	1
1:A:40:MET:HB2	1:A:79:TYR:CE2	0.50	2.42	29	9
1:A:8:THR:O	1:A:8:THR:CG2	0.50	2.59	22	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:SER:O	1:A:67:VAL:HG23	0.50	2.07	16	1
1:A:11:GLU:O	1:A:12:GLY:C	0.50	2.54	33	21
1:A:9:PRO:HA	1:A:21:ILE:CG1	0.50	2.36	33	15
1:A:4:LEU:HB2	1:A:25:PHE:CE1	0.49	2.41	10	7
1:A:17:ALA:H	1:A:101:VAL:HG13	0.49	1.68	27	3
1:A:58:SER:O	1:A:67:VAL:HG12	0.49	2.06	30	2
1:A:8:THR:N	1:A:9:PRO:HD3	0.49	2.22	21	35
1:A:18:PRO:O	1:A:19:ALA:CB	0.49	2.58	35	1
1:A:57:VAL:HG22	1:A:68:ILE:CG1	0.49	2.37	27	1
1:A:4:LEU:HB3	1:A:25:PHE:CZ	0.49	2.43	31	1
1:A:41:THR:O	1:A:41:THR:CG2	0.48	2.61	23	8
1:A:58:SER:O	1:A:67:VAL:CG1	0.48	2.61	25	2
1:A:10:ALA:H	1:A:97:VAL:HG11	0.48	1.68	1	3
1:A:79:TYR:CD1	1:A:99:PHE:CE1	0.48	3.01	8	3
1:A:69:THR:O	1:A:69:THR:CG2	0.48	2.62	4	6
1:A:58:SER:O	1:A:67:VAL:CG2	0.48	2.62	16	2
1:A:24:HIS:C	1:A:25:PHE:CG	0.48	2.91	23	5
1:A:5:VAL:HG12	1:A:6:SER:N	0.48	2.24	4	3
1:A:93:ILE:HG23	1:A:93:ILE:O	0.48	2.08	22	1
1:A:4:LEU:C	1:A:4:LEU:CD2	0.48	2.87	32	1
1:A:41:THR:O	1:A:42:ALA:C	0.48	2.56	9	5
1:A:83:TRP:CZ2	1:A:95:GLY:HA3	0.47	2.45	11	30
1:A:25:PHE:CD1	1:A:25:PHE:N	0.47	2.83	23	2
1:A:4:LEU:HB2	1:A:83:TRP:CZ3	0.47	2.45	8	1
1:A:79:TYR:HB2	1:A:99:PHE:CE2	0.47	2.44	11	5
1:A:21:ILE:O	1:A:67:VAL:HG23	0.47	2.10	32	1
1:A:23:LEU:CD1	1:A:68:ILE:CD1	0.46	2.94	11	2
1:A:83:TRP:N	1:A:95:GLY:O	0.46	2.48	21	4
1:A:4:LEU:HD23	1:A:25:PHE:CE2	0.46	2.45	12	2
1:A:4:LEU:HD22	1:A:4:LEU:C	0.46	2.35	14	2
1:A:66:MET:C	1:A:67:VAL:HG23	0.46	2.36	17	2
1:A:38:LEU:CD1	1:A:81:VAL:HG23	0.46	2.40	22	1
1:A:42:ALA:HB2	1:A:78:THR:H	0.46	1.70	12	2
1:A:100:LYS:N	1:A:100:LYS:CD	0.46	2.79	16	1
1:A:99:PHE:CD1	1:A:99:PHE:O	0.46	2.68	20	5
1:A:10:ALA:O	1:A:11:GLU:C	0.46	2.58	26	12
1:A:83:TRP:CH2	1:A:95:GLY:HA3	0.46	2.46	6	3
1:A:16:ALA:HA	1:A:101:VAL:HG13	0.46	1.87	17	3
1:A:15:GLY:O	1:A:16:ALA:HB2	0.46	2.11	24	2
1:A:4:LEU:HB2	1:A:25:PHE:CD2	0.46	2.46	1	2
1:A:51:MET:O	1:A:52:ALA:C	0.45	2.60	25	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LEU:CD2	1:A:53:VAL:HG11	0.45	2.31	22	1
1:A:24:HIS:ND1	1:A:65:THR:OG1	0.45	2.50	13	3
1:A:66:MET:O	1:A:67:VAL:CG2	0.45	2.64	17	1
1:A:75:THR:O	1:A:76:ALA:C	0.45	2.60	15	6
1:A:4:LEU:HA	1:A:25:PHE:CE1	0.45	2.47	12	2
1:A:9:PRO:HG3	1:A:97:VAL:HG21	0.44	1.87	26	3
1:A:66:MET:N	1:A:66:MET:HE3	0.44	2.27	15	1
1:A:4:LEU:HD11	1:A:7:SER:CB	0.44	2.43	21	1
1:A:10:ALA:HB1	1:A:99:PHE:CB	0.44	2.43	26	1
1:A:80:LYS:CE	1:A:96:SER:CB	0.44	2.96	25	1
1:A:82:ASP:OD1	1:A:82:ASP:N	0.43	2.51	12	4
1:A:99:PHE:CD1	1:A:99:PHE:C	0.43	2.96	15	3
1:A:4:LEU:HD12	1:A:83:TRP:CZ2	0.43	2.48	20	1
1:A:38:LEU:CD1	1:A:81:VAL:CG2	0.43	2.97	22	1
1:A:5:VAL:HG11	1:A:26:SER:H	0.43	1.72	33	1
1:A:4:LEU:HB3	1:A:83:TRP:CH2	0.43	2.49	27	3
1:A:16:ALA:C	1:A:101:VAL:HG13	0.43	2.39	18	1
1:A:83:TRP:CE2	1:A:95:GLY:HA3	0.43	2.49	27	6
1:A:22:GLU:OE2	1:A:24:HIS:NE2	0.43	2.51	11	1
1:A:5:VAL:HG11	1:A:26:SER:CB	0.43	2.44	33	1
1:A:83:TRP:O	1:A:95:GLY:N	0.42	2.51	27	1
1:A:22:GLU:C	1:A:23:LEU:HG	0.42	2.39	15	9
1:A:4:LEU:CD2	1:A:6:SER:O	0.42	2.67	23	2
1:A:41:THR:HG21	1:A:80:LYS:HD3	0.42	1.90	10	1
1:A:40:MET:HE3	1:A:79:TYR:OH	0.42	2.15	18	1
1:A:25:PHE:CE2	1:A:93:ILE:HD13	0.42	2.49	26	1
1:A:5:VAL:HG21	1:A:26:SER:N	0.42	2.29	33	2
1:A:4:LEU:CB	1:A:25:PHE:CE2	0.42	3.03	23	2
1:A:23:LEU:HB3	1:A:25:PHE:CE1	0.42	2.50	23	1
1:A:18:PRO:O	1:A:19:ALA:C	0.42	2.63	11	2
1:A:4:LEU:HD12	1:A:83:TRP:CH2	0.41	2.50	5	1
1:A:23:LEU:HD12	1:A:68:ILE:CD1	0.41	2.46	27	1
1:A:40:MET:N	1:A:51:MET:O	0.41	2.50	8	1
1:A:78:THR:OG1	1:A:100:LYS:CD	0.41	2.68	10	1
1:A:58:SER:O	1:A:67:VAL:O	0.41	2.39	23	1
1:A:66:MET:C	1:A:67:VAL:CG2	0.41	2.93	26	1
1:A:4:LEU:HD22	1:A:5:VAL:C	0.41	2.40	14	1
1:A:53:VAL:HG22	1:A:54:LYS:H	0.41	1.75	22	1
1:A:41:THR:C	1:A:42:ALA:O	0.41	2.64	4	3
1:A:17:ALA:HB2	1:A:101:VAL:CG2	0.41	2.45	6	1
1:A:84:ARG:HA	1:A:94:THR:HG22	0.41	1.93	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:THR:O	1:A:42:ALA:O	0.41	2.39	22	3
1:A:93:ILE:O	1:A:93:ILE:HG23	0.41	2.16	11	1
1:A:80:LYS:HG3	1:A:98:THR:CB	0.41	2.46	16	1
1:A:9:PRO:CA	1:A:21:ILE:HG12	0.41	2.46	18	1
1:A:8:THR:N	1:A:9:PRO:CD	0.41	2.83	21	4
1:A:41:THR:HG23	1:A:41:THR:O	0.41	2.16	24	1
1:A:40:MET:CB	1:A:79:TYR:CD2	0.41	3.04	34	1
1:A:40:MET:SD	1:A:40:MET:O	0.40	2.79	11	1
1:A:75:THR:C	1:A:76:ALA:O	0.40	2.65	16	3
1:A:55:ALA:HB2	1:A:70:PRO:HB3	0.40	1.91	7	1
1:A:83:TRP:HE1	1:A:97:VAL:HG23	0.40	1.76	17	1
1:A:4:LEU:CD1	1:A:4:LEU:H	0.40	2.30	28	1
1:A:83:TRP:CE3	1:A:83:TRP:C	0.40	2.99	27	1
1:A:17:ALA:CB	1:A:74:LEU:HB2	0.40	2.47	28	1
1:A:36:ALA:O	1:A:37:LYS:CG	0.40	2.70	11	1
1:A:10:ALA:O	1:A:12:GLY:N	0.40	2.55	26	1
1:A:11:GLU:CA	1:A:97:VAL:HG13	0.40	2.46	27	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	70/102 (69%)	58±2 (83±3%)	7±2 (10±3%)	4±1 (6±1%)	2	18
All	All	2450/3570 (69%)	2039 (83%)	257 (10%)	154 (6%)	2	18

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

Mol	Chain	Res	Type	Models (Total)
1	A	10	ALA	35
1	A	9	PRO	34
1	A	5	VAL	31
1	A	76	ALA	21
1	A	11	GLU	13

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Mol	Chain	Res	Type	Models (Total)
1	A	42	ALA	8
1	A	4	LEU	4
1	A	16	ALA	4
1	A	17	ALA	2
1	A	15	GLY	2

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	54/81 (67%)	37±2 (69±4%)	17±2 (31±4%)	1	15
All	All	1890/2835 (67%)	1306 (69%)	584 (31%)	1	15

All 33 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	4	LEU	35
1	A	11	GLU	35
1	A	21	ILE	35
1	A	69	THR	35
1	A	72	SER	33
1	A	80	LYS	33
1	A	96	SER	33
1	A	68	ILE	31
1	A	20	LYS	28
1	A	13	SER	27
1	A	22	GLU	23
1	A	37	LYS	20
1	A	66	MET	19
1	A	6	SER	18
1	A	40	MET	17
1	A	102	LYS	15
1	A	26	SER	15
1	A	51	MET	14
1	A	53	VAL	13
1	A	64	LYS	13

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Mol	Chain	Res	Type	Models (Total)
1	A	84	ARG	12
1	A	54	LYS	12
1	A	67	VAL	11
1	A	82	ASP	11
1	A	65	THR	8
1	A	78	THR	8
1	A	57	VAL	7
1	A	100	LYS	6
1	A	93	ILE	5
1	A	41	THR	4
1	A	8	THR	4
1	A	58	SER	3
1	A	79	TYR	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

No chemical shift data were provided