



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 02:43 AM UTC

PDB ID : 1KMG / pdb_00001kmg
Title : The Solution Structure Of Monomeric Copper-free Superoxide Dismutase
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Deposited on : 2001-12-15

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

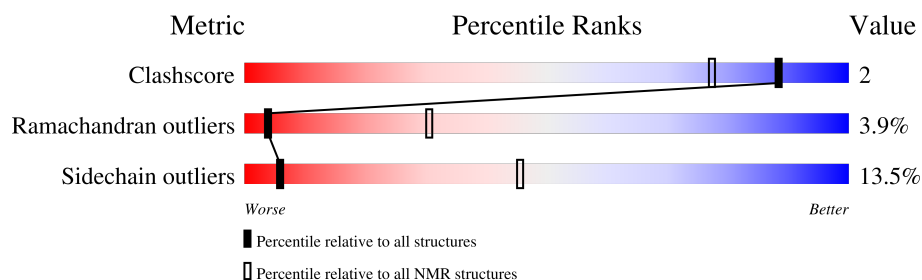
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	153	 77% 13% • 9%

2 Ensemble composition and analysis

This entry contains 35 models. Model 22 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:50, A:60-A:107, A:111-A:153 (139)	0.79	22

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 7 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2193 atoms, of which 1080 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Superoxide Dismutase.

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

There are 5 discrepancies between the modelled and reference sequences:

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

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

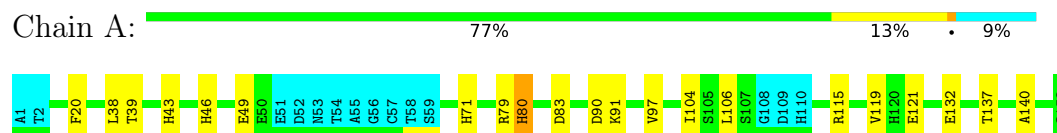
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Superoxide Dismutase

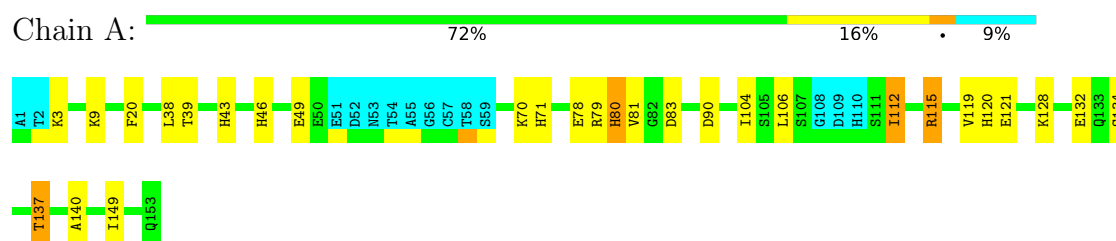


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

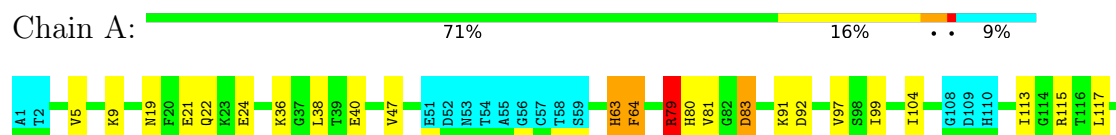
4.2.1 Score per residue for model 1

- Molecule 1: Superoxide Dismutase



4.2.2 Score per residue for model 2

- Molecule 1: Superoxide Dismutase

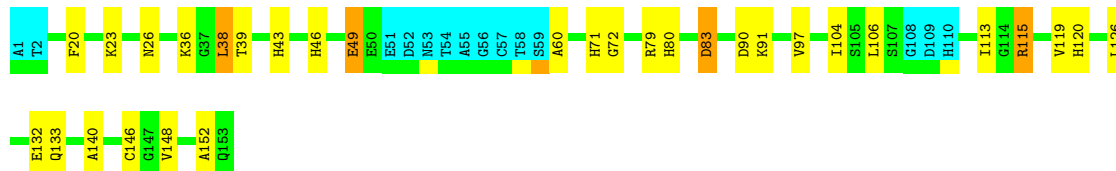




4.2.3 Score per residue for model 3

- Molecule 1: Superoxide Dismutase

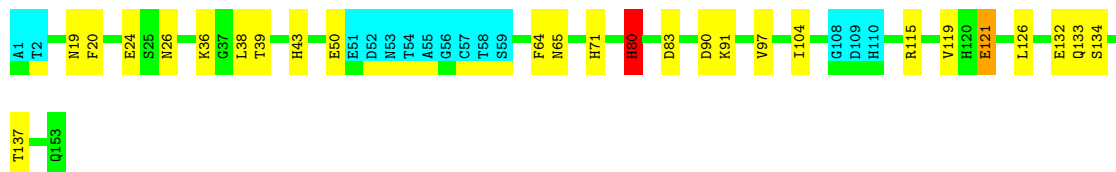
Chain A: 71% 18% 9%



4.2.4 Score per residue for model 4

- Molecule 1: Superoxide Dismutase

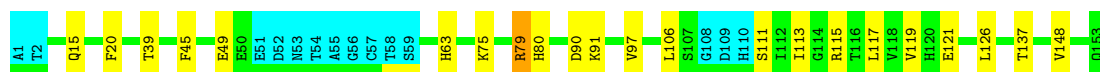
Chain A: 74% 16% 9%



4.2.5 Score per residue for model 5

- Molecule 1: Superoxide Dismutase

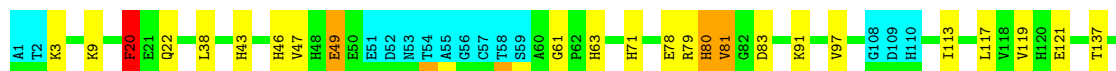
Chain A: 76% 14% 9%



4.2.6 Score per residue for model 6

- Molecule 1: Superoxide Dismutase

Chain A: 75% 14% 9%



Q153

4.2.7 Score per residue for model 7

- Molecule 1: Superoxide Dismutase

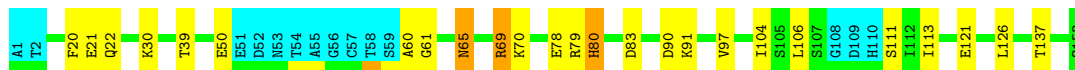
Chain A:  76% 14% 9%



4.2.8 Score per residue for model 8

- Molecule 1: Superoxide Dismutase

Chain A:  75% 14% 9%



4.2.9 Score per residue for model 9

- Molecule 1: Superoxide Dismutase

Chain A:  76% 14% 9%



4.2.10 Score per residue for model 10

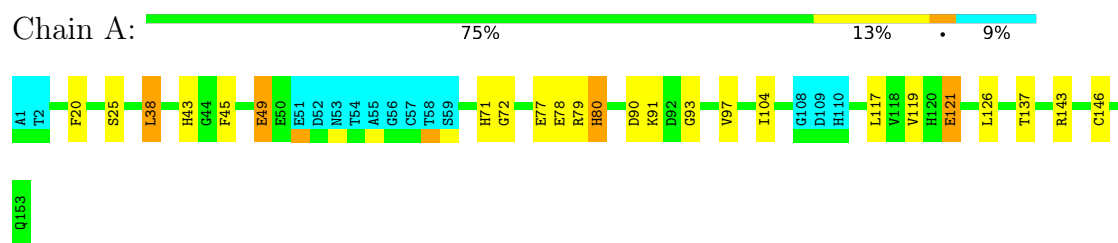
- Molecule 1: Superoxide Dismutase

Chain A:  73% 16% 9%



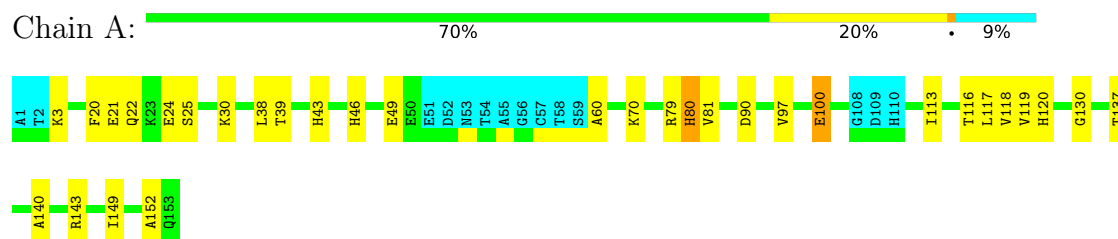
4.2.11 Score per residue for model 11

- Molecule 1: Superoxide Dismutase



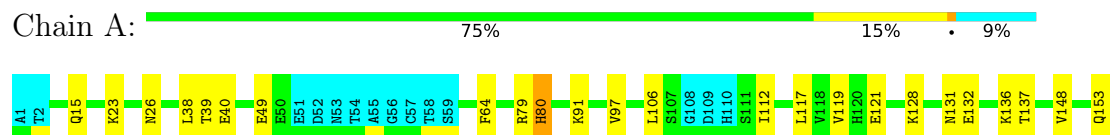
4.2.12 Score per residue for model 12

- Molecule 1: Superoxide Dismutase



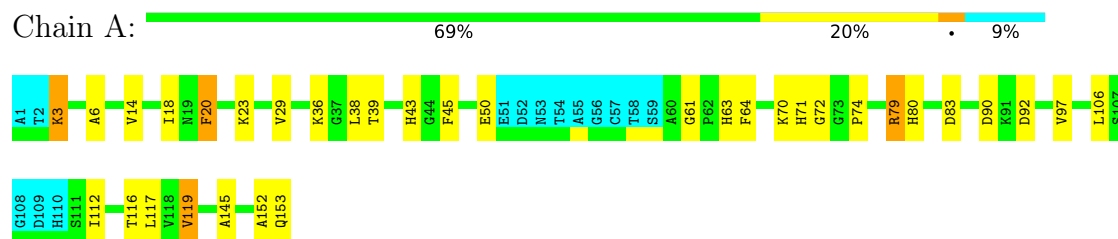
4.2.13 Score per residue for model 13

- Molecule 1: Superoxide Dismutase



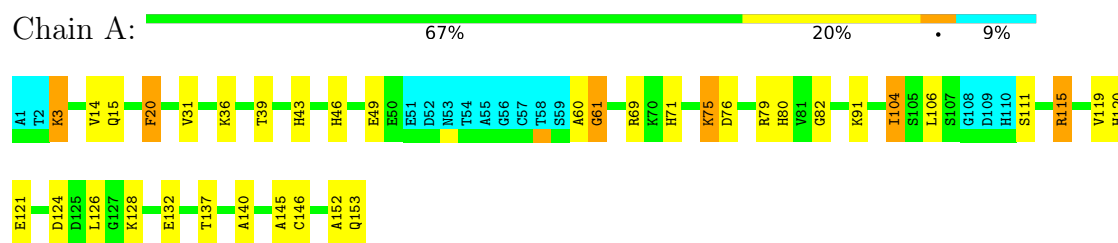
4.2.14 Score per residue for model 14

- Molecule 1: Superoxide Dismutase



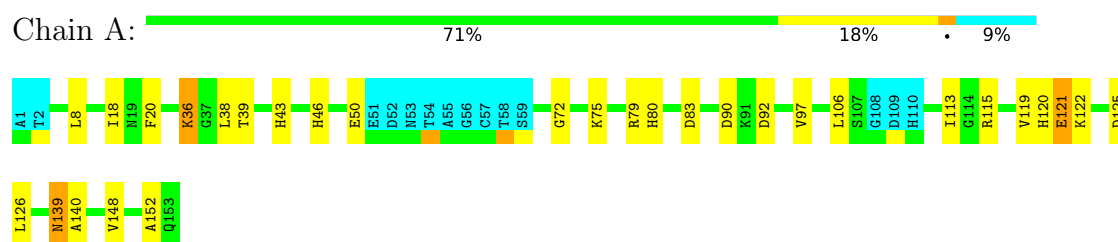
4.2.15 Score per residue for model 15

- Molecule 1: Superoxide Dismutase



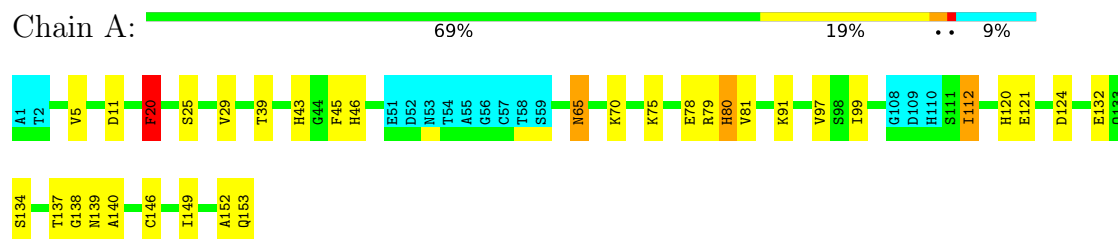
4.2.16 Score per residue for model 16

- Molecule 1: Superoxide Dismutase



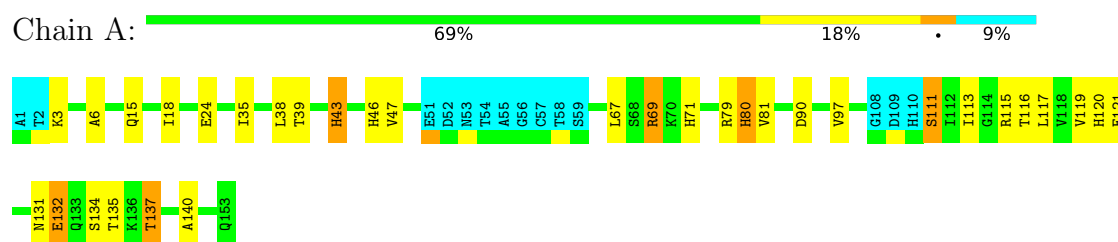
4.2.17 Score per residue for model 17

- Molecule 1: Superoxide Dismutase



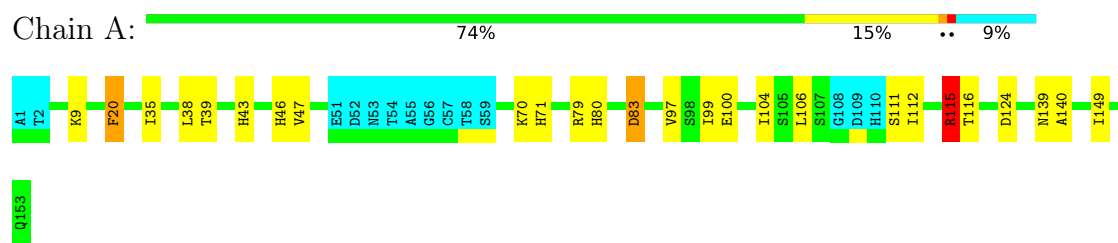
4.2.18 Score per residue for model 18

- Molecule 1: Superoxide Dismutase



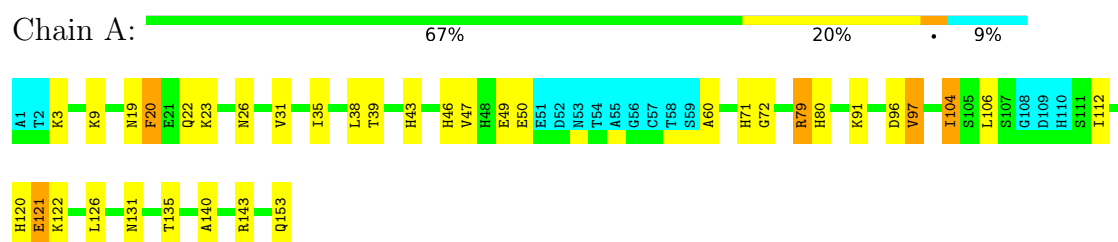
4.2.19 Score per residue for model 19

- Molecule 1: Superoxide Dismutase



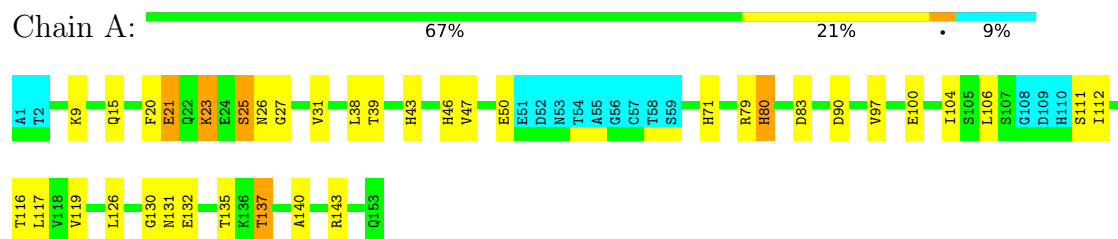
4.2.20 Score per residue for model 20

- Molecule 1: Superoxide Dismutase



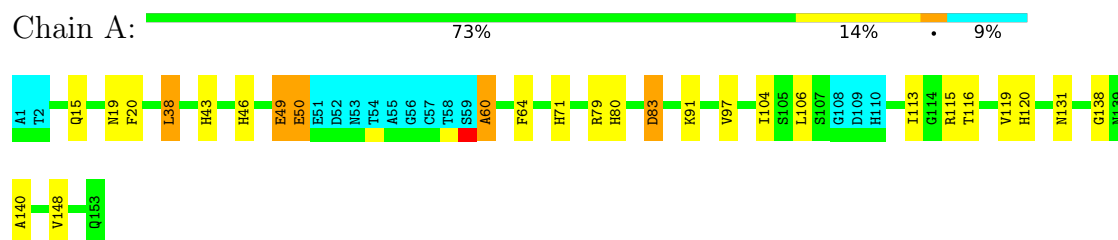
4.2.21 Score per residue for model 21

- Molecule 1: Superoxide Dismutase



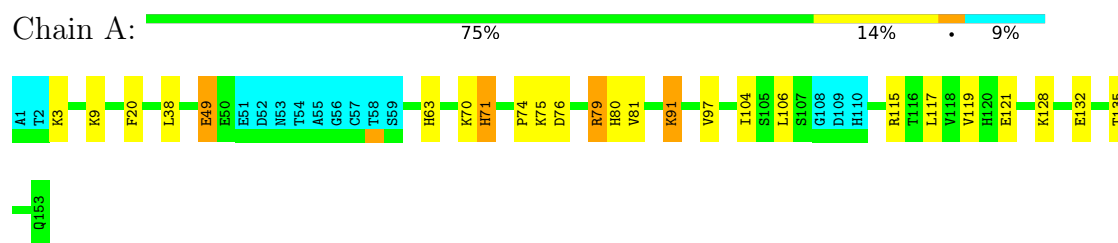
4.2.22 Score per residue for model 22 (medoid)

- Molecule 1: Superoxide Dismutase



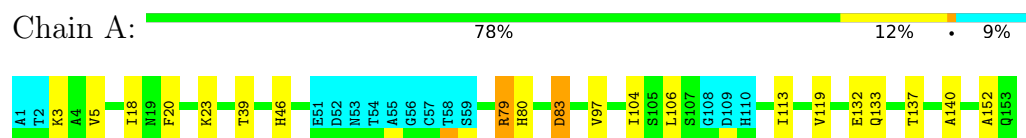
4.2.23 Score per residue for model 23

- Molecule 1: Superoxide Dismutase



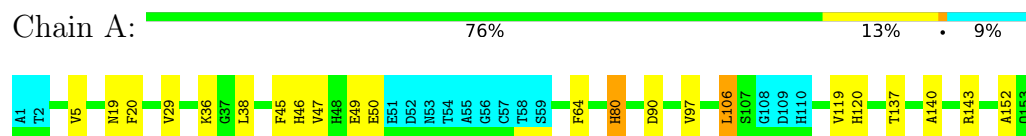
4.2.24 Score per residue for model 24

- Molecule 1: Superoxide Dismutase



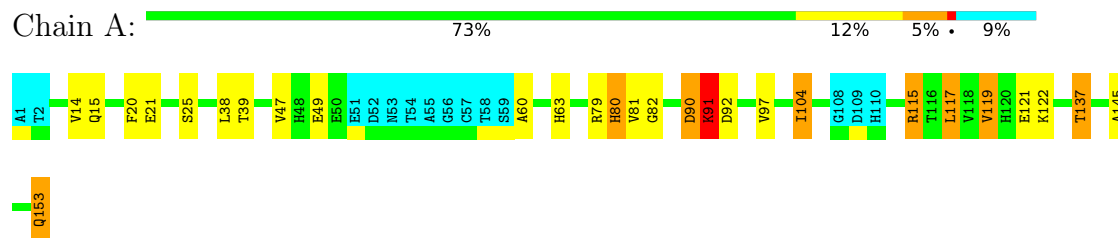
4.2.25 Score per residue for model 25

- Molecule 1: Superoxide Dismutase



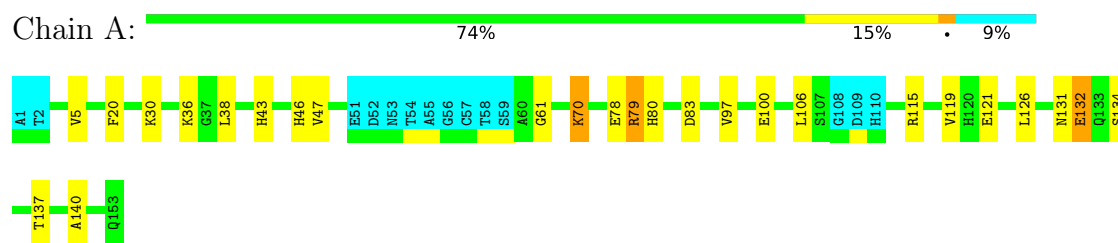
4.2.26 Score per residue for model 26

- Molecule 1: Superoxide Dismutase



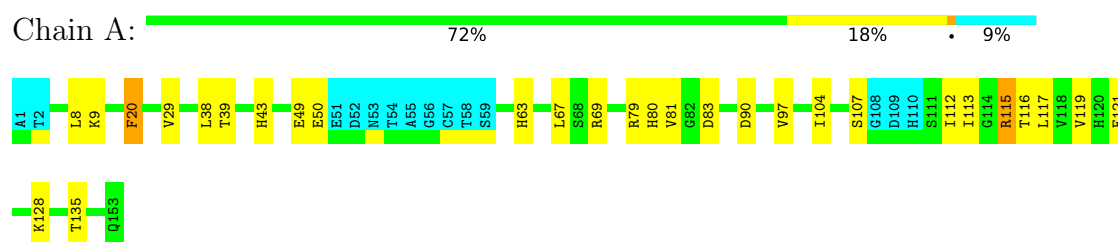
4.2.27 Score per residue for model 27

- Molecule 1: Superoxide Dismutase



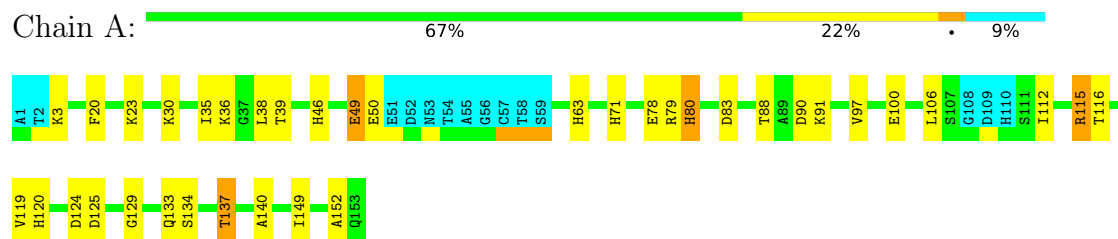
4.2.28 Score per residue for model 28

- Molecule 1: Superoxide Dismutase



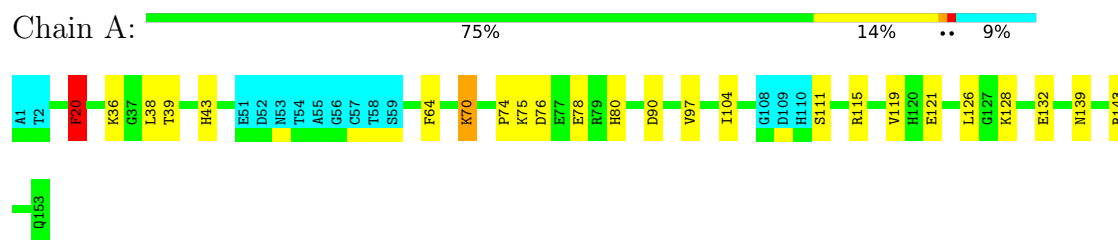
4.2.29 Score per residue for model 29

- Molecule 1: Superoxide Dismutase



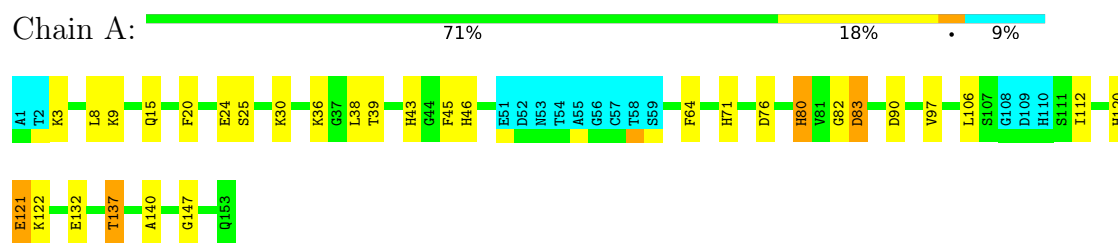
4.2.30 Score per residue for model 30

- Molecule 1: Superoxide Dismutase



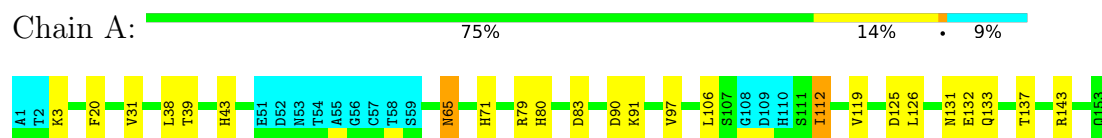
4.2.31 Score per residue for model 31

- Molecule 1: Superoxide Dismutase



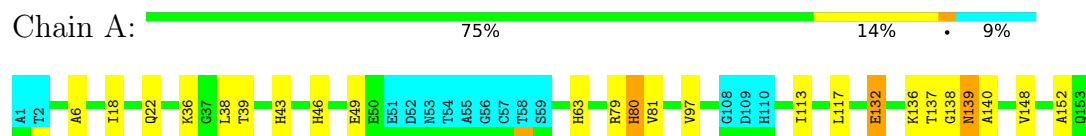
4.2.32 Score per residue for model 32

- Molecule 1: Superoxide Dismutase



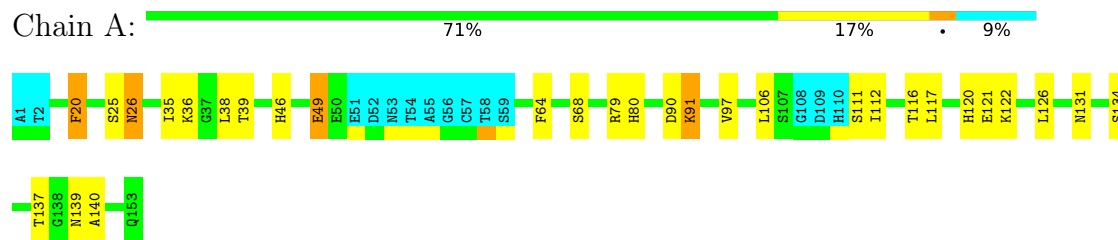
4.2.33 Score per residue for model 33

- Molecule 1: Superoxide Dismutase



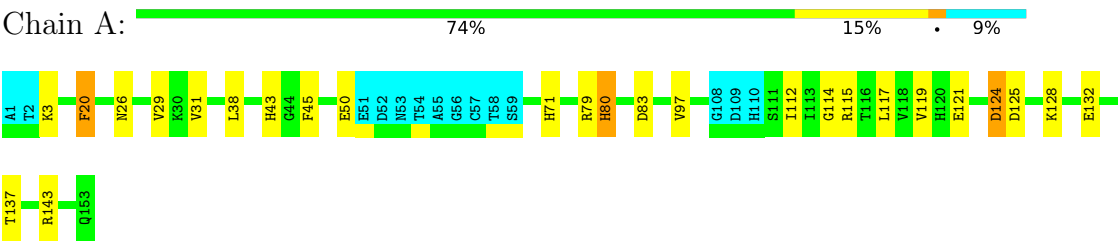
4.2.34 Score per residue for model 34

- Molecule 1: Superoxide Dismutase



4.2.35 Score per residue for model 35

● Molecule 1: Superoxide Dismutase



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 35 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
DIANA	structure solution	1.5
Amber	refinement	5.0

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	0.61±0.01	0±0/1034 (0.0± 0.0%)	1.32±0.03	2±1/1392 (0.2± 0.1%)
All	All	0.61	0/36190 (0.0%)	1.32	77/48720 (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	3.7±1.5
All	All	0	131

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	20	PHE	CA-CB-CG	8.53	122.33	113.80	6	4
1	A	83	ASP	CA-CB-CG	8.15	120.75	112.60	16	18
1	A	65	ASN	CA-CB-CG	6.82	119.42	112.60	32	3
1	A	64	PHE	CA-CB-CG	6.60	120.40	113.80	14	4
1	A	71	HIS	CB-CG-CD2	-6.31	123.00	131.20	19	17
1	A	128	LYS	CA-C-N	5.91	125.67	121.65	30	1
1	A	128	LYS	C-N-CA	5.91	125.67	121.65	30	1
1	A	60	ALA	N-CA-C	5.86	118.56	110.35	22	1
1	A	63	HIS	CA-CB-CG	5.69	119.49	113.80	2	2
1	A	61	GLY	CA-C-N	5.66	126.91	119.84	15	2
1	A	61	GLY	C-N-CA	5.66	126.91	119.84	15	2
1	A	76	ASP	CA-C-N	5.63	128.14	120.54	30	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	76	ASP	C-N-CA	5.63	128.14	120.54	30	2
1	A	139	ASN	CA-CB-CG	5.54	118.14	112.60	16	1
1	A	124	ASP	CA-CB-CG	5.43	118.03	112.60	35	2
1	A	81	VAL	CB-CA-C	5.26	119.91	111.29	6	1
1	A	63	HIS	CB-CG-CD2	-5.22	124.42	131.20	5	3
1	A	80	HIS	CB-CG-CD2	-5.19	124.45	131.20	4	1
1	A	78	GLU	CA-C-N	5.17	131.41	121.54	17	1
1	A	78	GLU	C-N-CA	5.17	131.41	121.54	17	1
1	A	81	VAL	CA-C-N	5.08	131.36	121.41	6	1
1	A	81	VAL	C-N-CA	5.08	131.36	121.41	6	1
1	A	135	THR	CA-C-N	5.08	127.34	120.38	23	1
1	A	135	THR	C-N-CA	5.08	127.34	120.38	23	1
1	A	132	GLU	CA-C-N	5.04	128.37	120.82	27	1
1	A	132	GLU	C-N-CA	5.04	128.37	120.82	27	1
1	A	137	THR	CB-CA-C	5.02	120.41	110.42	26	1
1	A	71	HIS	CB-CG-ND1	5.00	130.20	122.70	19	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	80	HIS	Sidechain	35
1	A	43	HIS	Sidechain	24
1	A	115	ARG	Sidechain	13
1	A	79	ARG	Sidechain,Peptide	11
1	A	20	PHE	Sidechain,Peptide	9
1	A	152	ALA	Peptide	7
1	A	143	ARG	Sidechain	5
1	A	82	GLY	Peptide	4
1	A	38	LEU	Peptide	3
1	A	83	ASP	Peptide	3
1	A	69	ARG	Sidechain	3
1	A	99	ILE	Peptide	2
1	A	96	ASP	Peptide	2
1	A	94	VAL	Peptide	1
1	A	75	LYS	Peptide	1
1	A	11	ASP	Peptide	1
1	A	35	ILE	Peptide	1
1	A	71	HIS	Sidechain	1
1	A	5	VAL	Peptide	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	68	SER	Peptide	1
1	A	91	LYS	Peptide	1
1	A	114	GLY	Peptide	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	1018	1005	1004	4±2
All	All	35665	35175	35140	134

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:HIS:CE1	1:A:140:ALA:HB2	0.67	2.25	1	19
1:A:47:VAL:HG11	1:A:115:ARG:CZ	0.58	2.28	26	1
1:A:20:PHE:CE1	1:A:112:ILE:HD11	0.57	2.34	32	1
1:A:50:GLU:HB2	1:A:60:ALA:HB2	0.55	1.79	22	1
1:A:5:VAL:HG23	1:A:152:ALA:HB2	0.54	1.78	24	4
1:A:14:VAL:HB	1:A:145:ALA:HB2	0.52	1.81	26	3
1:A:20:PHE:CZ	1:A:112:ILE:HD11	0.52	2.40	32	1
1:A:119:VAL:CG1	1:A:145:ALA:HB3	0.52	2.35	14	2
1:A:20:PHE:CE1	1:A:31:VAL:HG22	0.51	2.41	10	5
1:A:3:LYS:O	1:A:152:ALA:HB3	0.49	2.07	24	1
1:A:104:ILE:C	1:A:104:ILE:HD12	0.49	2.33	26	5
1:A:47:VAL:HG11	1:A:115:ARG:NE	0.49	2.23	26	1
1:A:120:HIS:CG	1:A:140:ALA:HB1	0.49	2.42	12	10
1:A:38:LEU:HD12	1:A:43:HIS:CD2	0.48	2.43	18	1
1:A:14:VAL:CB	1:A:145:ALA:HB2	0.48	2.37	26	1
1:A:38:LEU:HD11	1:A:119:VAL:HG21	0.48	1.84	18	1
1:A:46:HIS:ND1	1:A:120:HIS:CD2	0.48	2.82	25	5
1:A:46:HIS:HE1	1:A:140:ALA:HB2	0.47	1.67	1	5
1:A:45:PHE:CE1	1:A:119:VAL:HG22	0.47	2.44	5	1
1:A:112:ILE:CD1	1:A:149:ILE:HG21	0.46	2.41	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LYS:NZ	1:A:92:ASP:OD2	0.46	2.48	16	1
1:A:80:HIS:CE1	1:A:137:THR:HA	0.46	2.46	35	17
1:A:8:LEU:CD1	1:A:117:LEU:HD12	0.45	2.42	28	1
1:A:45:PHE:CZ	1:A:117:LEU:HD21	0.45	2.47	11	1
1:A:112:ILE:O	1:A:115:ARG:HB2	0.45	2.12	19	1
1:A:20:PHE:CZ	1:A:29:VAL:HG11	0.45	2.46	14	2
1:A:120:HIS:CB	1:A:140:ALA:HB1	0.45	2.41	15	2
1:A:38:LEU:HD11	1:A:119:VAL:CG2	0.45	2.41	18	1
1:A:64:PHE:CD2	1:A:81:VAL:HG13	0.45	2.47	2	1
1:A:20:PHE:CD2	1:A:29:VAL:HG11	0.44	2.48	35	1
1:A:45:PHE:CE2	1:A:117:LEU:HD21	0.44	2.47	35	1
1:A:117:LEU:HD13	1:A:118:VAL:N	0.44	2.27	12	1
1:A:20:PHE:C	1:A:20:PHE:CD1	0.44	2.96	17	1
1:A:71:HIS:CG	1:A:138:GLY:HA2	0.44	2.48	22	1
1:A:8:LEU:HD23	1:A:147:GLY:N	0.43	2.27	31	1
1:A:38:LEU:HD12	1:A:43:HIS:CG	0.43	2.48	18	1
1:A:46:HIS:ND1	1:A:63:HIS:CE1	0.43	2.86	6	1
1:A:112:ILE:HG12	1:A:149:ILE:HG21	0.42	1.90	17	1
1:A:3:LYS:NZ	1:A:153:GLN:O	0.42	2.52	14	3
1:A:6:ALA:HB3	1:A:18:ILE:HB	0.42	1.90	18	3
1:A:115:ARG:O	1:A:149:ILE:HG22	0.42	2.13	1	2
1:A:20:PHE:CD2	1:A:31:VAL:HG22	0.42	2.50	32	1
1:A:112:ILE:HD12	1:A:112:ILE:C	0.42	2.40	1	1
1:A:132:GLU:OE1	1:A:136:LYS:NZ	0.42	2.52	13	1
1:A:70:LYS:NZ	1:A:78:GLU:OE1	0.41	2.53	8	2
1:A:20:PHE:CG	1:A:149:ILE:HD11	0.41	2.50	19	1
1:A:96:ASP:CG	1:A:97:VAL:N	0.41	2.77	20	1
1:A:76:ASP:OD2	1:A:128:LYS:NZ	0.41	2.53	23	1
1:A:106:LEU:HD13	1:A:106:LEU:H	0.41	1.74	25	1
1:A:121:GLU:OE2	1:A:122:LYS:NZ	0.41	2.53	16	2
1:A:20:PHE:CD1	1:A:29:VAL:CG1	0.41	3.04	17	1
1:A:47:VAL:HG12	1:A:117:LEU:HA	0.41	1.93	26	1
1:A:70:LYS:NZ	1:A:78:GLU:OE2	0.41	2.54	27	2
1:A:21:GLU:OE1	1:A:23:LYS:NZ	0.40	2.54	21	1
1:A:91:LYS:NZ	1:A:92:ASP:OD1	0.40	2.54	26	1
1:A:30:LYS:NZ	1:A:100:GLU:CD	0.40	2.80	29	1
1:A:30:LYS:NZ	1:A:100:GLU:OE1	0.40	2.55	27	2
1:A:132:GLU:OE2	1:A:136:LYS:NZ	0.40	2.54	33	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	138/153 (90%)	104±3 (75±2%)	29±3 (21±2%)	5±2 (4±1%)	4	30
All	All	4830/5355 (90%)	3631 (75%)	1013 (21%)	186 (4%)	4	30

All 33 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	90	ASP	19
1	A	79	ARG	18
1	A	121	GLU	18
1	A	49	GLU	14
1	A	91	LYS	10
1	A	113	ILE	9
1	A	132	GLU	7
1	A	64	PHE	7
1	A	50	GLU	7
1	A	25	SER	7
1	A	81	VAL	6
1	A	60	ALA	6
1	A	72	GLY	6
1	A	26	ASN	6
1	A	134	SER	4
1	A	63	HIS	4
1	A	131	ASN	4
1	A	61	GLY	4
1	A	74	PRO	4
1	A	111	SER	4
1	A	133	GLN	3
1	A	139	ASN	3
1	A	40	GLU	2
1	A	38	LEU	2
1	A	130	GLY	2
1	A	138	GLY	2
1	A	126	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	93	GLY	1
1	A	23	LYS	1
1	A	27	GLY	1
1	A	82	GLY	1
1	A	107	SER	1
1	A	129	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	108/118 (92%)	93±3 (87±3%)	15±3 (13±3%)	6	45
All	All	3780/4130 (92%)	3271 (87%)	509 (13%)	6	45

All 68 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	97	VAL	32
1	A	38	LEU	27
1	A	39	THR	25
1	A	119	VAL	25
1	A	20	PHE	22
1	A	106	LEU	21
1	A	104	ILE	14
1	A	137	THR	13
1	A	36	LYS	13
1	A	126	LEU	13
1	A	112	ILE	12
1	A	117	LEU	12
1	A	132	GLU	12
1	A	91	LYS	12
1	A	3	LYS	11
1	A	79	ARG	10
1	A	49	GLU	10
1	A	9	LYS	9
1	A	115	ARG	9

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Mol	Chain	Res	Type	Models (Total)
1	A	121	GLU	8
1	A	47	VAL	8
1	A	15	GLN	8
1	A	75	LYS	8
1	A	116	THR	8
1	A	135	THR	7
1	A	139	ASN	7
1	A	70	LYS	7
1	A	128	LYS	6
1	A	19	ASN	6
1	A	22	GLN	6
1	A	24	GLU	6
1	A	23	LYS	6
1	A	148	VAL	6
1	A	50	GLU	6
1	A	83	ASP	5
1	A	21	GLU	5
1	A	113	ILE	5
1	A	146	CYS	5
1	A	111	SER	5
1	A	35	ILE	5
1	A	45	PHE	5
1	A	124	ASP	5
1	A	131	ASN	5
1	A	65	ASN	4
1	A	78	GLU	4
1	A	143	ARG	4
1	A	153	GLN	4
1	A	125	ASP	4
1	A	92	ASP	3
1	A	30	LYS	3
1	A	69	ARG	3
1	A	100	GLU	3
1	A	81	VAL	3
1	A	134	SER	3
1	A	122	LYS	3
1	A	26	ASN	2
1	A	133	GLN	2
1	A	18	ILE	2
1	A	67	LEU	2
1	A	25	SER	2
1	A	77	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	149	ILE	1
1	A	76	ASP	1
1	A	8	LEU	1
1	A	99	ILE	1
1	A	29	VAL	1
1	A	90	ASP	1
1	A	88	THR	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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