



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 05:48 AM UTC

PDB ID : 1CEJ / pdb_00001cej
Title : SOLUTION STRUCTURE OF AN EGF MODULE PAIR FROM THE PLASMODIUM FALCIPARUM MEROZOITE SURFACE PROTEIN 1
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Deposited on : 1999-03-08

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

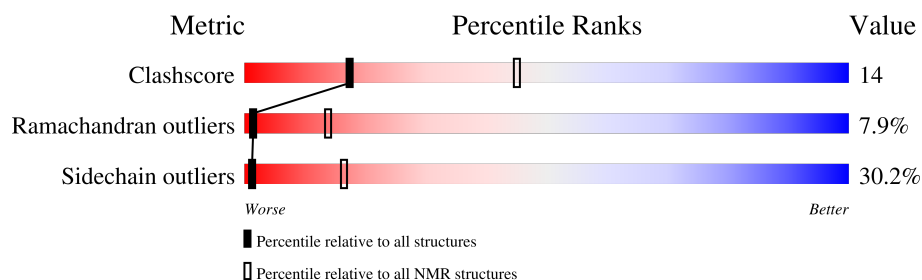
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

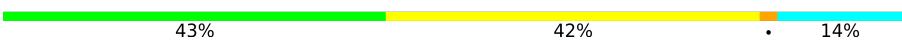
The overall completeness of chemical shifts assignment was not calculated.

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	96	

2 Ensemble composition and analysis

This entry contains 32 models. Model 18 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:5-A:65, A:72-A:93 (83)	1.21	18

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 5 clusters and 6 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1397 atoms, of which 663 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (MEROZOITE SURFACE PROTEIN 1).

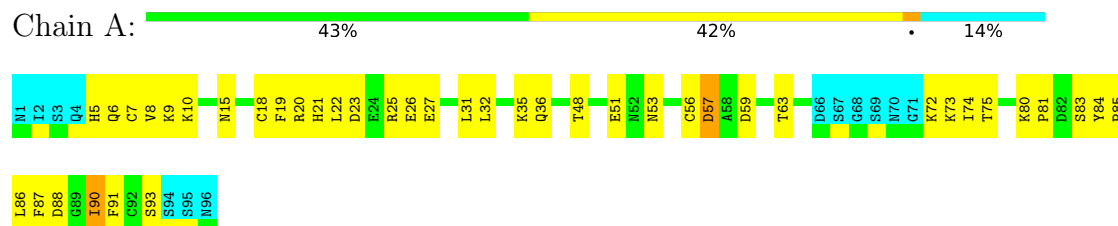
Mol	Chain	Residues	Atoms						Trace
1	A	96	Total	C	H	N	O	S	0
			1397	434	663	130	158	12	

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: PROTEIN (MEROZOITE SURFACE PROTEIN 1)

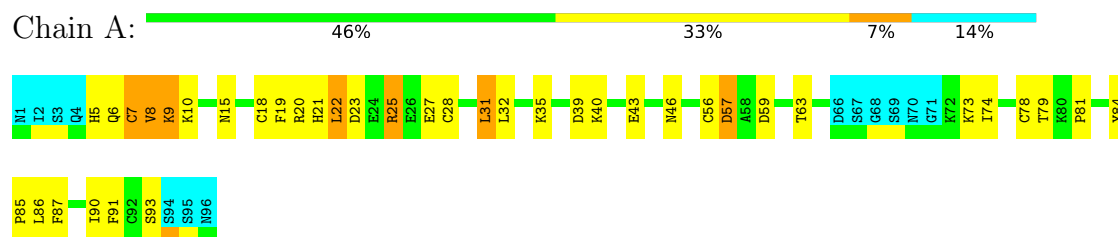


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

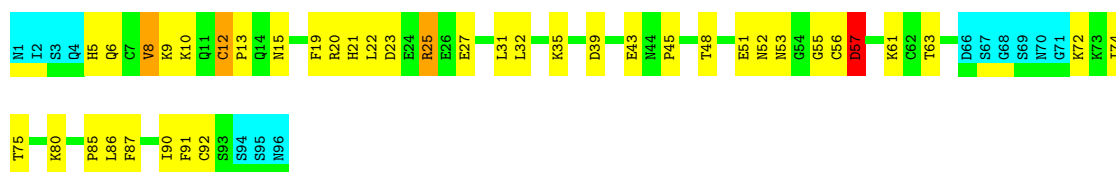
- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



4.2.2 Score per residue for model 2

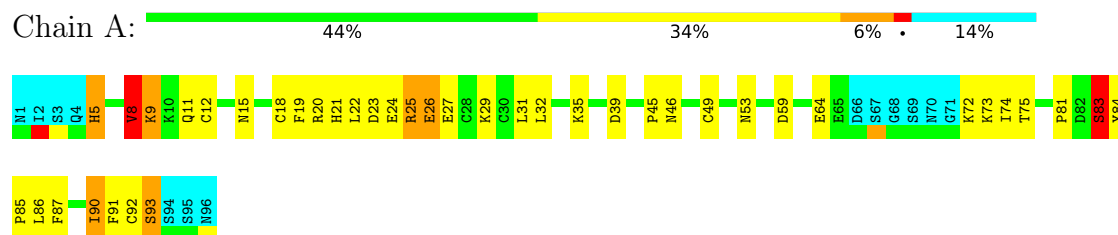
- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)





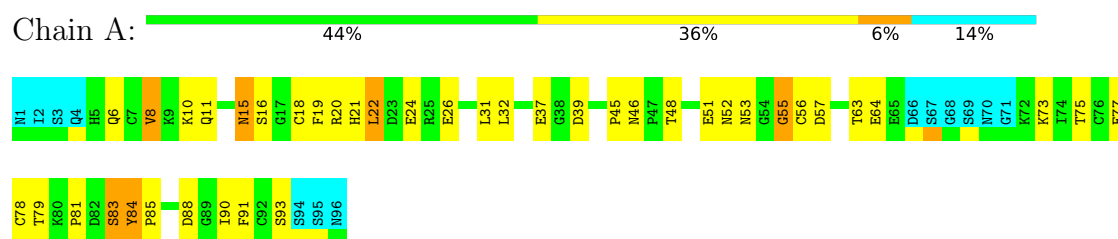
4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



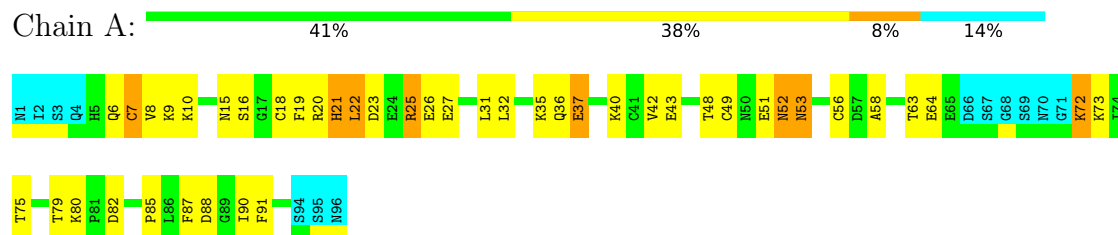
4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



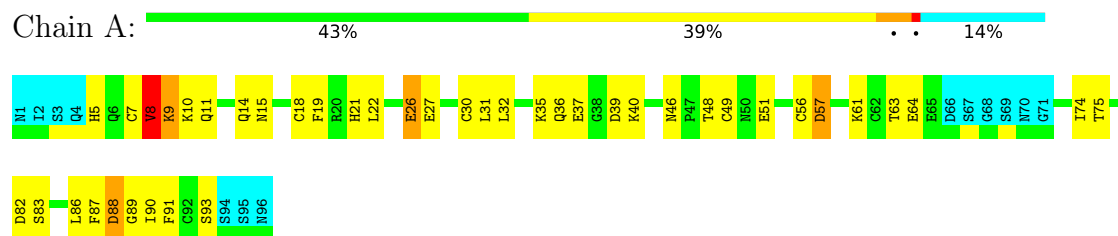
4.2.5 Score per residue for model 5

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



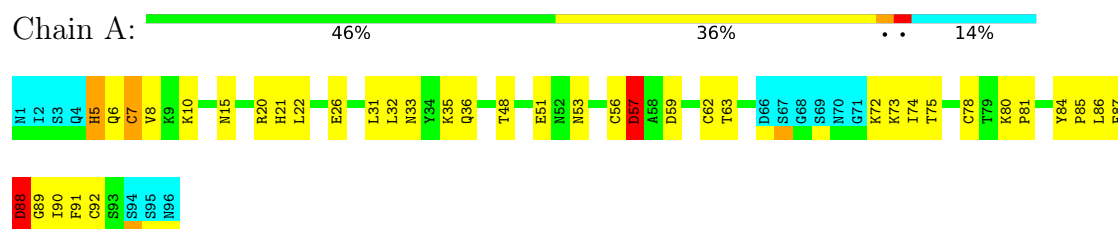
4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



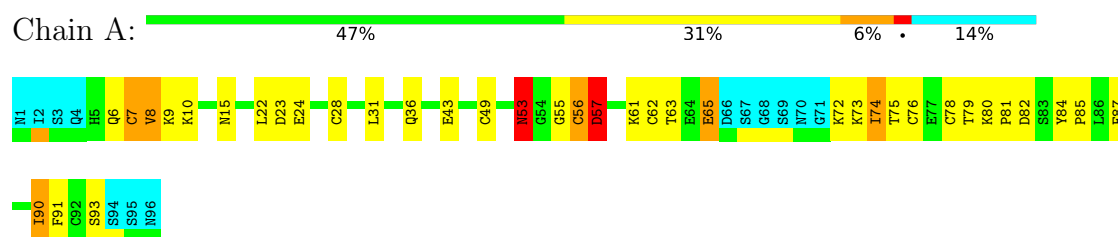
4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



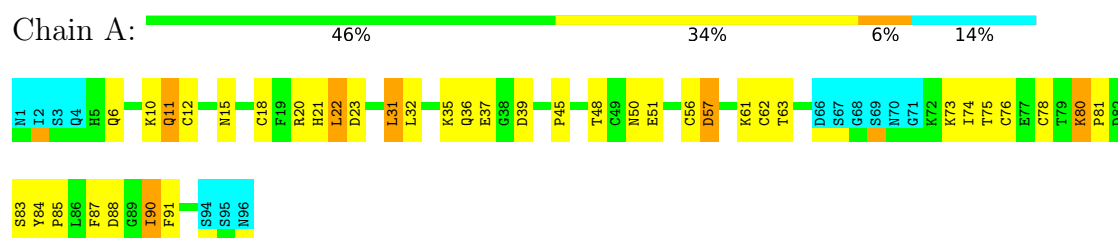
4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



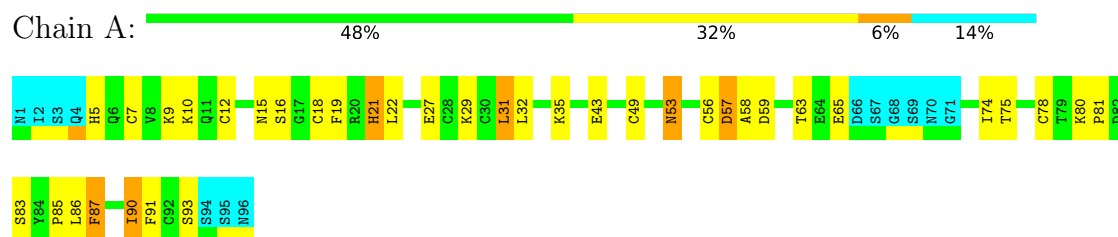
4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



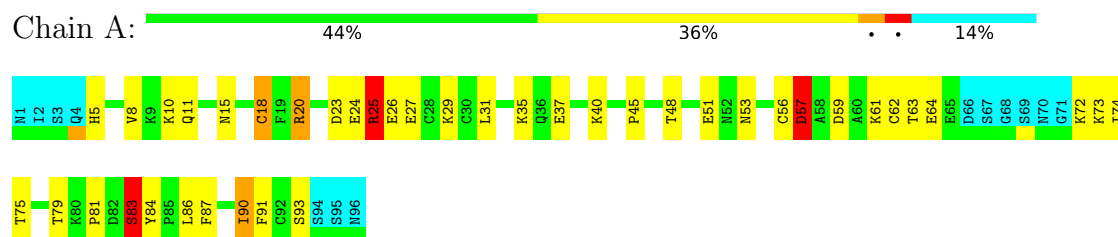
4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



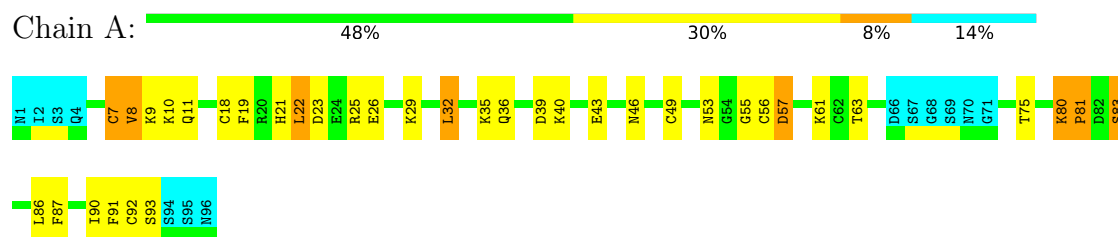
4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



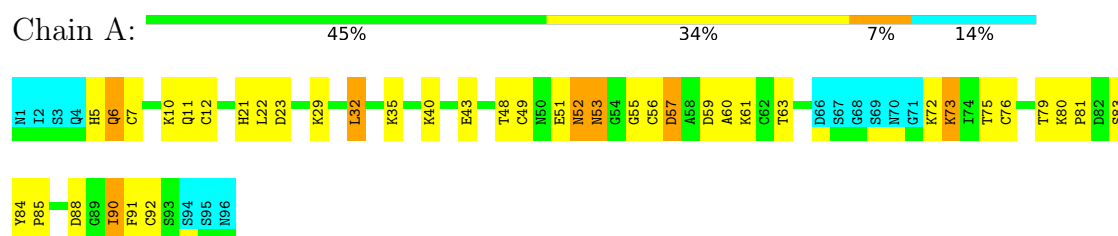
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



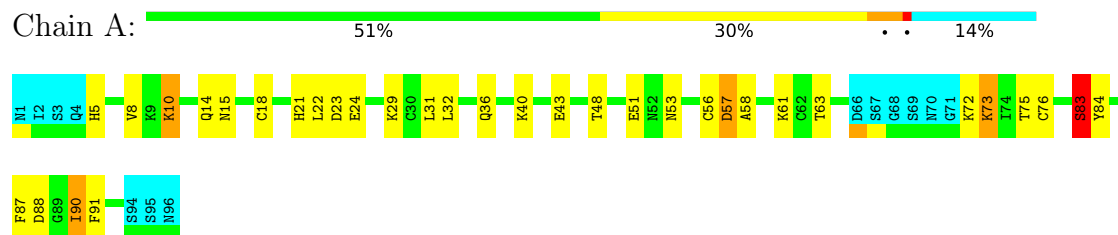
4.2.19 Score per residue for model 19

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



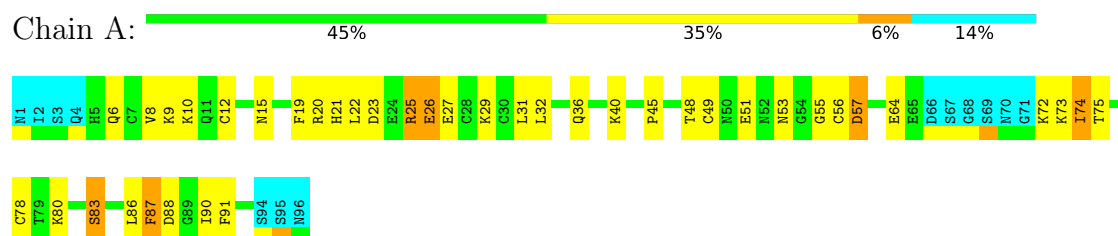
4.2.20 Score per residue for model 20

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



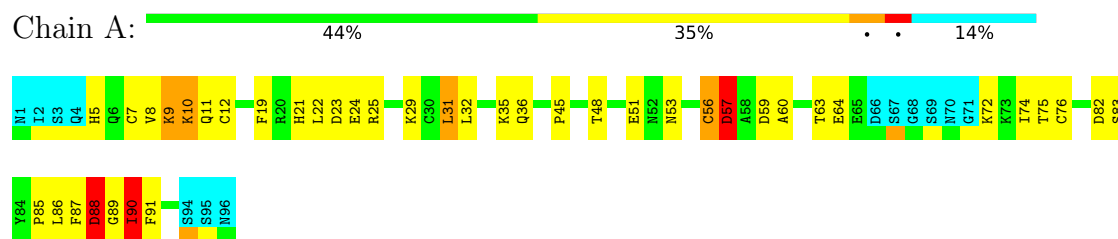
4.2.21 Score per residue for model 21

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



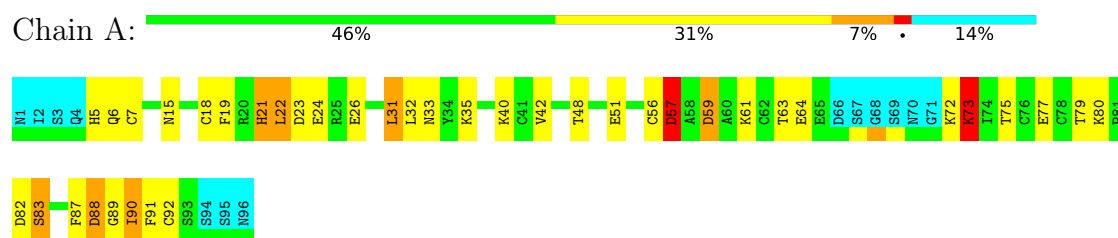
4.2.22 Score per residue for model 22

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



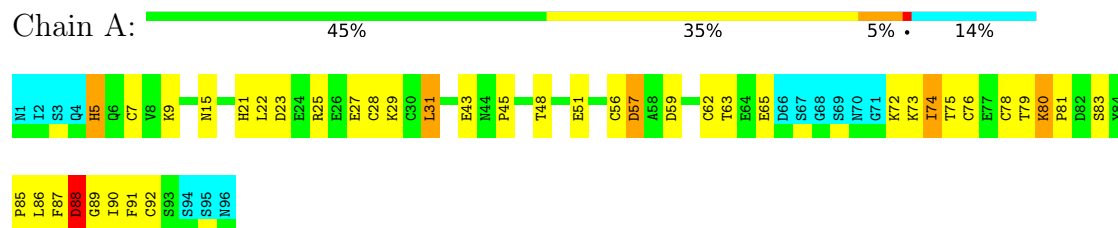
4.2.23 Score per residue for model 23

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



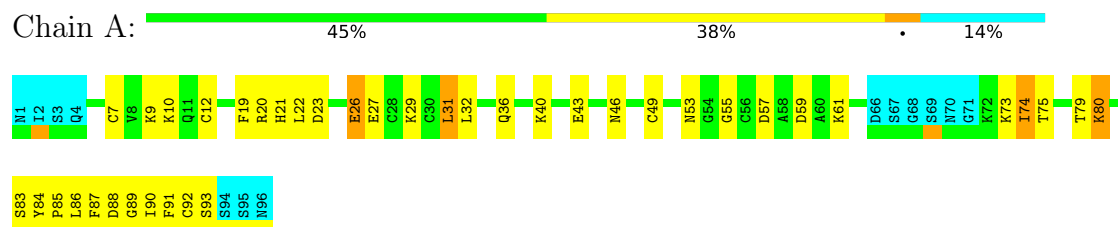
4.2.24 Score per residue for model 24

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



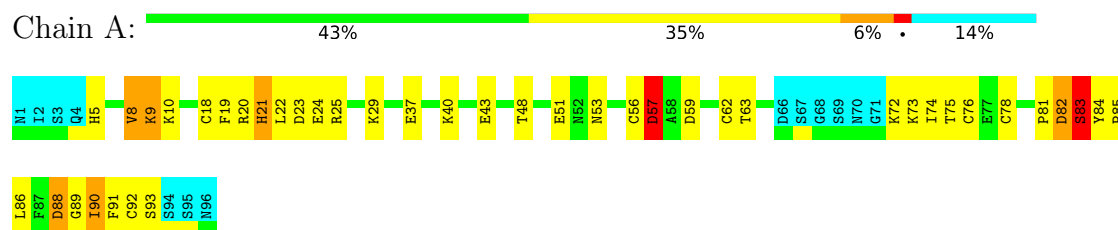
4.2.25 Score per residue for model 25

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



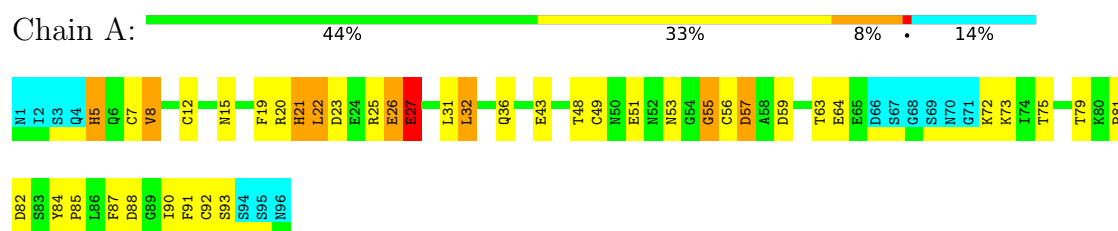
4.2.26 Score per residue for model 26

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



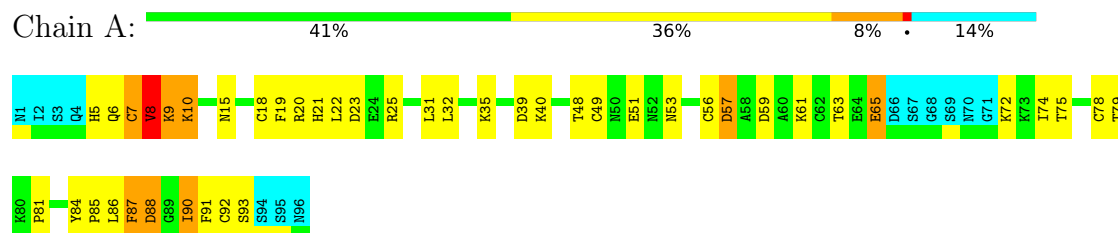
4.2.27 Score per residue for model 27

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



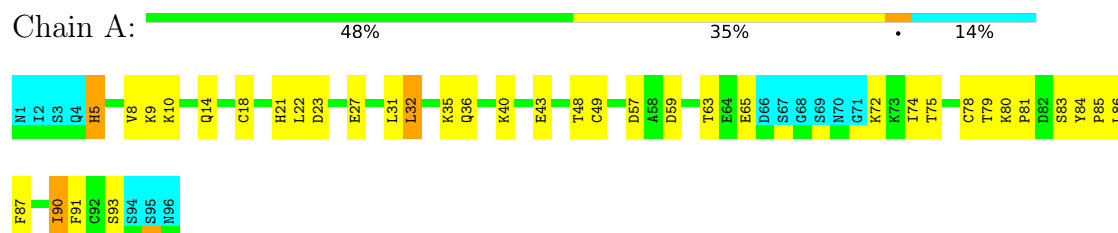
4.2.28 Score per residue for model 28

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



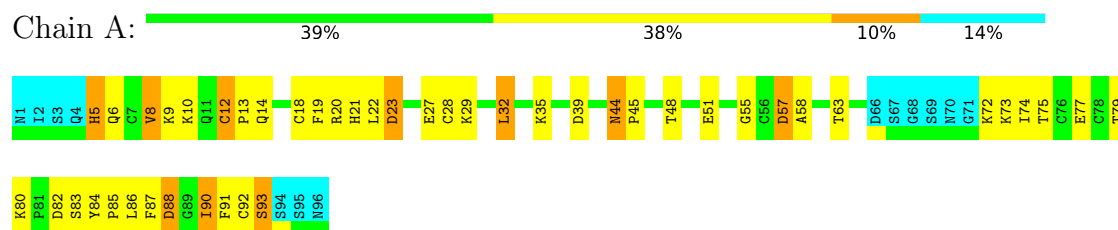
4.2.29 Score per residue for model 29

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



4.2.30 Score per residue for model 30

- Molecule 1: PROTEIN (MEROZOITE SURFACE PROTEIN 1)



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 32 were deposited, based on the following criterion: *NO RESTRAINT VIOLATIONS, ENERGY*.

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

Software name	Classification	Version
X-PLOR	refinement	3.843
X-PLOR	structure solution	3.843

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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	0.62±0.01	0±0/658 (0.0± 0.0%)	1.39±0.02	1±1/885 (0.1± 0.1%)
All	All	0.62	0/21056 (0.0%)	1.39	30/28320 (0.1%)

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	7	CYS	CB-CA-C	-5.47	109.28	115.79	16	1
1	A	12	CYS	CA-C-N	5.32	126.49	119.84	30	2
1	A	12	CYS	C-N-CA	5.32	126.49	119.84	30	2
1	A	55	GLY	N-CA-C	-5.27	108.21	114.48	17	1
1	A	84	TYR	CA-C-N	5.22	126.37	119.84	16	11
1	A	84	TYR	C-N-CA	5.22	126.37	119.84	16	11
1	A	87	PHE	CA-CB-CG	-5.11	108.69	113.80	10	2

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	646	589	589	17±4
All	All	20672	18848	18848	536

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:LEU:HD21	1:A:58:ALA:HB1	1.03	1.27	5	1
1:A:19:PHE:CE2	1:A:22:LEU:HD13	0.85	2.07	23	1
1:A:90:ILE:HD12	1:A:91:PHE:CE2	0.81	2.10	8	22
1:A:31:LEU:HD21	1:A:87:PHE:CE1	0.80	2.12	14	3
1:A:48:THR:HG21	1:A:51:GLU:CG	0.78	2.09	30	8
1:A:31:LEU:HD21	1:A:87:PHE:CE2	0.77	2.14	8	3
1:A:32:LEU:HD12	1:A:90:ILE:HG23	0.75	1.58	27	1
1:A:22:LEU:H	1:A:22:LEU:HD22	0.74	1.42	1	3
1:A:15:ASN:HA	1:A:31:LEU:HD12	0.73	1.61	15	24
1:A:22:LEU:HD12	1:A:22:LEU:H	0.73	1.44	16	7
1:A:55:GLY:O	1:A:90:ILE:HG22	0.71	1.84	25	6
1:A:90:ILE:HD11	1:A:91:PHE:CE2	0.70	2.21	23	1
1:A:5:HIS:NE2	1:A:86:LEU:HD21	0.69	2.02	7	1
1:A:86:LEU:HD12	1:A:91:PHE:CB	0.68	2.18	22	10
1:A:48:THR:HG23	1:A:51:GLU:HG2	0.68	1.65	7	8
1:A:8:VAL:HG13	1:A:26:GLU:OE1	0.68	1.89	13	1
1:A:48:THR:HG21	1:A:51:GLU:HG3	0.67	1.66	13	7
1:A:15:ASN:CA	1:A:31:LEU:HD12	0.66	2.20	5	12
1:A:31:LEU:HD23	1:A:90:ILE:CD1	0.66	2.20	12	8
1:A:31:LEU:HD21	1:A:87:PHE:CD1	0.65	2.26	14	2
1:A:5:HIS:HB2	1:A:86:LEU:HD11	0.65	1.67	14	1
1:A:87:PHE:CD1	1:A:90:ILE:HD11	0.65	2.26	32	1
1:A:32:LEU:HD21	1:A:90:ILE:HG23	0.64	1.69	22	1
1:A:86:LEU:HD12	1:A:91:PHE:HB2	0.64	1.69	25	8
1:A:22:LEU:HD21	1:A:58:ALA:CB	0.64	2.14	5	1
1:A:22:LEU:HD12	1:A:25:ARG:HB3	0.63	1.70	2	1
1:A:22:LEU:HD21	1:A:59:ASP:OD2	0.63	1.94	24	1
1:A:90:ILE:HD12	1:A:91:PHE:CE1	0.63	2.29	26	1
1:A:32:LEU:HG	1:A:90:ILE:HG22	0.63	1.70	32	1
1:A:48:THR:HG22	1:A:51:GLU:HG3	0.62	1.71	17	2
1:A:19:PHE:CZ	1:A:22:LEU:HD13	0.62	2.28	23	1
1:A:22:LEU:HD21	1:A:59:ASP:HB2	0.62	1.69	16	2
1:A:32:LEU:CD1	1:A:90:ILE:HG23	0.62	2.23	27	3
1:A:22:LEU:HD11	1:A:59:ASP:OD1	0.62	1.94	27	1
1:A:8:VAL:HG11	1:A:20:ARG:HH11	0.62	1.55	32	1
1:A:49:CYS:SG	1:A:74:ILE:HD12	0.62	2.35	29	1
1:A:8:VAL:HG22	1:A:9:LYS:H	0.61	1.55	8	1
1:A:8:VAL:HG12	1:A:9:LYS:H	0.61	1.55	28	3
1:A:8:VAL:HG11	1:A:20:ARG:NH1	0.61	2.10	32	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:LEU:HD23	1:A:22:LEU:N	0.61	2.10	27	3
1:A:32:LEU:HD21	1:A:76:CYS:SG	0.60	2.36	19	1
1:A:8:VAL:HG23	1:A:26:GLU:OE2	0.59	1.97	4	1
1:A:86:LEU:HD12	1:A:91:PHE:CE2	0.59	2.32	15	1
1:A:87:PHE:CD2	1:A:90:ILE:HD11	0.59	2.32	30	6
1:A:19:PHE:CE2	1:A:22:LEU:HD12	0.58	2.33	26	2
1:A:48:THR:HG23	1:A:49:CYS:N	0.57	2.15	17	7
1:A:22:LEU:N	1:A:22:LEU:HD12	0.57	2.15	19	8
1:A:31:LEU:HD22	1:A:87:PHE:CG	0.56	2.35	22	3
1:A:57:ASP:HB3	1:A:60:ALA:HB2	0.56	1.78	19	1
1:A:90:ILE:HD12	1:A:91:PHE:CZ	0.56	2.35	19	3
1:A:10:LYS:HZ3	1:A:28:CYS:N	0.56	1.98	16	1
1:A:48:THR:HA	1:A:74:ILE:HD11	0.55	1.78	24	1
1:A:31:LEU:HD21	1:A:87:PHE:CZ	0.54	2.37	14	1
1:A:86:LEU:HD12	1:A:91:PHE:HB3	0.54	1.78	3	3
1:A:8:VAL:HG21	1:A:25:ARG:CD	0.54	2.32	27	1
1:A:22:LEU:HD13	1:A:22:LEU:N	0.54	2.15	5	1
1:A:48:THR:HG21	1:A:51:GLU:HG2	0.54	1.79	30	6
1:A:86:LEU:HD21	1:A:93:SER:O	0.54	2.02	12	2
1:A:8:VAL:HG23	1:A:9:LYS:N	0.54	2.18	21	1
1:A:21:HIS:NE2	1:A:22:LEU:HD11	0.54	2.17	25	2
1:A:31:LEU:HD23	1:A:90:ILE:HD11	0.54	1.79	2	1
1:A:90:ILE:HD12	1:A:91:PHE:HE1	0.53	1.62	26	1
1:A:90:ILE:HD12	1:A:91:PHE:HE2	0.53	1.61	9	4
1:A:56:CYS:O	1:A:57:ASP:O	0.53	2.26	27	2
1:A:22:LEU:HD12	1:A:22:LEU:N	0.53	2.18	16	1
1:A:31:LEU:HD21	1:A:87:PHE:CD2	0.53	2.38	8	3
1:A:79:THR:O	1:A:79:THR:HG22	0.53	2.02	30	1
1:A:37:GLU:OE1	1:A:42:VAL:HG11	0.53	2.03	32	2
1:A:32:LEU:HG	1:A:90:ILE:HG21	0.53	1.80	20	2
1:A:86:LEU:HD12	1:A:91:PHE:CG	0.53	2.39	14	1
1:A:48:THR:HG22	1:A:51:GLU:CG	0.53	2.34	17	2
1:A:19:PHE:CE1	1:A:91:PHE:CD1	0.53	2.97	32	2
1:A:8:VAL:HG21	1:A:25:ARG:HD3	0.52	1.80	27	1
1:A:8:VAL:HG12	1:A:9:LYS:N	0.52	2.20	18	3
1:A:32:LEU:HD21	1:A:90:ILE:CG2	0.51	2.34	22	1
1:A:79:THR:O	1:A:79:THR:HG23	0.51	2.05	19	8
1:A:19:PHE:CD1	1:A:91:PHE:CD1	0.51	2.98	30	14
1:A:19:PHE:CE1	1:A:21:HIS:CD2	0.51	2.99	2	3
1:A:63:THR:OG1	1:A:75:THR:HG23	0.51	2.05	15	1
1:A:79:THR:HG23	1:A:79:THR:O	0.50	2.06	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:CYS:O	1:A:57:ASP:C	0.49	2.55	15	17
1:A:57:ASP:OD1	1:A:60:ALA:HB2	0.49	2.07	22	1
1:A:19:PHE:HE2	1:A:22:LEU:HD12	0.49	1.66	10	1
1:A:21:HIS:CE1	1:A:22:LEU:HD11	0.49	2.42	11	1
1:A:5:HIS:CD2	1:A:86:LEU:HD11	0.48	2.43	29	1
1:A:74:ILE:O	1:A:74:ILE:HG22	0.48	2.08	15	5
1:A:19:PHE:CZ	1:A:21:HIS:NE2	0.48	2.81	32	6
1:A:5:HIS:H	1:A:5:HIS:CD2	0.48	2.26	7	1
1:A:22:LEU:N	1:A:22:LEU:HD13	0.48	2.24	1	2
1:A:19:PHE:CZ	1:A:22:LEU:HD12	0.48	2.44	26	1
1:A:48:THR:HG22	1:A:49:CYS:N	0.48	2.23	29	2
1:A:7:CYS:C	1:A:8:VAL:HG12	0.47	2.34	6	1
1:A:19:PHE:CD1	1:A:91:PHE:CE1	0.47	3.01	30	1
1:A:22:LEU:HD22	1:A:22:LEU:N	0.47	2.21	1	2
1:A:21:HIS:C	1:A:23:ASP:H	0.47	2.16	31	1
1:A:21:HIS:H	1:A:26:GLU:CB	0.46	2.24	5	1
1:A:9:LYS:H	1:A:9:LYS:CD	0.46	2.23	22	1
1:A:5:HIS:CD2	1:A:21:HIS:CE1	0.46	3.03	11	1
1:A:5:HIS:CD2	1:A:19:PHE:CZ	0.46	3.03	27	1
1:A:32:LEU:HG	1:A:90:ILE:HG23	0.46	1.87	30	1
1:A:32:LEU:CD1	1:A:90:ILE:HG22	0.46	2.40	15	1
1:A:19:PHE:CG	1:A:91:PHE:CD1	0.46	3.04	2	2
1:A:86:LEU:HD23	1:A:86:LEU:N	0.46	2.26	15	1
1:A:87:PHE:CB	1:A:90:ILE:HD11	0.46	2.41	28	1
1:A:87:PHE:CG	1:A:90:ILE:HD11	0.46	2.45	30	3
1:A:10:LYS:HZ1	1:A:27:GLU:CA	0.46	2.24	11	1
1:A:31:LEU:CD2	1:A:87:PHE:CD2	0.46	2.99	5	3
1:A:21:HIS:N	1:A:21:HIS:CD2	0.46	2.84	26	2
1:A:5:HIS:CE1	1:A:21:HIS:ND1	0.46	2.84	32	2
1:A:86:LEU:CD1	1:A:91:PHE:CE2	0.45	2.99	15	1
1:A:85:PRO:O	1:A:86:LEU:HD23	0.45	2.11	26	1
1:A:19:PHE:CD2	1:A:20:ARG:N	0.45	2.85	27	1
1:A:48:THR:CG2	1:A:51:GLU:CG	0.45	2.94	17	6
1:A:5:HIS:CD2	1:A:86:LEU:CD1	0.45	2.99	29	2
1:A:22:LEU:H	1:A:22:LEU:CD2	0.45	2.20	18	3
1:A:91:PHE:O	1:A:91:PHE:CG	0.45	2.70	15	1
1:A:19:PHE:CG	1:A:20:ARG:N	0.45	2.84	5	1
1:A:21:HIS:CD2	1:A:21:HIS:N	0.45	2.85	6	2
1:A:5:HIS:NE2	1:A:21:HIS:CE1	0.45	2.85	11	1
1:A:21:HIS:CE1	1:A:25:ARG:HE	0.45	2.30	1	1
1:A:90:ILE:CD1	1:A:91:PHE:CE2	0.45	3.00	10	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:HIS:CE1	1:A:22:LEU:CD1	0.45	3.00	23	1
1:A:87:PHE:HB2	1:A:90:ILE:HD11	0.45	1.88	28	1
1:A:8:VAL:O	1:A:8:VAL:HG12	0.45	2.12	16	1
1:A:5:HIS:CB	1:A:86:LEU:HD11	0.44	2.41	14	1
1:A:87:PHE:CD2	1:A:90:ILE:CD1	0.44	3.00	13	2
1:A:53:ASN:C	1:A:53:ASN:OD1	0.44	2.60	28	2
1:A:31:LEU:CD2	1:A:87:PHE:CD1	0.44	3.00	9	1
1:A:55:GLY:HA2	1:A:90:ILE:HG22	0.44	1.89	18	1
1:A:32:LEU:HD12	1:A:88:ASP:HB2	0.44	1.89	28	1
1:A:48:THR:CG2	1:A:49:CYS:N	0.44	2.80	17	4
1:A:10:LYS:HZ1	1:A:26:GLU:C	0.44	2.21	11	1
1:A:48:THR:HG23	1:A:51:GLU:CG	0.44	2.39	7	3
1:A:22:LEU:CD1	1:A:58:ALA:HB3	0.44	2.42	10	1
1:A:22:LEU:N	1:A:22:LEU:CD2	0.44	2.81	30	5
1:A:83:SER:C	1:A:84:TYR:CD1	0.43	2.96	4	2
1:A:22:LEU:HD21	1:A:59:ASP:OD1	0.43	2.13	15	1
1:A:56:CYS:SG	1:A:60:ALA:HB3	0.43	2.53	22	1
1:A:31:LEU:HD22	1:A:87:PHE:CD2	0.43	2.48	29	1
1:A:53:ASN:OD1	1:A:53:ASN:C	0.43	2.61	15	8
1:A:21:HIS:O	1:A:22:LEU:HD12	0.43	2.14	9	2
1:A:86:LEU:CG	1:A:91:PHE:CE2	0.43	3.02	15	1
1:A:5:HIS:CG	1:A:86:LEU:HD11	0.43	2.49	24	1
1:A:90:ILE:O	1:A:91:PHE:CG	0.43	2.71	30	3
1:A:90:ILE:O	1:A:91:PHE:CD1	0.43	2.72	30	14
1:A:31:LEU:HD21	1:A:87:PHE:HE2	0.43	1.69	5	1
1:A:35:LYS:HG3	1:A:42:VAL:HG23	0.43	1.90	16	2
1:A:31:LEU:CD2	1:A:90:ILE:HD11	0.43	2.42	2	1
1:A:21:HIS:C	1:A:23:ASP:N	0.43	2.76	31	4
1:A:5:HIS:CD2	1:A:5:HIS:N	0.43	2.85	7	1
1:A:90:ILE:C	1:A:91:PHE:CD1	0.43	2.97	26	2
1:A:21:HIS:CE1	1:A:25:ARG:HH21	0.42	2.32	1	1
1:A:20:ARG:O	1:A:21:HIS:CG	0.42	2.73	17	5
1:A:86:LEU:HD12	1:A:91:PHE:CD2	0.42	2.49	26	1
1:A:20:ARG:C	1:A:21:HIS:CD2	0.42	2.97	3	4
1:A:53:ASN:ND2	1:A:56:CYS:N	0.42	2.67	8	1
1:A:83:SER:O	1:A:84:TYR:CD1	0.42	2.72	30	5
1:A:5:HIS:CD2	1:A:86:LEU:HD21	0.42	2.50	7	1
1:A:5:HIS:CE1	1:A:86:LEU:HD21	0.42	2.49	7	1
1:A:90:ILE:HD12	1:A:91:PHE:CD2	0.42	2.50	22	1
1:A:87:PHE:O	1:A:88:ASP:CB	0.42	2.68	23	4
1:A:84:TYR:CD1	1:A:84:TYR:N	0.42	2.84	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ASN:HD22	1:A:56:CYS:C	0.42	2.22	19	4
1:A:80:LYS:CB	1:A:81:PRO:CD	0.42	2.98	18	4
1:A:32:LEU:HD21	1:A:55:GLY:O	0.42	2.14	32	2
1:A:53:ASN:HD22	1:A:57:ASP:C	0.42	2.23	26	3
1:A:6:GLN:O	1:A:7:CYS:C	0.42	2.63	7	1
1:A:21:HIS:CG	1:A:22:LEU:N	0.42	2.88	10	1
1:A:35:LYS:HB2	1:A:35:LYS:HZ3	0.42	1.73	15	1
1:A:19:PHE:CE1	1:A:57:ASP:OD1	0.42	2.72	27	1
1:A:57:ASP:CA	1:A:90:ILE:O	0.42	2.68	30	1
1:A:84:TYR:H	1:A:93:SER:H	0.42	1.58	13	1
1:A:87:PHE:CD1	1:A:90:ILE:CD1	0.42	3.00	32	1
1:A:5:HIS:N	1:A:5:HIS:ND1	0.41	2.67	2	1
1:A:86:LEU:CD1	1:A:91:PHE:CZ	0.41	3.02	15	1
1:A:20:ARG:HA	1:A:26:GLU:HB2	0.41	1.92	25	2
1:A:22:LEU:HD21	1:A:59:ASP:CB	0.41	2.44	16	1
1:A:31:LEU:CD2	1:A:87:PHE:CG	0.41	3.03	24	1
1:A:20:ARG:C	1:A:22:LEU:H	0.41	2.23	27	1
1:A:83:SER:O	1:A:84:TYR:CD2	0.41	2.74	14	3
1:A:86:LEU:N	1:A:86:LEU:CD2	0.41	2.82	15	1
1:A:48:THR:CA	1:A:74:ILE:HD11	0.41	2.45	24	1
1:A:51:GLU:O	1:A:52:ASN:C	0.41	2.63	19	4
1:A:18:CYS:O	1:A:91:PHE:CD1	0.41	2.74	14	1
1:A:8:VAL:O	1:A:8:VAL:HG13	0.41	2.15	1	1
1:A:19:PHE:CZ	1:A:57:ASP:OD1	0.41	2.73	4	6
1:A:8:VAL:HG13	1:A:9:LYS:N	0.41	2.29	26	2
1:A:86:LEU:O	1:A:87:PHE:CD2	0.41	2.74	21	1
1:A:5:HIS:CE1	1:A:18:CYS:O	0.41	2.74	3	1
1:A:53:ASN:HD22	1:A:56:CYS:N	0.41	2.13	8	1
1:A:31:LEU:HD22	1:A:87:PHE:CD1	0.41	2.51	27	1
1:A:57:ASP:HA	1:A:90:ILE:O	0.41	2.14	30	1
1:A:26:GLU:O	1:A:27:GLU:CB	0.41	2.69	27	1
1:A:81:PRO:O	1:A:82:ASP:CB	0.41	2.69	26	1
1:A:83:SER:O	1:A:93:SER:CB	0.41	2.69	30	1
1:A:12:CYS:CB	1:A:13:PRO:CD	0.40	2.99	2	1
1:A:10:LYS:CD	1:A:11:GLN:N	0.40	2.84	15	1
1:A:53:ASN:HD22	1:A:58:ALA:CA	0.40	2.29	20	1
1:A:21:HIS:NE2	1:A:22:LEU:CD1	0.40	2.84	21	2
1:A:65:GLU:CD	1:A:65:GLU:H	0.40	2.24	28	1
1:A:5:HIS:CD2	1:A:5:HIS:O	0.40	2.74	29	1
1:A:22:LEU:H	1:A:22:LEU:CD1	0.40	2.29	29	1
1:A:90:ILE:C	1:A:91:PHE:CG	0.40	2.99	30	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LYS:NZ	1:A:26:GLU:CG	0.40	2.84	6	1
1:A:22:LEU:N	1:A:22:LEU:CD1	0.40	2.85	6	1
1:A:35:LYS:CE	1:A:42:VAL:CG2	0.40	3.00	11	1
1:A:5:HIS:ND1	1:A:6:GLN:N	0.40	2.70	19	1
1:A:29:LYS:NZ	1:A:53:ASN:ND2	0.40	2.69	19	1
1:A:10:LYS:CB	1:A:10:LYS:NZ	0.40	2.84	20	1
1:A:19:PHE:CE2	1:A:21:HIS:NE2	0.40	2.85	21	1
1:A:8:VAL:HG13	1:A:26:GLU:OE2	0.40	2.16	32	1
1:A:31:LEU:CD2	1:A:90:ILE:CD1	0.40	2.99	27	1
1:A:86:LEU:C	1:A:87:PHE:CD1	0.40	2.99	10	1
1:A:57:ASP:HB3	1:A:60:ALA:CB	0.40	2.47	12	1
1:A:80:LYS:N	1:A:80:LYS:CD	0.40	2.84	21	1
1:A:52:ASN:O	1:A:53:ASN:CB	0.40	2.70	12	1
1:A:20:ARG:CG	1:A:25:ARG:N	0.40	2.85	14	1
1:A:22:LEU:HD21	1:A:59:ASP:CG	0.40	2.40	15	1
1:A:44:ASN:HD22	1:A:45:PRO:CD	0.40	2.29	30	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	83/96 (86%)	58±3 (69±4%)	19±3 (23±4%)	7±2 (8±2%)	1	14
All	All	2656/3072 (86%)	1843 (69%)	603 (23%)	210 (8%)	1	14

All 37 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	57	ASP	23
1	A	85	PRO	23
1	A	8	VAL	16
1	A	81	PRO	16
1	A	83	SER	12
1	A	45	PRO	10

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Mol	Chain	Res	Type	Models (Total)
1	A	7	CYS	9
1	A	88	ASP	9
1	A	89	GLY	9
1	A	31	LEU	7
1	A	6	GLN	7
1	A	55	GLY	7
1	A	87	PHE	5
1	A	93	SER	5
1	A	25	ARG	4
1	A	73	LYS	4
1	A	21	HIS	4
1	A	9	LYS	3
1	A	20	ARG	3
1	A	5	HIS	3
1	A	11	GLN	3
1	A	26	GLU	3
1	A	65	GLU	3
1	A	12	CYS	3
1	A	10	LYS	3
1	A	23	ASP	2
1	A	27	GLU	2
1	A	13	PRO	2
1	A	92	CYS	2
1	A	78	CYS	1
1	A	72	LYS	1
1	A	53	ASN	1
1	A	47	PRO	1
1	A	14	GLN	1
1	A	90	ILE	1
1	A	58	ALA	1
1	A	38	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	76/87 (87%)	53±3 (70±4%)	23±3 (30±4%)	1 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2432/2784 (87%)	1697 (70%)	735 (30%)	1 16

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	63	THR	29
1	A	75	THR	28
1	A	10	LYS	24
1	A	72	LYS	24
1	A	23	ASP	22
1	A	35	LYS	22
1	A	74	ILE	21
1	A	88	ASP	21
1	A	32	LEU	19
1	A	73	LYS	19
1	A	57	ASP	18
1	A	59	ASP	17
1	A	93	SER	17
1	A	36	GLN	17
1	A	27	GLU	16
1	A	43	GLU	16
1	A	83	SER	16
1	A	90	ILE	16
1	A	18	CYS	15
1	A	40	LYS	15
1	A	80	LYS	15
1	A	29	LYS	15
1	A	7	CYS	14
1	A	25	ARG	14
1	A	5	HIS	13
1	A	9	LYS	13
1	A	78	CYS	13
1	A	61	LYS	13
1	A	64	GLU	13
1	A	24	GLU	12
1	A	39	ASP	11
1	A	92	CYS	11
1	A	53	ASN	11
1	A	21	HIS	11
1	A	82	ASP	11
1	A	12	CYS	10

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Mol	Chain	Res	Type	Models (Total)
1	A	11	GLN	10
1	A	28	CYS	9
1	A	46	ASN	9
1	A	26	GLU	9
1	A	6	GLN	9
1	A	56	CYS	9
1	A	22	LEU	8
1	A	8	VAL	7
1	A	49	CYS	7
1	A	37	GLU	7
1	A	76	CYS	7
1	A	16	SER	6
1	A	62	CYS	6
1	A	52	ASN	5
1	A	77	GLU	5
1	A	14	GLN	5
1	A	79	THR	4
1	A	65	GLU	4
1	A	20	ARG	3
1	A	33	ASN	3
1	A	50	ASN	3
1	A	84	TYR	2
1	A	30	CYS	2
1	A	15	ASN	1
1	A	86	LEU	1
1	A	91	PHE	1
1	A	44	ASN	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 oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided