



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 02:23 PM UTC

PDB ID : 1BA9 / pdb_00001ba9
Title : THE SOLUTION STRUCTURE OF REDUCED MONOMERIC SUPEROXIDE DISMUTASE, NMR, 36 STRUCTURES
Authors : Banci, L.; Benedetto, M.; Bertini, I.; Del Conte, R.; Piccioli, M.; Viezzoli, M.S.
Deposited on : 1998-04-24

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

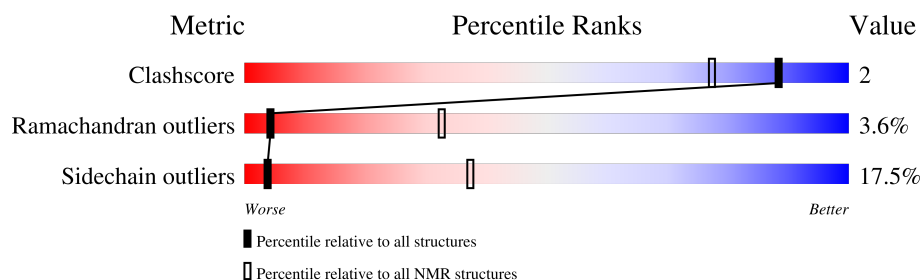
1 Overall quality at a glance

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	153	72% 13% 15%

2 Ensemble composition and analysis

This entry contains 36 models. Model 30 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:3-A:21, A:28-A:49, A:62-A:106, A:110-A:153 (130)	0.59	30

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 5 single-model clusters were found.

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2194 atoms, of which 1080 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms						Trace
1	A	153	Total	C	H	N	O	S	0
			2192	678	1080	204	228	2	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	CYS	engineered mutation	UNP P00441
A	50	GLU	PHE	engineered mutation	UNP P00441
A	51	GLU	GLY	engineered mutation	UNP P00441
A	111	SER	CYS	engineered mutation	UNP P00441
A	133	GLN	GLU	engineered mutation	UNP P00441

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

- Molecule 3 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

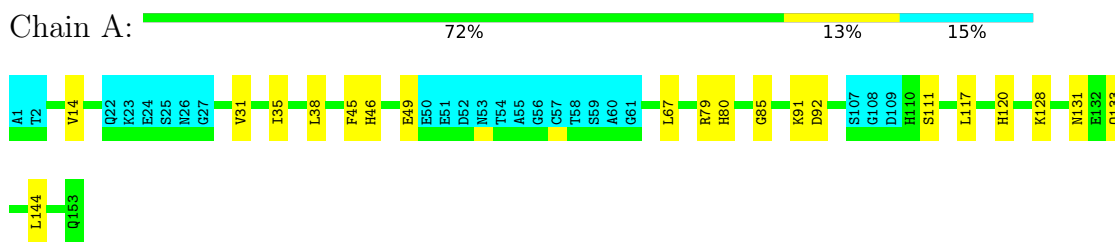
Mol	Chain	Residues	Atoms	
3	A	1	Total	Cu
			1	1

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: SUPEROXIDE DISMUTASE

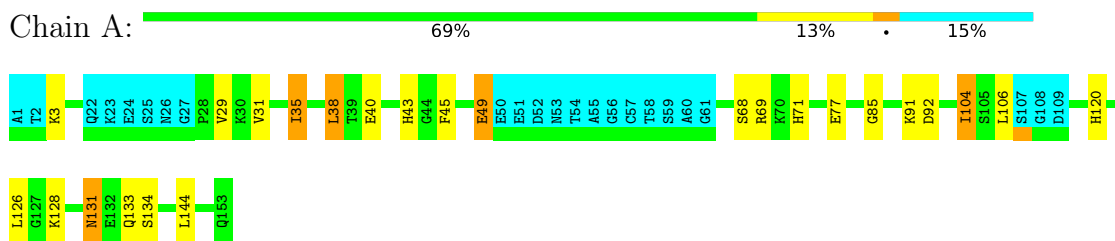


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

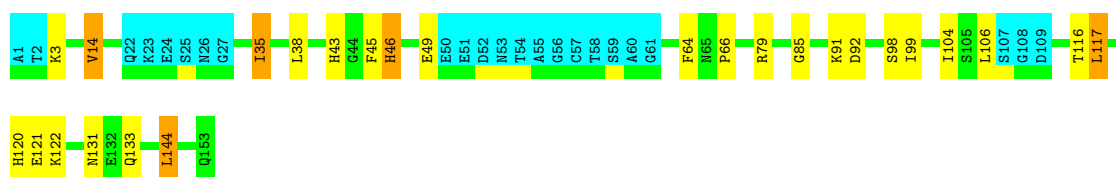
• Molecule 1: SUPEROXIDE DISMUTASE



4.2.2 Score per residue for model 2

• Molecule 1: SUPEROXIDE DISMUTASE

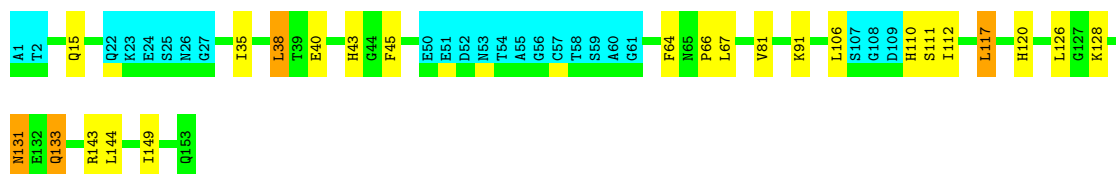




4.2.3 Score per residue for model 3

- Molecule 1: SUPEROXIDE DISMUTASE

Chain A: 69% 13% 15%



4.2.4 Score per residue for model 4

- Molecule 1: SUPEROXIDE DISMUTASE

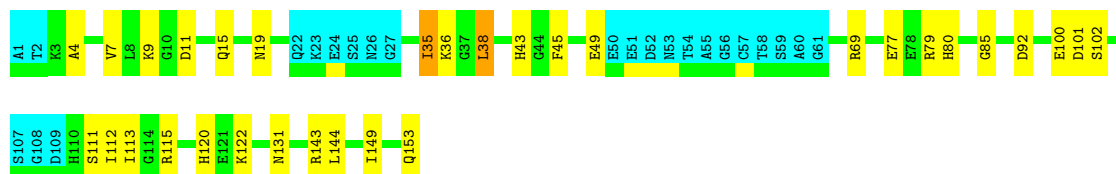
Chain A: 67% 16% 15%



4.2.5 Score per residue for model 5

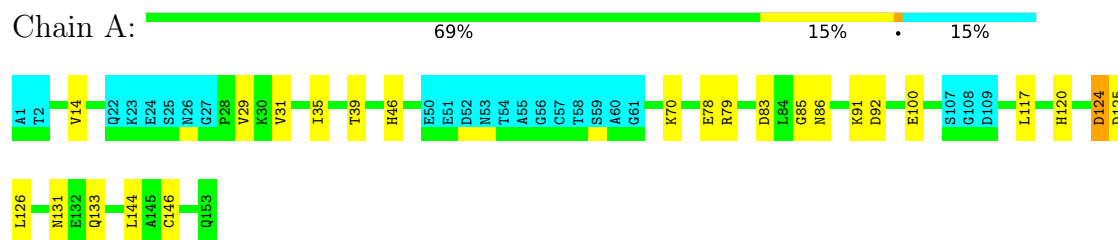
- Molecule 1: SUPEROXIDE DISMUTASE

Chain A: 64% 20% 15%



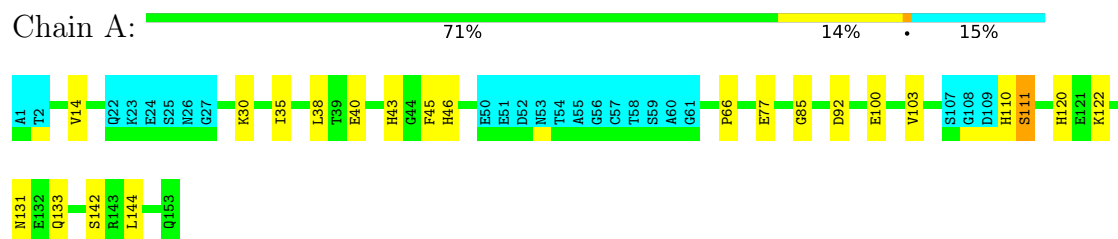
4.2.6 Score per residue for model 6

- Molecule 1: SUPEROXIDE DISMUTASE



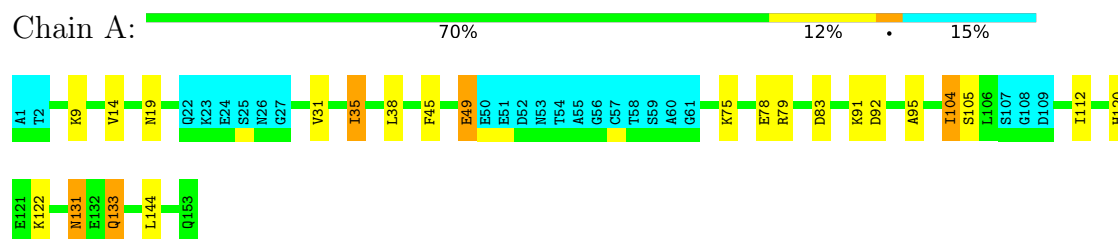
4.2.7 Score per residue for model 7

- Molecule 1: SUPEROXIDE DISMUTASE



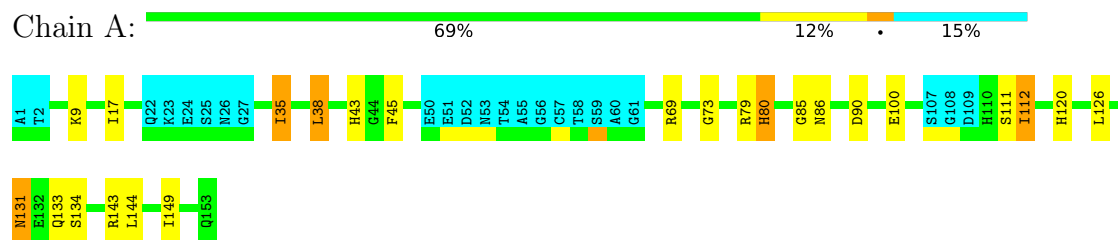
4.2.8 Score per residue for model 8

- Molecule 1: SUPEROXIDE DISMUTASE



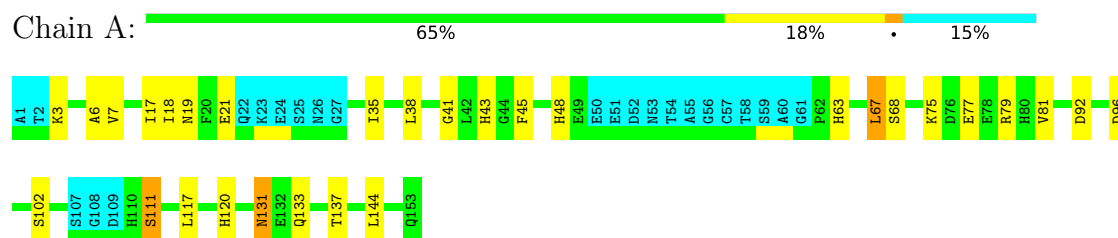
4.2.9 Score per residue for model 9

- Molecule 1: SUPEROXIDE DISMUTASE



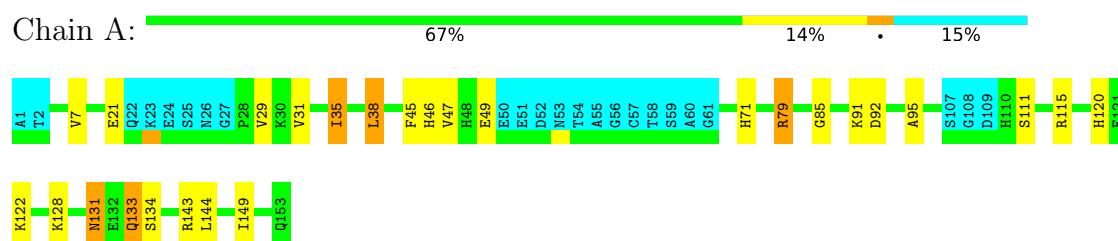
4.2.10 Score per residue for model 10

• Molecule 1: SUPEROXIDE DISMUTASE



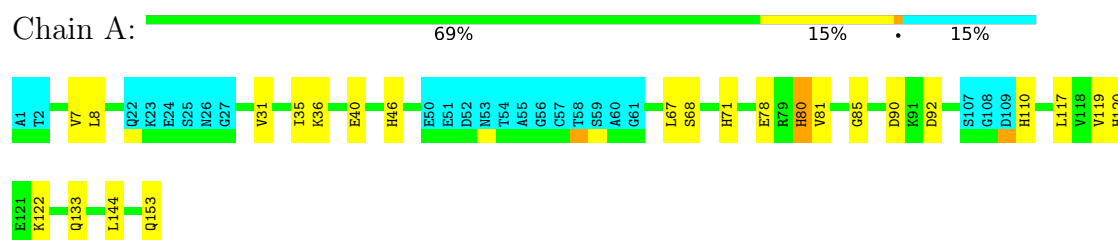
4.2.11 Score per residue for model 11

• Molecule 1: SUPEROXIDE DISMUTASE



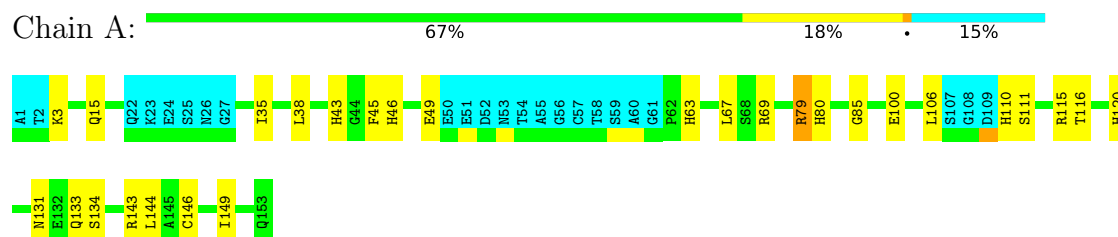
4.2.12 Score per residue for model 12

• Molecule 1: SUPEROXIDE DISMUTASE



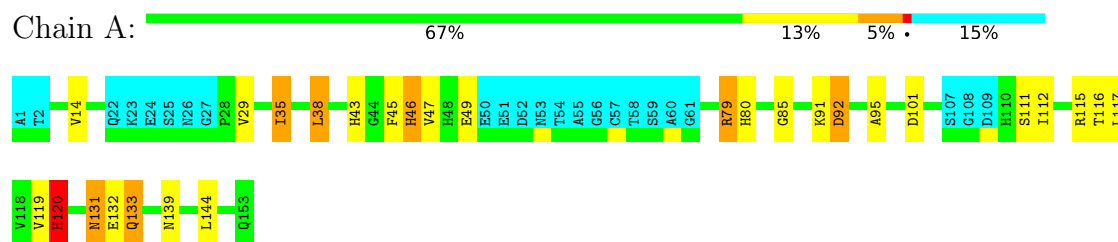
4.2.13 Score per residue for model 13

• Molecule 1: SUPEROXIDE DISMUTASE



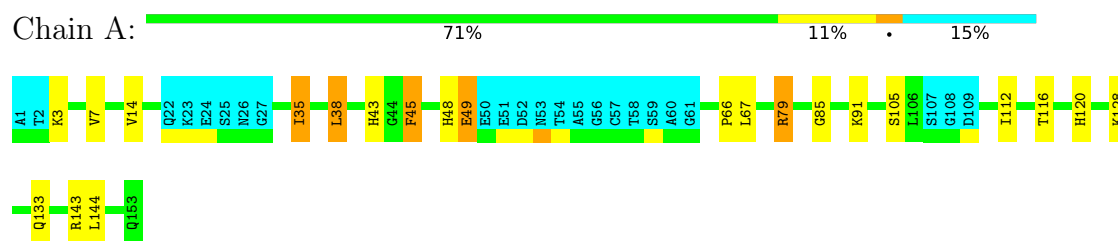
4.2.14 Score per residue for model 14

• Molecule 1: SUPEROXIDE DISMUTASE



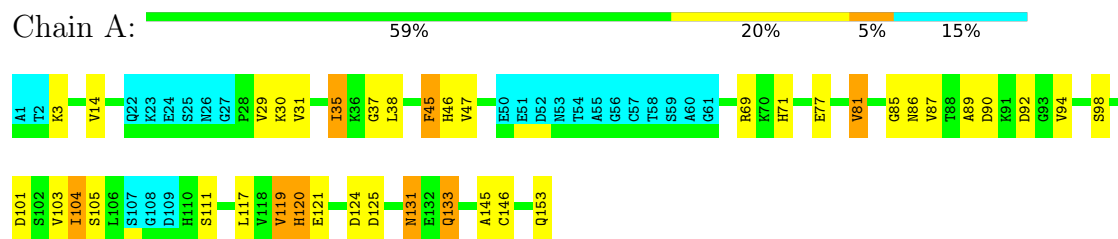
4.2.15 Score per residue for model 15

• Molecule 1: SUPEROXIDE DISMUTASE



4.2.16 Score per residue for model 16

• Molecule 1: SUPEROXIDE DISMUTASE



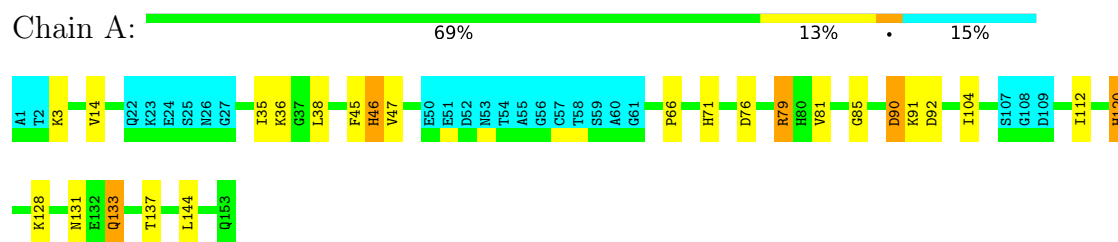
4.2.17 Score per residue for model 17

• Molecule 1: SUPEROXIDE DISMUTASE



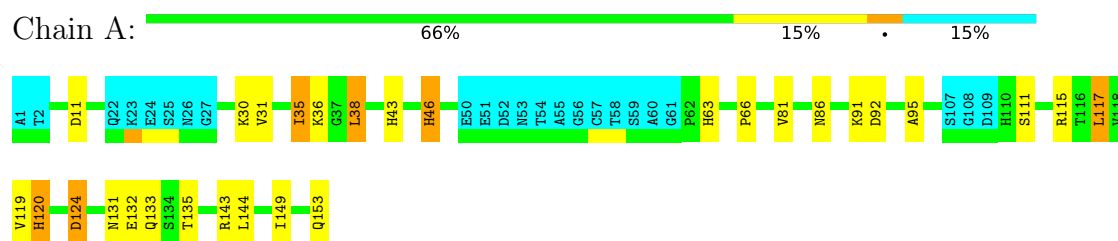
4.2.18 Score per residue for model 18

- Molecule 1: SUPEROXIDE DISMUTASE



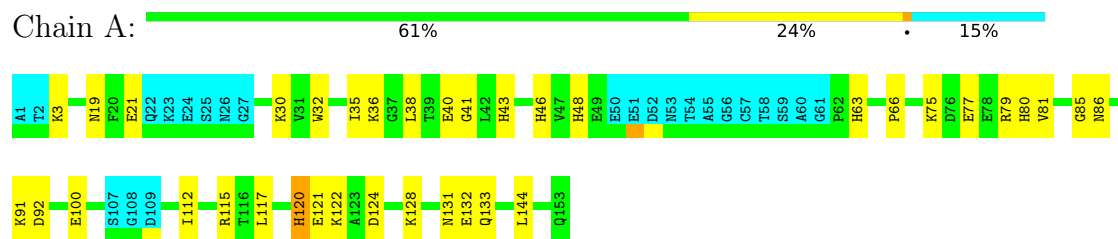
4.2.19 Score per residue for model 19

- Molecule 1: SUPEROXIDE DISMUTASE



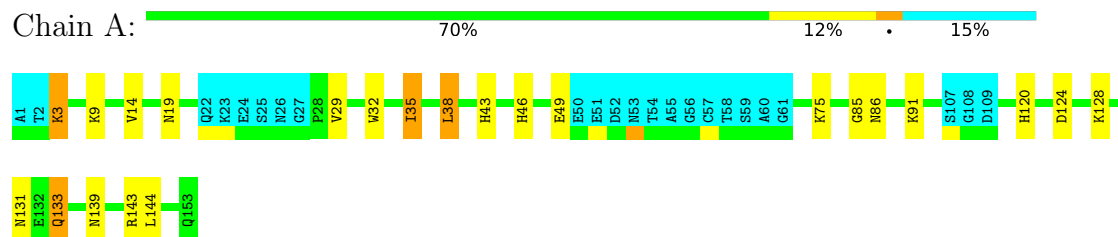
4.2.20 Score per residue for model 20

- Molecule 1: SUPEROXIDE DISMUTASE



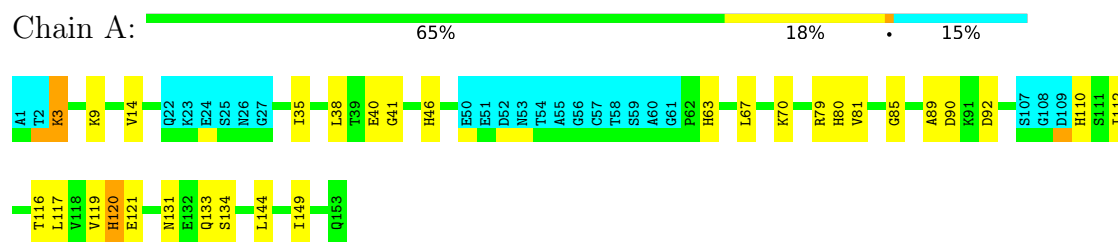
4.2.21 Score per residue for model 21

- Molecule 1: SUPEROXIDE DISMUTASE



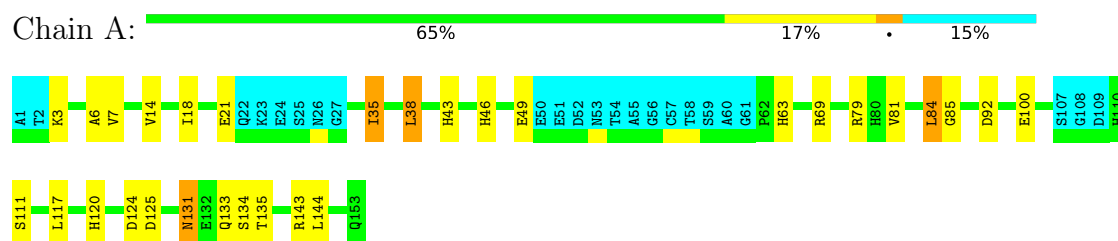
4.2.22 Score per residue for model 22

• Molecule 1: SUPEROXIDE DISMUTASE



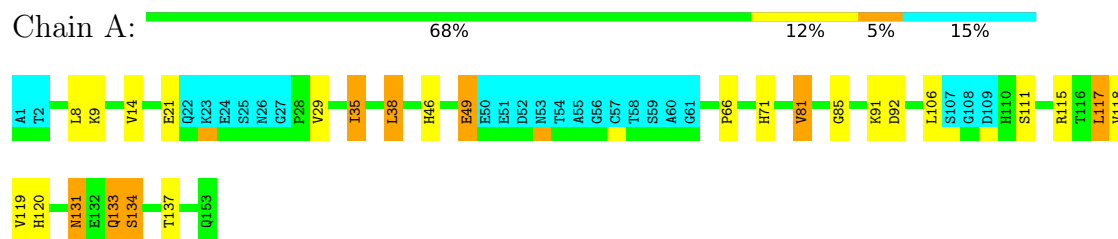
4.2.23 Score per residue for model 23

• Molecule 1: SUPEROXIDE DISMUTASE



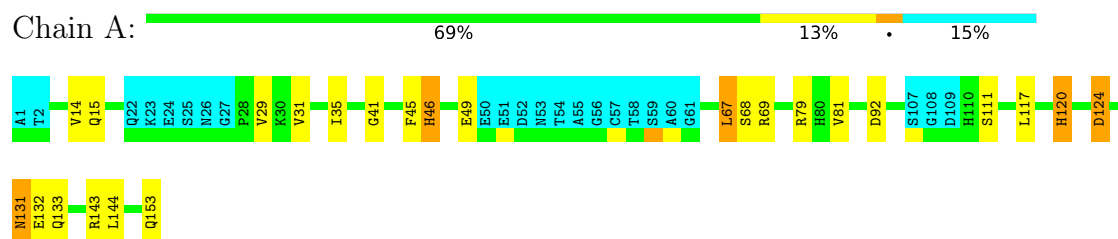
4.2.24 Score per residue for model 24

• Molecule 1: SUPEROXIDE DISMUTASE



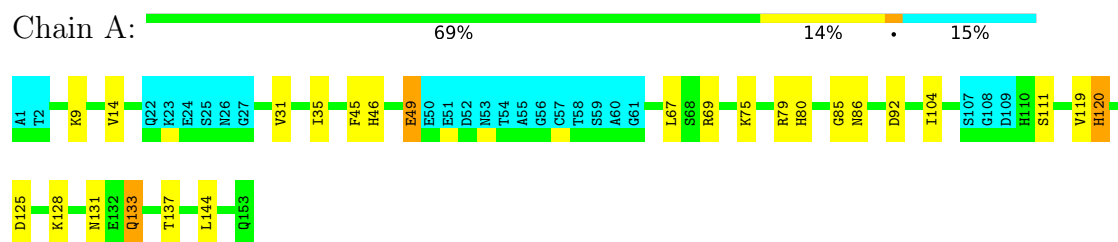
4.2.25 Score per residue for model 25

• Molecule 1: SUPEROXIDE DISMUTASE



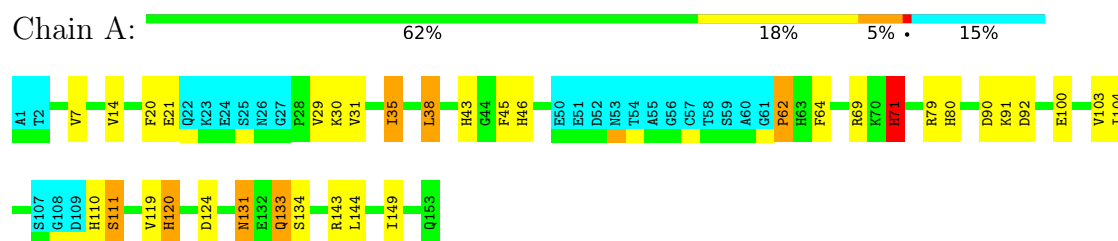
4.2.26 Score per residue for model 26

• Molecule 1: SUPEROXIDE DISMUTASE



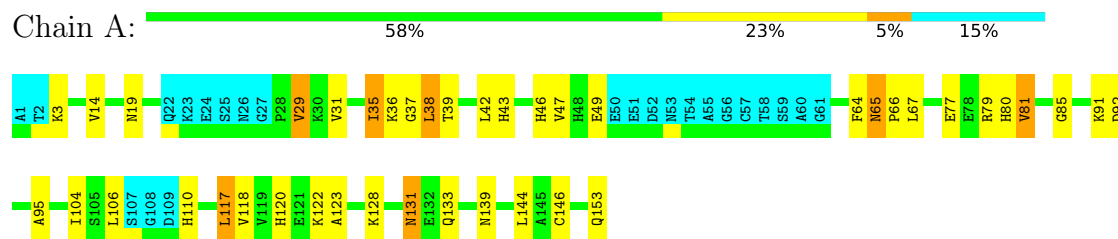
4.2.27 Score per residue for model 27

• Molecule 1: SUPEROXIDE DISMUTASE



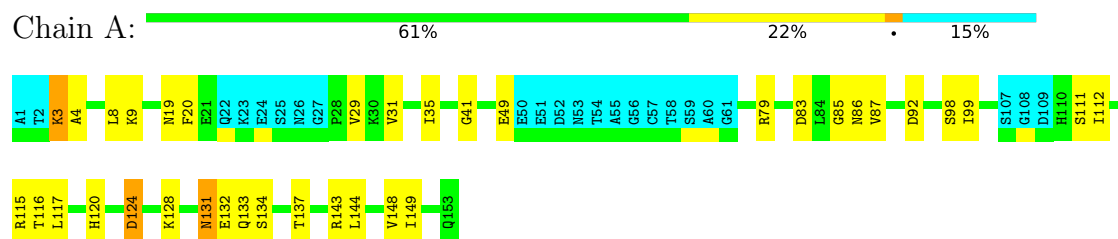
4.2.28 Score per residue for model 28

• Molecule 1: SUPEROXIDE DISMUTASE



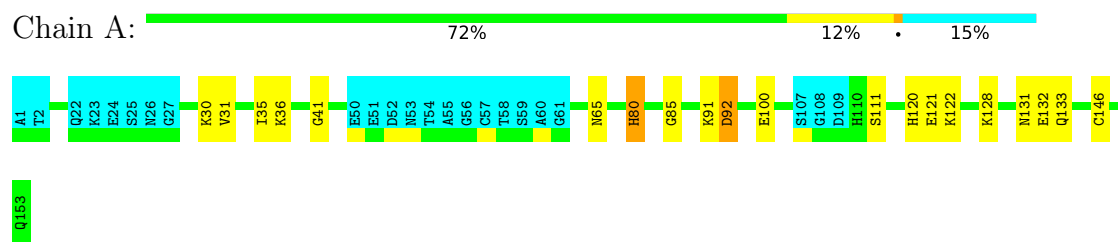
4.2.29 Score per residue for model 29

• Molecule 1: SUPEROXIDE DISMUTASE



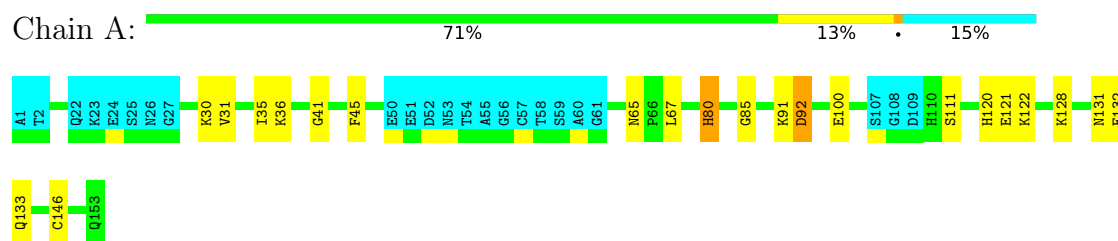
4.2.30 Score per residue for model 30 (medoid)

- Molecule 1: SUPEROXIDE DISMUTASE



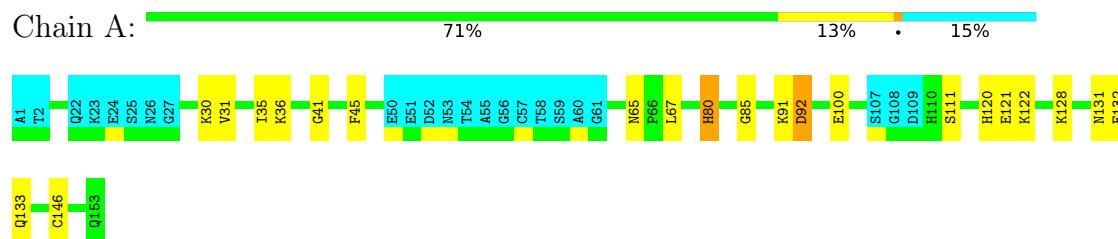
4.2.31 Score per residue for model 31

- Molecule 1: SUPEROXIDE DISMUTASE



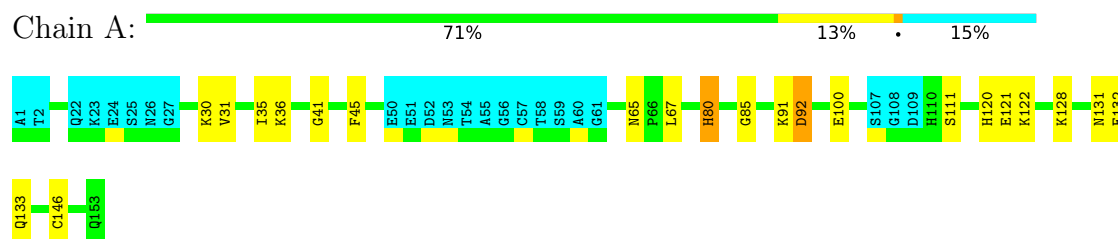
4.2.32 Score per residue for model 32

- Molecule 1: SUPEROXIDE DISMUTASE



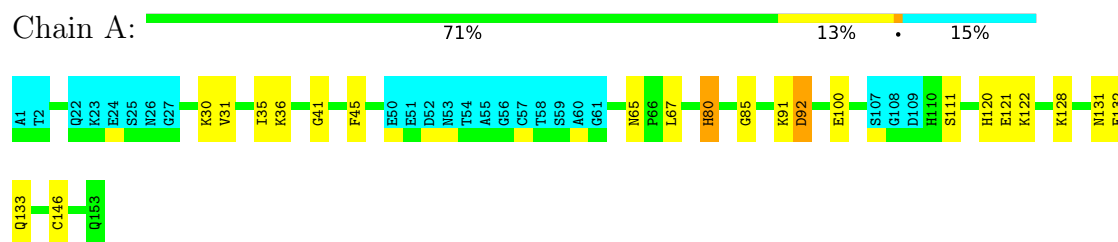
4.2.33 Score per residue for model 33

- Molecule 1: SUPEROXIDE DISMUTASE



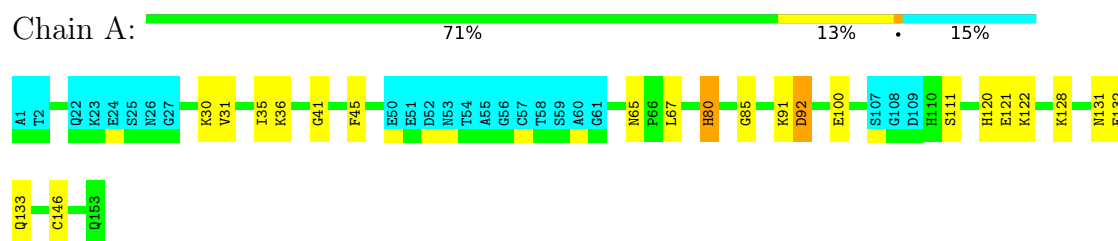
4.2.34 Score per residue for model 34

- Molecule 1: SUPEROXIDE DISMUTASE



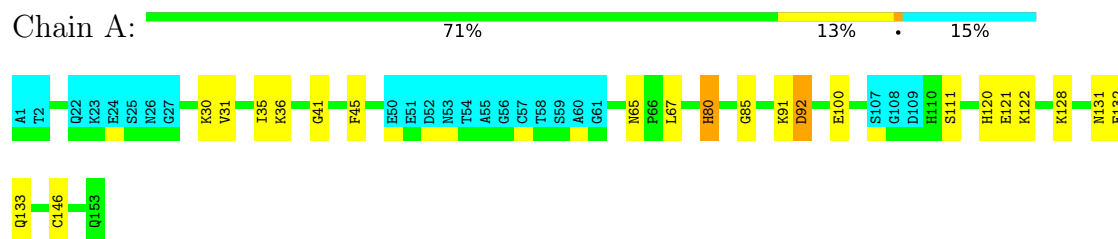
4.2.35 Score per residue for model 35

- Molecule 1: SUPEROXIDE DISMUTASE



4.2.36 Score per residue for model 36

- Molecule 1: SUPEROXIDE DISMUTASE



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORTION ANGLES DYNAMIC (DYANA)*.

Of the 36 calculated structures, 36 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
Amber	refinement	4.0
XEASY (ETH	structure solution	(ETH
ZURICH)	structure solution	

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: CU1, ZN

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	0.65±0.01	0±0/976 (0.0± 0.0%)	1.28±0.03	2±1/1314 (0.2± 0.1%)
All	All	0.65	0/35136 (0.0%)	1.28	71/47304 (0.2%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.2	0.8±0.7
All	All	1	28

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	120	HIS	CB-CG-CD2	-8.71	119.87	131.20	20	36
1	A	124	ASP	CA-CB-CG	7.47	120.07	112.60	29	3
1	A	41	GLY	N-CA-C	-6.43	104.52	111.21	10	12
1	A	63	HIS	CA-CB-CG	5.85	119.65	113.80	23	2
1	A	64	PHE	CA-CB-CG	5.82	119.62	113.80	27	3
1	A	71	HIS	CB-CG-CD2	-5.67	123.83	131.20	27	2
1	A	133	GLN	CA-C-N	5.63	128.62	120.79	11	1
1	A	133	GLN	C-N-CA	5.63	128.62	120.79	11	1
1	A	104	ILE	CA-CB-CG1	5.54	119.82	110.40	8	1
1	A	48	HIS	CB-CG-CD2	-5.21	124.43	131.20	10	3
1	A	124	ASP	CB-CA-C	5.10	118.17	109.80	19	1
1	A	90	ASP	CA-C-N	5.09	128.82	120.63	18	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	90	ASP	C-N-CA	5.09	128.82	120.63	18	1
1	A	80	HIS	CB-CG-CD2	-5.08	124.59	131.20	4	2
1	A	68	SER	CA-C-O	5.05	120.87	117.94	10	1
1	A	120	HIS	CB-CG-ND1	5.02	130.22	122.70	20	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	62	PRO	CA	1

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	80	HIS	Sidechain,Peptide	11
1	A	71	HIS	Sidechain	8
1	A	115	ARG	Sidechain	4
1	A	45	PHE	Sidechain	2
1	A	64	PHE	Sidechain	1
1	A	79	ARG	Sidechain	1
1	A	62	PRO	Peptide	1

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	959	952	951	4±2
All	All	34596	34272	34236	130

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ILE:HG21	1:A:38:LEU:HD23	0.71	1.61	1	12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LEU:HD12	1:A:43:HIS:CE1	0.63	2.27	2	14
1:A:14:VAL:HG23	1:A:38:LEU:HD22	0.62	1.70	2	1
1:A:117:LEU:CD1	1:A:149:ILE:HD11	0.62	2.24	22	1
1:A:117:LEU:HD13	1:A:149:ILE:HD11	0.60	1.74	22	1
1:A:42:LEU:HG	1:A:123:ALA:HB2	0.57	1.76	4	3
1:A:35:ILE:HG22	1:A:95:ALA:H	0.56	1.60	17	6
1:A:8:LEU:HD11	1:A:117:LEU:HD23	0.53	1.80	24	1
1:A:112:ILE:HG12	1:A:149:ILE:HG21	0.51	1.82	9	1
1:A:14:VAL:HG21	1:A:144:LEU:HB3	0.51	1.82	2	1
1:A:81:VAL:HG13	1:A:104:ILE:HG22	0.50	1.82	16	1
1:A:131:ASN:ND2	1:A:134:SER:H	0.49	2.06	23	4
1:A:45:PHE:CE1	1:A:117:LEU:HD12	0.49	2.42	16	1
1:A:115:ARG:HG2	1:A:149:ILE:HD12	0.48	1.86	13	1
1:A:115:ARG:HB2	1:A:149:ILE:HD12	0.47	1.85	11	2
1:A:70:LYS:NZ	1:A:78:GLU:OE2	0.47	2.47	6	1
1:A:46:HIS:CE1	1:A:63:HIS:CE1	0.46	3.03	19	2
1:A:115:ARG:CG	1:A:149:ILE:HD12	0.46	2.40	13	1
1:A:38:LEU:HD23	1:A:89:ALA:HB2	0.46	1.87	16	2
1:A:35:ILE:HG21	1:A:38:LEU:HD22	0.46	1.86	11	1
1:A:4:ALA:HB3	1:A:20:PHE:HB2	0.46	1.88	29	1
1:A:35:ILE:CG2	1:A:38:LEU:HD23	0.45	2.41	2	2
1:A:35:ILE:O	1:A:94:VAL:HG13	0.45	2.11	16	1
1:A:45:PHE:CZ	1:A:117:LEU:HD22	0.45	2.46	2	1
1:A:46:HIS:O	1:A:117:LEU:HD23	0.45	2.12	2	1
1:A:20:PHE:CE1	1:A:31:VAL:HG22	0.45	2.47	27	1
1:A:117:LEU:HD13	1:A:118:VAL:N	0.45	2.26	28	1
1:A:117:LEU:HD12	1:A:149:ILE:HD11	0.45	1.87	3	1
1:A:6:ALA:HB3	1:A:18:ILE:HB	0.44	1.89	10	2
1:A:131:ASN:ND2	1:A:131:ASN:C	0.44	2.75	25	12
1:A:91:LYS:NZ	1:A:92:ASP:OD1	0.44	2.50	14	1
1:A:73:GLY:HA3	1:A:126:LEU:HD22	0.43	1.90	9	1
1:A:38:LEU:HD23	1:A:43:HIS:CG	0.43	2.48	13	1
1:A:76:ASP:OD1	1:A:128:LYS:NZ	0.43	2.51	17	1
1:A:84:LEU:N	1:A:84:LEU:HD22	0.43	2.28	23	1
1:A:36:LYS:NZ	1:A:92:ASP:OD2	0.43	2.52	30	8
1:A:43:HIS:CE1	1:A:121:GLU:O	0.42	2.72	20	2
1:A:69:ARG:NH2	1:A:77:GLU:OE2	0.42	2.53	16	1
1:A:115:ARG:O	1:A:149:ILE:HD12	0.42	2.14	17	1
1:A:3:LYS:NZ	1:A:21:GLU:OE2	0.42	2.52	23	1
1:A:30:LYS:NZ	1:A:100:GLU:OE2	0.42	2.46	27	2
1:A:131:ASN:HD22	1:A:131:ASN:C	0.42	2.23	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ILE:HG21	1:A:38:LEU:HB2	0.42	1.92	23	1
1:A:65:ASN:N	1:A:66:PRO:CD	0.42	2.83	28	1
1:A:65:ASN:HD21	1:A:80:HIS:CD2	0.42	2.33	30	7
1:A:17:ILE:HD12	1:A:17:ILE:N	0.42	2.30	10	1
1:A:46:HIS:CE1	1:A:120:HIS:CD2	0.41	3.08	18	3
1:A:4:ALA:HB2	1:A:113:ILE:CD1	0.41	2.45	5	1
1:A:125:ASP:OD2	1:A:128:LYS:NZ	0.41	2.51	26	1
1:A:38:LEU:HD21	1:A:43:HIS:CG	0.41	2.50	23	1
1:A:76:ASP:OD2	1:A:128:LYS:NZ	0.41	2.53	18	1
1:A:8:LEU:CD1	1:A:117:LEU:HD23	0.41	2.46	12	1
1:A:45:PHE:C	1:A:46:HIS:CG	0.41	2.98	17	1
1:A:110:HIS:O	1:A:111:SER:C	0.41	2.64	27	2
1:A:46:HIS:NE2	1:A:124:ASP:OD2	0.41	2.54	21	1
1:A:45:PHE:CE1	1:A:117:LEU:HD22	0.41	2.51	2	1
1:A:38:LEU:HD12	1:A:43:HIS:NE2	0.41	2.31	10	1
1:A:131:ASN:C	1:A:131:ASN:HD22	0.41	2.24	14	1
1:A:4:ALA:HB2	1:A:113:ILE:HD11	0.40	1.93	17	1
1:A:119:VAL:CG1	1:A:145:ALA:HB3	0.40	2.46	16	1
1:A:117:LEU:HD12	1:A:149:ILE:CD1	0.40	2.47	19	1
1:A:71:HIS:HE2	1:A:124:ASP:CG	0.40	2.24	27	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	129/153 (84%)	109±3 (84±2%)	16±3 (12±2%)	5±2 (4±1%)	4	32
All	All	4644/5508 (84%)	3909 (84%)	568 (12%)	167 (4%)	4	32

All 26 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	85	GLY	29
1	A	111	SER	23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	14	VAL	18
1	A	79	ARG	18
1	A	66	PRO	10
1	A	132	GLU	10
1	A	133	GLN	9
1	A	80	HIS	8
1	A	49	GLU	7
1	A	120	HIS	7
1	A	3	LYS	4
1	A	81	VAL	3
1	A	110	HIS	3
1	A	67	LEU	2
1	A	68	SER	2
1	A	37	GLY	2
1	A	87	VAL	2
1	A	38	LEU	2
1	A	104	ILE	1
1	A	125	ASP	1
1	A	105	SER	1
1	A	134	SER	1
1	A	62	PRO	1
1	A	65	ASN	1
1	A	8	LEU	1
1	A	9	LYS	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	102/118 (86%)	84±4 (82±4%)	18±4 (17±4%)	4	37
All	All	3652/4248 (86%)	3014 (83%)	638 (17%)	4	37

All 76 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	35	ILE	36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	133	GLN	35
1	A	131	ASN	33
1	A	92	ASP	30
1	A	144	LEU	27
1	A	45	PHE	23
1	A	91	LYS	21
1	A	46	HIS	19
1	A	31	VAL	18
1	A	67	LEU	17
1	A	122	LYS	16
1	A	38	LEU	15
1	A	128	LYS	15
1	A	100	GLU	14
1	A	49	GLU	13
1	A	117	LEU	13
1	A	143	ARG	12
1	A	146	CYS	12
1	A	29	VAL	11
1	A	3	LYS	11
1	A	81	VAL	11
1	A	112	ILE	11
1	A	30	LYS	10
1	A	124	ASP	9
1	A	86	ASN	9
1	A	121	GLU	9
1	A	40	GLU	8
1	A	69	ARG	8
1	A	104	ILE	8
1	A	9	LYS	8
1	A	19	ASN	8
1	A	119	VAL	8
1	A	90	ASP	7
1	A	7	VAL	7
1	A	77	GLU	6
1	A	106	LEU	6
1	A	153	GLN	6
1	A	75	LYS	6
1	A	79	ARG	6
1	A	134	SER	5
1	A	137	THR	5
1	A	47	VAL	5
1	A	36	LYS	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	116	THR	5
1	A	126	LEU	4
1	A	15	GLN	4
1	A	21	GLU	4
1	A	139	ASN	4
1	A	101	ASP	4
1	A	98	SER	3
1	A	83	ASP	3
1	A	103	VAL	3
1	A	105	SER	3
1	A	32	TRP	3
1	A	99	ILE	2
1	A	110	HIS	2
1	A	111	SER	2
1	A	11	ASP	2
1	A	102	SER	2
1	A	39	THR	2
1	A	125	ASP	2
1	A	78	GLU	2
1	A	63	HIS	2
1	A	132	GLU	2
1	A	70	LYS	2
1	A	115	ARG	2
1	A	135	THR	2
1	A	149	ILE	2
1	A	68	SER	1
1	A	142	SER	1
1	A	17	ILE	1
1	A	96	ASP	1
1	A	84	LEU	1
1	A	118	VAL	1
1	A	64	PHE	1
1	A	148	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 [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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