



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:00 AM BST

PDB ID : 2KV1
Title : Insights into Function, Catalytic Mechanism and Fold Evolution of Mouse Selenoprotein Methionine Sulfoxide Reductase B1 through Structural Analysis
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Deposited on : 2010-03-04

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

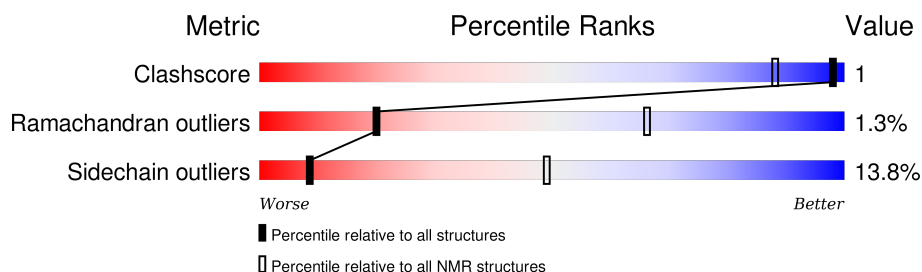
1 Overall quality at a glance

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	124	<div> <div>63%</div> <div>9%</div> <div>28%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:18-A:106 (89)	1.07	9

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1877 atoms, of which 903 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Methionine-R-sulfoxide reductase B1.

Mol	Chain	Residues	Atoms						Trace
1	A	124	Total	C	H	N	O	S	0
			1876	615	903	175	175	8	

There are 9 discrepancies between the modelled and reference sequences:

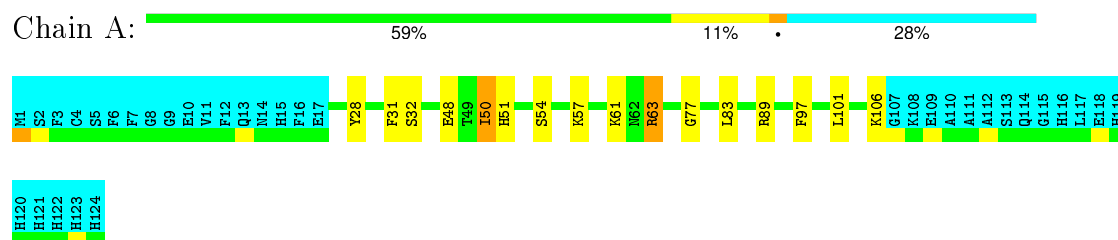
Chain	Residue	Modelled	Actual	Comment	Reference
A	95	CYS	SEC	ENGINEERED MUTATION	UNP Q9JLC3
A	117	LEU	-	EXPRESSION TAG	UNP Q9JLC3
A	118	GLU	-	EXPRESSION TAG	UNP Q9JLC3
A	119	HIS	-	EXPRESSION TAG	UNP Q9JLC3
A	120	HIS	-	EXPRESSION TAG	UNP Q9JLC3
A	121	HIS	-	EXPRESSION TAG	UNP Q9JLC3
A	122	HIS	-	EXPRESSION TAG	UNP Q9JLC3
A	123	HIS	-	EXPRESSION TAG	UNP Q9JLC3
A	124	HIS	-	EXPRESSION TAG	UNP Q9JLC3

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

Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

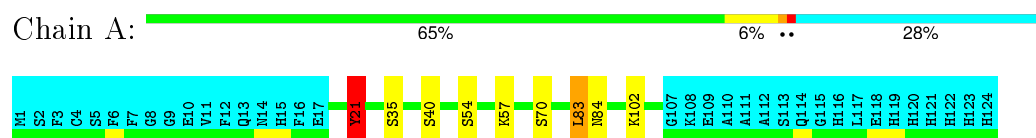
4.2.3 Score per residue for model 3

- Molecule 1: Methionine-R-sulfoxide reductase B1



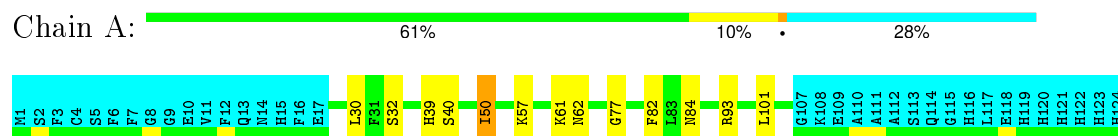
4.2.4 Score per residue for model 4

- Molecule 1: Methionine-R-sulfoxide reductase B1



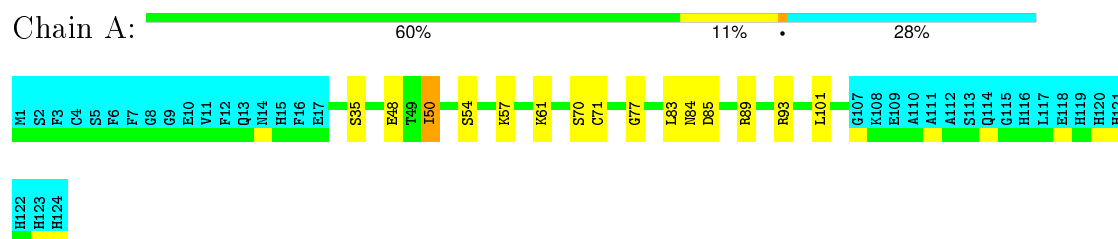
4.2.5 Score per residue for model 5

- Molecule 1: Methionine-R-sulfoxide reductase B1



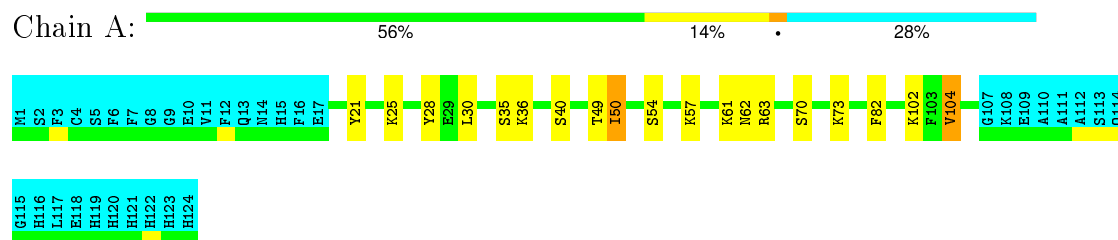
4.2.6 Score per residue for model 6

- Molecule 1: Methionine-R-sulfoxide reductase B1



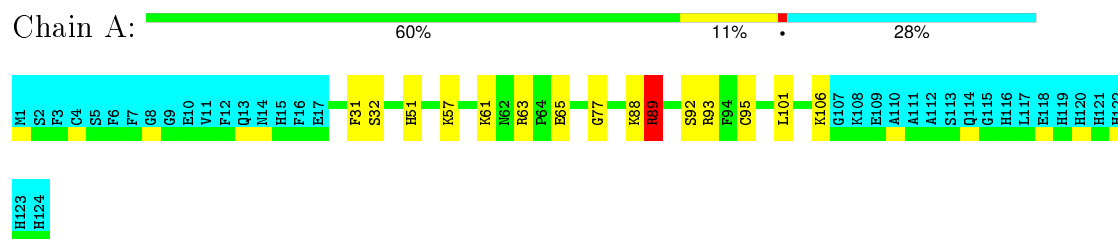
4.2.7 Score per residue for model 7

- Molecule 1: Methionine-R-sulfoxide reductase B1



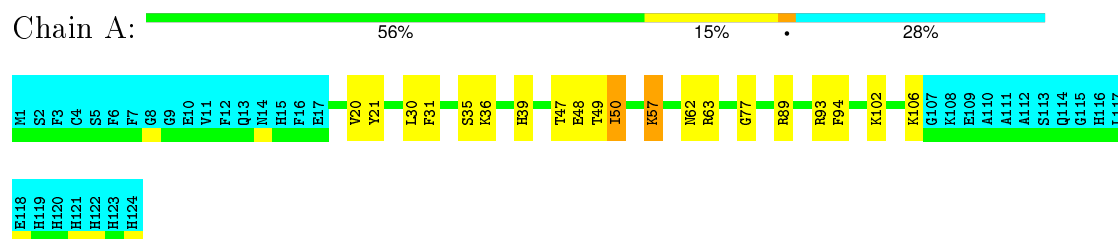
4.2.8 Score per residue for model 8

- Molecule 1: Methionine-R-sulfoxide reductase B1



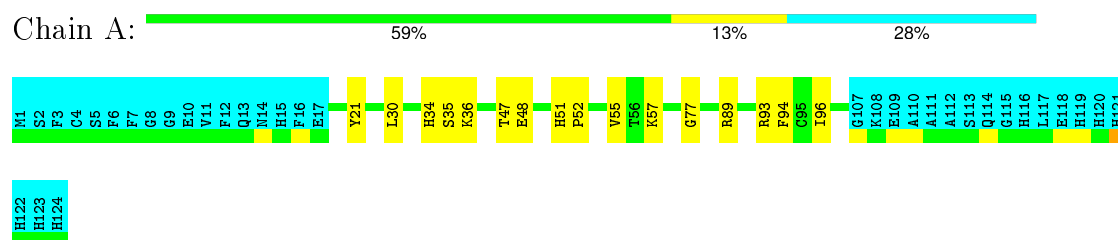
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Methionine-R-sulfoxide reductase B1



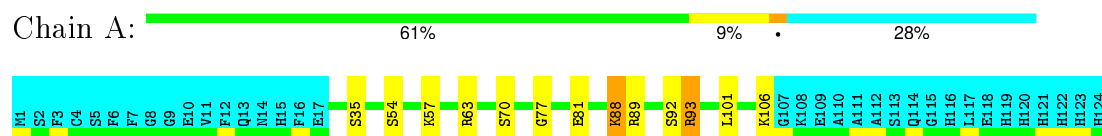
4.2.10 Score per residue for model 10

- Molecule 1: Methionine-R-sulfoxide reductase B1



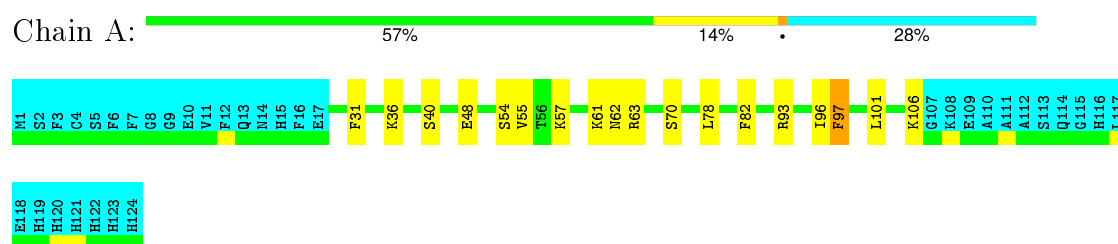
4.2.11 Score per residue for model 11

- Molecule 1: Methionine-R-sulfoxide reductase B1



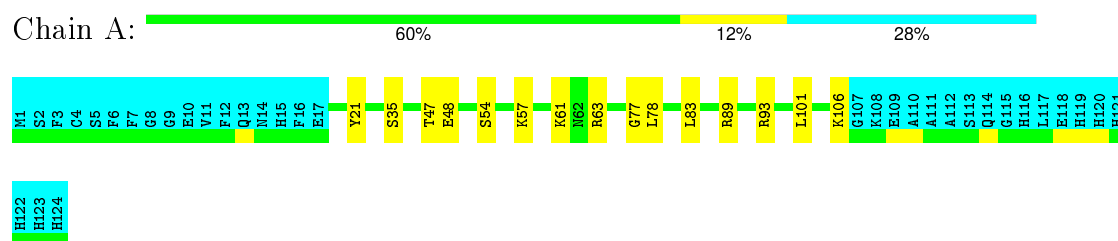
4.2.12 Score per residue for model 12

- Molecule 1: Methionine-R-sulfoxide reductase B1



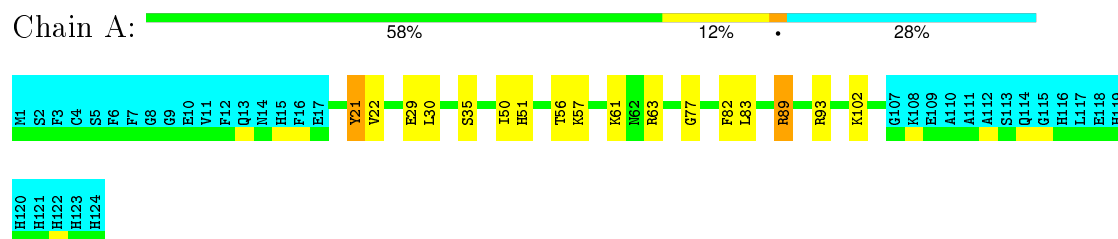
4.2.13 Score per residue for model 13

- Molecule 1: Methionine-R-sulfoxide reductase B1



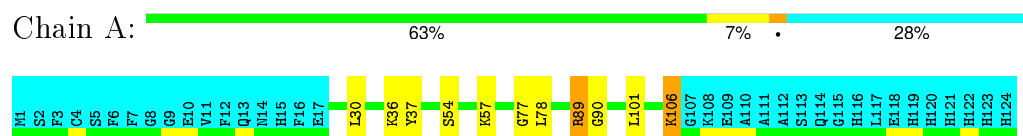
4.2.14 Score per residue for model 14

- Molecule 1: Methionine-R-sulfoxide reductase B1



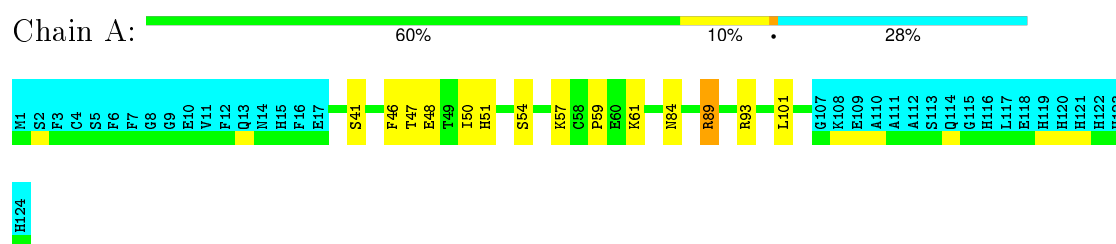
4.2.15 Score per residue for model 15

- Molecule 1: Methionine-R-sulfoxide reductase B1



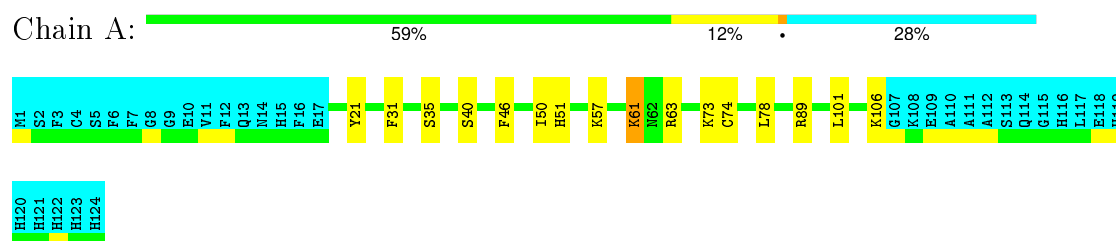
4.2.16 Score per residue for model 16

- Molecule 1: Methionine-R-sulfoxide reductase B1



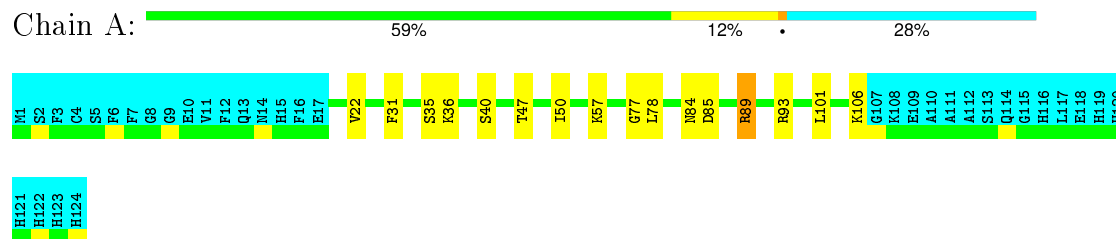
4.2.17 Score per residue for model 17

- Molecule 1: Methionine-R-sulfoxide reductase B1



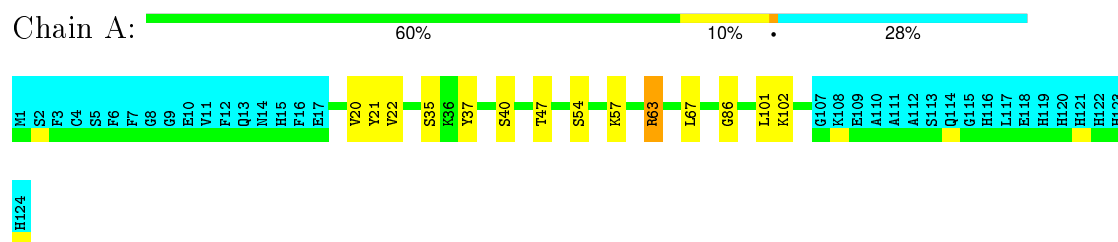
4.2.18 Score per residue for model 18

- Molecule 1: Methionine-R-sulfoxide reductase B1



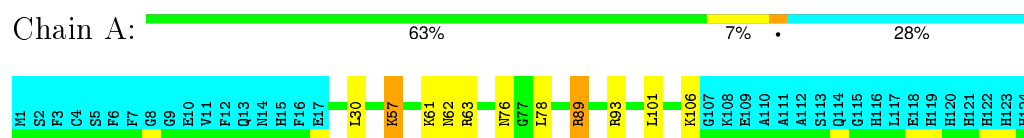
4.2.19 Score per residue for model 19

- Molecule 1: Methionine-R-sulfoxide reductase B1



4.2.20 Score per residue for model 20

- Molecule 1: Methionine-R-sulfoxide reductase B1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 96 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
AMBER	geometry optimization	10
CYANA	refinement	2.1

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 i

6.1 Standard geometry i

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	0.71±0.01	0±0/711 (0.0±0.0%)	1.16±0.03	2±1/960 (0.2±0.1%)
All	All	0.71	0/14220 (0.0%)	1.16	48/19200 (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	1.1±0.9
All	All	0	23

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	89	ARG	NE-CZ-NH1	9.55	125.08	120.30	14	13
1	A	63	ARG	NE-CZ-NH1	8.45	124.53	120.30	19	10
1	A	93	ARG	NE-CZ-NH1	7.79	124.20	120.30	14	12
1	A	89	ARG	NE-CZ-NH2	-6.00	117.30	120.30	20	3
1	A	74	CYS	N-CA-CB	-5.61	100.50	110.60	17	1
1	A	37	TYR	CB-CG-CD2	-5.58	117.65	121.00	19	1
1	A	71	CYS	CA-CB-SG	-5.53	104.04	114.00	6	1
1	A	21	TYR	CA-CB-CG	5.44	123.74	113.40	4	1
1	A	89	ARG	CD-NE-CZ	5.37	131.12	123.60	20	1
1	A	61	LYS	C-N-CA	5.10	134.44	121.70	20	2
1	A	63	ARG	NE-CZ-NH2	-5.09	117.75	120.30	8	1
1	A	106	LYS	CB-CA-C	5.07	120.55	110.40	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	104	VAL	CA-CB-CG2	5.04	118.46	110.90	7	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	89	ARG	Peptide	3
1	A	63	ARG	Sidechain	3
1	A	21	TYR	Sidechain	2
1	A	37	TYR	Sidechain	2
1	A	88	LYS	Peptide	2
1	A	30	LEU	Peptide	1
1	A	86	GLY	Peptide	1
1	A	28	TYR	Sidechain	1
1	A	55	VAL	Peptide	1
1	A	34	HIS	Peptide	1
1	A	101	LEU	Peptide	1
1	A	91	GLN	Peptide	1
1	A	90	GLY	Peptide	1
1	A	76	ASN	Peptide	1
1	A	59	PRO	Peptide	1
1	A	93	ARG	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	688	665	665	1±1
All	All	13780	13300	13300	15

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:ILE:HD12	1:A:50:ILE:H	0.60	1.57	7	2
1:A:51:HIS:CD2	1:A:55:VAL:HG21	0.58	2.33	10	1
1:A:50:ILE:H	1:A:50:ILE:HD12	0.55	1.61	3	4
1:A:20:VAL:HG22	1:A:21:TYR:H	0.52	1.64	9	2
1:A:52:PRO:O	1:A:55:VAL:HG22	0.48	2.09	10	1
1:A:57:LYS:HE2	1:A:57:LYS:H	0.43	1.73	9	1
1:A:57:LYS:HE3	1:A:57:LYS:H	0.42	1.73	20	1
1:A:78:LEU:H	1:A:78:LEU:HD22	0.42	1.74	18	1
1:A:30:LEU:O	1:A:30:LEU:HD12	0.41	2.16	14	1
1:A:83:LEU:HD23	1:A:84:ASN:H	0.41	1.76	4	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	89/124 (72%)	78±3 (88±3%)	10±3 (11±3%)	1±1 (1±1%)	20	66
All	All	1780/2480 (72%)	1558 (88%)	199 (11%)	23 (1%)	20	66

All 9 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	77	GLY	13
1	A	92	SER	3
1	A	86	GLY	1
1	A	88	LYS	1
1	A	89	ARG	1
1	A	106	LYS	1
1	A	78	LEU	1
1	A	97	PHE	1
1	A	41	SER	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	78/106 (74%)	67±3 (86±4%)	11±3 (14±4%)	8 49
All	All	1560/2120 (74%)	1344 (86%)	216 (14%)	8 49

All 44 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	57	LYS	20
1	A	101	LEU	14
1	A	35	SER	12
1	A	61	LYS	11
1	A	106	LYS	11
1	A	54	SER	10
1	A	50	ILE	9
1	A	40	SER	8
1	A	21	TYR	7
1	A	48	GLU	7
1	A	31	PHE	6
1	A	62	ASN	6
1	A	36	LYS	6
1	A	102	LYS	6
1	A	47	THR	6
1	A	51	HIS	5
1	A	89	ARG	5
1	A	30	LEU	5
1	A	83	LEU	5
1	A	22	VAL	5
1	A	70	SER	5
1	A	78	LEU	4
1	A	82	PHE	4
1	A	84	ASN	4
1	A	93	ARG	3
1	A	32	SER	3
1	A	46	PHE	3
1	A	96	ILE	2
1	A	81	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	97	PHE	2
1	A	94	PHE	2
1	A	73	LYS	2
1	A	39	HIS	2
1	A	25	LYS	2
1	A	49	THR	2
1	A	85	ASP	2
1	A	56	THR	1
1	A	65	GLU	1
1	A	104	VAL	1
1	A	67	LEU	1
1	A	95	CYS	1
1	A	28	TYR	1
1	A	63	ARG	1
1	A	29	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided