



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:11 PM BST

PDB ID : 1L3N
Title : The Solution Structure of Reduced Dimeric Copper Zinc SOD: the Structural Effects of Dimerization
Authors : Banci, L.; Bertini, I.; Cramaro, F.; Del Conte, R.; Viezzoli, M.S.
Deposited on : 2002-02-28

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

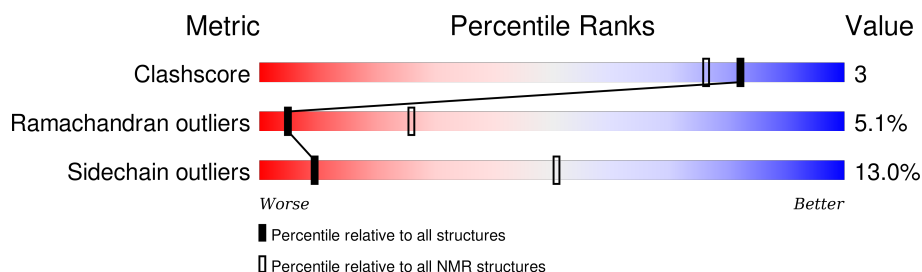
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	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	 88% 12% •
1	B	153	 80% 16% •

2 Ensemble composition and analysis ⓘ

This entry contains 30 models. Model 15 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:1-A:153, B:1-B:23, B:27-B:107, B:111-B:153 (300)	0.56	15

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4378 atoms, of which 2156 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
			2187	679	1078	203	225	2	
1	B	153	Total	C	H	N	O	S	0
			2187	679	1078	203	225	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 COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

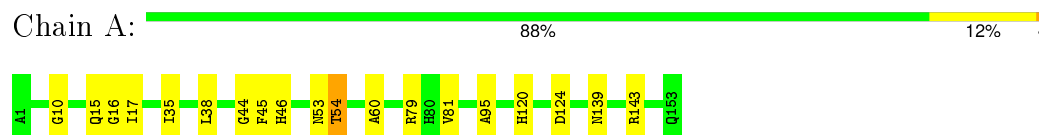
Mol	Chain	Residues	Atoms	
3	B	1	Total	Zn
			1	1
3	A	1	Total	Zn
			1	1

4 Residue-property plots [i](#)

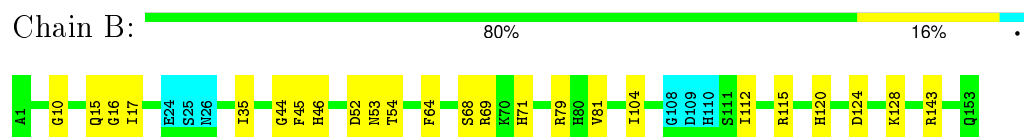
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA 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]

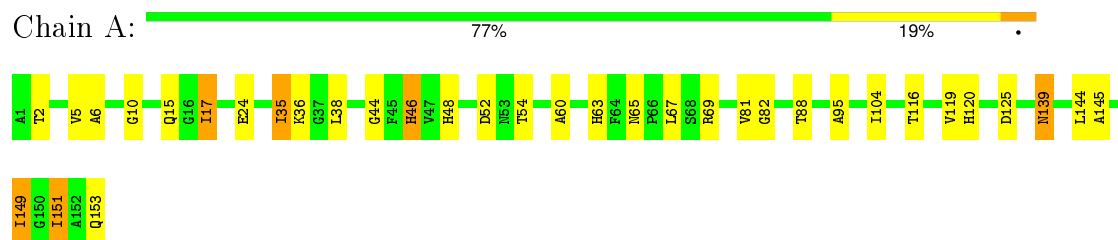


4.2 Scores per residue for each member of the ensemble

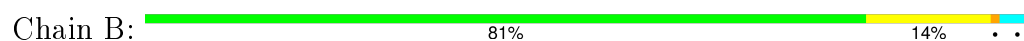
Colouring as in section 4.1 above.

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

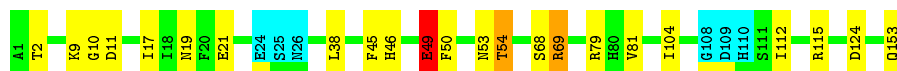
- Molecule 1: superoxide dismutase [Cu-Zn]

Chain A: 84% 15%



- Molecule 1: superoxide dismutase [Cu-Zn]

Chain B: 81% 13%



4.2.3 Score per residue for model 3

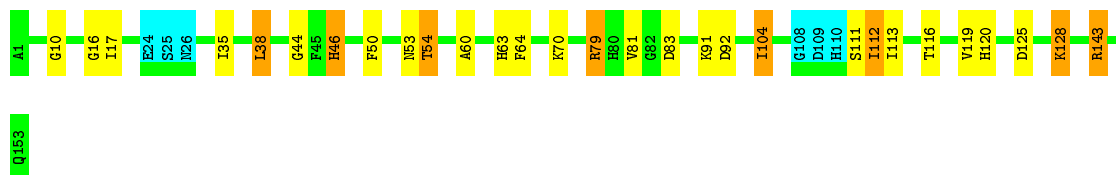
- Molecule 1: superoxide dismutase [Cu-Zn]

Chain A: 83% 15%



- Molecule 1: superoxide dismutase [Cu-Zn]

Chain B: 77% 14% 5%



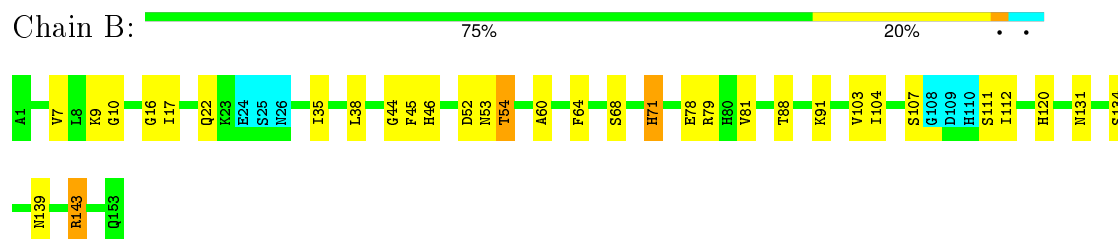
4.2.4 Score per residue for model 4

- Molecule 1: superoxide dismutase [Cu-Zn]

Chain A: 80% 18%

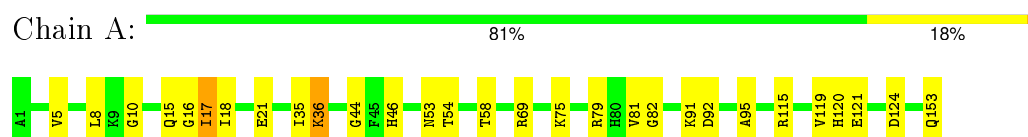


- Molecule 1: superoxide dismutase [Cu-Zn]

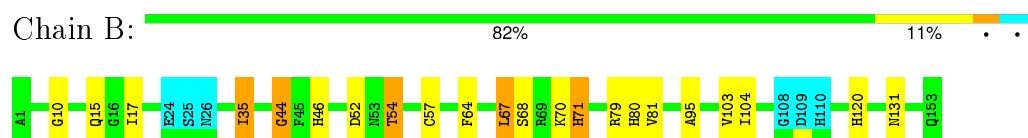


4.2.5 Score per residue for model 5

- Molecule 1: superoxide dismutase [Cu-Zn]

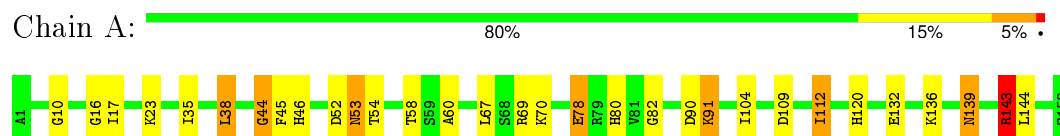


- Molecule 1: superoxide dismutase [Cu-Zn]

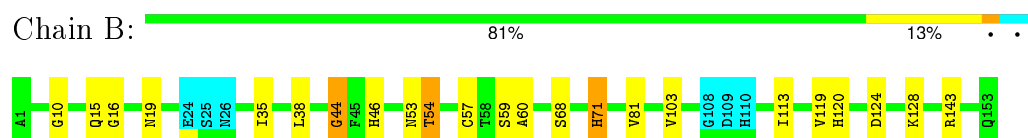


4.2.6 Score per residue for model 6

- Molecule 1: superoxide dismutase [Cu-Zn]

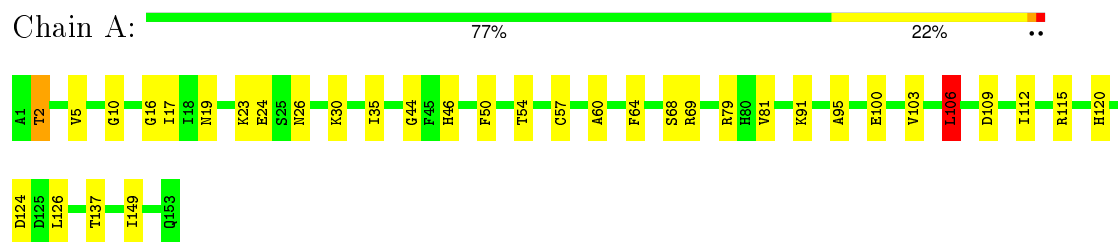


- Molecule 1: superoxide dismutase [Cu-Zn]

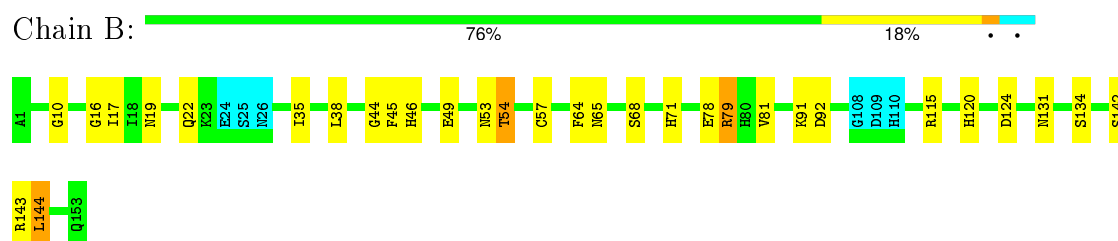


4.2.7 Score per residue for model 7

- Molecule 1: superoxide dismutase [Cu-Zn]

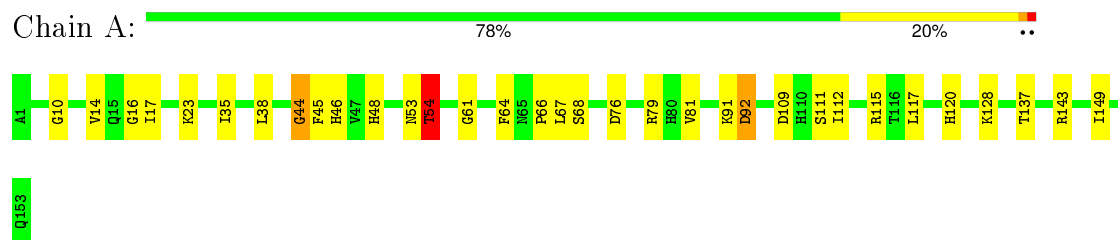


- Molecule 1: superoxide dismutase [Cu-Zn]

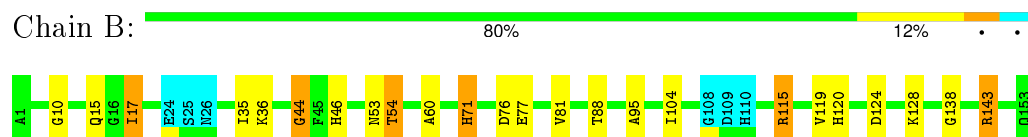


4.2.8 Score per residue for model 8

- Molecule 1: superoxide dismutase [Cu-Zn]

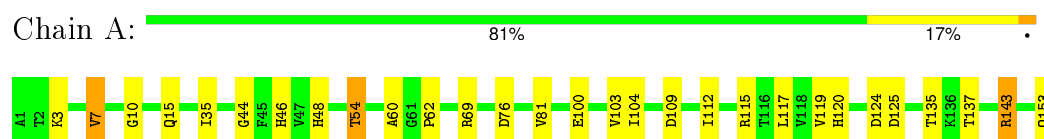


- Molecule 1: superoxide dismutase [Cu-Zn]

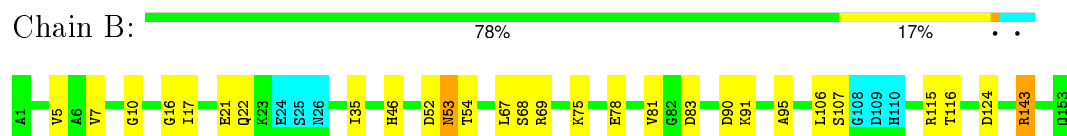


4.2.9 Score per residue for model 9

- Molecule 1: superoxide dismutase [Cu-Zn]

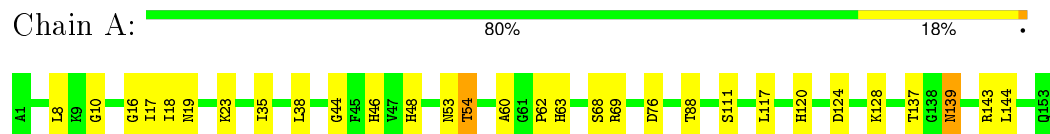


- Molecule 1: superoxide dismutase [Cu-Zn]

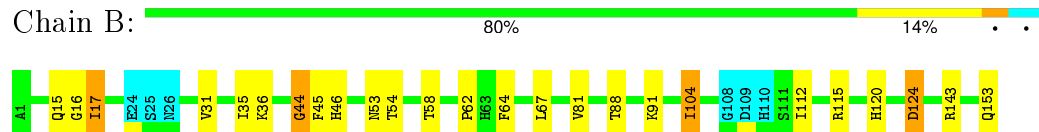


4.2.10 Score per residue for model 10

- Molecule 1: superoxide dismutase [Cu-Zn]

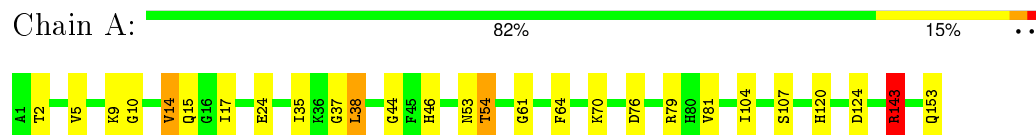


- Molecule 1: superoxide dismutase [Cu-Zn]

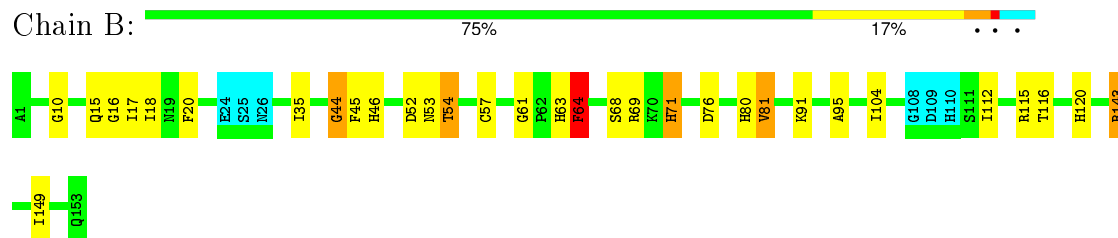


4.2.11 Score per residue for model 11

- Molecule 1: superoxide dismutase [Cu-Zn]

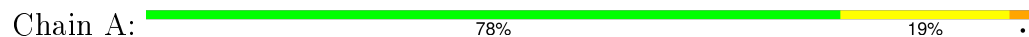


- Molecule 1: superoxide dismutase [Cu-Zn]




4.2.12 Score per residue for model 12

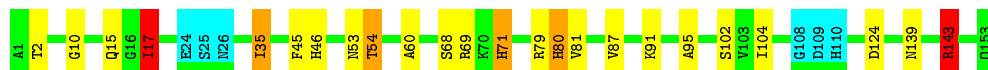
- Molecule 1: superoxide dismutase [Cu-Zn]





- Molecule 1: superoxide dismutase [Cu-Zn]

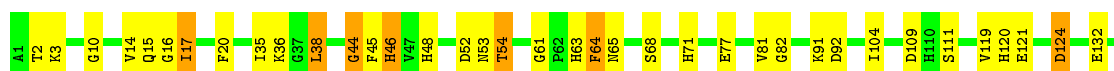
Chain B: 



4.2.13 Score per residue for model 13

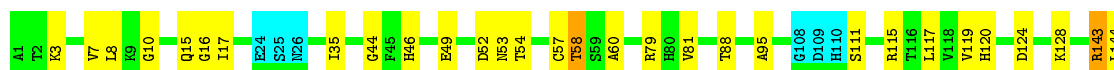
- Molecule 1: superoxide dismutase [Cu-Zn]

Chain A: 




- Molecule 1: superoxide dismutase [Cu-Zn]

Chain B: 



4.2.14 Score per residue for model 14

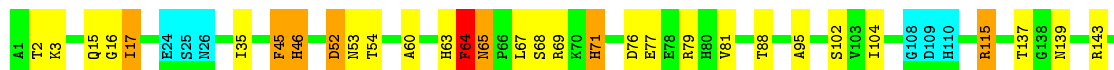
- Molecule 1: superoxide dismutase [Cu-Zn]

Chain A: 



- Molecule 1: superoxide dismutase [Cu-Zn]

Chain B: 





4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: superoxide dismutase [Cu-Zn]

Chain A: 79% 18%



- Molecule 1: superoxide dismutase [Cu-Zn]

Chain B: 78% 14%



4.2.16 Score per residue for model 16

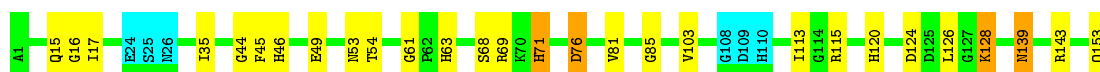
- Molecule 1: superoxide dismutase [Cu-Zn]

Chain A: 84% 14%



- Molecule 1: superoxide dismutase [Cu-Zn]

Chain B: 78% 16%



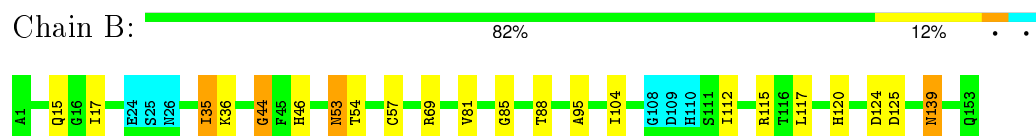
4.2.17 Score per residue for model 17

- Molecule 1: superoxide dismutase [Cu-Zn]

Chain A: 80% 18%

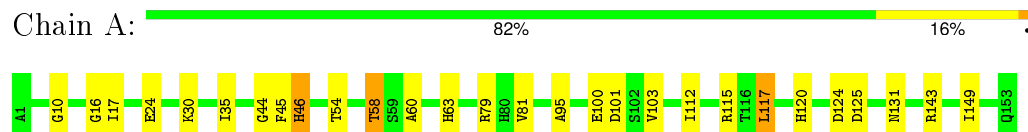


- Molecule 1: superoxide dismutase [Cu-Zn]

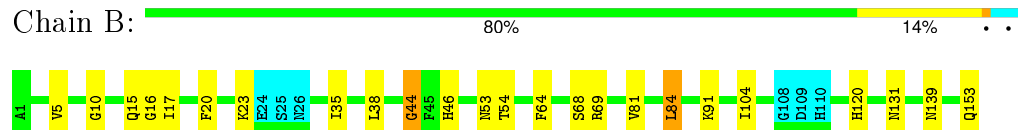


4.2.18 Score per residue for model 18

- Molecule 1: superoxide dismutase [Cu-Zn]

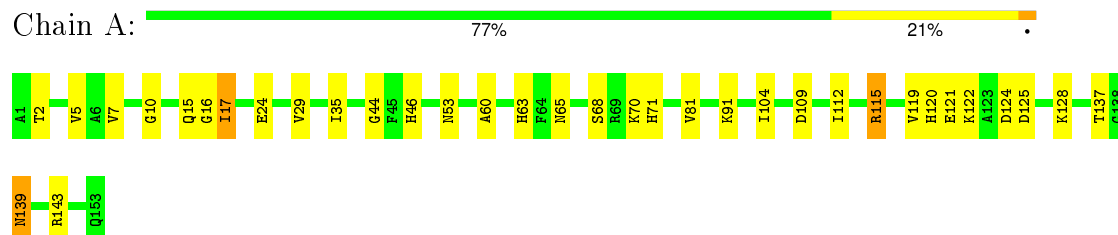


- Molecule 1: superoxide dismutase [Cu-Zn]

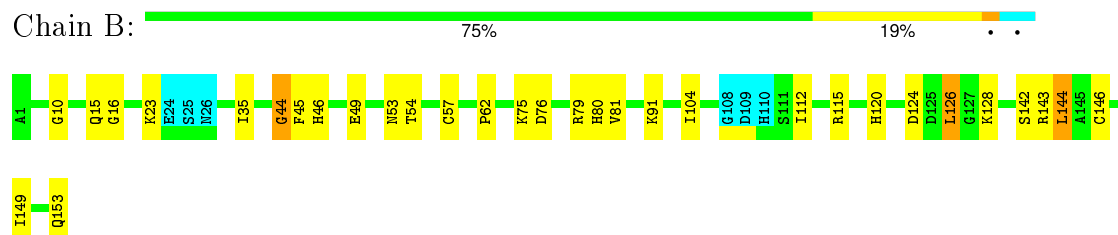


4.2.19 Score per residue for model 19

- Molecule 1: superoxide dismutase [Cu-Zn]

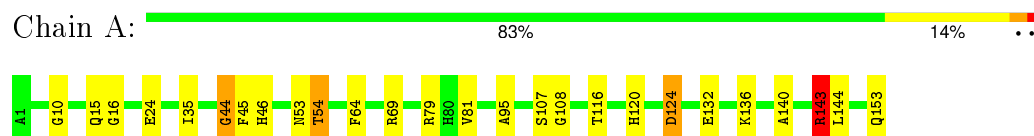


- Molecule 1: superoxide dismutase [Cu-Zn]

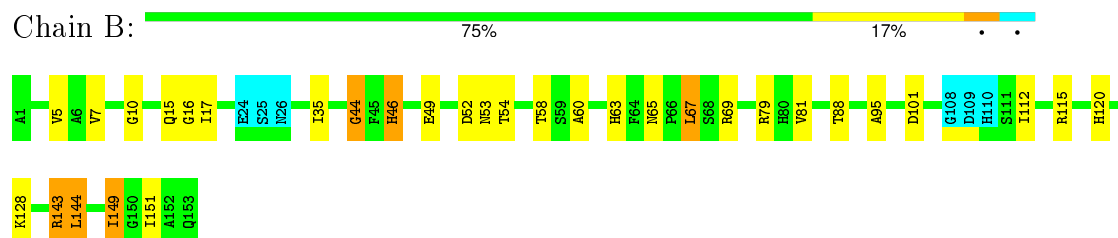


4.2.20 Score per residue for model 20

- Molecule 1: superoxide dismutase [Cu-Zn]

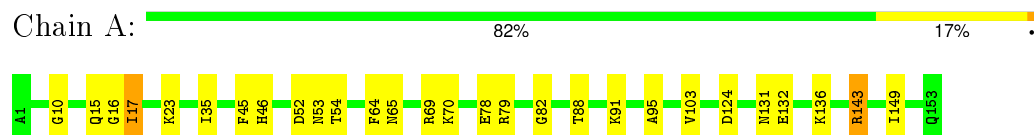


- Molecule 1: superoxide dismutase [Cu-Zn]

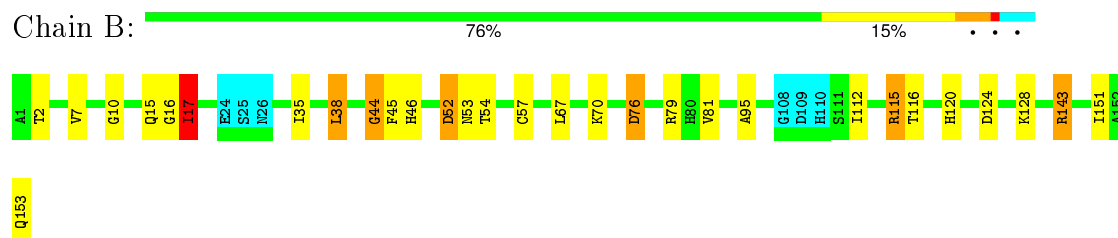


4.2.21 Score per residue for model 21

- Molecule 1: superoxide dismutase [Cu-Zn]

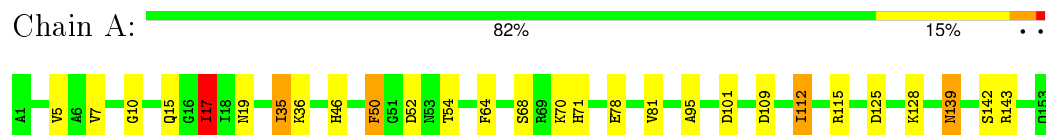


- Molecule 1: superoxide dismutase [Cu-Zn]

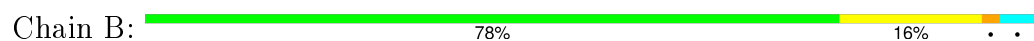


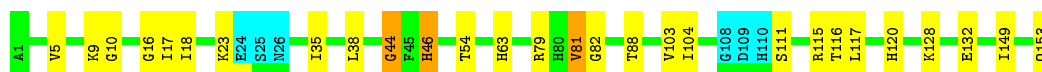
4.2.22 Score per residue for model 22

- Molecule 1: superoxide dismutase [Cu-Zn]



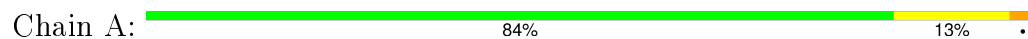
- Molecule 1: superoxide dismutase [Cu-Zn]



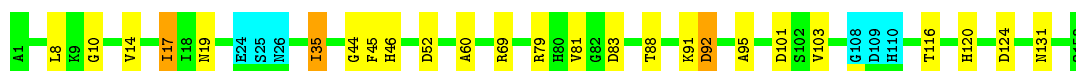
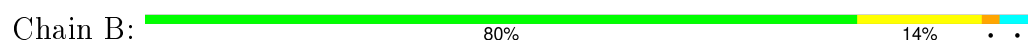


4.2.23 Score per residue for model 23

- Molecule 1: superoxide dismutase [Cu-Zn]

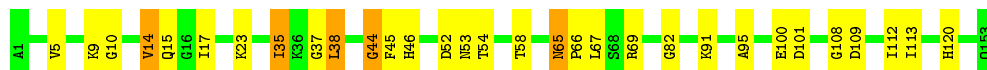
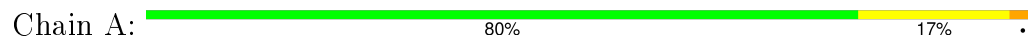


- Molecule 1: superoxide dismutase [Cu-Zn]

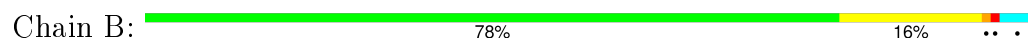


4.2.24 Score per residue for model 24

- Molecule 1: superoxide dismutase [Cu-Zn]

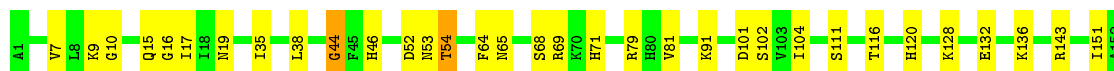
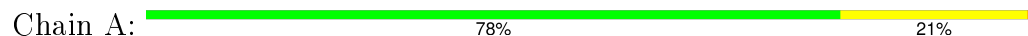


- Molecule 1: superoxide dismutase [Cu-Zn]

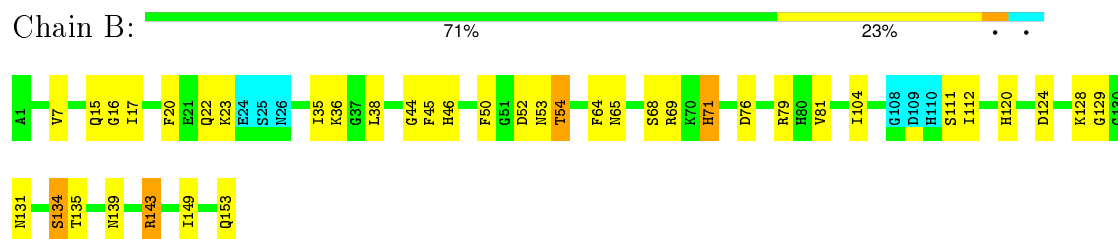


4.2.25 Score per residue for model 25

- Molecule 1: superoxide dismutase [Cu-Zn]

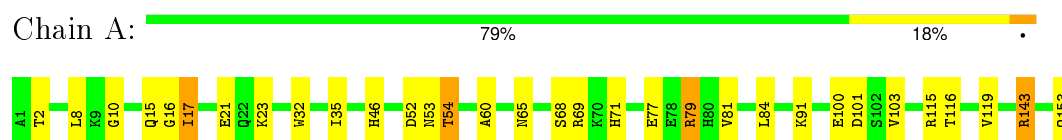


- Molecule 1: superoxide dismutase [Cu-Zn]

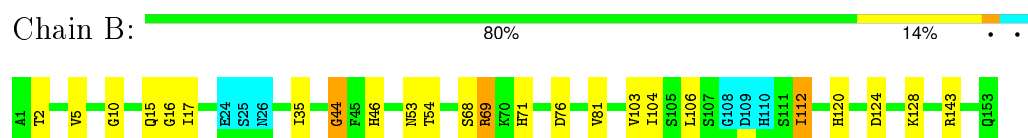


4.2.26 Score per residue for model 26

- Molecule 1: superoxide dismutase [Cu-Zn]

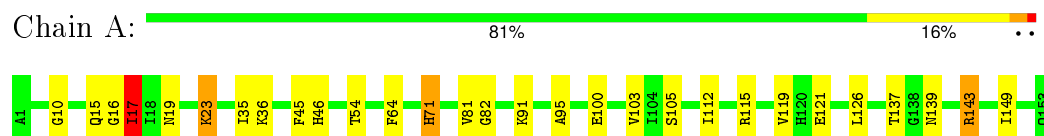


- Molecule 1: superoxide dismutase [Cu-Zn]

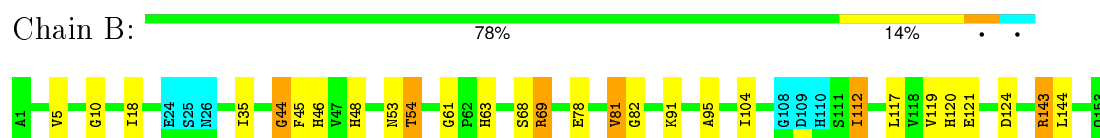


4.2.27 Score per residue for model 27

- Molecule 1: superoxide dismutase [Cu-Zn]

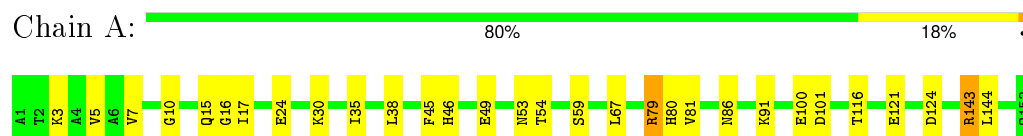


- Molecule 1: superoxide dismutase [Cu-Zn]

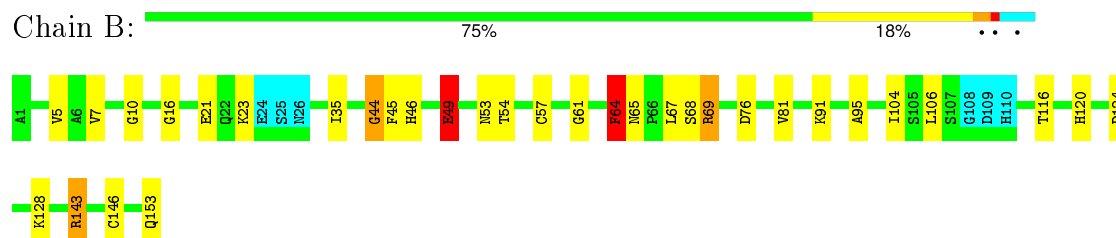


4.2.28 Score per residue for model 28

- Molecule 1: superoxide dismutase [Cu-Zn]

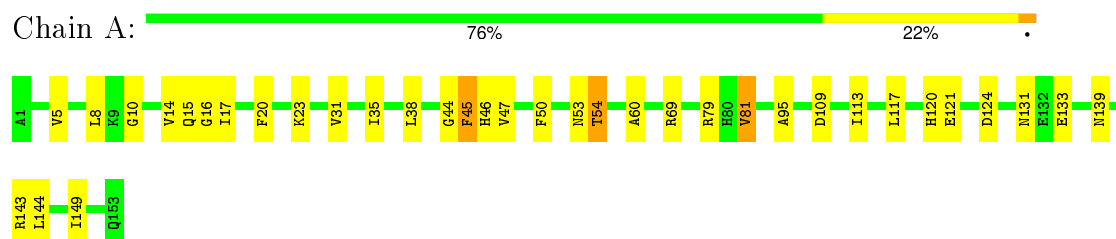


- Molecule 1: superoxide dismutase [Cu-Zn]

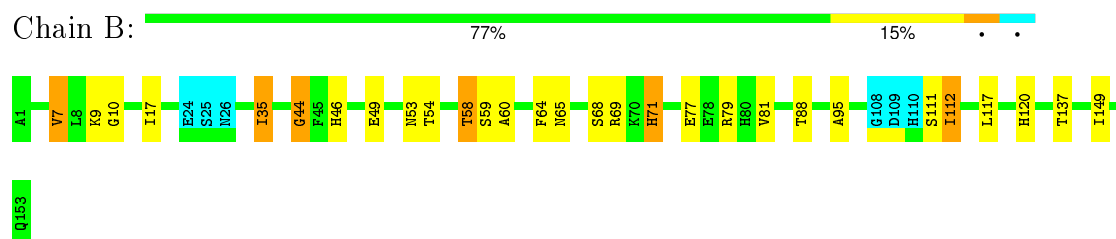


4.2.29 Score per residue for model 29

- Molecule 1: superoxide dismutase [Cu-Zn]

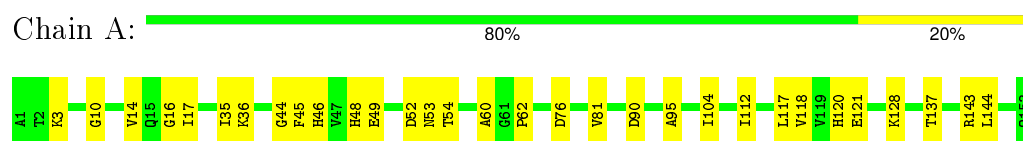


- Molecule 1: superoxide dismutase [Cu-Zn]

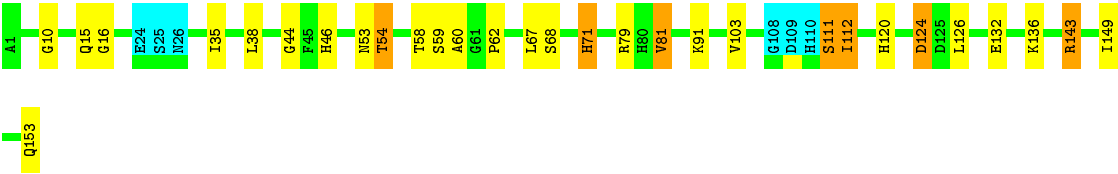


4.2.30 Score per residue for model 30

- 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: *simulated annealing and restrained energy minimization in vacuum*.

Of the 1400 calculated structures, 30 were deposited, based on the following criterion: *structure with the lowest energy target function*.

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

Software name	Classification	Version
CALIBA	structure solution	
GLOMSA	structure solution	
DYANA	structure solution	
AMBER	refinement	

No chemical shift data was provided. 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, CU1

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	0.50±0.01	0±0/1127 (0.0±0.0%)	1.02±0.02	0±0/1519 (0.0±0.0%)
1	B	0.51±0.01	0±0/1081 (0.0±0.0%)	1.03±0.02	1±1/1457 (0.0±0.0%)
All	All	0.51	0/66240 (0.0%)	1.03	23/89280 (0.0%)

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	1.7±1.0
1	B	0.0±0.0	1.7±1.1
All	All	0	102

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	B	143	ARG	NE-CZ-NH1	7.99	124.30	120.30	27	6
1	A	115	ARG	NE-CZ-NH2	-7.55	116.53	120.30	19	1
1	B	69	ARG	NE-CZ-NH1	7.12	123.86	120.30	17	2
1	A	143	ARG	NE-CZ-NH1	7.00	123.80	120.30	11	3
1	B	69	ARG	NE-CZ-NH2	-6.58	117.01	120.30	29	4
1	B	115	ARG	NE-CZ-NH2	-6.14	117.23	120.30	14	3
1	B	69	ARG	CD-NE-CZ	5.40	131.16	123.60	17	1
1	A	79	ARG	NE-CZ-NH2	-5.38	117.61	120.30	15	1
1	A	50	PHE	CB-CG-CD2	-5.35	117.06	120.80	22	1
1	A	79	ARG	NE-CZ-NH1	5.22	122.91	120.30	15	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	64	PHE	Sidechain	11
1	B	64	PHE	Sidechain	11
1	A	115	ARG	Sidechain	10
1	A	69	ARG	Sidechain	9
1	B	115	ARG	Sidechain	9
1	A	143	ARG	Sidechain	9
1	B	71	HIS	Sidechain	7
1	B	69	ARG	Sidechain	5
1	B	79	ARG	Sidechain	5
1	B	143	ARG	Sidechain	4
1	B	50	PHE	Sidechain	3
1	A	45	PHE	Sidechain	3
1	B	20	PHE	Sidechain	3
1	A	50	PHE	Sidechain	3
1	A	48	HIS	Sidechain	2
1	B	45	PHE	Sidechain	2
1	A	79	ARG	Sidechain	2
1	A	20	PHE	Sidechain	1
1	A	71	HIS	Sidechain	1
1	B	46	HIS	Sidechain	1
1	B	80	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	1109	1078	1077	8±2
1	B	1064	1047	1046	7±2
All	All	65310	63750	63690	396

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ILE:CG2	1:B:54:THR:HG22	0.85	2.01	24	5
1:B:16:GLY:HA2	1:B:35:ILE:HG22	0.77	1.55	9	18
1:A:16:GLY:HA2	1:A:35:ILE:HG22	0.77	1.56	27	20
1:A:54:THR:HG22	1:B:17:ILE:HG22	0.77	1.55	10	7
1:A:54:THR:HG22	1:B:17:ILE:CG2	0.76	2.10	5	8
1:A:16:GLY:CA	1:A:35:ILE:HG22	0.66	2.20	26	21
1:A:17:ILE:CG2	1:B:54:THR:HG23	0.65	2.22	11	7
1:A:35:ILE:CG1	1:A:95:ALA:HB3	0.64	2.23	12	11
1:A:17:ILE:HG22	1:B:54:THR:HG23	0.64	1.70	22	5
1:A:44:GLY:HA3	1:A:120:HIS:HB2	0.63	1.70	15	21
1:A:17:ILE:HG22	1:B:54:THR:HG22	0.62	1.69	24	2
1:B:16:GLY:CA	1:B:35:ILE:HG22	0.61	2.25	20	14
1:B:35:ILE:HG12	1:B:95:ALA:HB3	0.61	1.72	29	13
1:A:38:LEU:HD13	1:A:38:LEU:H	0.60	1.57	4	1
1:B:111:SER:O	1:B:112:ILE:HG23	0.59	1.98	29	1
1:A:38:LEU:N	1:A:38:LEU:HD13	0.59	2.12	13	1
1:B:38:LEU:HD13	1:B:38:LEU:N	0.58	2.12	21	1
1:A:38:LEU:HD13	1:A:38:LEU:N	0.58	2.13	4	3
1:B:44:GLY:HA3	1:B:120:HIS:HB2	0.57	1.77	10	24
1:A:35:ILE:HG12	1:A:95:ALA:HB3	0.57	1.74	15	11
1:A:54:THR:HG23	1:B:17:ILE:CG2	0.57	2.30	4	5
1:B:35:ILE:CG1	1:B:95:ALA:HB3	0.55	2.30	9	10
1:B:124:ASP:HB2	1:B:126:LEU:CD2	0.55	2.30	30	1
1:B:104:ILE:HD13	1:B:104:ILE:C	0.55	2.22	3	1
1:A:117:LEU:CD1	1:A:149:ILE:HD11	0.55	2.31	15	1
1:B:81:VAL:HG13	1:B:82:GLY:H	0.54	1.63	27	2
1:A:14:VAL:HG13	1:A:38:LEU:HD12	0.54	1.78	13	3
1:A:7:VAL:HG21	1:B:53:ASN:HB3	0.54	1.80	25	3
1:A:5:VAL:HG11	1:B:52:ASP:HA	0.54	1.80	23	1
1:B:38:LEU:H	1:B:38:LEU:HD13	0.53	1.62	21	1
1:B:16:GLY:HA3	1:B:35:ILE:HG22	0.53	1.80	26	1
1:A:5:VAL:HG11	1:B:52:ASP:CA	0.52	2.33	23	1
1:A:54:THR:HG23	1:B:17:ILE:HG22	0.51	1.83	18	2
1:A:35:ILE:CD1	1:A:95:ALA:HB3	0.51	2.36	30	8
1:A:35:ILE:HD11	1:A:95:ALA:HB3	0.50	1.82	30	7
1:A:81:VAL:HG13	1:A:82:GLY:H	0.50	1.65	2	2
1:A:6:ALA:HB2	1:A:149:ILE:HG12	0.49	1.83	1	1
1:B:7:VAL:HG12	1:B:17:ILE:HG23	0.49	1.84	21	1
1:A:17:ILE:CG2	1:B:54:THR:CG2	0.49	2.91	15	11
1:A:84:LEU:HD13	1:A:84:LEU:C	0.49	2.28	26	1
1:A:8:LEU:HD21	1:A:117:LEU:HB3	0.49	1.84	10	1
1:B:35:ILE:C	1:B:35:ILE:HD12	0.49	2.27	3	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ILE:HD12	1:A:35:ILE:C	0.48	2.28	6	1
1:B:35:ILE:HD12	1:B:45:PHE:CZ	0.47	2.45	12	1
1:B:84:LEU:C	1:B:84:LEU:HD12	0.47	2.29	18	1
1:A:117:LEU:HD11	1:A:149:ILE:HD11	0.47	1.85	3	1
1:A:53:ASN:HB3	1:B:7:VAL:HG21	0.47	1.87	29	2
1:A:46:HIS:CG	1:A:63:HIS:CE1	0.46	3.03	15	6
1:A:121:GLU:HA	1:A:144:LEU:HD22	0.46	1.86	30	1
1:B:71:HIS:HB2	1:B:80:HIS:CE1	0.46	2.45	5	3
1:A:38:LEU:HD12	1:A:38:LEU:N	0.46	2.25	10	4
1:B:38:LEU:HD12	1:B:38:LEU:N	0.46	2.25	2	5
1:B:64:PHE:CD1	1:B:64:PHE:N	0.46	2.81	14	1
1:A:63:HIS:CD2	1:A:137:THR:HG22	0.46	2.46	10	2
1:B:49:GLU:CG	1:B:50:PHE:N	0.46	2.79	2	1
1:B:45:PHE:CE1	1:B:87:VAL:HG13	0.46	2.46	15	1
1:A:8:LEU:HD21	1:A:117:LEU:CB	0.46	2.40	10	1
1:B:35:ILE:CD1	1:B:95:ALA:HB3	0.45	2.40	21	3
1:B:35:ILE:HD11	1:B:95:ALA:HB3	0.45	1.87	21	2
1:A:38:LEU:N	1:A:38:LEU:HD12	0.45	2.27	25	3
1:B:38:LEU:N	1:B:38:LEU:HD12	0.45	2.26	6	3
1:B:49:GLU:CG	1:B:50:PHE:H	0.45	2.25	2	1
1:A:117:LEU:N	1:A:117:LEU:HD12	0.45	2.26	3	1
1:B:5:VAL:O	1:B:149:ILE:HG23	0.45	2.11	20	1
1:B:46:HIS:CG	1:B:63:HIS:CE1	0.45	3.05	27	4
1:B:36:LYS:NZ	1:B:92:ASP:OD2	0.45	2.50	24	1
1:A:106:LEU:H	1:A:106:LEU:HD13	0.44	1.72	7	1
1:B:47:VAL:HG12	1:B:115:ARG:HH11	0.44	1.72	1	1
1:A:20:PHE:CD2	1:A:31:VAL:HG12	0.44	2.47	29	1
1:B:8:LEU:HD21	1:B:117:LEU:HB2	0.44	1.88	13	1
1:B:85:GLY:CA	1:B:126:LEU:HD21	0.44	2.42	16	1
1:A:36:LYS:NZ	1:A:92:ASP:OD2	0.44	2.51	23	2
1:A:144:LEU:N	1:A:144:LEU:CD2	0.44	2.81	15	2
1:A:30:LYS:NZ	1:A:100:GLU:OE1	0.44	2.51	28	3
1:B:104:ILE:HD12	1:B:104:ILE:C	0.44	2.32	4	1
1:B:129:GLY:HA3	1:B:134:SER:CB	0.43	2.43	25	1
1:B:35:ILE:HD13	1:B:35:ILE:N	0.43	2.28	12	1
1:B:121:GLU:HA	1:B:144:LEU:HD22	0.43	1.90	27	1
1:B:49:GLU:CG	1:B:61:GLY:HA3	0.43	2.44	28	1
1:A:35:ILE:HD13	1:A:38:LEU:HD23	0.43	1.91	6	1
1:A:44:GLY:HA2	1:A:124:ASP:OD2	0.43	2.13	11	3
1:B:35:ILE:HD13	1:B:38:LEU:HD23	0.43	1.89	3	1
1:B:46:HIS:NE2	1:B:124:ASP:OD2	0.43	2.52	15	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:LYS:NZ	1:A:100:GLU:OE2	0.43	2.51	27	1
1:A:76:ASP:OD1	1:A:128:LYS:NZ	0.43	2.52	30	1
1:B:144:LEU:N	1:B:144:LEU:CD2	0.42	2.81	7	1
1:B:75:LYS:HG3	1:B:126:LEU:HD12	0.42	1.91	19	1
1:B:76:ASP:OD1	1:B:128:LYS:NZ	0.42	2.52	28	5
1:B:47:VAL:HG12	1:B:115:ARG:NH1	0.42	2.29	1	1
1:B:45:PHE:CZ	1:B:84:LEU:HB3	0.42	2.49	15	1
1:B:76:ASP:OD2	1:B:128:LYS:NZ	0.42	2.52	26	3
1:B:144:LEU:CD2	1:B:144:LEU:N	0.42	2.82	19	2
1:A:91:LYS:NZ	1:A:92:ASP:OD1	0.42	2.53	8	1
1:A:54:THR:CG2	1:B:17:ILE:CG2	0.42	2.98	2	7
1:A:124:ASP:CB	1:A:140:ALA:HB2	0.42	2.44	20	1
1:A:76:ASP:OD2	1:A:128:LYS:NZ	0.42	2.53	8	2
1:B:70:LYS:NZ	1:B:76:ASP:OD2	0.42	2.53	21	1
1:A:119:VAL:CG1	1:A:145:ALA:HB3	0.42	2.44	1	1
1:A:117:LEU:HD11	1:A:149:ILE:CG1	0.42	2.45	18	1
1:A:124:ASP:HB3	1:A:140:ALA:HB2	0.42	1.92	20	1
1:B:91:LYS:NZ	1:B:92:ASP:OD1	0.42	2.53	23	1
1:B:117:LEU:HD11	1:B:149:ILE:CG1	0.42	2.45	22	1
1:A:132:GLU:OE2	1:A:136:LYS:NZ	0.41	2.54	25	4
1:A:47:VAL:HG12	1:A:117:LEU:HD22	0.41	1.92	29	1
1:A:46:HIS:NE2	1:A:124:ASP:OD2	0.41	2.53	13	1
1:A:125:ASP:OD1	1:A:128:LYS:NZ	0.41	2.53	19	1
1:B:49:GLU:CD	1:B:61:GLY:HA3	0.41	2.35	16	1
1:A:79:ARG:CD	1:A:79:ARG:H	0.41	2.29	26	1
1:A:90:ASP:OD2	1:A:91:LYS:NZ	0.41	2.52	6	1
1:B:125:ASP:OD1	1:B:128:LYS:NZ	0.41	2.54	3	1
1:A:121:GLU:CD	1:A:122:LYS:HZ3	0.41	2.19	19	1
1:B:90:ASP:OD2	1:B:91:LYS:NZ	0.41	2.54	9	1
1:A:70:LYS:NZ	1:A:78:GLU:OE2	0.41	2.52	22	2
1:B:8:LEU:HD23	1:B:147:GLY:N	0.41	2.30	13	1
1:A:132:GLU:OE1	1:A:136:LYS:NZ	0.41	2.53	20	2
1:A:78:GLU:N	1:A:78:GLU:CD	0.41	2.74	3	1
1:A:101:ASP:OD1	1:A:102:SER:N	0.41	2.54	25	1
1:A:5:VAL:CG1	1:B:52:ASP:HB2	0.41	2.45	14	1
1:A:30:LYS:NZ	1:A:100:GLU:OE2	0.40	2.55	18	1
1:A:7:VAL:HG12	1:A:17:ILE:HG23	0.40	1.92	22	1
1:B:104:ILE:CD1	1:B:104:ILE:H	0.40	2.29	10	1
1:B:71:HIS:CD2	1:B:138:GLY:CA	0.40	3.05	8	1
1:B:46:HIS:HE2	1:B:124:ASP:CG	0.40	2.19	10	1
1:A:23:LYS:NZ	1:A:24:GLU:OE2	0.40	2.54	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:45:PHE:CD1	1:B:87:VAL:HG22	0.40	2.51	12	1
1:A:48:HIS:CD2	1:A:118:VAL:CG2	0.40	3.05	30	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%)	117±3 (78±2%)	26±3 (17±2%)	8±2 (5±2%)	5	25
1	B	145/153 (95%)	113±5 (78±3%)	25±4 (17±3%)	7±2 (5±1%)	5	26
All	All	8880/9180 (97%)	6910 (78%)	1514 (17%)	456 (5%)	5	26

All 71 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	81	VAL	30
1	A	10	GLY	28
1	B	10	GLY	24
1	A	81	VAL	23
1	A	60	ALA	18
1	B	68	SER	18
1	B	44	GLY	15
1	A	143	ARG	14
1	B	112	ILE	13
1	B	71	HIS	13
1	B	60	ALA	13
1	A	82	GLY	11
1	A	139	ASN	11
1	B	143	ARG	11
1	B	103	VAL	10
1	A	44	GLY	10
1	A	2	THR	9
1	A	68	SER	9
1	A	109	ASP	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	103	VAL	8
1	A	111	SER	8
1	A	17	ILE	8
1	A	112	ILE	7
1	B	149	ILE	7
1	B	57	CYS	7
1	A	71	HIS	7
1	A	149	ILE	7
1	B	111	SER	6
1	B	49	GLU	6
1	B	52	ASP	5
1	B	17	ILE	5
1	A	62	PRO	4
1	A	64	PHE	4
1	A	48	HIS	4
1	B	2	THR	4
1	A	80	HIS	4
1	B	113	ILE	4
1	A	57	CYS	3
1	B	62	PRO	3
1	A	61	GLY	3
1	B	63	HIS	3
1	B	139	ASN	3
1	B	64	PHE	3
1	A	108	GLY	3
1	B	58	THR	3
1	B	67	LEU	2
1	A	49	GLU	2
1	B	61	GLY	2
1	A	65	ASN	2
1	A	113	ILE	2
1	A	37	GLY	2
1	A	79	ARG	2
1	A	58	THR	2
1	B	83	ASP	2
1	A	126	LEU	2
1	A	66	PRO	2
1	A	14	VAL	2
1	A	151	ILE	1
1	B	14	VAL	1
1	A	54	THR	1
1	B	126	LEU	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	53	ASN	1
1	B	80	HIS	1
1	B	65	ASN	1
1	B	78	GLU	1
1	A	106	LEU	1
1	A	104	ILE	1
1	B	48	HIS	1
1	B	85	GLY	1
1	A	107	SER	1
1	B	106	LEU	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%)	102±3 (87±2%)	15±3 (13±2%)	9	51
1	B	112/117 (96%)	97±3 (87±3%)	15±3 (13±3%)	9	51
All	All	6870/7020 (98%)	5977 (87%)	893 (13%)	9	51

All 147 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	46	HIS	30
1	B	46	HIS	28
1	B	53	ASN	26
1	A	54	THR	24
1	A	15	GLN	21
1	B	54	THR	21
1	B	15	GLN	20
1	B	143	ARG	18
1	A	53	ASN	18
1	B	124	ASP	18
1	B	104	ILE	17
1	A	124	ASP	15
1	B	153	GLN	14
1	B	79	ARG	13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	45	PHE	13
1	B	91	LYS	13
1	A	45	PHE	13
1	A	79	ARG	13
1	A	143	ARG	12
1	A	24	GLU	12
1	A	91	LYS	12
1	A	5	VAL	11
1	A	153	GLN	11
1	B	69	ARG	11
1	A	52	ASP	11
1	B	88	THR	10
1	A	144	LEU	10
1	A	104	ILE	10
1	A	23	LYS	10
1	B	52	ASP	9
1	B	128	LYS	9
1	A	139	ASN	9
1	B	67	LEU	8
1	A	121	GLU	8
1	A	67	LEU	8
1	A	119	VAL	8
1	A	35	ILE	8
1	A	116	THR	8
1	A	88	THR	8
1	B	139	ASN	8
1	B	7	VAL	7
1	B	5	VAL	7
1	A	3	LYS	7
1	A	36	LYS	7
1	A	65	ASN	7
1	B	116	THR	7
1	B	115	ARG	7
1	A	137	THR	7
1	B	112	ILE	6
1	B	65	ASN	6
1	B	35	ILE	6
1	B	119	VAL	6
1	A	69	ARG	6
1	B	131	ASN	6
1	A	17	ILE	6
1	A	7	VAL	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	49	GLU	5
1	B	76	ASP	5
1	A	14	VAL	5
1	A	112	ILE	5
1	B	36	LYS	5
1	A	38	LEU	5
1	A	19	ASN	5
1	A	125	ASP	5
1	A	101	ASP	5
1	A	58	THR	5
1	B	17	ILE	4
1	B	23	LYS	4
1	A	70	LYS	4
1	A	78	GLU	4
1	B	9	LYS	4
1	B	64	PHE	4
1	A	21	GLU	4
1	A	9	LYS	4
1	A	131	ASN	4
1	B	144	LEU	4
1	B	58	THR	4
1	B	19	ASN	4
1	A	117	LEU	4
1	A	100	GLU	4
1	A	18	ILE	4
1	B	22	GLN	4
1	A	115	ARG	4
1	B	21	GLU	4
1	B	117	LEU	3
1	A	76	ASP	3
1	B	146	CYS	3
1	B	59	SER	3
1	A	133	GLU	3
1	A	92	ASP	3
1	B	38	LEU	3
1	B	151	ILE	3
1	B	18	ILE	3
1	A	8	LEU	3
1	B	81	VAL	3
1	A	2	THR	3
1	B	134	SER	3
1	A	86	ASN	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	78	GLU	3
1	B	92	ASP	3
1	B	142	SER	3
1	B	132	GLU	3
1	B	77	GLU	3
1	B	102	SER	3
1	A	77	GLU	2
1	B	101	ASP	2
1	A	59	SER	2
1	B	57	CYS	2
1	A	30	LYS	2
1	B	137	THR	2
1	B	3	LYS	2
1	B	70	LYS	2
1	B	106	LEU	2
1	A	68	SER	2
1	B	111	SER	2
1	B	2	THR	2
1	A	106	LEU	2
1	A	105	SER	2
1	A	151	ILE	2
1	A	75	LYS	2
1	A	128	LYS	2
1	B	107	SER	2
1	A	135	THR	2
1	A	81	VAL	1
1	B	135	THR	1
1	A	107	SER	1
1	B	75	LYS	1
1	B	83	ASP	1
1	A	90	ASP	1
1	A	29	VAL	1
1	B	87	VAL	1
1	B	68	SER	1
1	B	31	VAL	1
1	B	8	LEU	1
1	A	22	GLN	1
1	A	47	VAL	1
1	A	132	GLU	1
1	B	11	ASP	1
1	A	25	SER	1
1	A	146	CYS	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	84	LEU	1
1	A	26	ASN	1
1	B	121	GLU	1
1	B	136	LYS	1
1	B	125	ASP	1
1	A	32	TRP	1
1	A	142	SER	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 carbohydrates in this entry.

6.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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