



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 08:12 PM BST

PDB ID : 2AF2
Title : Solution structure of disulfide reduced and copper depleted Human Superoxide Dismutase
Authors : Banci, L.; Bertini, I.; Cantini, F.; D'Amelio, N.; Gaggelli, E.; Structural Proteomics in Europe (SPINE)
Deposited on : 2005-07-25

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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

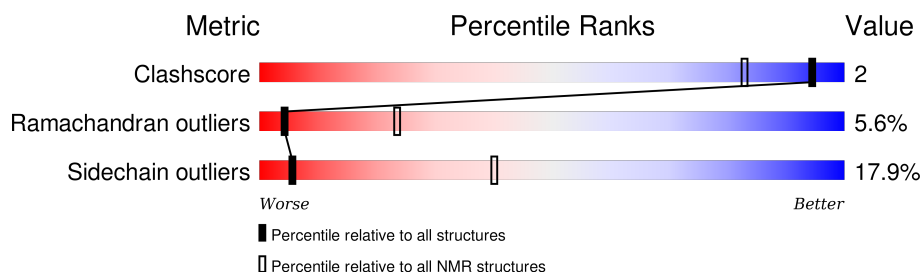
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 85%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	 85% 14% ..
1	B	153	 84% 12% ..

2 Ensemble composition and analysis ⓘ

This entry contains 30 models. Model 23 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:2-A:153, B:1-B:54, B:60-B:153 (300)	1.12	23

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 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4375 atoms, of which 2157 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms						Trace
1	A	153	Total	C	H	N	O	S	0
			2188	679	1080	203	224	2	
1	B	153	Total	C	H	N	O	S	0
			2185	679	1077	203	224	2	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	CYS	ENGINEERED	UNP P00441
A	111	SER	CYS	ENGINEERED	UNP P00441
B	6	ALA	CYS	ENGINEERED	UNP P00441
B	111	SER	CYS	ENGINEERED	UNP P00441

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

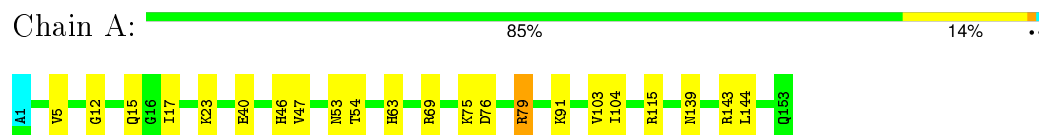
Mol	Chain	Residues	Atoms	
2	B	1	Total	Zn
			1	1
2	A	1	Total	Zn
			1	1

4 Residue-property plots

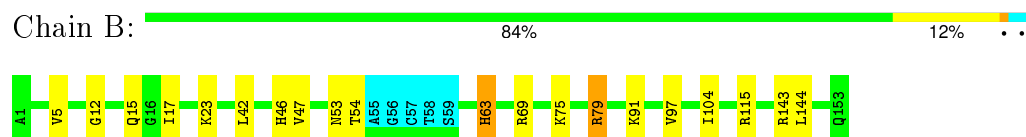
4.1 Average score per residue in the NMR ensemble

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: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]

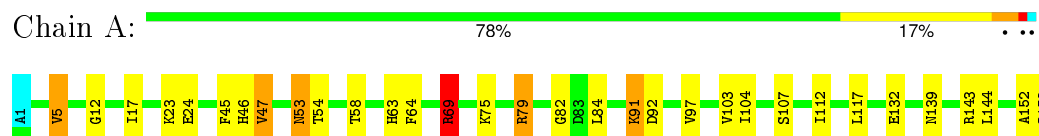


4.2 Scores per residue for each member of the ensemble

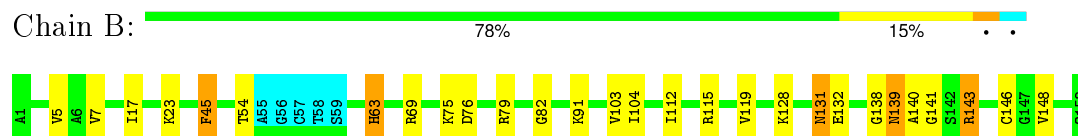
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Superoxide dismutase [Cu-Zn]

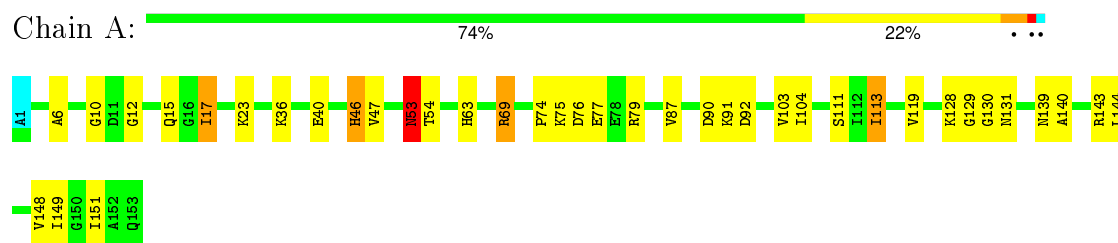


- Molecule 1: Superoxide dismutase [Cu-Zn]

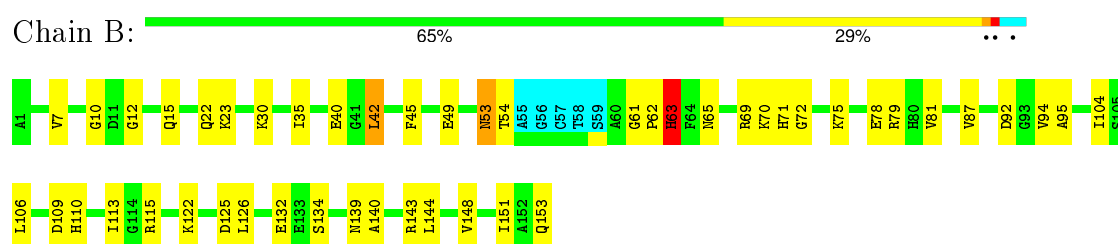


4.2.2 Score per residue for model 2

- Molecule 1: Superoxide dismutase [Cu-Zn]

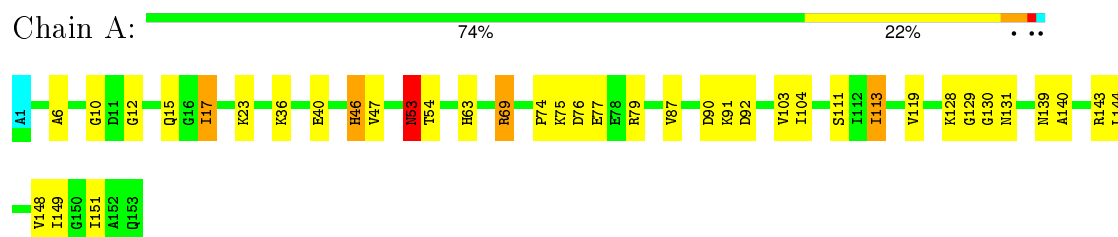


- Molecule 1: Superoxide dismutase [Cu-Zn]

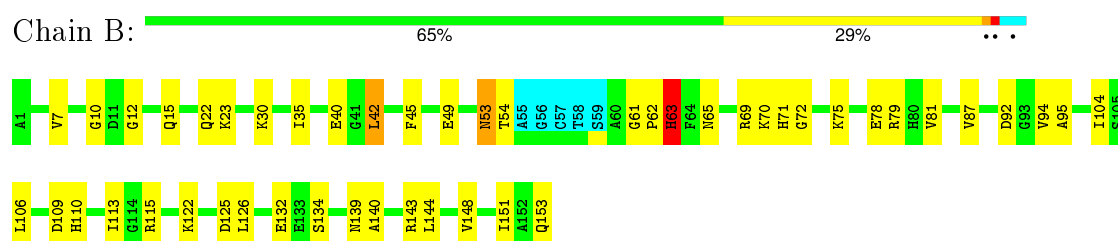


4.2.3 Score per residue for model 3

- Molecule 1: Superoxide dismutase [Cu-Zn]

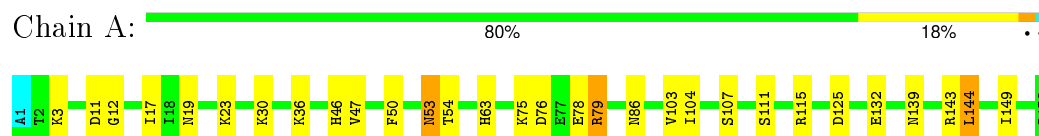


- Molecule 1: Superoxide dismutase [Cu-Zn]

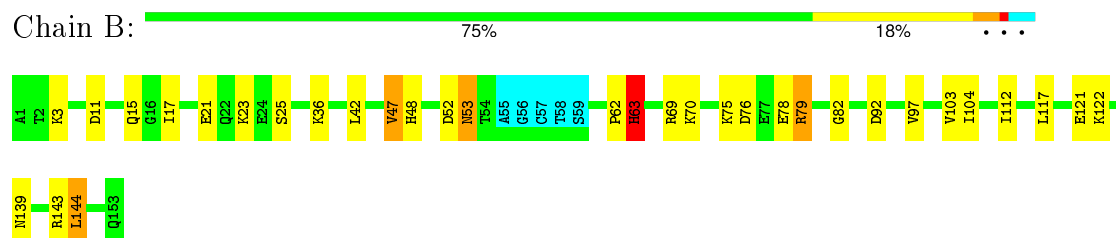


4.2.4 Score per residue for model 4

- Molecule 1: Superoxide dismutase [Cu-Zn]

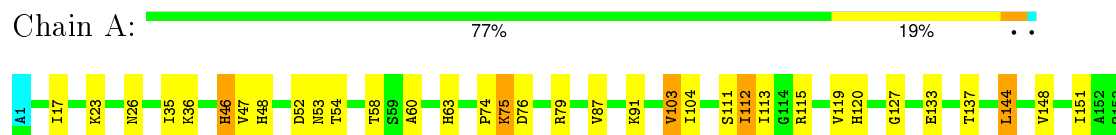


- Molecule 1: Superoxide dismutase [Cu-Zn]

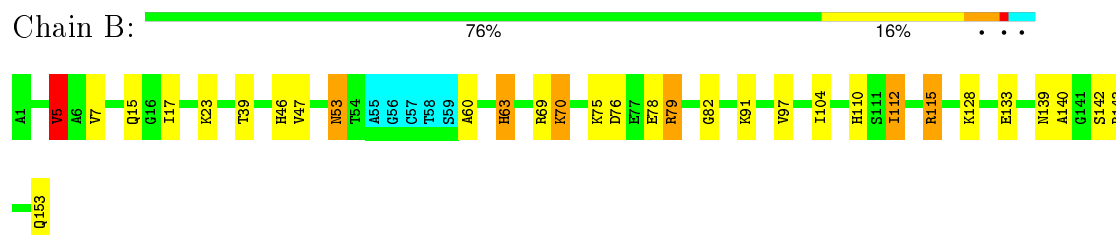


4.2.5 Score per residue for model 5

- Molecule 1: Superoxide dismutase [Cu-Zn]

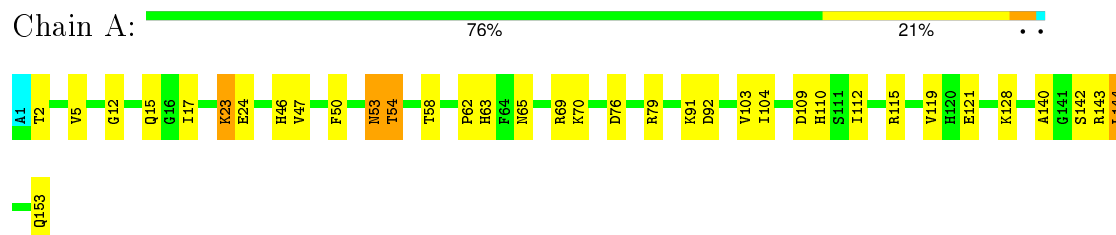


- Molecule 1: Superoxide dismutase [Cu-Zn]

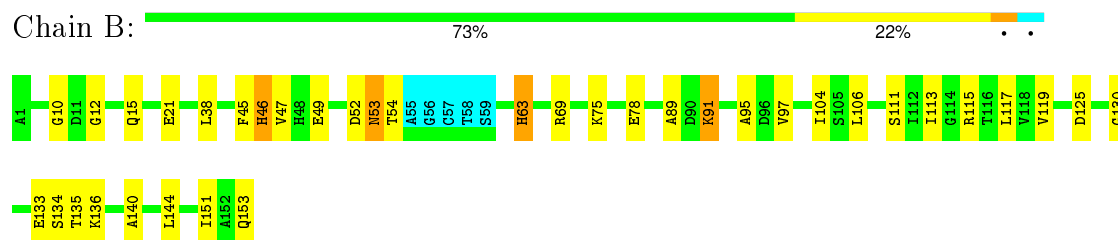


4.2.6 Score per residue for model 6

- Molecule 1: Superoxide dismutase [Cu-Zn]

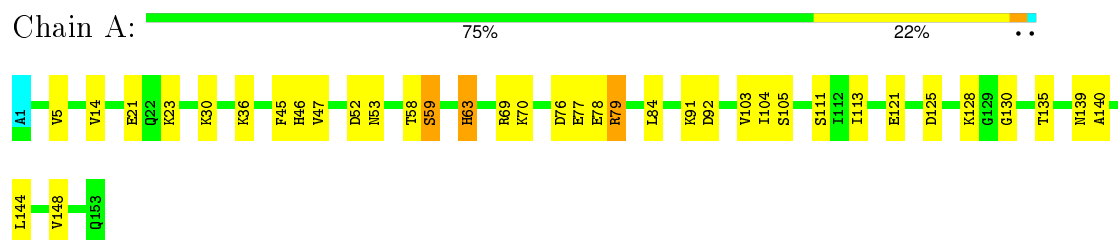


- Molecule 1: Superoxide dismutase [Cu-Zn]

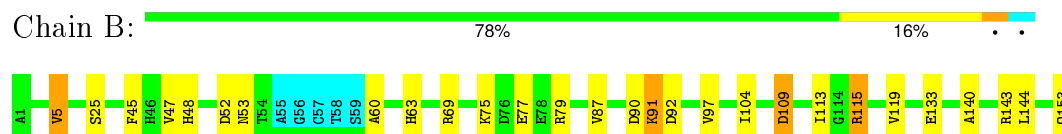


4.2.7 Score per residue for model 7

- Molecule 1: Superoxide dismutase [Cu-Zn]

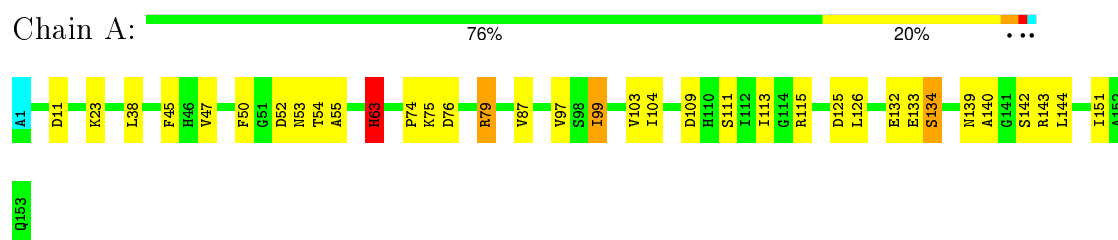


- Molecule 1: Superoxide dismutase [Cu-Zn]

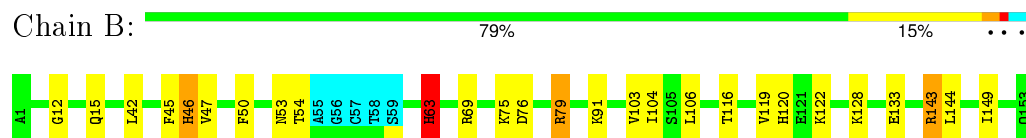


4.2.8 Score per residue for model 8

- Molecule 1: Superoxide dismutase [Cu-Zn]

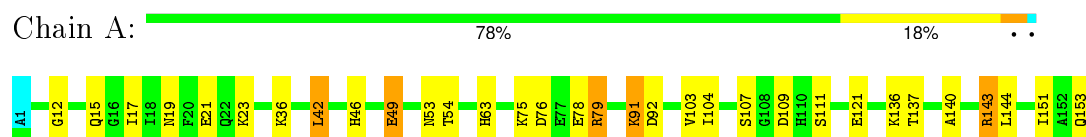


- Molecule 1: Superoxide dismutase [Cu-Zn]

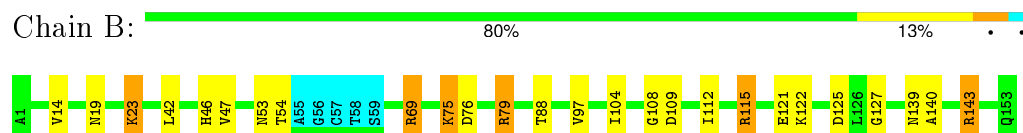


4.2.9 Score per residue for model 9

- Molecule 1: Superoxide dismutase [Cu-Zn]

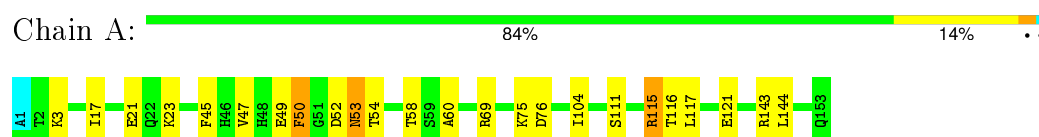


- Molecule 1: Superoxide dismutase [Cu-Zn]

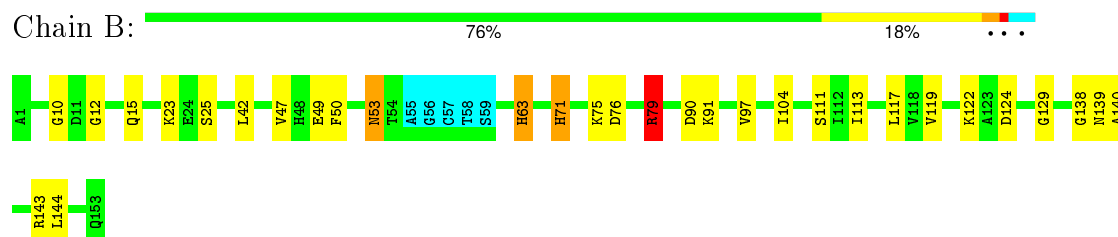


4.2.10 Score per residue for model 10

- Molecule 1: Superoxide dismutase [Cu-Zn]

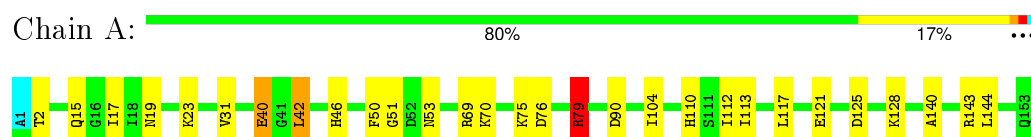


- Molecule 1: Superoxide dismutase [Cu-Zn]

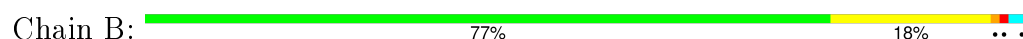


4.2.11 Score per residue for model 11

- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]

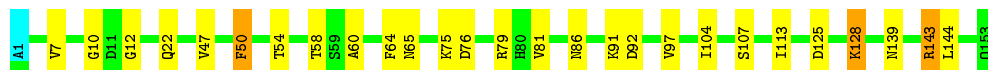




4.2.12 Score per residue for model 12

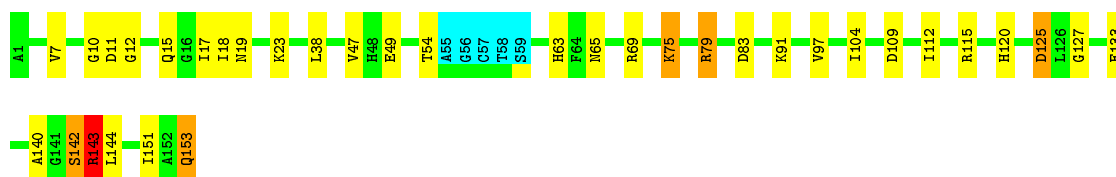
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A: 82% 16% ..



- Molecule 1: Superoxide dismutase [Cu-Zn]

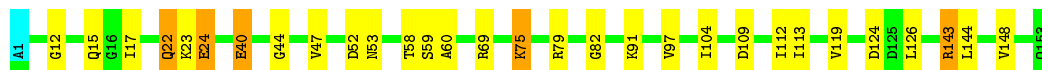
Chain B: 74% 19% ..



4.2.13 Score per residue for model 13

- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A: 80% 16% ..



- Molecule 1: Superoxide dismutase [Cu-Zn]

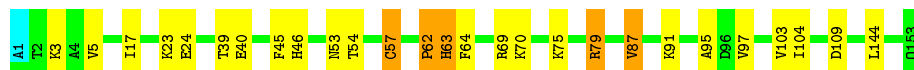
Chain B: 78% 16% ..



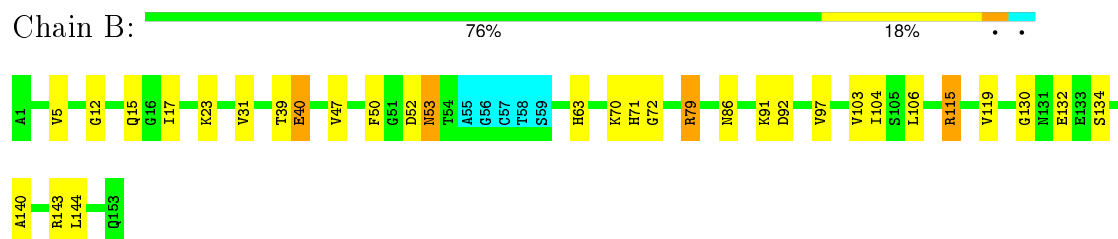
4.2.14 Score per residue for model 14

- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A: 82% 14% ..

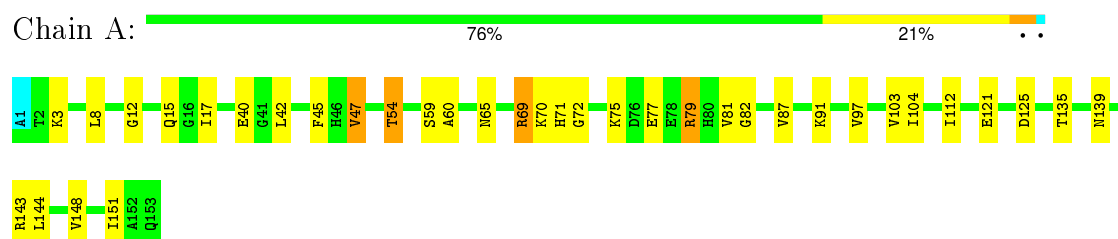


- Molecule 1: Superoxide dismutase [Cu-Zn]

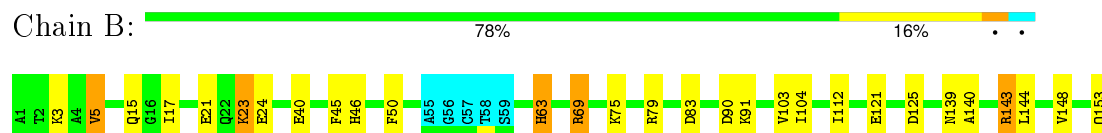


4.2.15 Score per residue for model 15

- Molecule 1: Superoxide dismutase [Cu-Zn]

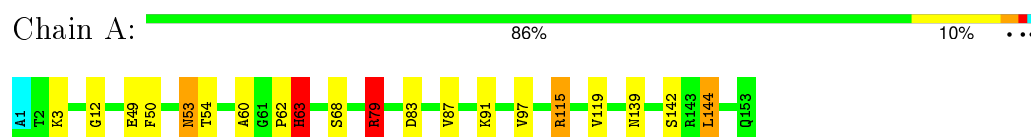


- Molecule 1: Superoxide dismutase [Cu-Zn]

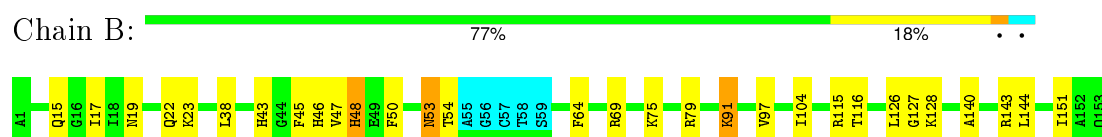


4.2.16 Score per residue for model 16

- Molecule 1: Superoxide dismutase [Cu-Zn]

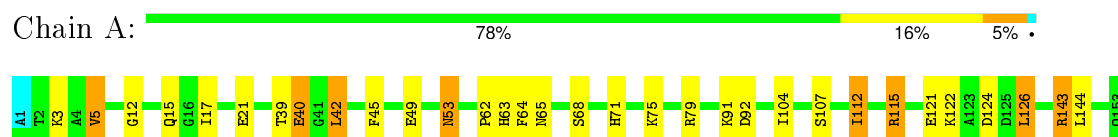


- Molecule 1: Superoxide dismutase [Cu-Zn]

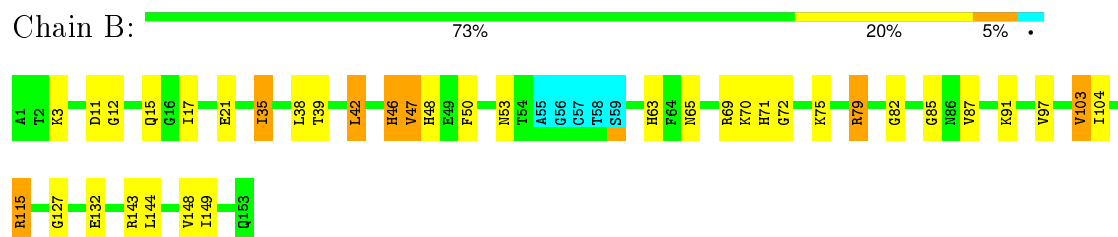


4.2.17 Score per residue for model 17

- Molecule 1: Superoxide dismutase [Cu-Zn]

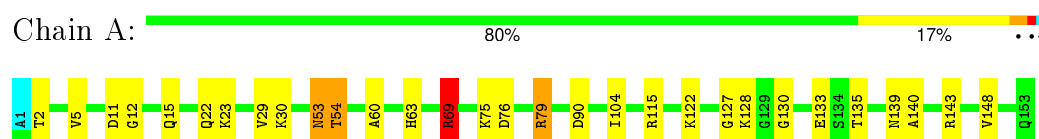


- Molecule 1: Superoxide dismutase [Cu-Zn]

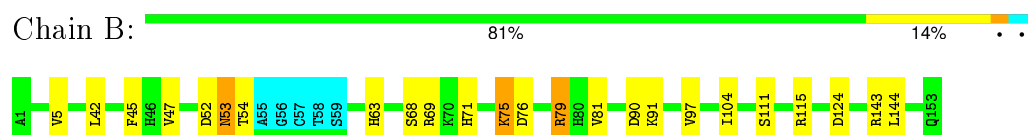


4.2.18 Score per residue for model 18

- Molecule 1: Superoxide dismutase [Cu-Zn]

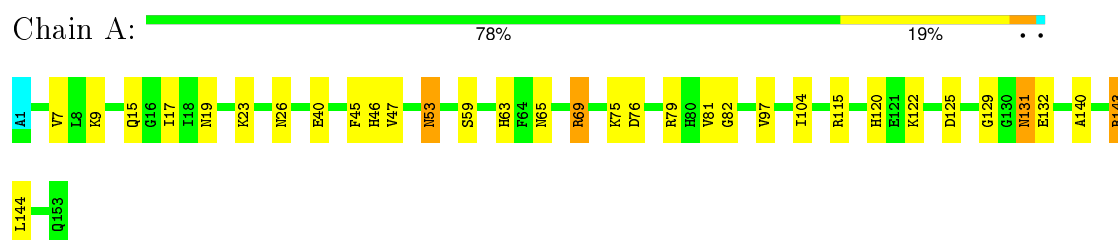


- Molecule 1: Superoxide dismutase [Cu-Zn]

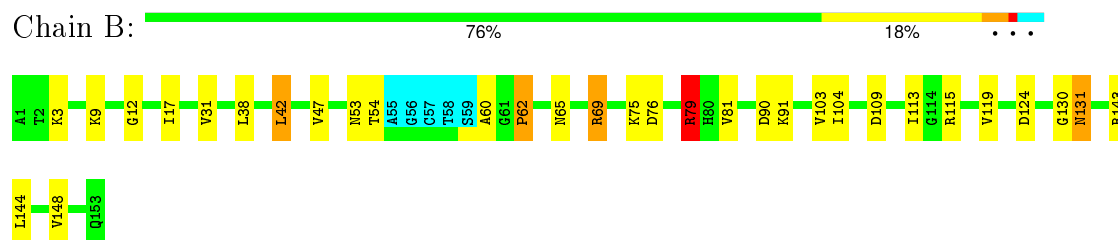


4.2.19 Score per residue for model 19

- Molecule 1: Superoxide dismutase [Cu-Zn]

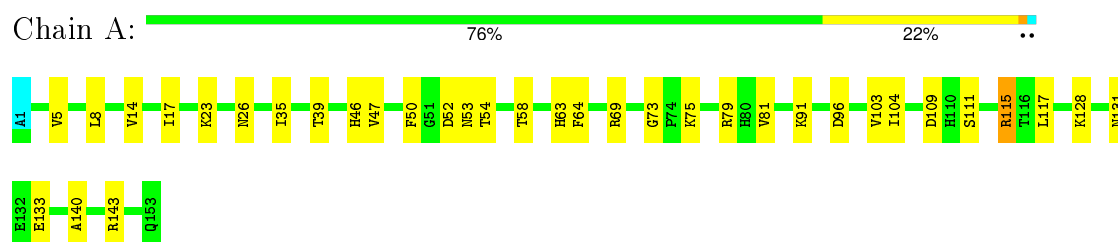


- Molecule 1: Superoxide dismutase [Cu-Zn]

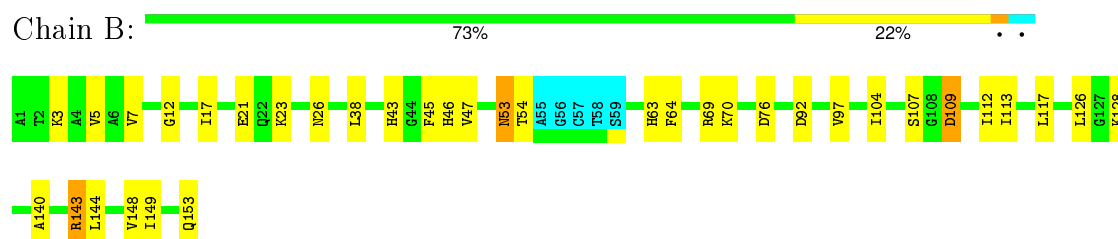


4.2.20 Score per residue for model 20

- Molecule 1: Superoxide dismutase [Cu-Zn]

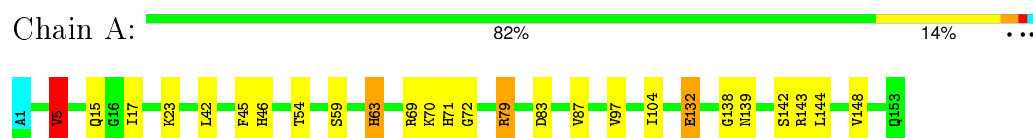


- Molecule 1: Superoxide dismutase [Cu-Zn]

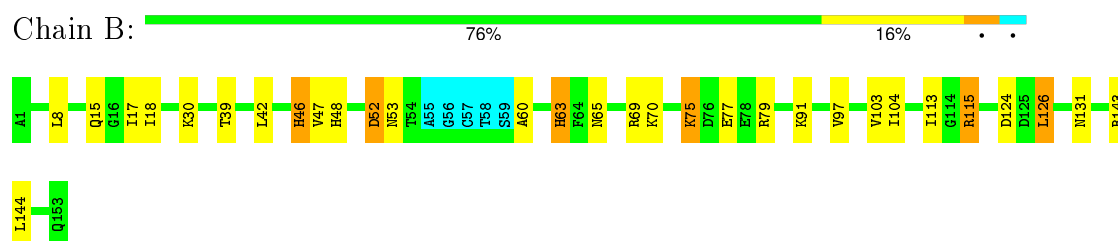


4.2.21 Score per residue for model 21

- Molecule 1: Superoxide dismutase [Cu-Zn]

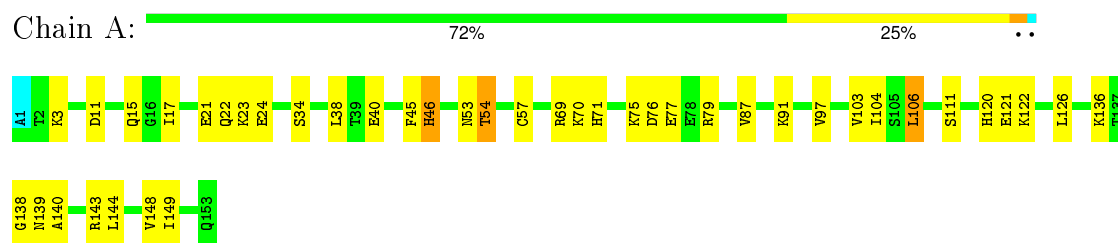


- Molecule 1: Superoxide dismutase [Cu-Zn]

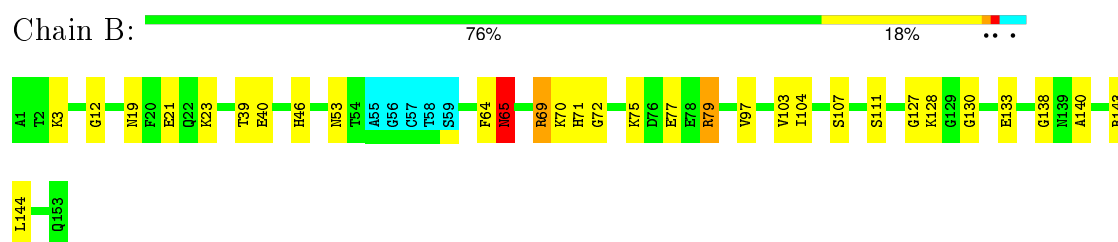


4.2.22 Score per residue for model 22

- Molecule 1: Superoxide dismutase [Cu-Zn]

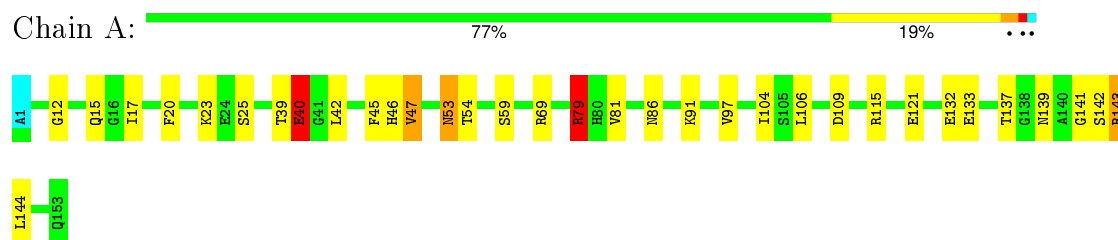


- Molecule 1: Superoxide dismutase [Cu-Zn]

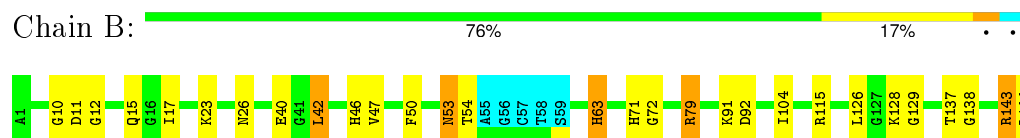


4.2.23 Score per residue for model 23 (medoid)

- Molecule 1: Superoxide dismutase [Cu-Zn]



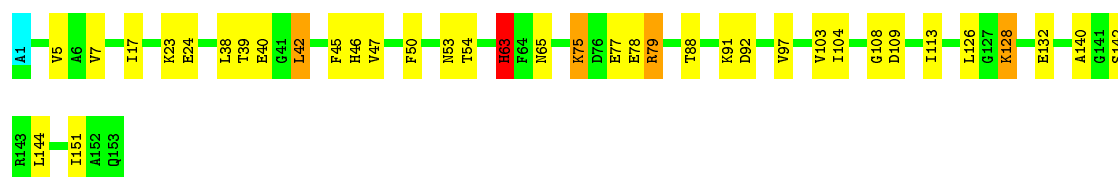
- Molecule 1: Superoxide dismutase [Cu-Zn]



4.2.24 Score per residue for model 24

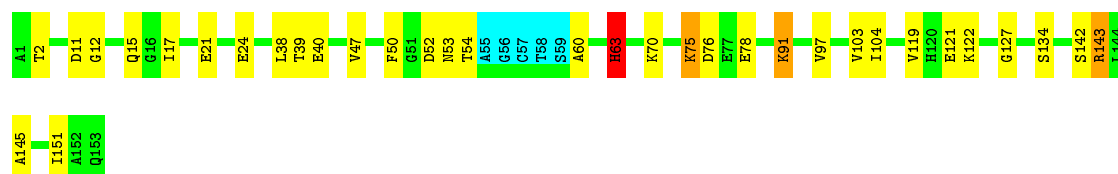
- Molecule 1: Superoxide dismutase [Cu-Zn]





- Molecule 1: Superoxide dismutase [Cu-Zn]

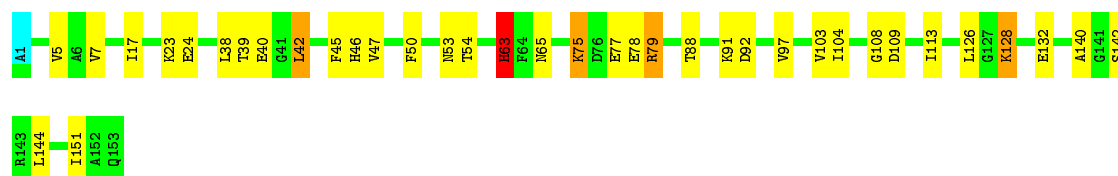
Chain B: 75% 20%



4.2.25 Score per residue for model 25

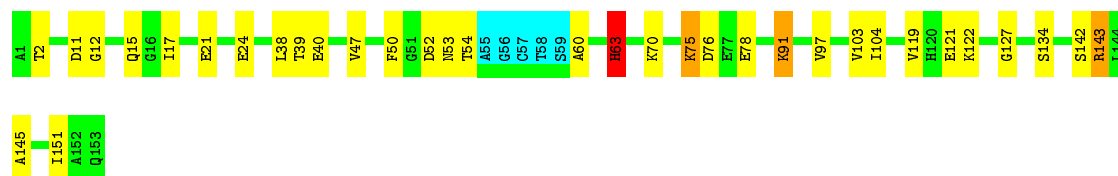
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A: 75% 21%



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B: 75% 20%



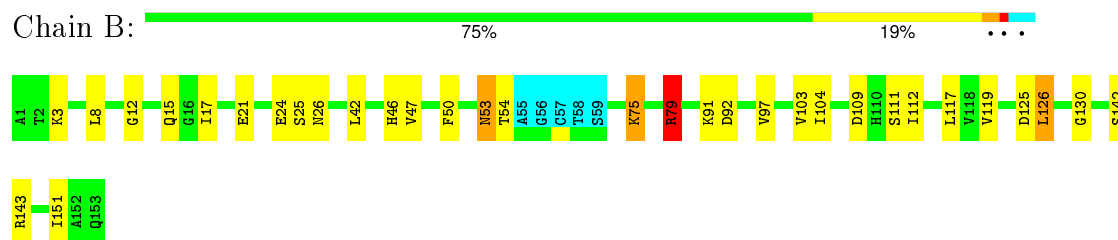
4.2.26 Score per residue for model 26

- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A: 79% 15% 5%

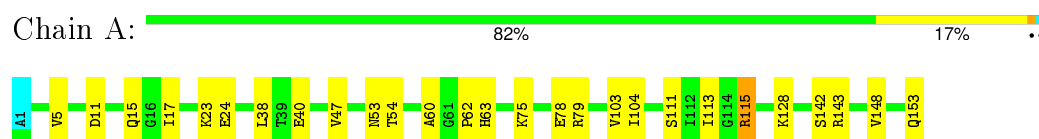


- Molecule 1: Superoxide dismutase [Cu-Zn]

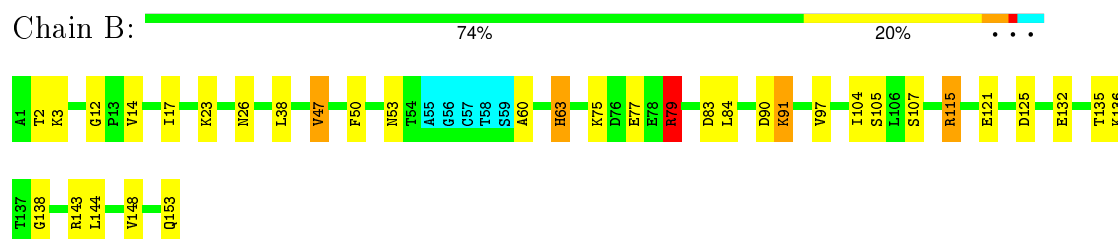


4.2.27 Score per residue for model 27

- Molecule 1: Superoxide dismutase [Cu-Zn]

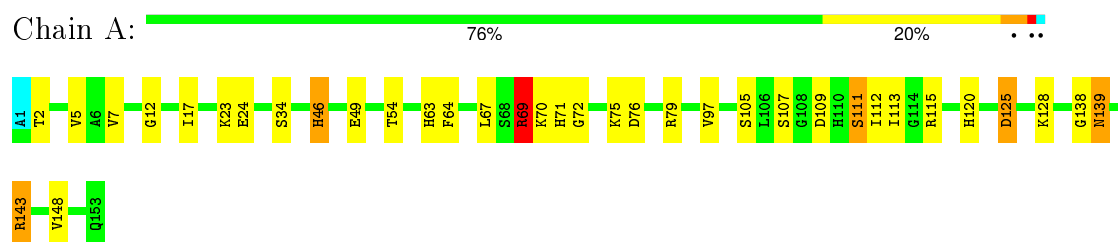


- Molecule 1: Superoxide dismutase [Cu-Zn]

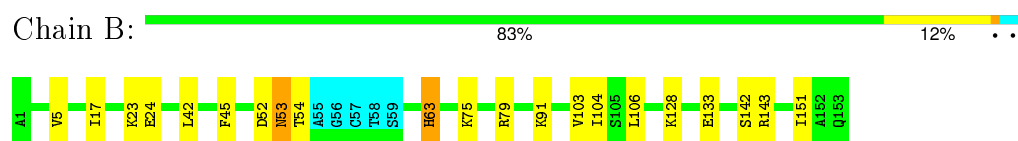


4.2.28 Score per residue for model 28

- Molecule 1: Superoxide dismutase [Cu-Zn]

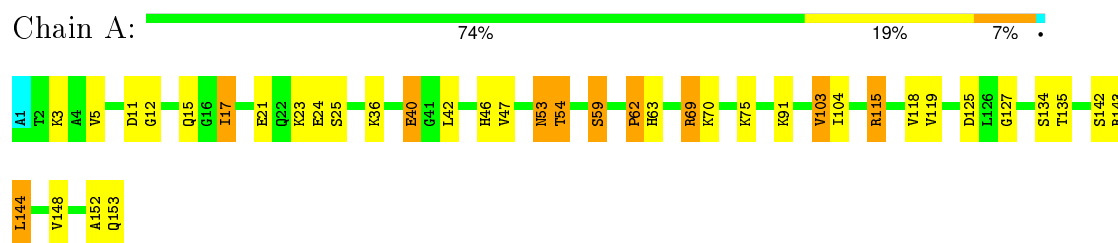


- Molecule 1: Superoxide dismutase [Cu-Zn]

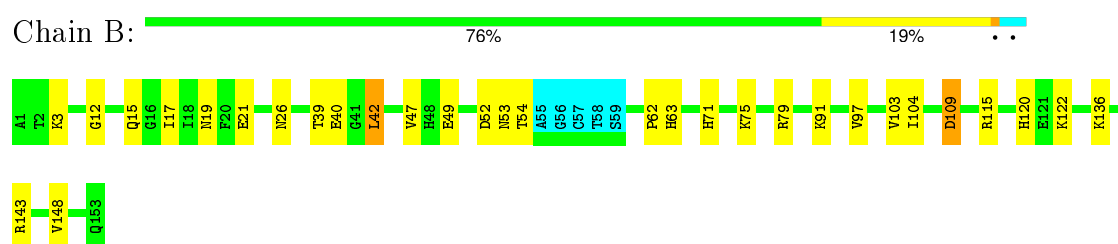


4.2.29 Score per residue for model 29

- Molecule 1: Superoxide dismutase [Cu-Zn]

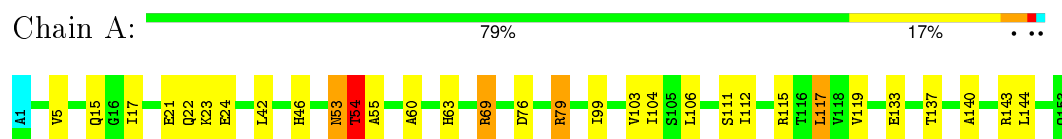


- Molecule 1: Superoxide dismutase [Cu-Zn]

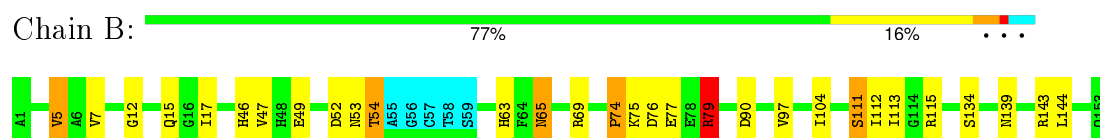


4.2.30 Score per residue for model 30

- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]



5 Refinement protocol and experimental data overview

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

Of the 600 calculated structures, 30 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
CYANA	structure solution	1.03
AMBER	refinement	8

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)	BMRB entry 6821
Number of chemical shift lists	1
Total number of shifts	3284
Number of shifts mapped to atoms	3284
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.62±0.01	0±0/1121 (0.0±0.0%)	1.19±0.03	3±1/1512 (0.2±0.1%)
1	B	0.62±0.01	0±0/1098 (0.0±0.0%)	1.20±0.03	3±1/1481 (0.2±0.1%)
All	All	0.62	0/66570 (0.0%)	1.19	172/89790 (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±0.0	0.7±0.7
1	B	0.0±0.0	1.2±1.0
All	All	0	58

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	79	ARG	NE-CZ-NH1	10.34	125.47	120.30	30	20
1	B	143	ARG	NE-CZ-NH1	9.41	125.01	120.30	4	15
1	B	115	ARG	NE-CZ-NH1	9.23	124.91	120.30	7	14
1	B	79	ARG	NE-CZ-NH1	8.87	124.74	120.30	21	18
1	B	115	ARG	NE-CZ-NH2	-8.42	116.09	120.30	11	4
1	A	69	ARG	NE-CZ-NH1	8.24	124.42	120.30	30	12
1	B	79	ARG	NE-CZ-NH2	-8.11	116.24	120.30	29	2
1	A	143	ARG	NE-CZ-NH1	7.86	124.23	120.30	26	9
1	B	69	ARG	NE-CZ-NH1	7.77	124.19	120.30	30	10
1	A	115	ARG	NE-CZ-NH2	-7.48	116.56	120.30	20	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	5	VAL	CG1-CB-CG2	7.34	122.64	110.90	13	2
1	A	115	ARG	NE-CZ-NH1	7.19	123.90	120.30	8	11
1	B	69	ARG	NE-CZ-NH2	-6.70	116.95	120.30	6	4
1	A	79	ARG	NE-CZ-NH2	-6.67	116.97	120.30	20	2
1	B	24	GLU	C-N-CA	6.50	137.96	121.70	26	1
1	B	119	VAL	CA-CB-CG1	6.41	120.52	110.90	24	6
1	B	52	ASP	N-CA-CB	6.40	122.11	110.60	21	1
1	A	69	ARG	NE-CZ-NH2	-6.26	117.17	120.30	13	7
1	B	47	VAL	CA-CB-CG2	6.04	119.96	110.90	17	1
1	A	69	ARG	CD-NE-CZ	5.97	131.96	123.60	10	1
1	A	5	VAL	CG1-CB-CG2	5.88	120.31	110.90	21	1
1	A	99	ILE	CA-CB-CG1	5.67	121.78	111.00	8	1
1	B	144	LEU	CB-CA-C	5.65	120.93	110.20	22	1
1	A	143	ARG	NE-CZ-NH2	-5.64	117.48	120.30	19	2
1	B	111	SER	C-N-CA	5.59	135.67	121.70	26	1
1	A	112	ILE	C-N-CA	5.53	135.52	121.70	5	3
1	A	119	VAL	CA-CB-CG1	5.44	119.06	110.90	16	3
1	A	2	THR	CA-CB-CG2	5.34	119.88	112.40	28	1
1	B	69	ARG	CD-NE-CZ	5.27	130.98	123.60	5	3
1	A	29	VAL	CA-CB-CG1	5.24	118.76	110.90	18	1
1	B	97	VAL	CA-CB-CG1	5.20	118.70	110.90	20	1
1	A	53	ASN	C-N-CA	5.18	134.64	121.70	26	1
1	A	47	VAL	CA-CB-CG1	5.17	118.66	110.90	23	1
1	A	125	ASP	CB-CG-OD1	5.17	122.95	118.30	28	1
1	A	128	LYS	CA-CB-CG	-5.16	102.06	113.40	27	3
1	B	81	VAL	CA-CB-CG1	5.13	118.59	110.90	2	2
1	A	117	LEU	CB-CG-CD1	5.11	119.69	111.00	30	1
1	A	128	LYS	CB-CG-CD	5.10	124.86	111.60	12	1
1	B	63	HIS	CA-CB-CG	5.04	122.17	113.60	11	1
1	A	54	THR	N-CA-C	5.04	124.61	111.00	18	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	69	ARG	Sidechain	10
1	B	115	ARG	Sidechain	8
1	B	69	ARG	Sidechain	8
1	B	63	HIS	Sidechain	7
1	B	79	ARG	Sidechain	7

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	115	ARG	Sidechain	6
1	B	71	HIS	Sidechain	3
1	A	79	ARG	Sidechain	2
1	A	63	HIS	Sidechain	2
1	B	143	ARG	Sidechain	2
1	A	143	ARG	Sidechain	1
1	B	50	PHE	Sidechain	1
1	A	46	HIS	Sidechain	1

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	1103	1073	1072	4±2
1	B	1080	1052	1054	4±2
All	All	65550	63750	63780	195

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:B:42:LEU:HD22	1:B:42:LEU:H	0.68	1.48	23	1
1:A:53:ASN:ND2	1:B:7:VAL:HG21	0.66	2.05	3	3
1:B:63:HIS:CD2	1:B:63:HIS:H	0.65	2.09	17	6
1:B:63:HIS:H	1:B:63:HIS:CD2	0.65	2.06	6	7
1:A:5:VAL:HG11	1:B:52:ASP:HA	0.64	1.69	6	3
1:A:54:THR:CG2	1:B:7:VAL:HG22	0.64	2.22	1	3
1:A:42:LEU:HD22	1:A:42:LEU:H	0.62	1.55	9	1
1:A:54:THR:HG22	1:B:7:VAL:HA	0.61	1.73	12	2
1:A:63:HIS:CD2	1:A:63:HIS:H	0.61	2.13	14	3
1:B:42:LEU:H	1:B:42:LEU:HD22	0.61	1.55	17	2
1:A:54:THR:HG22	1:B:5:VAL:HG23	0.61	1.71	15	1
1:B:91:LYS:HE2	1:B:91:LYS:H	0.60	1.57	16	2
1:A:52:ASP:HA	1:B:5:VAL:HG21	0.58	1.75	20	4
1:A:47:VAL:HG23	1:A:82:GLY:HA2	0.57	1.75	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:VAL:HG13	1:A:144:LEU:CD2	0.57	2.29	5	1
1:A:115:ARG:NE	1:A:116:THR:H	0.56	1.98	10	1
1:B:42:LEU:H	1:B:42:LEU:HD23	0.55	1.62	10	5
1:A:120:HIS:CE1	1:A:143:ARG:HE	0.55	2.20	19	1
1:A:45:PHE:CE1	1:A:117:LEU:HD11	0.54	2.38	10	2
1:B:42:LEU:CD2	1:B:42:LEU:H	0.54	2.16	23	2
1:A:119:VAL:HG13	1:A:144:LEU:HD22	0.53	1.80	5	2
1:A:53:ASN:HD21	1:A:148:VAL:CG2	0.52	2.17	3	2
1:A:5:VAL:HG21	1:B:52:ASP:HA	0.52	1.82	21	3
1:A:42:LEU:HD13	1:A:42:LEU:H	0.51	1.66	17	2
1:B:48:HIS:CG	1:B:116:THR:HG23	0.51	2.40	16	1
1:A:113:ILE:HD13	1:A:149:ILE:HG22	0.51	1.82	3	2
1:B:42:LEU:HD23	1:B:42:LEU:H	0.51	1.66	8	3
1:A:17:ILE:HD13	1:B:54:THR:HG23	0.50	1.83	3	2
1:A:42:LEU:H	1:A:42:LEU:HD23	0.50	1.66	23	1
1:A:87:VAL:HG22	1:A:95:ALA:HB1	0.50	1.84	14	1
1:A:7:VAL:HA	1:B:54:THR:HG22	0.49	1.82	28	3
1:A:42:LEU:H	1:A:42:LEU:HD13	0.49	1.67	25	1
1:B:38:LEU:HD23	1:B:38:LEU:H	0.49	1.67	25	2
1:B:46:HIS:O	1:B:117:LEU:HD22	0.48	2.08	20	2
1:A:54:THR:CG2	1:B:5:VAL:HG23	0.48	2.37	15	1
1:A:22:GLN:CB	1:A:106:LEU:HD13	0.48	2.39	30	1
1:B:71:HIS:CG	1:B:72:GLY:N	0.48	2.82	14	6
1:B:46:HIS:CE1	1:B:48:HIS:CD2	0.48	3.02	17	2
1:A:46:HIS:NE2	1:A:63:HIS:CD2	0.47	2.82	26	1
1:A:49:GLU:H	1:A:49:GLU:CD	0.47	2.12	17	1
1:A:91:LYS:H	1:A:91:LYS:HE2	0.47	1.69	9	1
1:B:112:ILE:HG23	1:B:149:ILE:HG21	0.47	1.86	20	1
1:A:14:VAL:HG11	1:A:144:LEU:HD11	0.47	1.87	7	1
1:A:5:VAL:CG1	1:B:52:ASP:HA	0.47	2.39	28	1
1:A:40:GLU:CD	1:A:40:GLU:H	0.46	2.14	23	1
1:A:44:GLY:O	1:A:119:VAL:HG13	0.46	2.10	13	1
1:A:35:ILE:HG21	1:A:119:VAL:HG11	0.46	1.87	5	1
1:A:46:HIS:CE1	1:A:63:HIS:CD2	0.46	3.03	3	3
1:A:7:VAL:CG2	1:B:54:THR:H	0.46	2.22	12	1
1:B:65:ASN:ND2	1:B:81:VAL:H	0.46	2.08	19	1
1:B:22:GLN:HB2	1:B:106:LEU:HD13	0.46	1.87	3	2
1:B:45:PHE:HB2	1:B:119:VAL:HG22	0.46	1.86	1	1
1:A:54:THR:HG22	1:B:7:VAL:HG22	0.45	1.86	1	3
1:A:151:ILE:N	1:A:151:ILE:HD12	0.45	2.26	25	2
1:A:53:ASN:O	1:A:54:THR:HG23	0.45	2.10	30	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:42:LEU:H	1:B:42:LEU:CD2	0.45	2.25	19	2
1:A:42:LEU:CD2	1:A:42:LEU:H	0.45	2.21	9	1
1:A:71:HIS:CG	1:A:72:GLY:N	0.45	2.85	21	3
1:A:22:GLN:CB	1:A:106:LEU:HD11	0.45	2.42	22	1
1:A:71:HIS:CD2	1:A:138:GLY:HA3	0.45	2.46	21	2
1:B:47:VAL:HG12	1:B:117:LEU:HB2	0.45	1.89	4	1
1:B:126:LEU:HD13	1:B:126:LEU:H	0.45	1.72	21	2
1:B:89:ALA:HB2	1:B:95:ALA:HB2	0.44	1.90	6	1
1:A:144:LEU:CD2	1:A:145:ALA:H	0.44	2.26	26	1
1:B:45:PHE:CE1	1:B:117:LEU:HD21	0.43	2.48	6	1
1:B:47:VAL:HG23	1:B:82:GLY:HA2	0.43	1.88	17	2
1:B:71:HIS:CD2	1:B:138:GLY:HA2	0.43	2.49	10	1
1:B:46:HIS:CD2	1:B:63:HIS:CD2	0.43	3.07	6	1
1:A:63:HIS:CE1	1:A:71:HIS:ND1	0.43	2.86	17	1
1:A:105:SER:H	1:A:111:SER:HB3	0.43	1.73	28	2
1:A:131:ASN:CG	1:A:132:GLU:H	0.43	2.16	19	1
1:A:22:GLN:HB3	1:A:106:LEU:HD11	0.43	1.89	22	1
1:A:38:LEU:HD23	1:A:144:LEU:HD11	0.43	1.88	22	1
1:A:63:HIS:H	1:A:63:HIS:CD2	0.43	2.30	29	1
1:A:5:VAL:CG1	1:A:152:ALA:HB2	0.43	2.42	1	1
1:A:63:HIS:CD2	1:A:63:HIS:N	0.43	2.86	14	2
1:B:63:HIS:N	1:B:63:HIS:CD2	0.43	2.86	5	1
1:B:47:VAL:HG12	1:B:115:ARG:HB3	0.43	1.91	27	1
1:B:35:ILE:HD13	1:B:87:VAL:HG21	0.42	1.90	17	1
1:B:38:LEU:HD13	1:B:43:HIS:CD2	0.42	2.49	16	2
1:A:67:LEU:HB3	1:A:69:ARG:HE	0.42	1.74	28	1
1:A:5:VAL:HG23	1:B:54:THR:HG22	0.42	1.89	1	1
1:A:63:HIS:N	1:A:63:HIS:CD2	0.42	2.87	29	3
1:B:63:HIS:CE1	1:B:71:HIS:CE1	0.42	3.08	10	1
1:A:62:PRO:C	1:A:63:HIS:CD2	0.42	2.93	6	2
1:A:23:LYS:H	1:A:23:LYS:CD	0.42	2.26	6	1
1:A:53:ASN:HB2	1:B:5:VAL:HG13	0.42	1.92	30	1
1:B:63:HIS:CE1	1:B:71:HIS:ND1	0.42	2.88	11	1
1:A:49:GLU:CD	1:A:49:GLU:H	0.42	2.18	26	1
1:A:54:THR:HG21	1:B:148:VAL:O	0.42	2.15	29	1
1:B:42:LEU:H	1:B:42:LEU:HD13	0.42	1.75	29	1
1:B:70:LYS:HE2	1:B:78:GLU:OE1	0.41	2.15	5	1
1:A:46:HIS:CG	1:A:63:HIS:CE1	0.41	3.08	28	1
1:B:124:ASP:CG	1:B:140:ALA:HB2	0.41	2.35	10	1
1:B:64:PHE:CG	1:B:65:ASN:N	0.41	2.88	22	1
1:A:53:ASN:CG	1:B:7:VAL:HG21	0.41	2.36	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:151:ILE:N	1:B:151:ILE:HD12	0.41	2.29	26	1
1:B:23:LYS:HZ2	1:B:24:GLU:CD	0.41	2.19	15	1
1:B:75:LYS:HE2	1:B:125:ASP:O	0.41	2.15	12	1
1:A:91:LYS:HZ3	1:A:91:LYS:H	0.41	1.57	1	1
1:B:131:ASN:HD21	1:B:139:ASN:ND2	0.41	2.13	1	1
1:A:6:ALA:O	1:B:54:THR:HG21	0.41	2.16	3	2
1:B:35:ILE:HB	1:B:95:ALA:HB3	0.41	1.91	3	2
1:B:47:VAL:HG23	1:B:82:GLY:C	0.41	2.36	4	1
1:B:151:ILE:HG22	1:B:153:GLN:H	0.41	1.76	12	1
1:B:132:GLU:CG	1:B:136:LYS:HE3	0.41	2.45	27	1
1:B:53:ASN:N	1:B:53:ASN:ND2	0.41	2.69	28	1
1:A:51:GLY:HA2	1:B:152:ALA:CA	0.41	2.46	11	1
1:B:63:HIS:CD2	1:B:63:HIS:N	0.41	2.88	3	2
1:B:47:VAL:CG2	1:B:82:GLY:HA2	0.41	2.46	17	1
1:B:8:LEU:CD2	1:B:117:LEU:HD12	0.40	2.46	26	1
1:A:134:SER:HA	1:A:139:ASN:HB2	0.40	1.93	8	1
1:B:46:HIS:CE1	1:B:120:HIS:CD2	0.40	3.10	8	1
1:A:46:HIS:CE1	1:A:120:HIS:CD2	0.40	3.09	5	3
1:B:120:HIS:CE1	1:B:143:ARG:HH11	0.40	2.34	12	1
1:A:5:VAL:HG11	1:B:52:ASP:CA	0.40	2.46	30	1
1:B:23:LYS:HE2	1:B:23:LYS:N	0.40	2.31	9	1
1:A:46:HIS:O	1:A:117:LEU:HD22	0.40	2.16	1	1
1:B:63:HIS:CE1	1:B:137:THR:O	0.40	2.74	23	1
1:A:47:VAL:HG23	1:A:82:GLY:CA	0.40	2.46	15	1
1:A:22:GLN:HE22	1:A:24:GLU:C	0.40	2.19	13	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	151/153 (99%)	115±5 (76±3%)	27±4 (18±3%)	9±3 (6±2%)	4	23
1	B	146/153 (95%)	112±4 (77±3%)	26±4 (18±3%)	8±2 (6±2%)	4	24
All	All	8910/9180 (97%)	6824 (77%)	1586 (18%)	500 (6%)	4	23

All 100 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	79	ARG	21
1	B	79	ARG	19
1	B	12	GLY	18
1	B	53	ASN	17
1	A	54	THR	16
1	A	12	GLY	16
1	A	53	ASN	16
1	B	103	VAL	14
1	A	140	ALA	14
1	A	103	VAL	14
1	B	140	ALA	13
1	A	113	ILE	12
1	B	75	LYS	10
1	B	113	ILE	9
1	A	60	ALA	9
1	B	54	THR	9
1	A	40	GLU	8
1	A	111	SER	8
1	B	60	ALA	7
1	A	59	SER	7
1	B	112	ILE	7
1	A	75	LYS	7
1	B	50	PHE	7
1	B	127	GLY	7
1	A	142	SER	7
1	B	63	HIS	7
1	B	40	GLU	6
1	B	130	GLY	6
1	A	78	GLU	6
1	B	10	GLY	6
1	B	91	LYS	6
1	A	109	ASP	6
1	B	111	SER	5
1	B	62	PRO	5
1	B	109	ASP	5
1	A	112	ILE	5
1	A	65	ASN	5
1	B	78	GLU	4
1	A	130	GLY	4
1	B	25	SER	4
1	B	65	ASN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	126	LEU	4
1	A	74	PRO	4
1	A	50	PHE	4
1	A	17	ILE	4
1	B	139	ASN	4
1	A	139	ASN	4
1	A	144	LEU	4
1	B	26	ASN	4
1	A	62	PRO	4
1	B	138	GLY	4
1	A	49	GLU	4
1	B	142	SER	3
1	B	126	LEU	3
1	A	10	GLY	3
1	A	63	HIS	3
1	A	129	GLY	3
1	B	129	GLY	3
1	B	77	GLU	3
1	A	127	GLY	3
1	A	132	GLU	3
1	A	57	CYS	2
1	A	108	GLY	2
1	B	5	VAL	2
1	B	74	PRO	2
1	B	145	ALA	2
1	A	68	SER	2
1	A	26	ASN	2
1	A	55	ALA	2
1	A	42	LEU	2
1	A	77	GLU	2
1	A	81	VAL	2
1	B	49	GLU	2
1	B	61	GLY	2
1	A	64	PHE	2
1	B	141	GLY	1
1	A	73	GLY	1
1	A	152	ALA	1
1	A	138	GLY	1
1	A	151	ILE	1
1	A	133	GLU	1
1	B	144	LEU	1
1	B	128	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	B	68	SER	1
1	B	132	GLU	1
1	A	39	THR	1
1	B	125	ASP	1
1	B	85	GLY	1
1	B	131	ASN	1
1	B	17	ILE	1
1	A	143	ARG	1
1	B	52	ASP	1
1	B	82	GLY	1
1	A	82	GLY	1
1	B	81	VAL	1
1	B	108	GLY	1
1	B	133	GLU	1
1	A	5	VAL	1
1	A	52	ASP	1
1	A	141	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	117/117 (100%)	96±4 (82±3%)	21±4 (18±3%)	5	39
1	B	114/117 (97%)	94±4 (82±3%)	20±4 (18±3%)	6	41
All	All	6930/7020 (99%)	5687 (82%)	1243 (18%)	5	40

All 185 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	B	104	ILE	30
1	A	104	ILE	28
1	A	23	LYS	26
1	A	144	LEU	23
1	B	53	ASN	22
1	B	97	VAL	21
1	A	17	ILE	21

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Mol	Chain	Res	Type	Models (Total)
1	B	47	VAL	21
1	B	91	LYS	21
1	B	75	LYS	21
1	B	15	GLN	21
1	B	143	ARG	21
1	B	144	LEU	20
1	A	75	LYS	20
1	A	53	ASN	20
1	B	63	HIS	20
1	A	91	LYS	19
1	A	47	VAL	19
1	B	17	ILE	19
1	A	143	ARG	19
1	B	23	LYS	18
1	A	46	HIS	18
1	A	63	HIS	17
1	A	76	ASP	16
1	A	15	GLN	16
1	A	97	VAL	14
1	B	70	LYS	13
1	A	40	GLU	12
1	B	76	ASP	12
1	B	46	HIS	12
1	A	24	GLU	11
1	A	139	ASN	11
1	A	128	LYS	11
1	B	45	PHE	11
1	B	153	GLN	11
1	A	45	PHE	11
1	A	70	LYS	10
1	A	148	VAL	10
1	A	92	ASP	10
1	B	21	GLU	10
1	A	3	LYS	9
1	B	128	LYS	9
1	A	125	ASP	9
1	A	87	VAL	9
1	B	151	ILE	9
1	A	121	GLU	9
1	B	42	LEU	9
1	B	39	THR	9
1	B	3	LYS	9

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Mol	Chain	Res	Type	Models (Total)
1	B	122	LYS	9
1	A	58	THR	8
1	A	50	PHE	8
1	A	42	LEU	8
1	B	109	ASP	8
1	A	103	VAL	8
1	B	5	VAL	8
1	B	92	ASP	8
1	A	5	VAL	8
1	B	148	VAL	8
1	A	54	THR	7
1	B	65	ASN	7
1	B	90	ASP	7
1	B	125	ASP	7
1	A	21	GLU	7
1	A	36	LYS	7
1	B	121	GLU	7
1	B	134	SER	7
1	B	133	GLU	7
1	A	151	ILE	6
1	A	133	GLU	6
1	B	11	ASP	6
1	B	50	PHE	6
1	B	139	ASN	6
1	A	153	GLN	6
1	A	11	ASP	6
1	A	107	SER	6
1	B	40	GLU	5
1	B	132	GLU	5
1	A	39	THR	5
1	B	38	LEU	5
1	A	77	GLU	5
1	A	135	THR	5
1	A	69	ARG	5
1	B	49	GLU	5
1	A	132	GLU	5
1	B	19	ASN	5
1	A	111	SER	5
1	A	115	ARG	4
1	B	142	SER	4
1	B	126	LEU	4
1	A	79	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	137	THR	4
1	A	90	ASP	4
1	B	54	THR	4
1	B	106	LEU	4
1	A	122	LYS	4
1	A	131	ASN	4
1	B	79	ARG	4
1	B	48	HIS	4
1	A	109	ASP	4
1	A	38	LEU	4
1	A	19	ASN	4
1	A	64	PHE	4
1	B	111	SER	3
1	B	30	LYS	3
1	B	69	ARG	3
1	B	87	VAL	3
1	A	117	LEU	3
1	B	110	HIS	3
1	A	126	LEU	3
1	B	116	THR	3
1	A	59	SER	3
1	B	24	GLU	3
1	A	2	THR	3
1	B	131	ASN	3
1	A	22	GLN	3
1	B	83	ASP	3
1	B	2	THR	3
1	B	124	ASP	3
1	A	149	ILE	3
1	A	86	ASN	3
1	B	107	SER	3
1	A	81	VAL	3
1	B	119	VAL	3
1	A	119	VAL	3
1	A	30	LYS	3
1	B	52	ASP	3
1	B	115	ARG	3
1	A	112	ILE	3
1	A	136	LYS	3
1	A	57	CYS	2
1	B	78	GLU	2
1	A	88	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	110	HIS	2
1	B	64	PHE	2
1	B	149	ILE	2
1	B	14	VAL	2
1	B	31	VAL	2
1	B	94	VAL	2
1	A	8	LEU	2
1	A	62	PRO	2
1	B	112	ILE	2
1	B	135	THR	2
1	A	25	SER	2
1	A	124	ASP	2
1	B	136	LYS	2
1	A	83	ASP	2
1	A	99	ILE	2
1	B	77	GLU	2
1	A	31	VAL	2
1	A	106	LEU	2
1	A	142	SER	2
1	B	18	ILE	2
1	A	84	LEU	2
1	B	86	ASN	2
1	A	34	SER	2
1	A	49	GLU	2
1	A	65	ASN	2
1	A	134	SER	2
1	A	35	ILE	1
1	A	96	ASP	1
1	B	88	THR	1
1	B	84	LEU	1
1	B	74	PRO	1
1	B	7	VAL	1
1	A	9	LYS	1
1	B	103	VAL	1
1	B	117	LEU	1
1	B	146	CYS	1
1	A	26	ASN	1
1	B	120	HIS	1
1	B	36	LYS	1
1	B	62	PRO	1
1	B	22	GLN	1
1	B	9	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	B	35	ILE	1
1	B	26	ASN	1
1	A	20	PHE	1
1	A	52	ASP	1
1	A	48	HIS	1
1	B	105	SER	1
1	A	118	VAL	1
1	A	14	VAL	1
1	A	7	VAL	1
1	B	8	LEU	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 carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6821

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	3284
Number of shifts mapped to atoms	3284
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	228	2.00 ± 0.09	Should be applied
$^{13}\text{C}_\beta$	224	2.49 ± 0.08	Should be applied
$^{13}\text{C}'$	306	2.57 ± 0.11	Should be applied
^{15}N	294	0.36 ± 0.21	None needed (< 0.5 ppm)

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 85%, i.e. 2831 atoms were assigned a chemical shift out of a possible 3338. 34 out of 46 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1401/1480 (95%)	589/590 (100%)	523/600 (87%)	289/290 (100%)
Sidechain	1346/1648 (82%)	885/954 (93%)	441/628 (70%)	20/66 (30%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	84/210 (40%)	82/116 (71%)	0/74 (0%)	2/20 (10%)
Overall	2831/3338 (85%)	1556/1660 (94%)	964/1302 (74%)	311/376 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 2870 atoms were assigned a chemical shift out of a possible 3382. 34 out of 46 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	1428/1510 (95%)	600/602 (100%)	534/612 (87%)	294/296 (99%)
Sidechain	1358/1662 (82%)	892/962 (93%)	446/634 (70%)	20/66 (30%)
Aromatic	84/210 (40%)	82/116 (71%)	0/74 (0%)	2/20 (10%)
Overall	2870/3382 (85%)	1574/1680 (94%)	980/1320 (74%)	316/382 (83%)

7.1.4 Statistically unusual chemical shifts ⓘ

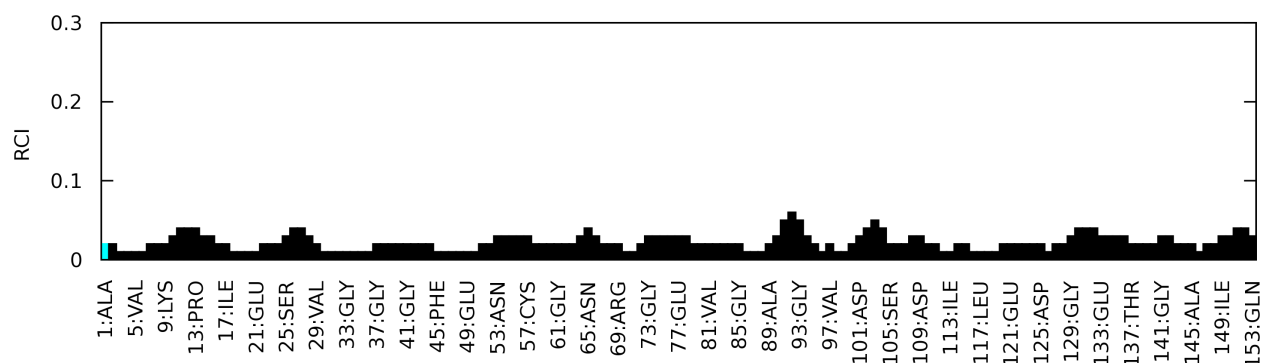
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	69	ARG	NE	128.81	92.63 – 76.73	27.8
1	B	69	ARG	NE	128.81	92.63 – 76.73	27.8
1	A	115	ARG	HD3	1.17	4.36 – 1.86	-7.8
1	B	115	ARG	HD3	1.17	4.36 – 1.86	-7.8
1	A	79	ARG	HG2	3.22	2.92 – 0.22	6.1
1	B	79	ARG	HG2	3.22	2.92 – 0.22	6.1
1	A	79	ARG	HG3	3.22	3.00 – 0.10	5.8
1	B	79	ARG	HG3	3.22	3.00 – 0.10	5.8
1	B	153	GLN	CG	27.38	39.38 – 28.18	-5.7
1	A	153	GLN	CG	27.38	39.38 – 28.18	-5.7

7.1.5 Random Coil Index (RCI) plots ⓘ

The images below report *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:



Random coil index (RCI) for chain B:

