Full wwPDB NMR Structure Validation Report (i)

Oct 31, 2021 – 09:07 AM EDT

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

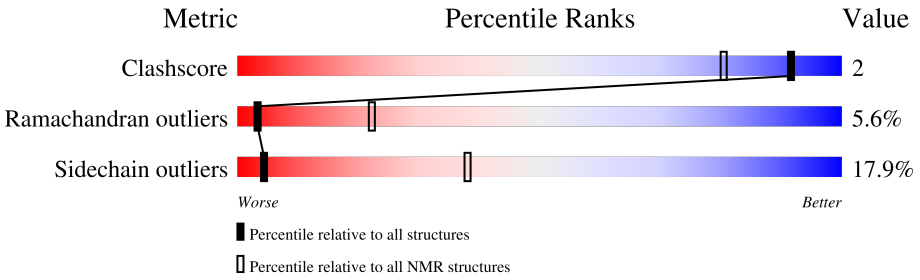
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=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 (i)

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 mutation	UNP P00441
A	111	SER	CYS	engineered mutation	UNP P00441
B	6	ALA	CYS	engineered mutation	UNP P00441
B	111	SER	CYS	engineered mutation	UNP P00441

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

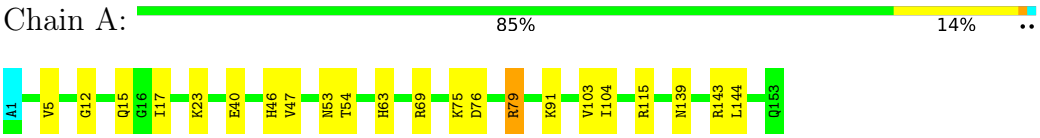
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1
2	B	1	Total	Zn
			1	1

4 Residue-property plots (i)

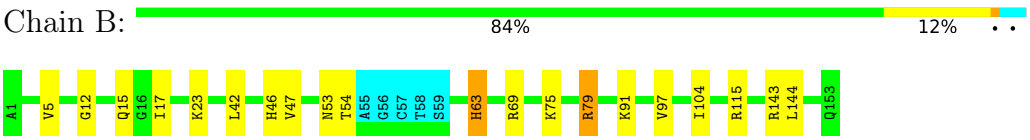
4.1 Average score per residue in the NMR ensemble

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 [Cu-Zn]



• Molecule 1: Superoxide dismutase [Cu-Zn]

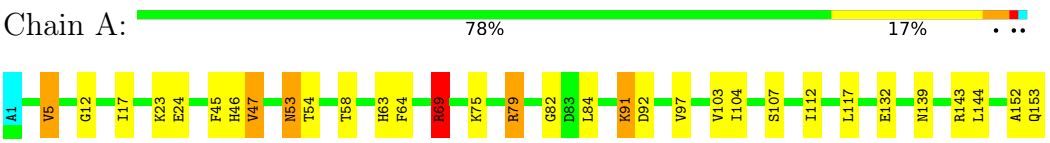


4.2 Scores per residue for each member of the ensemble

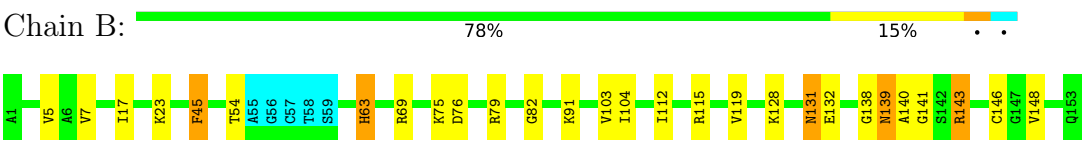
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Superoxide dismutase [Cu-Zn]



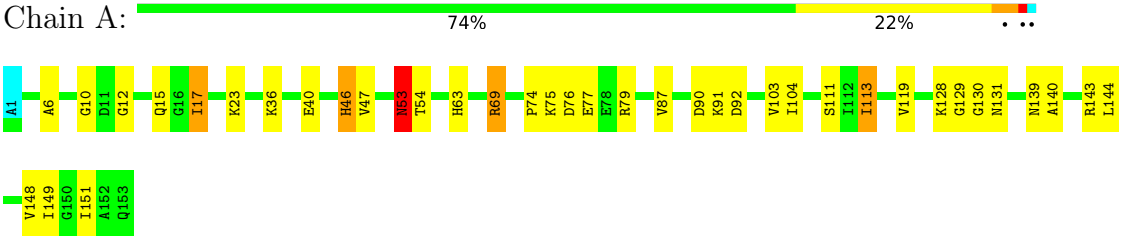
• Molecule 1: Superoxide dismutase [Cu-Zn]



4.2.2 Score per residue for model 2

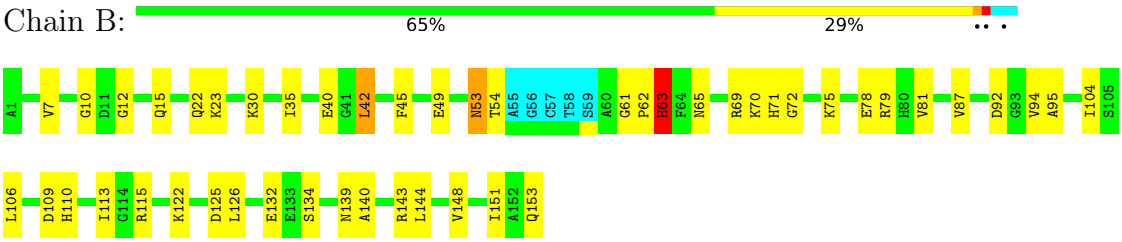
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

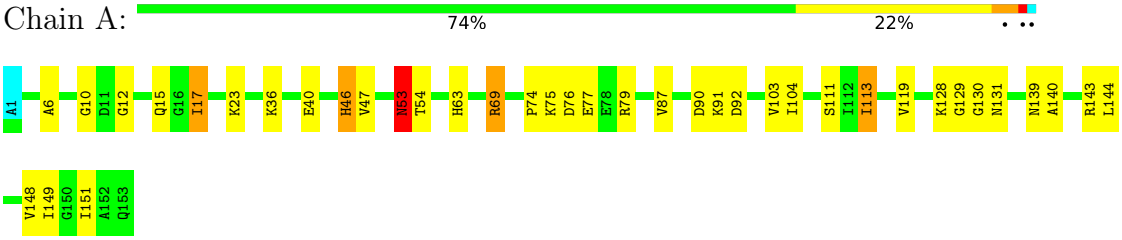
Chain B:



4.2.3 Score per residue for model 3

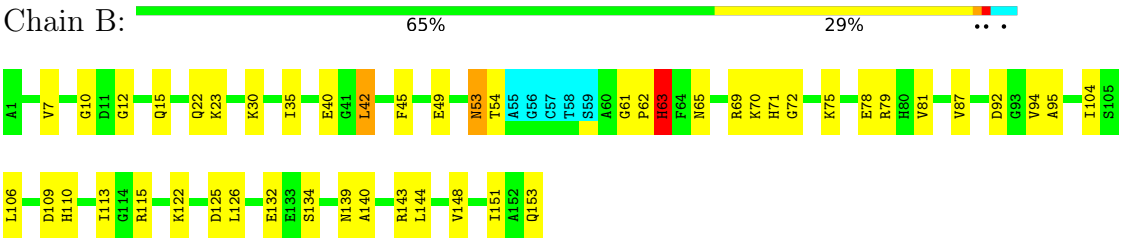
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



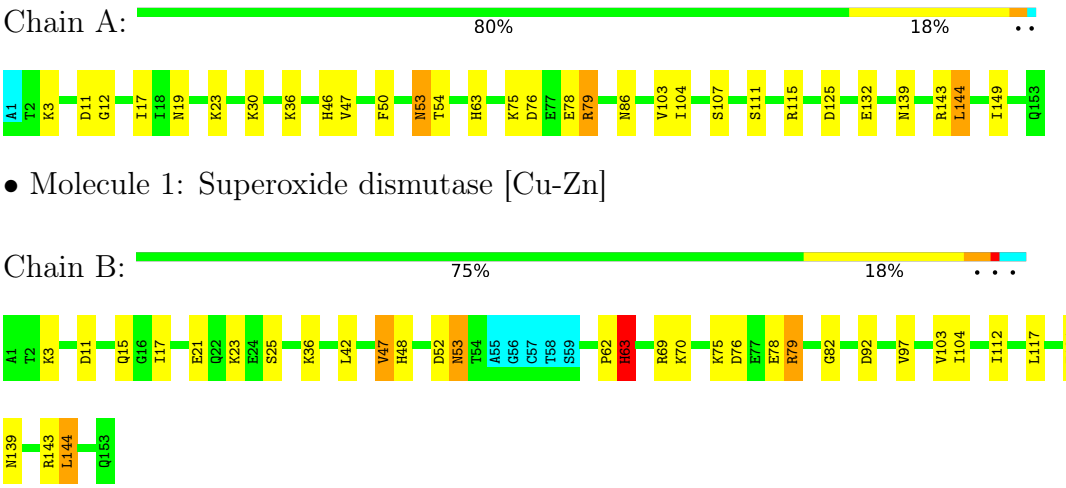
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:



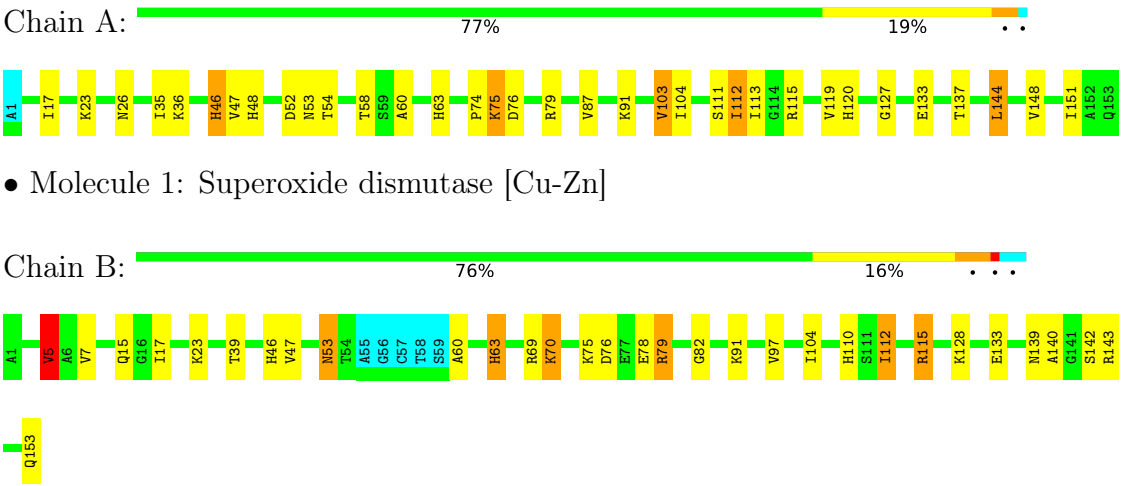
4.2.4 Score per residue for model 4

• Molecule 1: Superoxide dismutase [Cu-Zn]



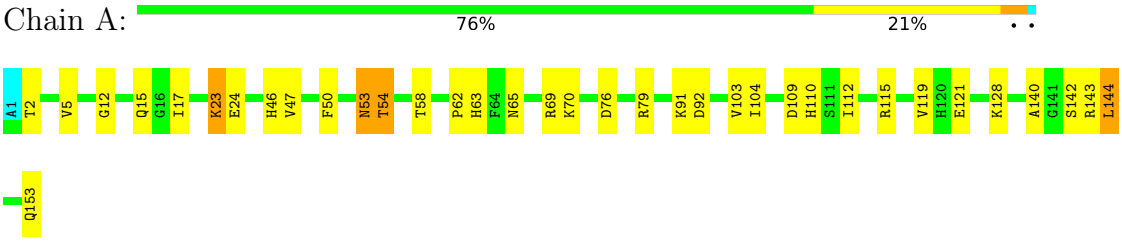
4.2.5 Score per residue for model 5

- Molecule 1: Superoxide dismutase [Cu-Zn]



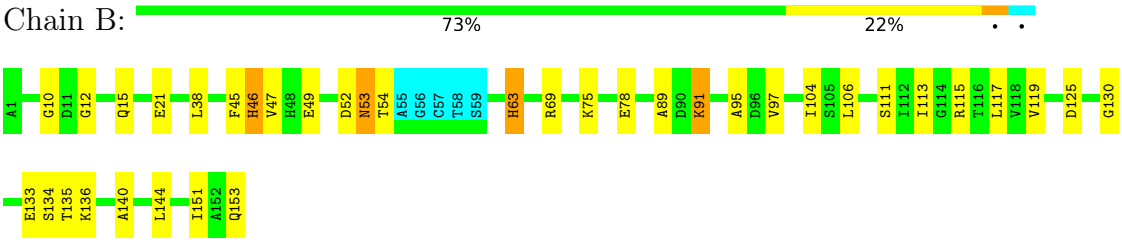
4.2.6 Score per residue for model 6

- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]

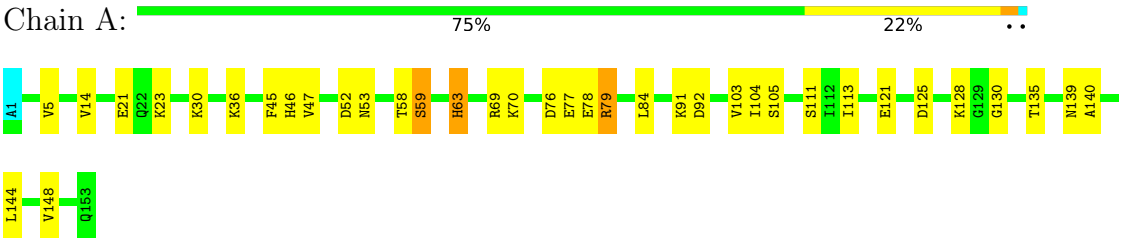
Chain B:



4.2.7 Score per residue for model 7

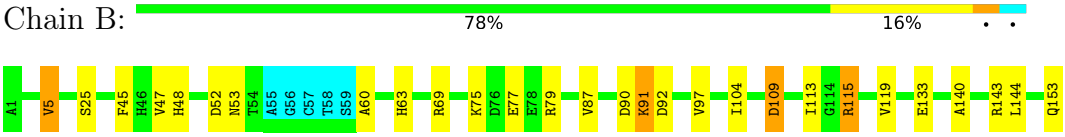
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



- Molecule 1: Superoxide dismutase [Cu-Zn]

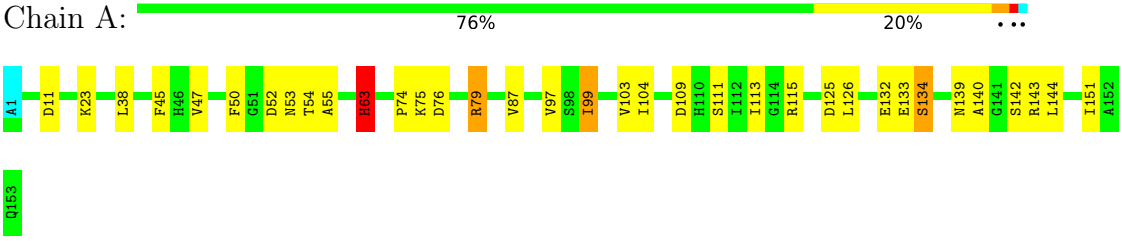
Chain B:



4.2.8 Score per residue for model 8

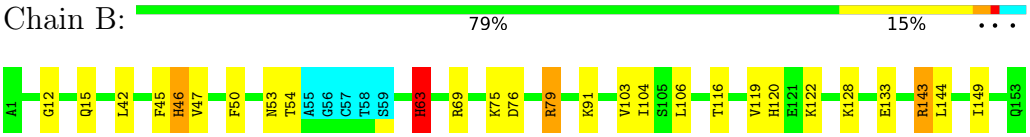
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



- Molecule 1: Superoxide dismutase [Cu-Zn]

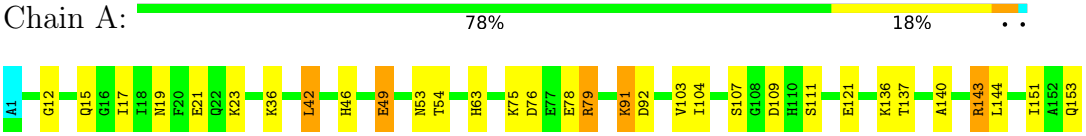
Chain B:



4.2.9 Score per residue for model 9

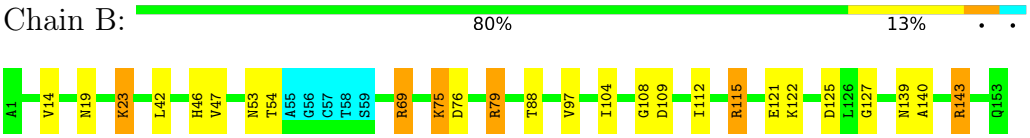
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

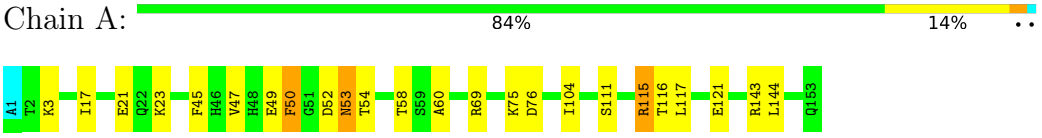
Chain B:



4.2.10 Score per residue for model 10

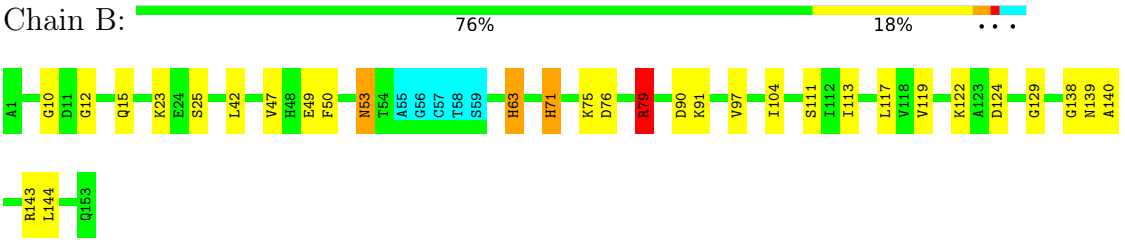
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

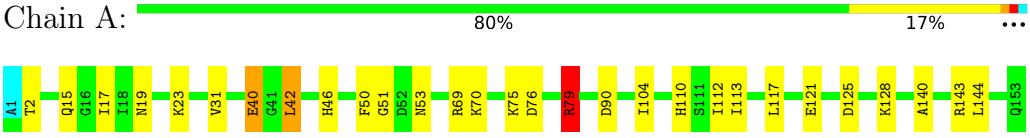
Chain B:



4.2.11 Score per residue for model 11

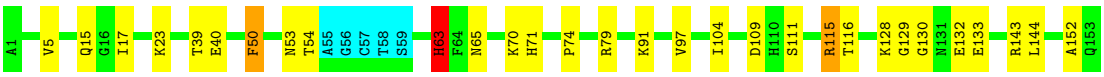
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

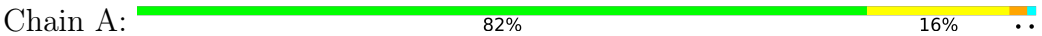
Chain B:

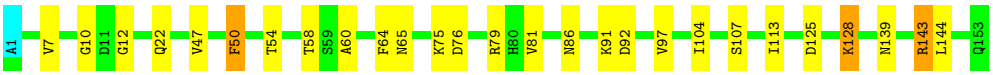


4.2.12 Score per residue for model 12

• Molecule 1: Superoxide dismutase [Cu-Zn]

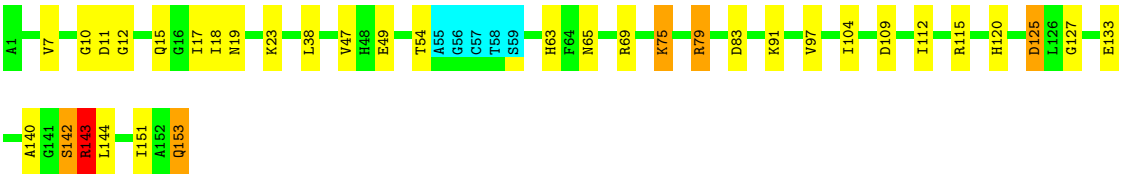
Chain A:





• Molecule 1: Superoxide dismutase [Cu-Zn]

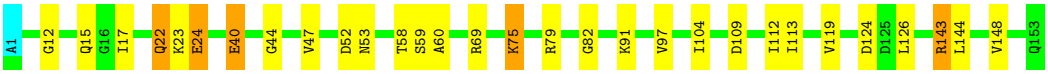
Chain B:



4.2.13 Score per residue for model 13

• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:

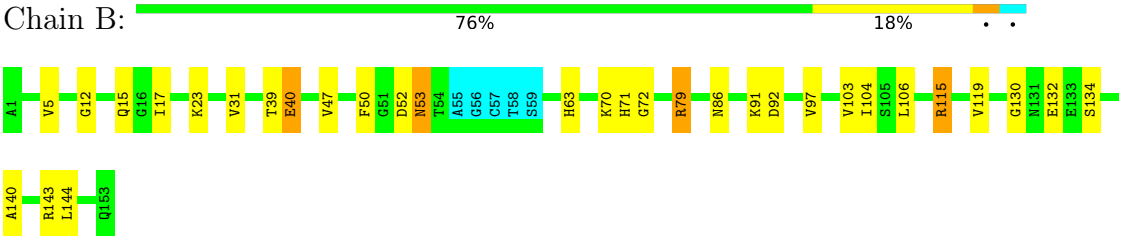
4.2.14 Score per residue for model 14

• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:

• Molecule 1: Superoxide dismutase [Cu-Zn]

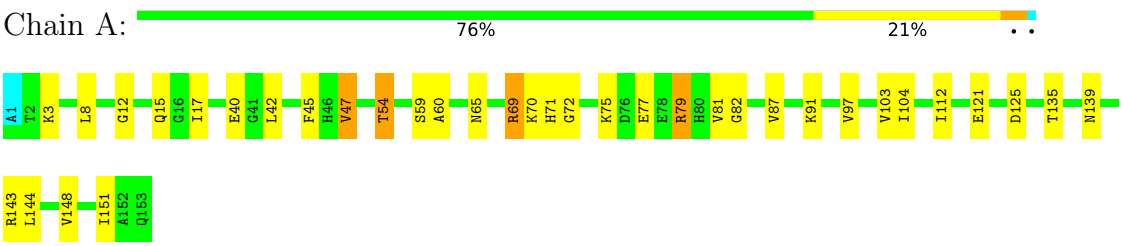
Chain B:



4.2.15 Score per residue for model 15

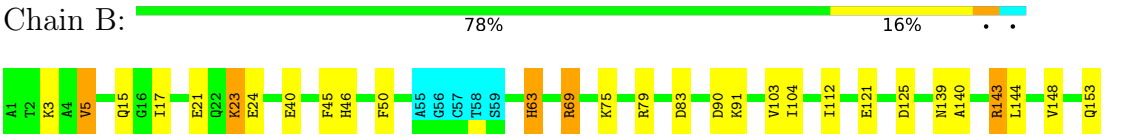
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

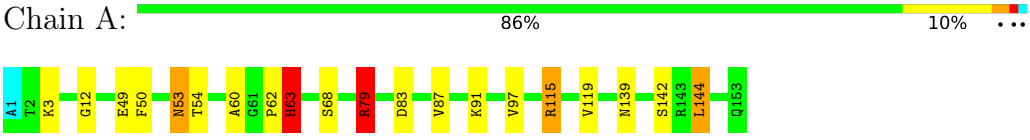
Chain B:



4.2.16 Score per residue for model 16

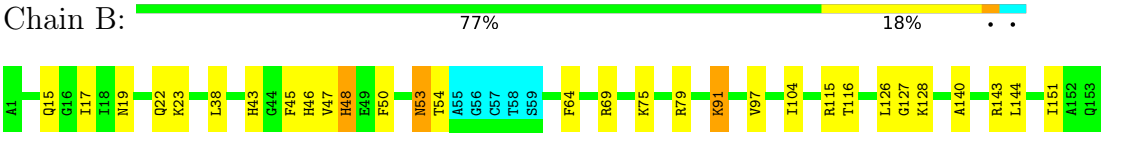
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

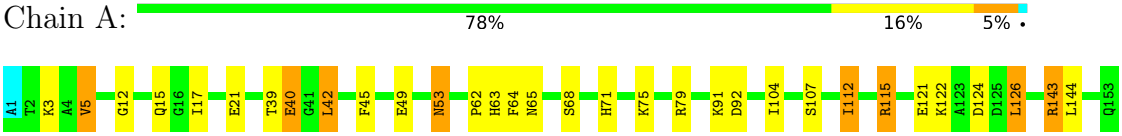
Chain B:



4.2.17 Score per residue for model 17

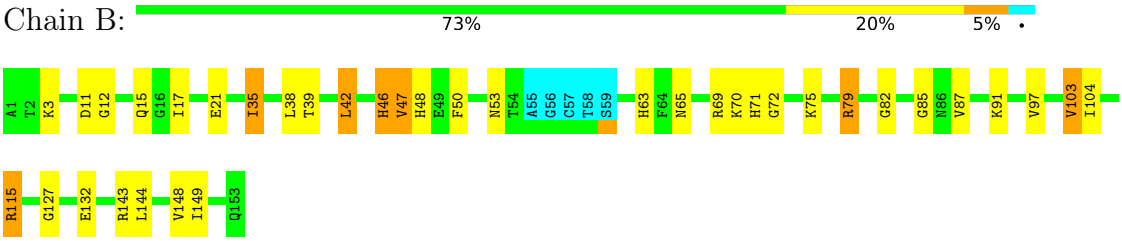
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

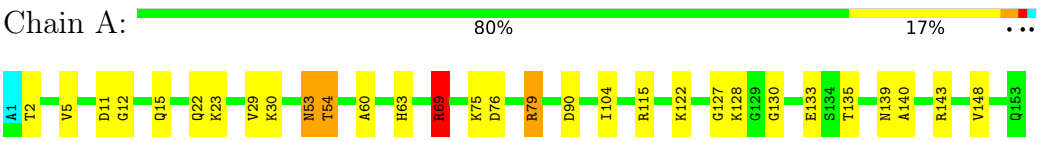
Chain B:



4.2.18 Score per residue for model 18

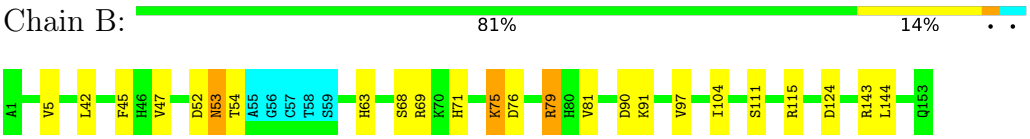
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

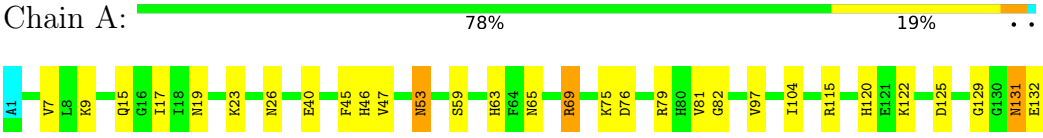
Chain B:



4.2.19 Score per residue for model 19

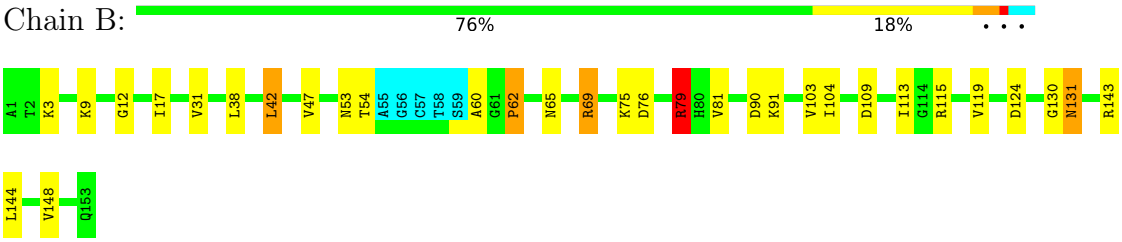
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

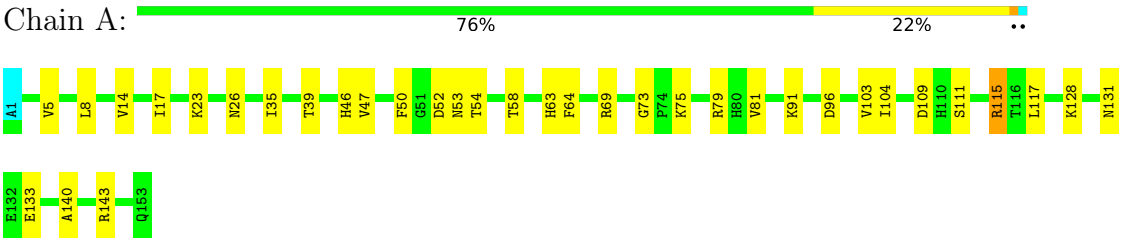
Chain B:



4.2.20 Score per residue for model 20

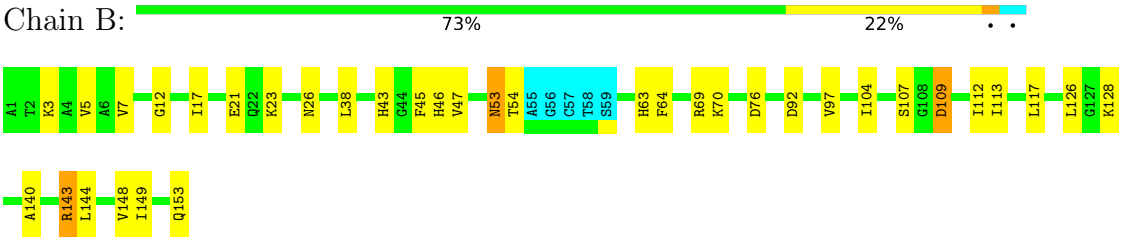
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



- Molecule 1: Superoxide dismutase [Cu-Zn]

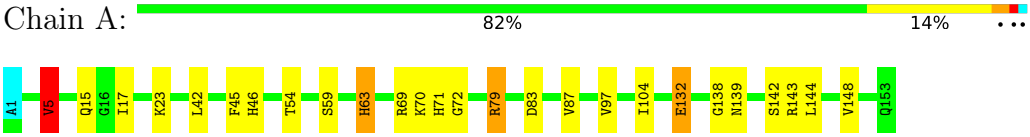
Chain B:



4.2.21 Score per residue for model 21

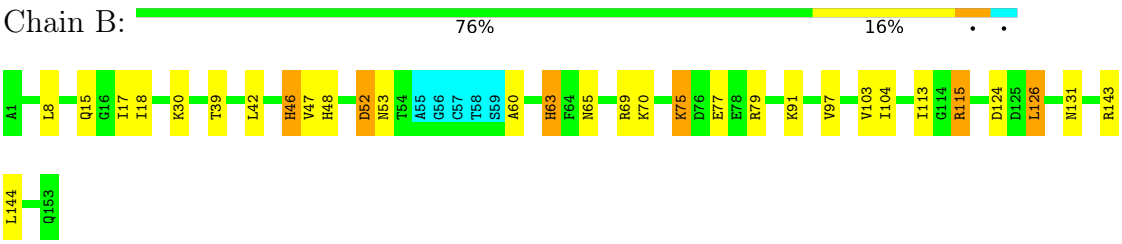
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



- Molecule 1: Superoxide dismutase [Cu-Zn]

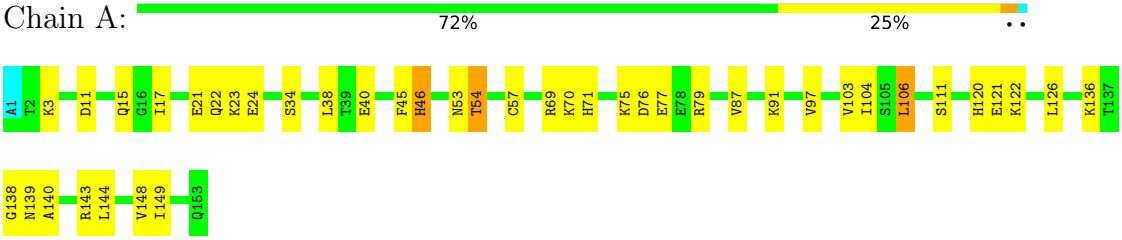
Chain B:



4.2.22 Score per residue for model 22

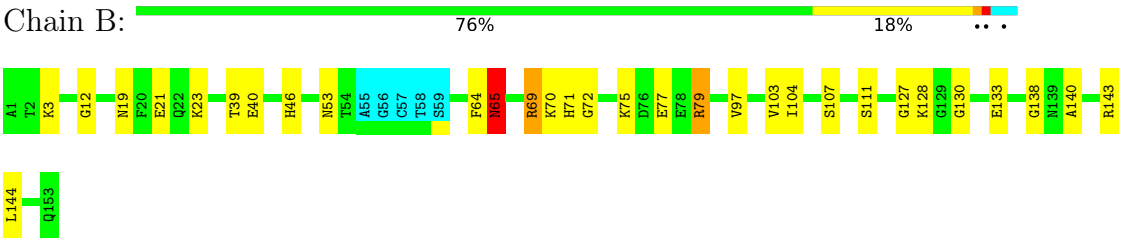
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

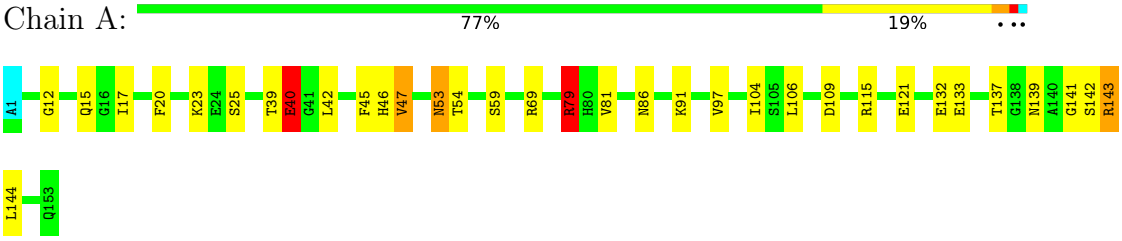
Chain B:



4.2.23 Score per residue for model 23 (medoid)

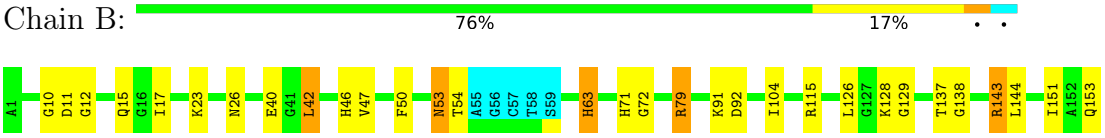
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

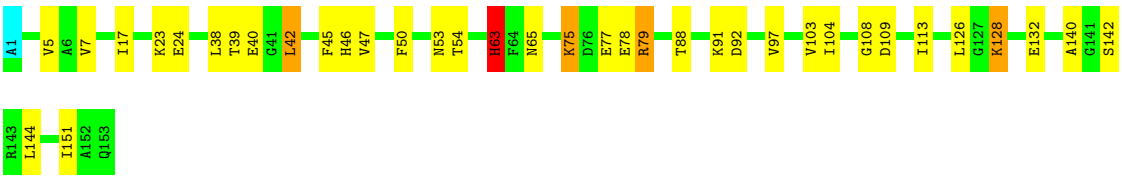
Chain B:



4.2.24 Score per residue for model 24

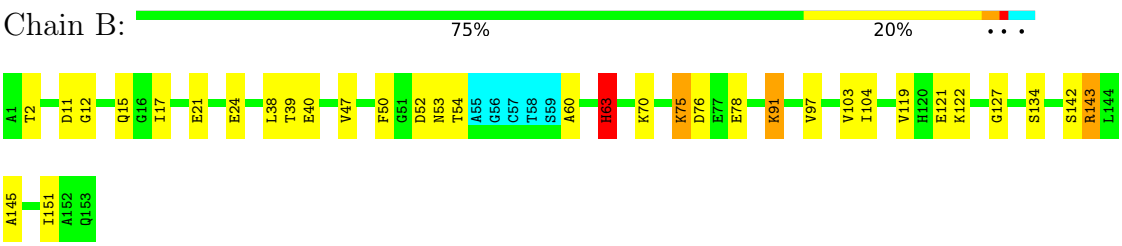
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

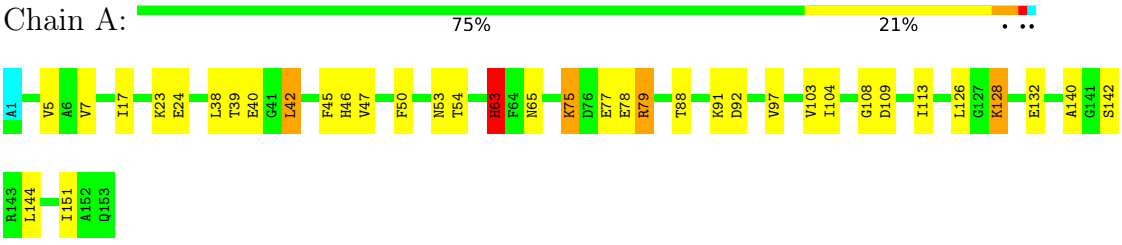
Chain B:



4.2.25 Score per residue for model 25

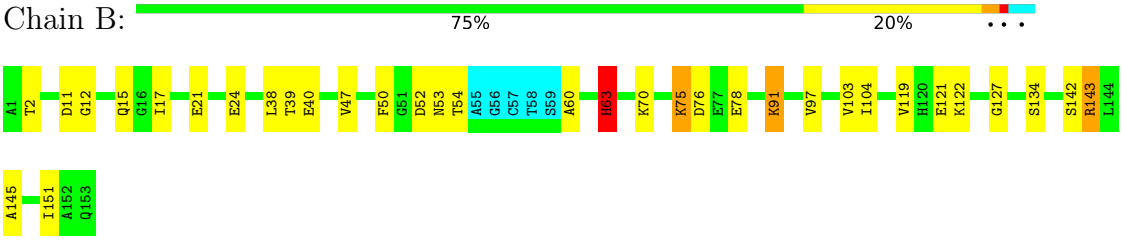
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

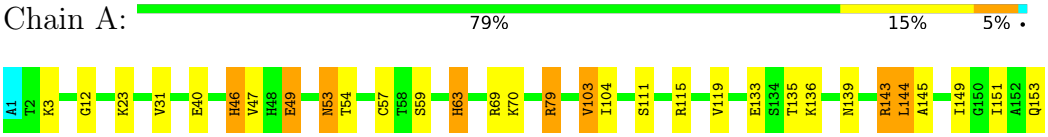
Chain B:



4.2.26 Score per residue for model 26

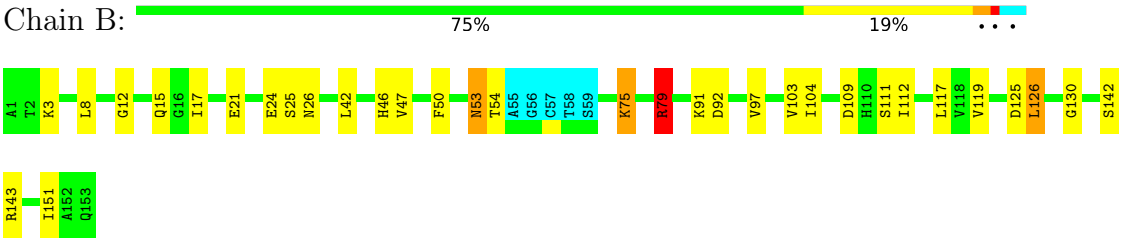
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

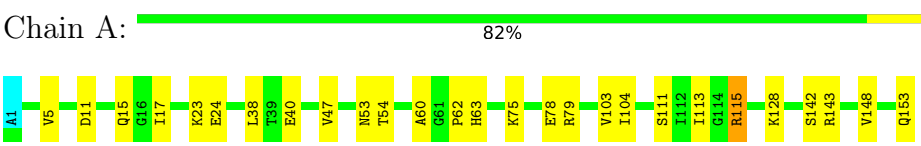
Chain B:



4.2.27 Score per residue for model 27

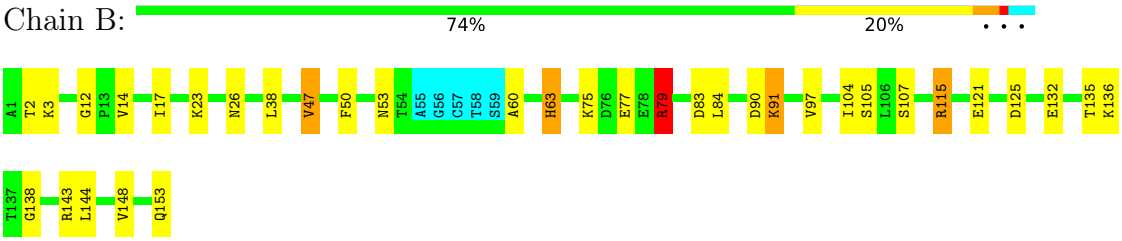
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



- Molecule 1: Superoxide dismutase [Cu-Zn]

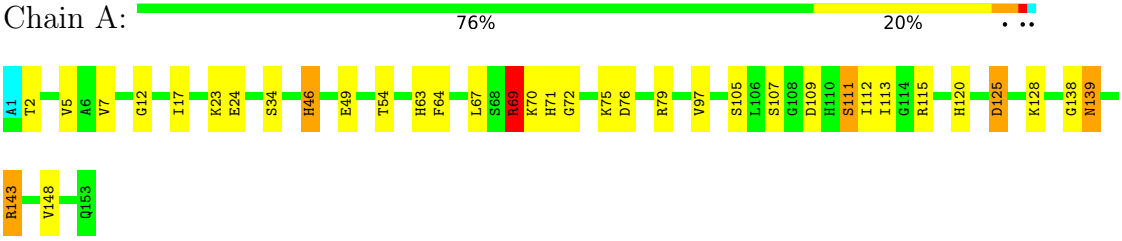
Chain B:



4.2.28 Score per residue for model 28

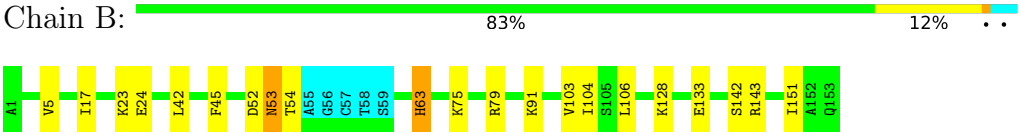
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



- Molecule 1: Superoxide dismutase [Cu-Zn]

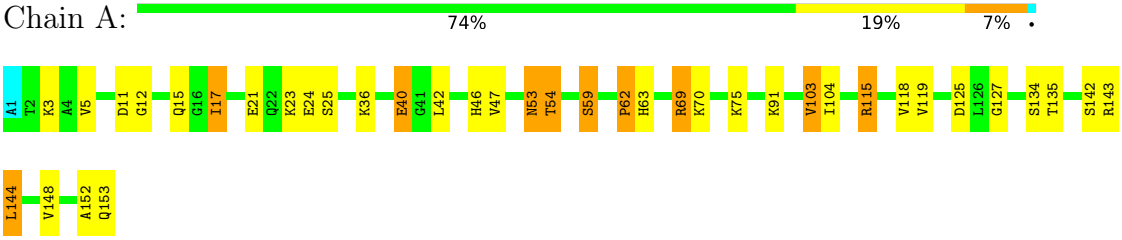
Chain B:



4.2.29 Score per residue for model 29

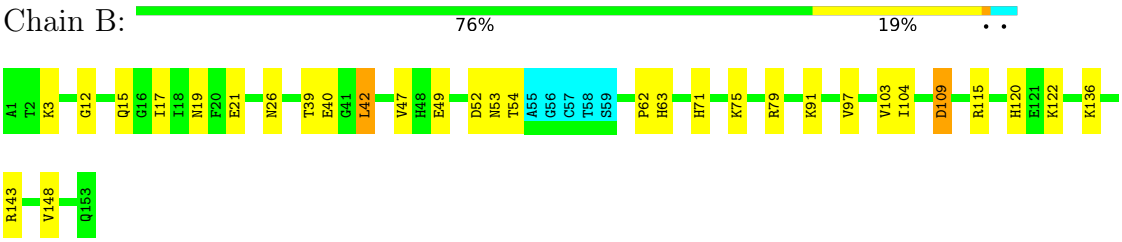
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

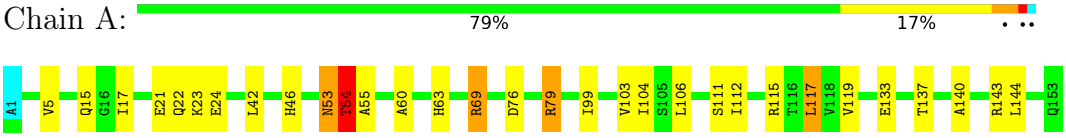
Chain B:



4.2.30 Score per residue for model 30

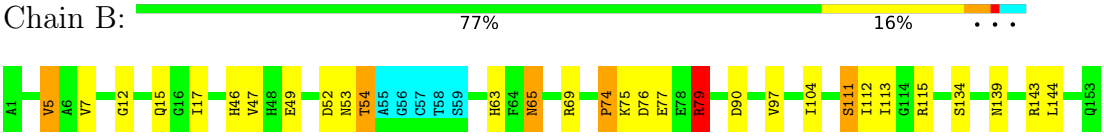
• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:



• Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, sumulated 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

No chemical shift data was provided.

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(^{o})	Ideal(^{o})	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(^{o})	Ideal(^{o})	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	69	ARG	Sidechain	8
1	B	115	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	63	HIS	Sidechain	2
1	B	143	ARG	Sidechain	2
1	A	79	ARG	Sidechain	2
1	B	50	PHE	Sidechain	1
1	A	46	HIS	Sidechain	1
1	A	143	ARG	Sidechain	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	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:H	1:B:42:LEU:HD22	0.68	1.48	23	3
1:A:53:ASN:ND2	1:B:7:VAL:HG21	0.66	2.05	2	3
1:B:63:HIS:H	1:B:63:HIS:CD2	0.65	2.09	17	8
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:H	1:A:42:LEU:HD22	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:H	1:A:63:HIS:CD2	0.61	2.13	14	4
1:A:54:THR:HG22	1:B:5:VAL:HG23	0.61	1.71	15	1
1:B:91:LYS:H	1:B:91:LYS:HE2	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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:42:LEU:H	1:B:42:LEU:HD23	0.55	1.62	10	8
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:H	1:B:42:LEU:CD2	0.54	2.16	23	4
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	2	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	3
1:A:113:ILE:HD13	1:A:149:ILE:HG22	0.51	1.82	2	2
1:B:48:HIS:CG	1:B:116:THR:HG23	0.51	2.40	16	1
1:A:17:ILE:HD13	1:B:54:THR:HG23	0.50	1.83	2	2
1:A:87:VAL:HG22	1:A:95:ALA:HB1	0.50	1.84	14	1
1:A:42:LEU:H	1:A:42:LEU:HD23	0.50	1.66	23	1
1:A:7:VAL:HA	1:B:54:THR:HG22	0.49	1.82	28	3
1:B:38:LEU:H	1:B:38:LEU:HD23	0.49	1.67	24	2
1:B:46:HIS:O	1:B:117:LEU:HD22	0.48	2.08	20	2
1:B:63:HIS:CD2	1:B:63:HIS:H	0.48	2.26	20	5
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	2
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:44:GLY:O	1:A:119:VAL:HG13	0.46	2.10	13	1
1:A:40:GLU:H	1:A:40:GLU:CD	0.46	2.14	23	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	2	3
1:A:7:VAL:CG2	1:B:54:THR:H	0.46	2.22	12	1
1:B:22:GLN:HB2	1:B:106:LEU:HD13	0.46	1.87	2	2
1:B:65:ASN:ND2	1:B:81:VAL:H	0.46	2.08	19	1
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:HD12	1:A:151:ILE:N	0.45	2.26	24	2
1:A:53:ASN:O	1:A:54:THR:HG23	0.45	2.10	30	1
1:A:42:LEU:H	1:A:42:LEU:CD2	0.45	2.21	9	1
1:A:71:HIS:CG	1:A:72:GLY:N	0.45	2.85	21	3
1:A:71:HIS:CD2	1:A:138:GLY:HA3	0.45	2.46	21	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:GLN:CB	1:A:106:LEU:HD11	0.45	2.42	22	1
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: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	5
1:B:63:HIS:CD2	1:B:63:HIS:N	0.43	2.86	5	3
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:B:63:HIS:CE1	1:B:71:HIS:CE1	0.42	3.08	10	1
1:A:23:LYS:H	1:A:23:LYS:CD	0.42	2.26	6	1
1:A:62:PRO:C	1:A:63:HIS:CD2	0.42	2.93	6	2
1:B:63:HIS:CE1	1:B:71:HIS:ND1	0.42	2.88	11	1
1:A:53:ASN:HB2	1:B:5:VAL:HG13	0.42	1.92	30	1
1:A:54:THR:HG21	1:B:148:VAL:O	0.42	2.15	29	1
1:B:42:LEU:HD13	1:B:42:LEU:H	0.42	1.75	29	1
1:B:70:LYS:HE2	1:B:78:GLU:OE1	0.41	2.15	5	1
1:B:124:ASP:CG	1:B:140:ALA:HB2	0.41	2.35	10	1
1:A:46:HIS:CG	1:A:63:HIS:CE1	0.41	3.08	28	1
1:A:53:ASN:CG	1:B:7:VAL:HG21	0.41	2.36	1	1
1:B:64:PHE:CG	1:B:65:ASN:N	0.41	2.88	22	1
1:B:23:LYS:HZ2	1:B:24:GLU:CD	0.41	2.19	15	1
1:B:151:ILE:HD12	1:B:151:ILE:N	0.41	2.29	26	1
1:A:91:LYS:H	1:A:91:LYS:HZ3	0.41	1.57	1	1
1:B:75:LYS:HE2	1:B:125:ASP:O	0.41	2.15	12	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	2	2
1:B:35:ILE:HB	1:B:95:ALA:HB3	0.41	1.91	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:47:VAL:HG23	1:B:82:GLY:C	0.41	2.36	4	1
1:A:51:GLY:HA2	1:B:152:ALA:CA	0.41	2.46	11	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:B:47:VAL:CG2	1:B:82:GLY:HA2	0.41	2.46	17	1
1:A:46:HIS:CE1	1:A:120:HIS:CD2	0.40	3.09	5	3
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:B:8:LEU:CD2	1:B:117:LEU:HD12	0.40	2.46	26	1
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:A:46:HIS:O	1:A:117:LEU:HD22	0.40	2.16	1	1
1:B:23:LYS:N	1:B:23:LYS:HE2	0.40	2.31	9	1
1:A:22:GLN:HE22	1:A:24:GLU:C	0.40	2.19	13	1
1:A:47:VAL:HG23	1:A:82:GLY:CA	0.40	2.46	15	1
1:B:63:HIS:CE1	1:B:137:THR:O	0.40	2.74	23	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	151/153 (99%)	115±5 (76±3%)	27±4 (18±3%)	9±3 (6±2%)	3	22
1	B	146/153 (95%)	112±4 (77±3%)	26±4 (18±3%)	8±2 (6±2%)	3	23
All	All	8910/9180 (97%)	6824 (77%)	1586 (18%)	500 (6%)	3	22

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

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Mol	Chain	Res	Type	Models (Total)
1	A	12	GLY	16
1	A	53	ASN	16
1	A	54	THR	16
1	B	103	VAL	14
1	A	103	VAL	14
1	A	140	ALA	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	112	ILE	7
1	A	75	LYS	7
1	B	60	ALA	7
1	A	142	SER	7
1	A	59	SER	7
1	B	63	HIS	7
1	B	127	GLY	7
1	B	50	PHE	7
1	B	10	GLY	6
1	B	40	GLU	6
1	A	78	GLU	6
1	B	130	GLY	6
1	B	91	LYS	6
1	A	109	ASP	6
1	B	62	PRO	5
1	A	65	ASN	5
1	A	112	ILE	5
1	B	111	SER	5
1	B	109	ASP	5
1	B	138	GLY	4
1	A	74	PRO	4
1	A	130	GLY	4
1	A	50	PHE	4
1	A	144	LEU	4
1	B	25	SER	4
1	B	78	GLU	4
1	B	139	ASN	4
1	A	17	ILE	4

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Mol	Chain	Res	Type	Models (Total)
1	A	126	LEU	4
1	A	49	GLU	4
1	A	62	PRO	4
1	A	139	ASN	4
1	B	65	ASN	4
1	B	26	ASN	4
1	A	10	GLY	3
1	A	129	GLY	3
1	B	126	LEU	3
1	A	132	GLU	3
1	A	127	GLY	3
1	B	77	GLU	3
1	A	63	HIS	3
1	B	129	GLY	3
1	B	142	SER	3
1	A	64	PHE	2
1	B	5	VAL	2
1	B	61	GLY	2
1	A	26	ASN	2
1	A	55	ALA	2
1	A	42	LEU	2
1	B	74	PRO	2
1	A	57	CYS	2
1	A	68	SER	2
1	A	81	VAL	2
1	A	77	GLU	2
1	A	108	GLY	2
1	B	145	ALA	2
1	B	49	GLU	2
1	B	82	GLY	1
1	B	141	GLY	1
1	B	144	LEU	1
1	A	151	ILE	1
1	A	52	ASP	1
1	B	133	GLU	1
1	B	108	GLY	1
1	A	39	THR	1
1	B	128	LYS	1
1	A	5	VAL	1
1	B	85	GLY	1
1	B	132	GLU	1
1	B	68	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	B	81	VAL	1
1	A	82	GLY	1
1	B	131	ASN	1
1	A	73	GLY	1
1	A	133	GLU	1
1	A	141	GLY	1
1	A	143	ARG	1
1	B	17	ILE	1
1	B	125	ASP	1
1	A	138	GLY	1
1	A	152	ALA	1
1	B	52	ASP	1

6.3.2 Protein sidechains (i)

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%)	4	37
1	B	114/117 (97%)	94±4 (82±3%)	20±4 (18±3%)	4	38
All	All	6930/7020 (99%)	5687 (82%)	1243 (18%)	4	38

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	A	17	ILE	21
1	B	75	LYS	21
1	B	91	LYS	21
1	B	143	ARG	21
1	B	15	GLN	21
1	B	47	VAL	21
1	B	97	VAL	21

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Mol	Chain	Res	Type	Models (Total)
1	A	53	ASN	20
1	A	75	LYS	20
1	B	63	HIS	20
1	B	144	LEU	20
1	A	47	VAL	19
1	A	91	LYS	19
1	A	143	ARG	19
1	B	17	ILE	19
1	B	23	LYS	18
1	A	46	HIS	18
1	A	63	HIS	17
1	A	15	GLN	16
1	A	76	ASP	16
1	A	97	VAL	14
1	B	70	LYS	13
1	B	76	ASP	12
1	B	46	HIS	12
1	A	40	GLU	12
1	A	24	GLU	11
1	A	139	ASN	11
1	B	45	PHE	11
1	A	128	LYS	11
1	B	153	GLN	11
1	A	45	PHE	11
1	A	92	ASP	10
1	B	21	GLU	10
1	A	148	VAL	10
1	A	70	LYS	10
1	B	128	LYS	9
1	A	87	VAL	9
1	B	42	LEU	9
1	B	122	LYS	9
1	B	151	ILE	9
1	A	3	LYS	9
1	A	125	ASP	9
1	B	3	LYS	9
1	B	39	THR	9
1	A	121	GLU	9
1	A	5	VAL	8
1	A	58	THR	8
1	A	103	VAL	8
1	B	148	VAL	8

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Mol	Chain	Res	Type	Models (Total)
1	B	92	ASP	8
1	B	109	ASP	8
1	B	5	VAL	8
1	A	50	PHE	8
1	A	42	LEU	8
1	A	36	LYS	7
1	B	65	ASN	7
1	B	125	ASP	7
1	B	134	SER	7
1	B	121	GLU	7
1	B	133	GLU	7
1	A	54	THR	7
1	A	21	GLU	7
1	B	90	ASP	7
1	A	107	SER	6
1	A	153	GLN	6
1	B	139	ASN	6
1	A	151	ILE	6
1	A	11	ASP	6
1	B	11	ASP	6
1	A	133	GLU	6
1	B	50	PHE	6
1	A	69	ARG	5
1	A	132	GLU	5
1	B	132	GLU	5
1	A	77	GLU	5
1	B	49	GLU	5
1	A	111	SER	5
1	B	38	LEU	5
1	A	135	THR	5
1	B	19	ASN	5
1	B	40	GLU	5
1	A	39	THR	5
1	A	90	ASP	4
1	A	131	ASN	4
1	A	19	ASN	4
1	B	48	HIS	4
1	B	79	ARG	4
1	A	137	THR	4
1	B	142	SER	4
1	A	109	ASP	4
1	A	115	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	B	106	LEU	4
1	A	38	LEU	4
1	B	54	THR	4
1	A	64	PHE	4
1	A	79	ARG	4
1	B	126	LEU	4
1	A	122	LYS	4
1	A	112	ILE	3
1	B	131	ASN	3
1	B	30	LYS	3
1	B	87	VAL	3
1	B	110	HIS	3
1	A	30	LYS	3
1	A	86	ASN	3
1	A	149	ILE	3
1	B	52	ASP	3
1	A	2	THR	3
1	B	115	ARG	3
1	B	119	VAL	3
1	A	59	SER	3
1	B	116	THR	3
1	A	136	LYS	3
1	B	69	ARG	3
1	A	117	LEU	3
1	B	111	SER	3
1	A	22	GLN	3
1	A	81	VAL	3
1	B	83	ASP	3
1	A	126	LEU	3
1	B	124	ASP	3
1	B	107	SER	3
1	B	2	THR	3
1	B	24	GLU	3
1	A	119	VAL	3
1	A	84	LEU	2
1	B	78	GLU	2
1	B	94	VAL	2
1	B	112	ILE	2
1	A	110	HIS	2
1	B	135	THR	2
1	B	136	LYS	2
1	A	99	ILE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	134	SER	2
1	B	149	ILE	2
1	A	49	GLU	2
1	B	14	VAL	2
1	A	31	VAL	2
1	B	18	ILE	2
1	A	124	ASP	2
1	B	86	ASN	2
1	A	57	CYS	2
1	A	62	PRO	2
1	B	31	VAL	2
1	A	8	LEU	2
1	A	65	ASN	2
1	A	83	ASP	2
1	A	142	SER	2
1	B	64	PHE	2
1	B	77	GLU	2
1	A	34	SER	2
1	A	106	LEU	2
1	A	25	SER	2
1	A	88	THR	2
1	B	146	CYS	1
1	B	36	LYS	1
1	A	48	HIS	1
1	B	88	THR	1
1	A	52	ASP	1
1	B	117	LEU	1
1	B	22	GLN	1
1	B	35	ILE	1
1	B	103	VAL	1
1	A	7	VAL	1
1	A	9	LYS	1
1	B	9	LYS	1
1	B	62	PRO	1
1	A	14	VAL	1
1	A	26	ASN	1
1	A	35	ILE	1
1	A	96	ASP	1
1	B	8	LEU	1
1	A	20	PHE	1
1	B	84	LEU	1
1	B	105	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	118	VAL	1
1	B	26	ASN	1
1	B	120	HIS	1
1	B	7	VAL	1
1	B	74	PRO	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 monosaccharides in this entry.

6.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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