



Full wwPDB NMR Structure Validation Report ⓘ

Nov 9, 2024 – 01:01 pm GMT

PDB ID : 1GL8
Title : Solution structure of thioredoxin m from spinach, oxidized form
Authors : Neira, J.L.; Gonzalez, C.; Toiron, C.; De-Prat-gay, G.; Rico, M.
Deposited on : 2001-08-30

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	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.39

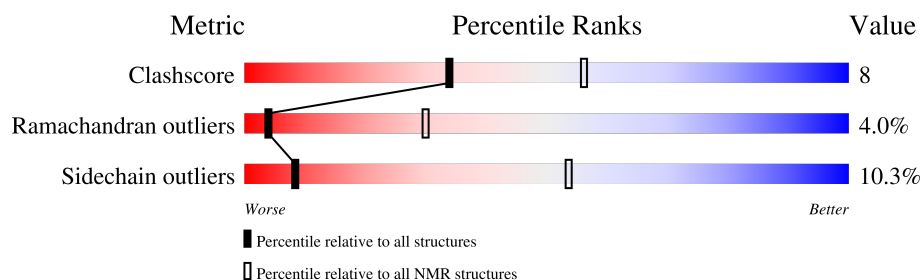
1 Overall quality at a glance

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	104	

2 Ensemble composition and analysis

This entry contains 25 models. Model 3 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:14-A:40, A:49-A:117 (96)	0.98	3

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 3 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1656 atoms, of which 835 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called THIOREDOXIN.

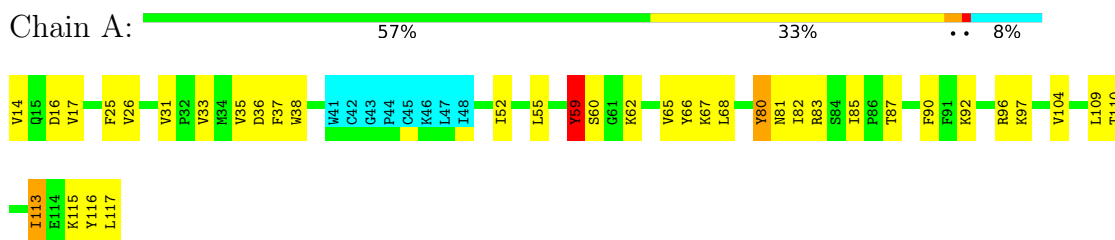
Mol	Chain	Residues	Atoms						Trace
1	A	104	Total	C	H	N	O	S	0
			1656	533	835	128	157	3	

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: THIOREDOXIN

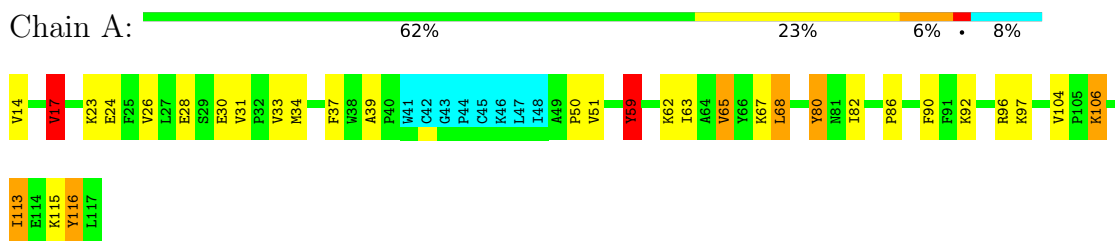


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

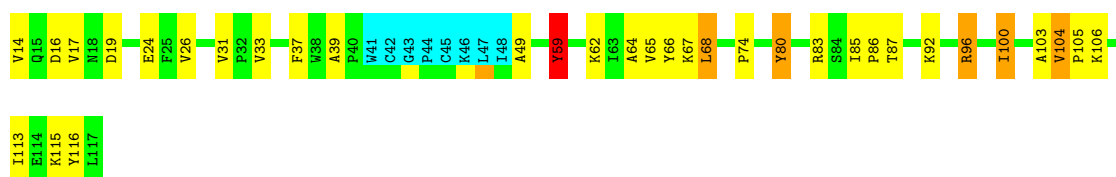
- Molecule 1: THIOREDOXIN



4.2.2 Score per residue for model 2

- Molecule 1: THIOREDOXIN

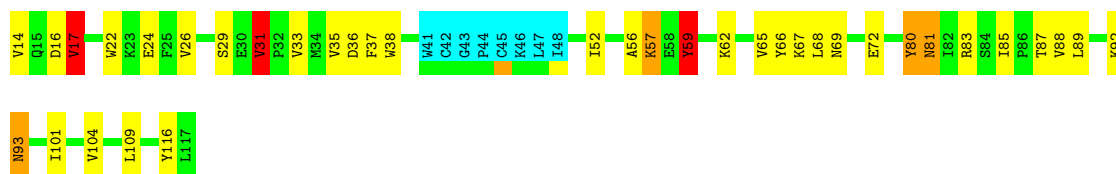




4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: THIOREDOXIN

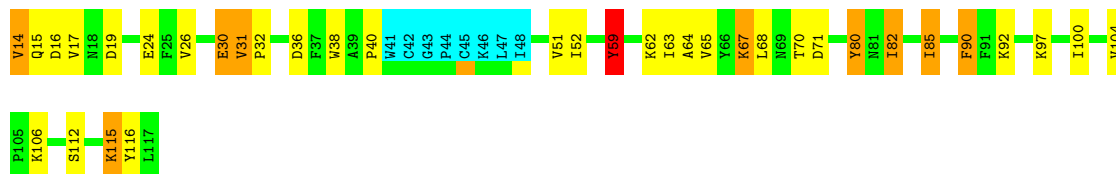
Chain A: 57% 29% 8%



4.2.4 Score per residue for model 4

- Molecule 1: THIOREDOXIN

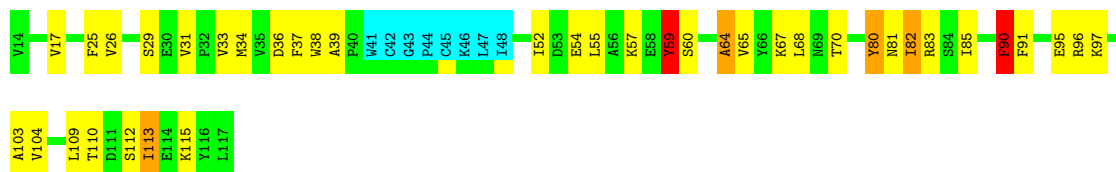
Chain A: 58% 25% 9% 8%



4.2.5 Score per residue for model 5

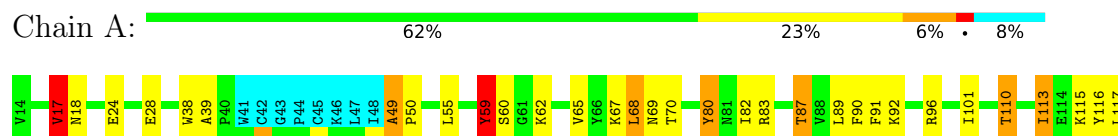
- Molecule 1: THIOREDOXIN

Chain A: 55% 32% 8%



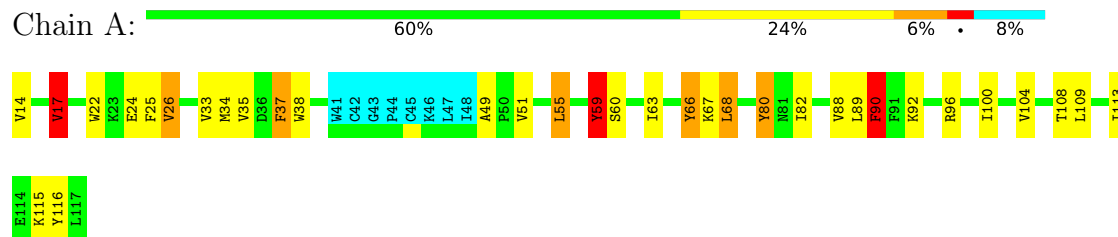
4.2.6 Score per residue for model 6

- Molecule 1: THIOREDOXIN



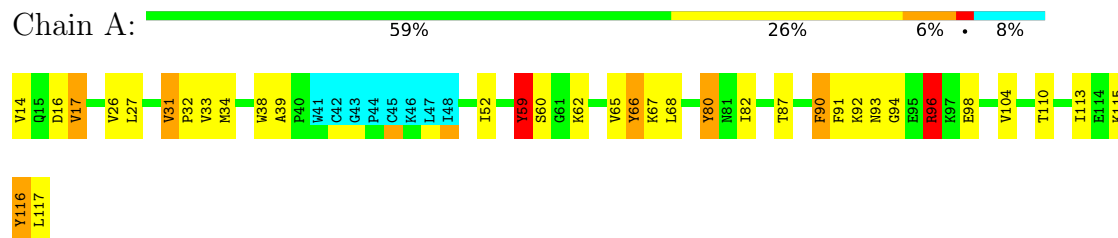
4.2.7 Score per residue for model 7

- Molecule 1: THIOREDOXIN



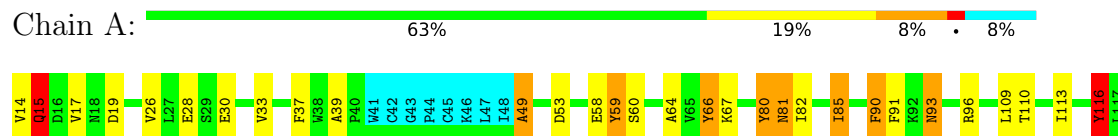
4.2.8 Score per residue for model 8

- Molecule 1: THIOREDOXIN



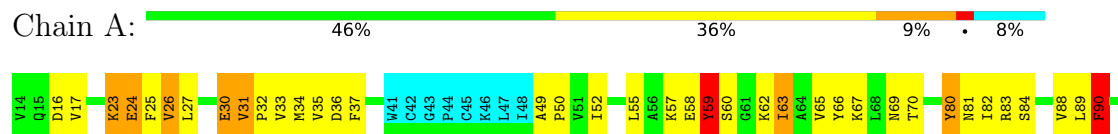
4.2.9 Score per residue for model 9

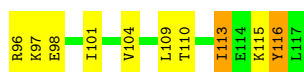
- Molecule 1: THIOREDOXIN



4.2.10 Score per residue for model 10

- Molecule 1: THIOREDOXIN

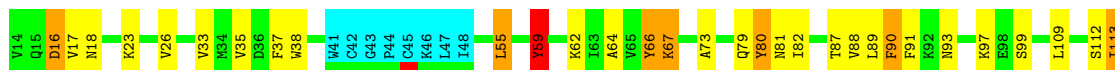




4.2.11 Score per residue for model 11

- Molecule 1: THIOREDOXIN

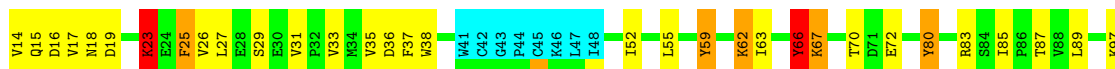
Chain A: 59% 23% 10% 8%



4.2.12 Score per residue for model 12

- Molecule 1: THIOREDOXIN

Chain A: 55% 28% 7% 8%



4.2.13 Score per residue for model 13

- Molecule 1: THIOREDOXIN

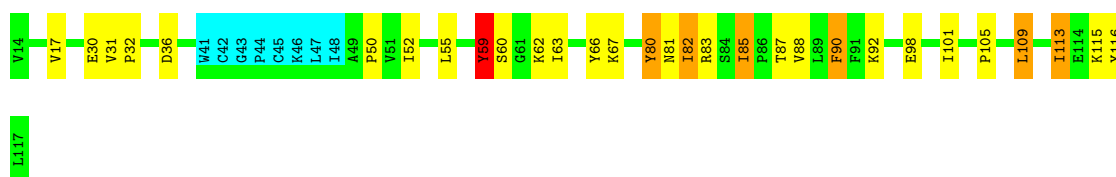
Chain A: 56% 29% 6% 8%



4.2.14 Score per residue for model 14

- Molecule 1: THIOREDOXIN

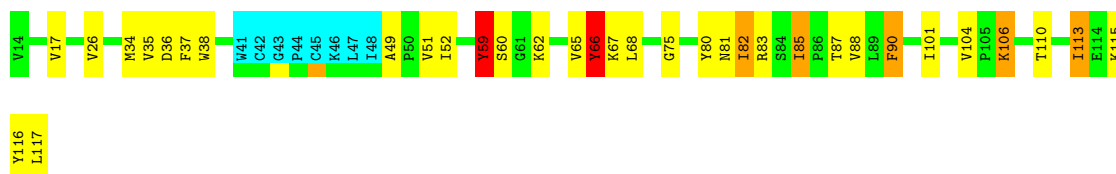
Chain A: 63% 22% 6% 8%



4.2.15 Score per residue for model 15

- Molecule 1: THIOREDOXIN

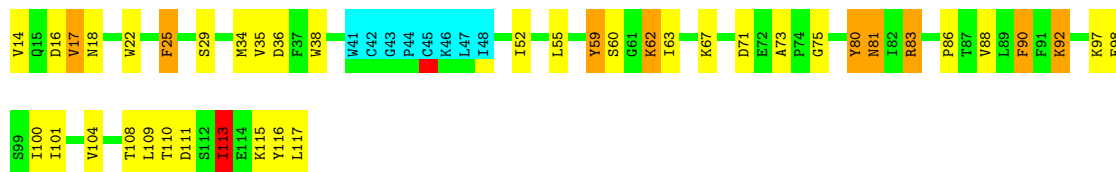
Chain A: 60% 26% 5% 8%



4.2.16 Score per residue for model 16

- Molecule 1: THIOREDOXIN

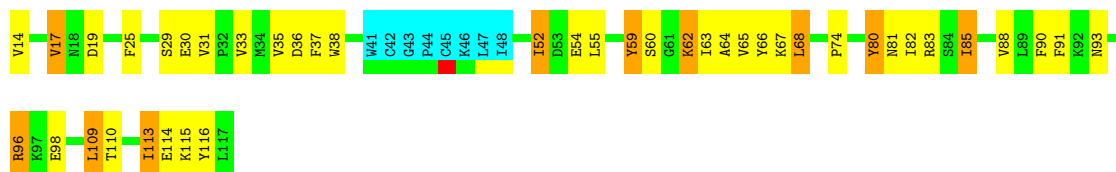
Chain A: 53% 30% 9% 8%



4.2.17 Score per residue for model 17

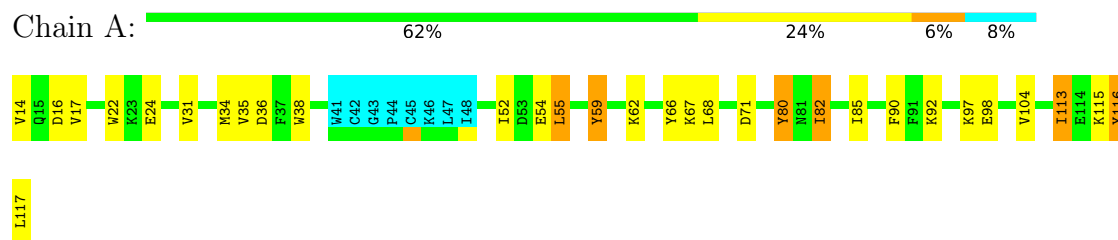
- Molecule 1: THIOREDOXIN

Chain A: 52% 31% 10% 8%



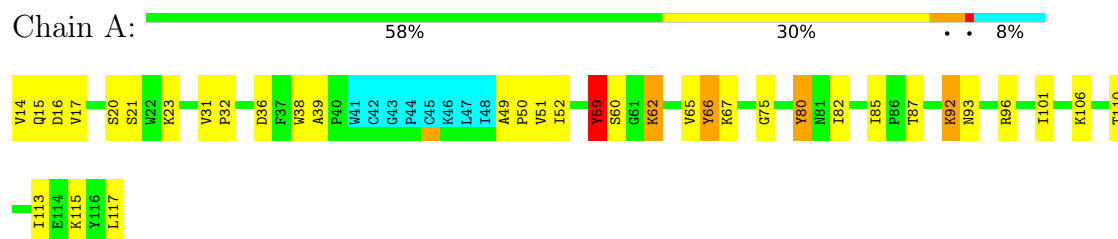
4.2.18 Score per residue for model 18

- Molecule 1: THIOREDOXIN



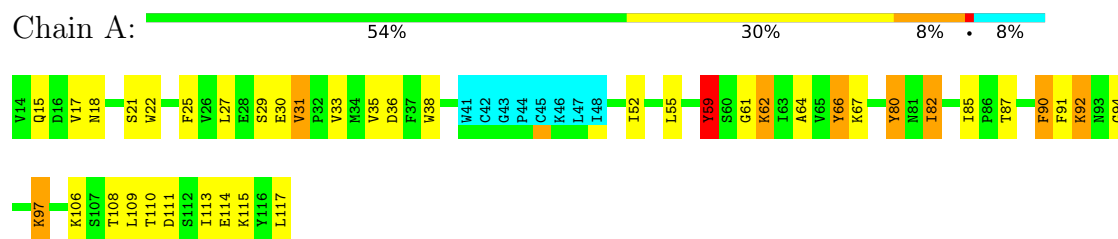
4.2.19 Score per residue for model 19

- Molecule 1: THIOREDOXIN



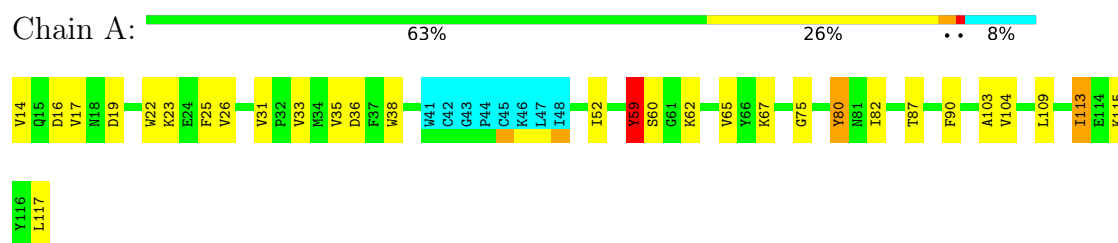
4.2.20 Score per residue for model 20

- Molecule 1: THIOREDOXIN



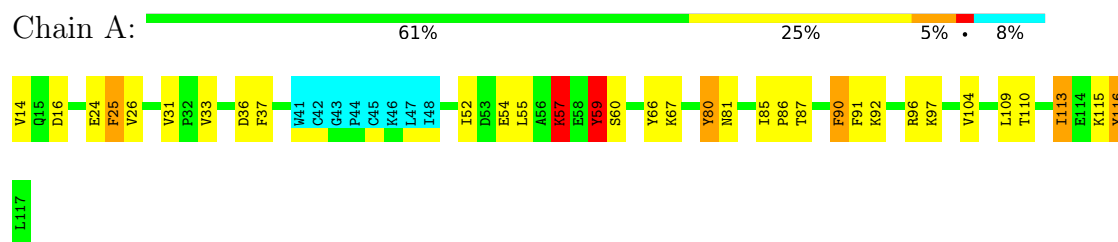
4.2.21 Score per residue for model 21

- Molecule 1: THIOREDOXIN



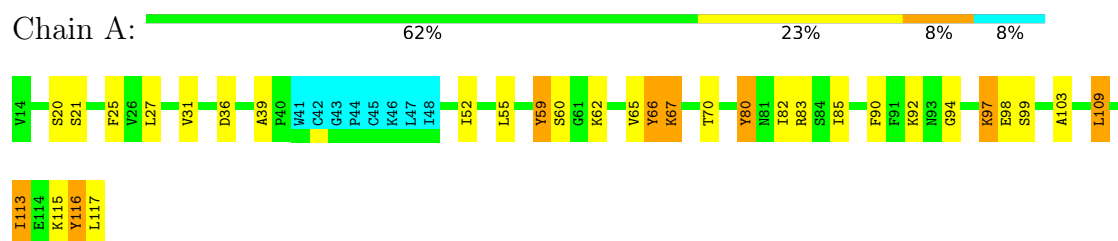
4.2.22 Score per residue for model 22

• Molecule 1: THIOREDOXIN



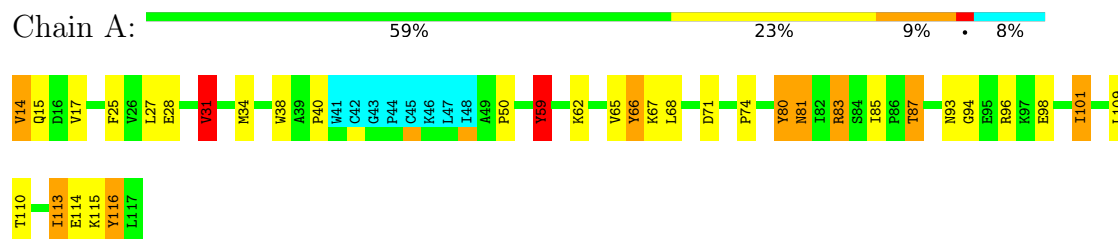
4.2.23 Score per residue for model 23

• Molecule 1: THIOREDOXIN



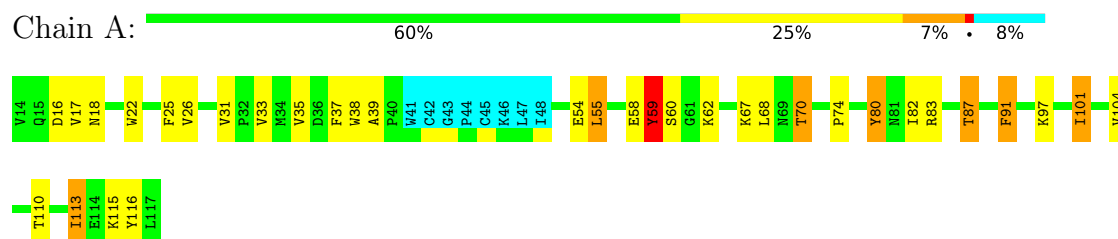
4.2.24 Score per residue for model 24

• Molecule 1: THIOREDOXIN



4.2.25 Score per residue for model 25

• Molecule 1: THIOREDOXIN



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *RESTRAINED MOLECULAR DYNAMICS*.

Of the 25 calculated structures, 25 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
GROMOS	refinement	
GROMOS	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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	0.80±0.01	0±0/776 (0.0± 0.0%)	1.44±0.14	7±3/1056 (0.7± 0.2%)
All	All	0.80	2/19400 (0.0%)	1.44	173/26400 (0.7%)

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	6.8±1.5
All	All	0	170

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	81	ASN	CG-ND2	-7.53	1.14	1.32	24	2

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	81	ASN	OD1-CG-ND2	-29.96	52.98	121.90	9	2
1	A	81	ASN	CB-CG-ND2	-17.38	74.98	116.70	9	1
1	A	59	TYR	CB-CG-CD2	-16.30	111.22	121.00	19	18
1	A	15	GLN	CG-CD-NE2	-13.02	85.46	116.70	9	1
1	A	66	TYR	CB-CG-CD2	-11.45	114.13	121.00	15	13
1	A	15	GLN	CG-CD-OE1	11.24	144.09	121.60	9	1
1	A	15	GLN	OE1-CD-NE2	-10.12	98.63	121.90	9	1
1	A	116	TYR	CB-CG-CD2	-9.96	115.03	121.00	7	11
1	A	80	TYR	CB-CG-CD2	-9.27	115.44	121.00	8	24
1	A	83	ARG	NE-CZ-NH1	9.02	124.81	120.30	24	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	59	TYR	CB-CG-CD1	-8.69	115.79	121.00	11	4
1	A	96	ARG	NE-CZ-NH1	8.53	124.57	120.30	24	3
1	A	25	PHE	CB-CG-CD2	-7.63	115.46	120.80	25	5
1	A	59	TYR	CD1-CG-CD2	7.57	126.23	117.90	24	3
1	A	23	LYS	CD-CE-NZ	-7.39	94.71	111.70	12	4
1	A	81	ASN	CA-CB-CG	-7.29	97.36	113.40	9	1
1	A	115	LYS	N-CA-CB	-7.15	97.73	110.60	23	23
1	A	57	LYS	CD-CE-NZ	-6.76	96.15	111.70	22	2
1	A	23	LYS	CA-CB-CG	-6.68	98.69	113.40	13	4
1	A	15	GLN	CA-CB-CG	-6.68	98.70	113.40	9	1
1	A	37	PHE	CB-CG-CD2	-6.51	116.24	120.80	12	5
1	A	116	TYR	CB-CG-CD1	-6.47	117.12	121.00	8	5
1	A	90	PHE	CB-CG-CD2	-6.37	116.34	120.80	9	7
1	A	113	ILE	N-CA-CB	5.95	124.47	110.80	22	3
1	A	80	TYR	CB-CG-CD1	-5.89	117.47	121.00	4	1
1	A	66	TYR	CB-CG-CD1	-5.80	117.52	121.00	12	1
1	A	31	VAL	CB-CA-C	5.73	122.28	111.40	13	4
1	A	113	ILE	CB-CA-C	-5.54	100.53	111.60	16	6
1	A	49	ALA	CB-CA-C	5.49	118.33	110.10	9	2
1	A	17	VAL	CA-CB-CG2	5.47	119.11	110.90	3	4
1	A	106	LYS	CD-CE-NZ	-5.46	99.15	111.70	1	1
1	A	59	TYR	CG-CD1-CE1	-5.45	116.94	121.30	24	1
1	A	110	THR	CA-CB-CG2	-5.38	104.87	112.40	6	1
1	A	30	GLU	CA-C-N	-5.31	105.51	117.20	10	1
1	A	83	ARG	CB-CG-CD	-5.30	97.82	111.60	16	1
1	A	81	ASN	N-CA-CB	-5.24	101.17	110.60	16	1
1	A	91	PHE	CB-CG-CD2	-5.21	117.16	120.80	22	1
1	A	97	LYS	CD-CE-NZ	-5.05	100.08	111.70	23	1
1	A	96	ARG	NE-CZ-NH2	-5.04	117.78	120.30	24	1
1	A	90	PHE	CA-C-N	-5.00	106.19	117.20	22	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	TYR	Sidechain	25
1	A	59	TYR	Sidechain,Mainchain	21
1	A	90	PHE	Sidechain	15
1	A	92	LYS	Mainchain	12
1	A	66	TYR	Sidechain	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	24	GLU	Mainchain	9
1	A	109	LEU	Mainchain	9
1	A	116	TYR	Sidechain	8
1	A	23	LYS	Mainchain	4
1	A	74	PRO	Mainchain	4
1	A	30	GLU	Mainchain	4
1	A	91	PHE	Sidechain	4
1	A	49	ALA	Mainchain	4
1	A	55	LEU	Mainchain	4
1	A	25	PHE	Mainchain,Sidechain	3
1	A	82	ILE	Mainchain	3
1	A	70	THR	Mainchain	3
1	A	26	VAL	Mainchain	2
1	A	64	ALA	Mainchain	2
1	A	81	ASN	Mainchain,Sidechain	2
1	A	114	GLU	Mainchain	2
1	A	86	PRO	Mainchain	1
1	A	100	ILE	Mainchain	1
1	A	22	TRP	Mainchain	1
1	A	29	SER	Mainchain	1
1	A	108	THR	Mainchain	1
1	A	15	GLN	Sidechain	1
1	A	93	ASN	Mainchain	1
1	A	18	ASN	Mainchain	1
1	A	95	GLU	Mainchain	1
1	A	17	VAL	Mainchain	1
1	A	61	GLY	Mainchain	1
1	A	67	LYS	Mainchain	1
1	A	83	ARG	Sidechain	1
1	A	16	ASP	Mainchain	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	759	772	756	12±4
All	All	18975	19300	18900	304

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:TYR:HB3	1:A:62:LYS:HB2	0.84	1.47	24	8
1:A:14:VAL:HG11	1:A:17:VAL:HG22	0.76	1.57	7	7
1:A:36:ASP:HB3	1:A:52:ILE:HG13	0.74	1.60	5	3
1:A:62:LYS:HB3	1:A:117:LEU:HD21	0.72	1.60	21	2
1:A:59:TYR:HE2	1:A:110:THR:HG23	0.70	1.47	8	3
1:A:81:ASN:HD21	1:A:83:ARG:NH1	0.68	1.87	15	1
1:A:36:ASP:HB3	1:A:52:ILE:HG12	0.67	1.66	14	9
1:A:59:TYR:OH	1:A:110:THR:HG23	0.66	1.89	19	4
1:A:25:PHE:O	1:A:29:SER:HB2	0.64	1.92	20	3
1:A:62:LYS:HD3	1:A:117:LEU:HD13	0.64	1.69	11	1
1:A:14:VAL:HG11	1:A:17:VAL:HB	0.63	1.70	21	4
1:A:92:LYS:HB2	1:A:97:LYS:HD2	0.62	1.69	4	2
1:A:98:GLU:HB2	1:A:116:TYR:OH	0.62	1.94	14	4
1:A:81:ASN:HD21	1:A:83:ARG:NH2	0.61	1.93	3	5
1:A:81:ASN:ND2	1:A:83:ARG:NH2	0.61	2.47	16	1
1:A:26:VAL:HG13	1:A:33:VAL:HG11	0.61	1.71	11	9
1:A:82:ILE:HD13	1:A:85:ILE:HD11	0.60	1.74	15	2
1:A:88:VAL:HG11	1:A:109:LEU:HD22	0.60	1.73	14	2
1:A:35:VAL:O	1:A:88:VAL:HA	0.59	1.97	10	6
1:A:59:TYR:CE2	1:A:110:THR:HG23	0.59	2.32	8	4
1:A:90:PHE:HE2	1:A:100:ILE:HG12	0.58	1.59	4	1
1:A:23:LYS:HG2	1:A:27:LEU:HD12	0.58	1.75	12	2
1:A:81:ASN:HD21	1:A:83:ARG:CZ	0.57	2.12	14	7
1:A:62:LYS:HD3	1:A:62:LYS:H	0.57	1.60	12	1
1:A:21:SER:HB2	1:A:25:PHE:HD2	0.57	1.59	23	1
1:A:33:VAL:HG22	1:A:64:ALA:HB3	0.57	1.75	13	3
1:A:27:LEU:HG	1:A:94:GLY:HA3	0.57	1.74	8	2
1:A:56:ALA:HB2	1:A:65:VAL:HG21	0.57	1.77	3	1
1:A:33:VAL:HB	1:A:91:PHE:HB2	0.57	1.76	5	4
1:A:59:TYR:HD1	1:A:62:LYS:HB2	0.57	1.60	23	1
1:A:55:LEU:HB3	1:A:59:TYR:OH	0.56	2.00	6	7
1:A:14:VAL:HG21	1:A:67:LYS:H	0.56	1.60	22	1
1:A:34:MET:HE1	1:A:113:ILE:HD12	0.55	1.76	24	4
1:A:110:THR:HA	1:A:113:ILE:HD12	0.55	1.77	17	2
1:A:59:TYR:CZ	1:A:113:ILE:HG13	0.55	2.35	18	5
1:A:89:LEU:HD22	1:A:96:ARG:HH11	0.55	1.62	13	1
1:A:52:ILE:HG23	1:A:65:VAL:HG22	0.55	1.78	17	1
1:A:14:VAL:HG11	1:A:67:LYS:HG2	0.55	1.78	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:VAL:HG13	1:A:93:ASN:HB2	0.55	1.78	3	2
1:A:36:ASP:HB2	1:A:52:ILE:HG12	0.55	1.79	10	3
1:A:22:TRP:HZ3	1:A:68:LEU:HD22	0.55	1.62	7	1
1:A:17:VAL:HG21	1:A:66:TYR:HB3	0.54	1.77	19	1
1:A:17:VAL:HG11	1:A:66:TYR:HB3	0.54	1.79	13	3
1:A:92:LYS:HB2	1:A:97:LYS:HE3	0.54	1.78	20	2
1:A:89:LEU:HD23	1:A:96:ARG:HD2	0.54	1.79	10	2
1:A:21:SER:HB3	1:A:25:PHE:HD2	0.53	1.63	20	1
1:A:14:VAL:HG11	1:A:17:VAL:HG23	0.53	1.78	19	1
1:A:62:LYS:HE3	1:A:117:LEU:HG	0.53	1.81	13	1
1:A:81:ASN:ND2	1:A:83:ARG:HH21	0.53	2.01	16	1
1:A:31:VAL:O	1:A:33:VAL:HG23	0.53	2.04	21	4
1:A:27:LEU:HD22	1:A:94:GLY:HA2	0.52	1.80	20	2
1:A:117:LEU:O	1:A:117:LEU:HD12	0.52	2.04	6	2
1:A:21:SER:HB3	1:A:25:PHE:CD2	0.52	2.40	20	1
1:A:59:TYR:HB2	1:A:62:LYS:HB2	0.51	1.82	13	1
1:A:62:LYS:HG2	1:A:63:ILE:H	0.51	1.65	12	1
1:A:55:LEU:HD22	1:A:59:TYR:OH	0.51	2.06	10	5
1:A:59:TYR:OH	1:A:113:ILE:HD13	0.51	2.06	9	1
1:A:109:LEU:O	1:A:113:ILE:HG23	0.51	2.05	10	2
1:A:51:VAL:HG13	1:A:106:LYS:HG3	0.50	1.83	1	1
1:A:40:PRO:HD2	1:A:71:ASP:OD1	0.49	2.08	24	2
1:A:62:LYS:HD2	1:A:63:ILE:H	0.49	1.67	17	1
1:A:26:VAL:O	1:A:33:VAL:HG21	0.49	2.08	12	2
1:A:34:MET:HE1	1:A:90:PHE:CE2	0.49	2.43	1	1
1:A:32:PRO:HB2	1:A:62:LYS:O	0.49	2.08	19	2
1:A:37:PHE:CE2	1:A:68:LEU:HD22	0.48	2.43	2	2
1:A:30:GLU:HB3	1:A:64:ALA:HB2	0.48	1.85	4	1
1:A:90:PHE:HD2	1:A:98:GLU:HB3	0.48	1.67	8	2
1:A:51:VAL:HG13	1:A:106:LYS:HG2	0.48	1.84	15	3
1:A:112:SER:HA	1:A:115:LYS:HE2	0.48	1.85	11	2
1:A:14:VAL:HG22	1:A:66:TYR:CD1	0.48	2.43	12	1
1:A:54:GLU:HA	1:A:57:LYS:HE2	0.48	1.84	22	2
1:A:110:THR:O	1:A:113:ILE:HD12	0.48	2.08	6	1
1:A:59:TYR:HE1	1:A:110:THR:HG23	0.47	1.69	9	1
1:A:62:LYS:HE3	1:A:117:LEU:HD13	0.47	1.85	20	1
1:A:26:VAL:HA	1:A:33:VAL:HG11	0.47	1.84	22	2
1:A:69:ASN:HB2	1:A:72:GLU:HB3	0.47	1.86	3	1
1:A:30:GLU:HB2	1:A:64:ALA:HB2	0.47	1.86	20	1
1:A:64:ALA:HB1	1:A:66:TYR:CZ	0.47	2.45	11	2
1:A:17:VAL:HG23	1:A:68:LEU:HB3	0.47	1.86	6	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:MET:SD	1:A:63:ILE:HG13	0.47	2.50	10	1
1:A:90:PHE:HB3	1:A:116:TYR:OH	0.47	2.08	15	4
1:A:22:TRP:HZ3	1:A:35:VAL:HG21	0.47	1.67	25	2
1:A:110:THR:HG22	1:A:114:GLU:OE1	0.47	2.09	24	1
1:A:59:TYR:HB2	1:A:62:LYS:HD2	0.47	1.86	23	2
1:A:90:PHE:CE2	1:A:100:ILE:HG12	0.47	2.43	4	1
1:A:82:ILE:HD13	1:A:85:ILE:HG23	0.47	1.88	14	1
1:A:22:TRP:CZ3	1:A:35:VAL:HG21	0.47	2.44	25	3
1:A:31:VAL:HG23	1:A:32:PRO:HD3	0.46	1.86	10	1
1:A:35:VAL:HG23	1:A:89:LEU:HB2	0.46	1.87	3	3
1:A:90:PHE:HE1	1:A:100:ILE:HD13	0.46	1.69	7	1
1:A:18:ASN:HA	1:A:73:ALA:HB2	0.46	1.88	16	2
1:A:62:LYS:HD2	1:A:63:ILE:N	0.46	2.25	17	1
1:A:110:THR:O	1:A:114:GLU:HG3	0.46	2.10	17	1
1:A:98:GLU:HB2	1:A:115:LYS:HE2	0.45	1.89	13	1
1:A:16:ASP:HB3	1:A:72:GLU:OE1	0.45	2.11	12	1
1:A:103:ALA:O	1:A:109:LEU:HD11	0.45	2.12	23	1
1:A:52:ILE:HD12	1:A:55:LEU:HD12	0.45	1.87	17	1
1:A:14:VAL:HG11	1:A:67:LYS:H	0.45	1.72	12	1
1:A:87:THR:HG23	1:A:101:ILE:HA	0.45	1.88	15	4
1:A:92:LYS:HG3	1:A:93:ASN:H	0.44	1.73	19	1
1:A:39:ALA:HB2	1:A:85:ILE:HG13	0.44	1.88	19	3
1:A:17:VAL:HG12	1:A:67:LYS:C	0.44	2.32	14	2
1:A:81:ASN:HD21	1:A:83:ARG:NE	0.44	2.10	17	1
1:A:82:ILE:C	1:A:82:ILE:HD13	0.44	2.33	4	1
1:A:49:ALA:N	1:A:50:PRO:HD3	0.44	2.28	6	1
1:A:14:VAL:CG1	1:A:67:LYS:H	0.44	2.26	12	1
1:A:25:PHE:HA	1:A:29:SER:HB3	0.44	1.90	17	1
1:A:55:LEU:HD22	1:A:59:TYR:HH	0.43	1.73	5	1
1:A:59:TYR:CE2	1:A:113:ILE:HG13	0.43	2.48	5	1
1:A:100:ILE:HG23	1:A:103:ALA:O	0.43	2.12	2	1
1:A:113:ILE:HG22	1:A:117:LEU:O	0.43	2.14	8	1
1:A:104:VAL:HA	1:A:109:LEU:HD11	0.43	1.89	12	1
1:A:35:VAL:HG12	1:A:66:TYR:HB2	0.43	1.90	13	2
1:A:62:LYS:HB3	1:A:117:LEU:HD13	0.43	1.90	18	1
1:A:31:VAL:HA	1:A:93:ASN:HB2	0.43	1.91	24	1
1:A:109:LEU:O	1:A:113:ILE:HD13	0.43	2.14	24	1
1:A:37:PHE:CE2	1:A:68:LEU:HD23	0.43	2.48	25	1
1:A:34:MET:HB2	1:A:63:ILE:HB	0.43	1.90	7	1
1:A:63:ILE:HD12	1:A:63:ILE:O	0.43	2.14	7	1
1:A:34:MET:HE2	1:A:90:PHE:HE2	0.43	1.74	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ASN:ND2	1:A:83:ARG:CZ	0.43	2.81	15	1
1:A:17:VAL:O	1:A:21:SER:HB2	0.43	2.14	20	1
1:A:32:PRO:O	1:A:63:ILE:HA	0.43	2.14	4	2
1:A:109:LEU:H	1:A:109:LEU:HD12	0.43	1.73	12	1
1:A:22:TRP:HH2	1:A:35:VAL:HG11	0.43	1.74	18	1
1:A:82:ILE:HD11	1:A:85:ILE:CD1	0.42	2.44	4	1
1:A:52:ILE:HG22	1:A:65:VAL:HG23	0.42	1.90	5	1
1:A:70:THR:HG21	1:A:85:ILE:HG12	0.42	1.91	12	2
1:A:59:TYR:CE1	1:A:110:THR:HG23	0.42	2.49	9	1
1:A:104:VAL:N	1:A:105:PRO:HD2	0.42	2.30	2	1
1:A:52:ILE:HG23	1:A:65:VAL:HB	0.42	1.91	3	1
1:A:59:TYR:OH	1:A:110:THR:CG2	0.42	2.68	24	1
1:A:51:VAL:O	1:A:55:LEU:HG	0.42	2.15	7	1
1:A:62:LYS:HG2	1:A:117:LEU:HD13	0.42	1.90	19	1
1:A:113:ILE:HD12	1:A:113:ILE:N	0.42	2.29	8	2
1:A:89:LEU:CD2	1:A:96:ARG:HD2	0.42	2.44	10	1
1:A:106:LYS:O	1:A:109:LEU:HB2	0.42	2.15	13	1
1:A:84:SER:OG	1:A:101:ILE:HG23	0.42	2.15	10	1
1:A:32:PRO:HG3	1:A:92:LYS:NZ	0.42	2.30	13	1
1:A:34:MET:HE1	1:A:90:PHE:HE2	0.42	1.74	13	1
1:A:52:ILE:HD11	1:A:109:LEU:HD23	0.42	1.90	5	1
1:A:59:TYR:O	1:A:62:LYS:HB3	0.41	2.15	12	1
1:A:108:THR:O	1:A:111:ASP:HB3	0.41	2.14	16	2
1:A:88:VAL:HG22	1:A:90:PHE:HE1	0.41	1.75	11	1
1:A:26:VAL:HG22	1:A:66:TYR:HD2	0.41	1.74	15	1
1:A:29:SER:HB3	1:A:31:VAL:HG22	0.41	1.92	5	1
1:A:59:TYR:HB3	1:A:62:LYS:CB	0.41	2.34	24	1
1:A:32:PRO:HB2	1:A:63:ILE:HG22	0.41	1.93	10	1
1:A:59:TYR:CE1	1:A:113:ILE:HD11	0.41	2.49	10	1
1:A:70:THR:HG21	1:A:85:ILE:HD11	0.41	1.92	23	1
1:A:38:TRP:O	1:A:70:THR:HG22	0.41	2.16	25	2
1:A:37:PHE:CE2	1:A:68:LEU:HD11	0.41	2.50	7	1
1:A:59:TYR:HB2	1:A:63:ILE:HG13	0.41	1.93	4	1
1:A:39:ALA:HB2	1:A:85:ILE:HG21	0.41	1.92	5	1
1:A:62:LYS:CD	1:A:63:ILE:H	0.41	2.29	16	1
1:A:22:TRP:CH2	1:A:35:VAL:HG21	0.41	2.51	20	1
1:A:103:ALA:HB1	1:A:109:LEU:HD21	0.41	1.92	21	1
1:A:63:ILE:HD13	1:A:65:VAL:HG13	0.41	1.92	1	1
1:A:24:GLU:O	1:A:28:GLU:HB2	0.40	2.15	1	1
1:A:52:ILE:O	1:A:65:VAL:HG11	0.40	2.16	8	1
1:A:59:TYR:HB2	1:A:62:LYS:HG3	0.40	1.93	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:LYS:HD3	1:A:67:LYS:O	0.40	2.17	11	1
1:A:113:ILE:HA	1:A:116:TYR:OH	0.40	2.17	9	1
1:A:90:PHE:HE2	1:A:100:ILE:HD13	0.40	1.76	16	1
1:A:34:MET:SD	1:A:52:ILE:HG13	0.40	2.56	8	1
1:A:91:PHE:CE1	1:A:96:ARG:HG3	0.40	2.52	17	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	94/104 (90%)	78±3 (83±3%)	12±3 (13±3%)	4±1 (4±1%)	4	30
All	All	2350/2600 (90%)	1959 (83%)	296 (13%)	95 (4%)	4	30

All 20 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	104	VAL	15
1	A	31	VAL	14
1	A	60	SER	12
1	A	16	ASP	10
1	A	37	PHE	6
1	A	50	PRO	5
1	A	85	ILE	4
1	A	18	ASN	4
1	A	82	ILE	4
1	A	75	GLY	4
1	A	93	ASN	3
1	A	17	VAL	3
1	A	26	VAL	2
1	A	49	ALA	2
1	A	105	PRO	2
1	A	83	ARG	1
1	A	101	ILE	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	96	ARG	1
1	A	15	GLN	1
1	A	62	LYS	1

6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/92 (92%)	76±2 (90±2%)	9±2 (10±2%)	8	53
All	All	2125/2300 (92%)	1907 (90%)	218 (10%)	8	53

All 47 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	67	LYS	22
1	A	113	ILE	19
1	A	82	ILE	14
1	A	68	LEU	13
1	A	87	THR	13
1	A	59	TYR	11
1	A	65	VAL	10
1	A	96	ARG	9
1	A	97	LYS	9
1	A	17	VAL	8
1	A	19	ASP	7
1	A	62	LYS	6
1	A	15	GLN	5
1	A	101	ILE	5
1	A	81	ASN	4
1	A	58	GLU	4
1	A	117	LEU	4
1	A	106	LYS	3
1	A	57	LYS	3
1	A	28	GLU	3
1	A	60	SER	3
1	A	25	PHE	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	85	ILE	3
1	A	54	GLU	3
1	A	30	GLU	2
1	A	16	ASP	2
1	A	14	VAL	2
1	A	69	ASN	2
1	A	109	LEU	2
1	A	63	ILE	2
1	A	99	SER	2
1	A	83	ARG	2
1	A	71	ASP	2
1	A	98	GLU	2
1	A	20	SER	2
1	A	31	VAL	1
1	A	95	GLU	1
1	A	112	SER	1
1	A	89	LEU	1
1	A	90	PHE	1
1	A	53	ASP	1
1	A	24	GLU	1
1	A	79	GLN	1
1	A	86	PRO	1
1	A	52	ILE	1
1	A	93	ASN	1
1	A	21	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 oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

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