WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 07:18 pm GMT

PDB ID	:	1OZO
Title	:	Three-dimensional solution structure of apo-S100P protein determined by NMR spectroscopy
Authors	:	Lee, Y.-C.; Volk, D.E.; Thiviyanathan, V.; Kleerekoper, Q.; Gribenko, A.V.; Zhang, S.; Gorenstein, D.G.; Makhatadze, G.I.; Luxon, B.A.
Deposited on	:	2003-04-09

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

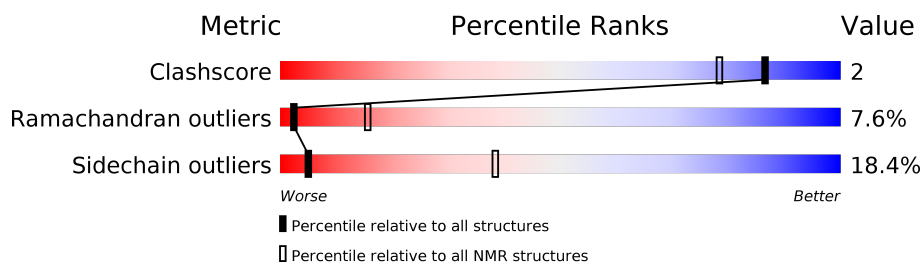|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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	Percentile Ranks	Value
Clashscore		2
Ramachandran outliers		7.6%
Sidechain outliers		18.4%

Worse — *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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

Mol	Chain	Length	Quality of chain
1	A	95	65% 15% • 17%
1	B	95	64% 13% • 19%

2 Ensemble composition and analysis ⓘ

This entry contains 16 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 15 as representative, based on the following criterion: *fewest violations,lowest energy*.

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:21, A:27-A:84, B:1-B:19, B:27-B:84 (156)	0.54	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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2918 atoms, of which 1462 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called S-100P protein.

Mol	Chain	Residues	Atoms						Trace
1	A	95	Total	C	H	N	O	S	0
			1459	462	731	114	148	4	
1	B	95	Total	C	H	N	O	S	0
			1459	462	731	114	148	4	

There are 6 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	THR	CONFLICT	UNP P25815
A	85	SER	CYS	CONFLICT	UNP P25815
A	92	THR	ALA	CONFLICT	UNP P25815
B	6	ALA	THR	CONFLICT	UNP P25815
B	85	SER	CYS	CONFLICT	UNP P25815
B	92	THR	ALA	CONFLICT	UNP P25815

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: S-100P protein

Chain A:

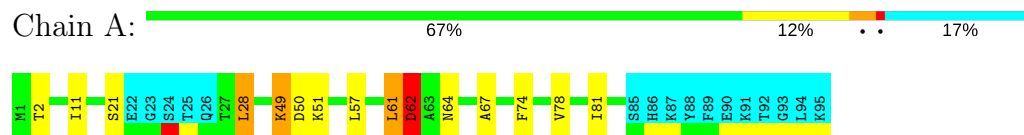• Molecule 1: S-100P protein
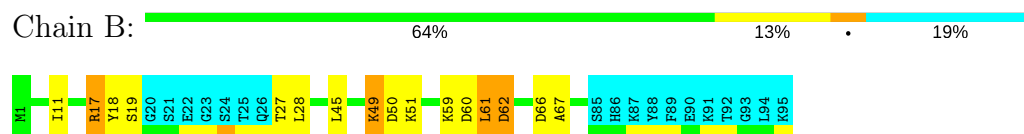
Chain B:

4.2 Scores per residue for each member of the ensemble

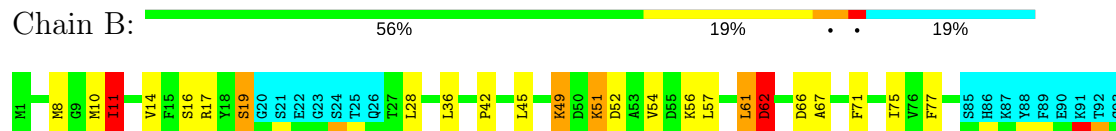Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

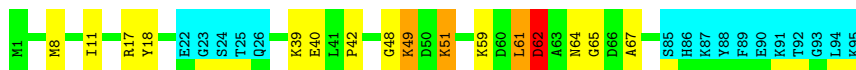• Molecule 1: S-100P protein

Chain A:

• Molecule 1: S-100P protein

Chain B:

L94 K95

4.2.2 Score per residue for model 2

• Molecule 1: S-100P protein

Chain A:

66% 13% 17%

M1 M8 I11 R17 Y18 E22 G23 S24 T25 Q26 K39 E40 L41 P42 G48 K49 D50 K51 K59 D60 L61 D62 A63 N64 G65 D66 A67 S85 H86 K87 Y88 F89 E90 K91 T92 G93 L94 K95

• Molecule 1: S-100P protein

Chain B:

56% 20% 19%

M1 E5 I11 V14 Y18 S19 G20 S21 E22 G23 S24 T25 Q26 T27 L28 L33 L36 E40 L41 P42 L45 K49 D50 K51 D52 L57 L58 K59 D60 L61 D62 G65 D66 A67 F77 V78 S85 H86 K87 Y88 F89 E90 K91 T92 G93 L94 K95
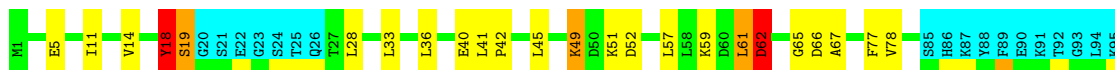
4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: S-100P protein

Chain A:

62% 20% 17%

M1 M8 I11 I12 D13 S16 R17 Y18 S19 G20 S21 E22 G23 S24 T25 Q26 K34 M37 L45 K49 D50 K51 D52 A53 L58 K59 D60 L61 D62 I81 S85 H86 K87 Y88 F89 E90 K91 T92 G93 L94 K95

• Molecule 1: S-100P protein

Chain B:

62% 15% 19%

M1 L4 I11 R17 G20 S21 E22 G23 S24 T25 Q26 V35 P42 S47 G48 K49 D50 K51 D52 L61 D62 A63 N64 G65 D66 A67 Q68 V69 V78 S85 H86 K87 Y88 F89 E90 K91 T92 G93 L94 K95

4.2.4 Score per residue for model 4

• Molecule 1: S-100P protein

Chain A:

60% 19% 17%

M1 M8 I11 R17 Y18 S19 G20 S21 E22 G23 S24 T25 Q26 T27 L28 M37 E38 K39 E40 L45 K49 D50 K51 K59 D60 L61 D62 A63 N64 G65 D66 A67 Q68 V69 S85 H86 K87 Y88 F89 E90 K91 T92 G93 L94 K95

• Molecule 1: S-100P protein

Chain B:

53% 20% 6% 19%
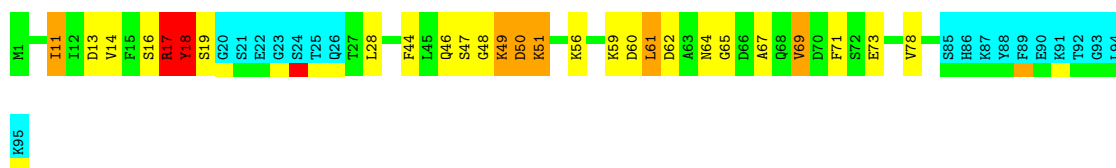
4.2.5 Score per residue for model 5

• Molecule 1: S-100P protein

Chain A:

• Molecule 1: S-100P protein

Chain B:

4.2.6 Score per residue for model 6

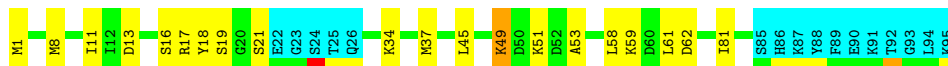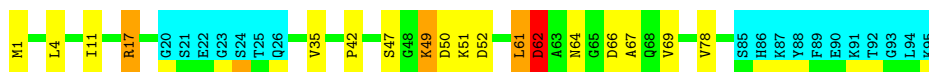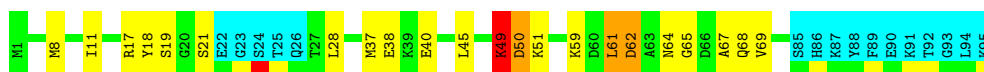• Molecule 1: S-100P protein

Chain A:

• Molecule 1: S-100P protein

Chain B:

4.2.7 Score per residue for model 7

• Molecule 1: S-100P protein

Chain A:

K95

• Molecule 1: S-100P protein

Chain B:

57%   18%   5% •   19%

M1 M8 I11 I12 D13 V14 F15 S16 R17 G20 S21 E22 G23 S24 T25 Q26 T27 L28 M37 E38 K39 L45 K49 D50 K51 L57 D60 L61 D62 A67 F74 I81 T82 S85 H86 K87 Y88 F89 E90 K91 T92 G93 L94 K95

4.2.8 Score per residue for model 8

• Molecule 1: S-100P protein

Chain A:

64%   13%   5% •   17%

M1 I11 R17 Y18 S21 E22 G23 S24 T25 Q26 T27 L28 T29 M37 L45 K49 D50 K51 K59 D60 L61 D62 A63 N64 A67 S85 H86 K87 Y88 F89 E90 K91 T92 G93 L94 K95

• Molecule 1: S-100P protein

Chain B:

54%   24%   • •   19%

M1 I11 R17 Y18 S19 G20 S21 E22 G23 S24 T25 Q26 T27 L28 L33 M37 L45 Q46 S47 G48 D52 A53 V54 K59 D60 L61 D62 A63 N64 G65 D66 A67 Q68 V69 D70 F71 I81 S85 H86 K87 Y88 F89 E90 K91 T92 G93 L94 K95

4.2.9 Score per residue for model 9

• Molecule 1: S-100P protein

Chain A:

57%   22%   •   17%

M1 L4 I11 S16 R17 Y18 S19 G20 S21 E22 G23 S24 T25 Q26 T27 L28 K34 L45 Q46 S47 G48 K49 D50 A53 K56 L57 L58 K59 D60 L61 D62 A63 N64 G65 D66 A67 Q68 V69 S85 H86 K87 Y88 F89 E90 K91 T92 G93 L94 K95

• Molecule 1: S-100P protein

Chain B:

63%   13%   5%   19%

M1 T2 I11 R17 Y18 S19 G20 S21 E22 G23 S24 T25 Q26 T27 L28 L45 G48 K49 D50 K51 D52 A53 K59 D60 L61 D62 A63 N64 A67 S85 H86 K87 Y88 F89 E90 K91 T92 G93 L94 K95
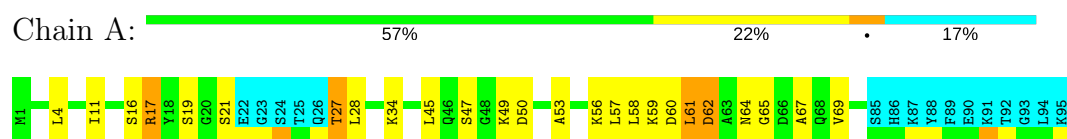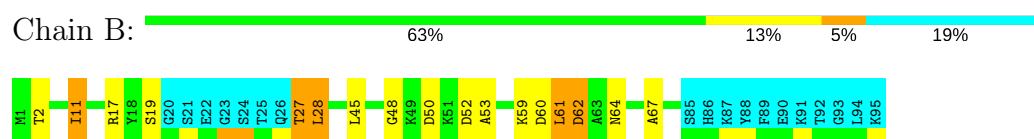
4.2.10 Score per residue for model 10
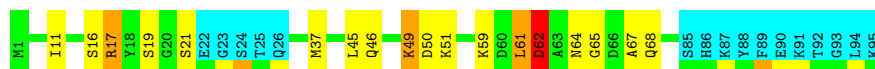
• Molecule 1: S-100P protein

Chain A:

66%   16%   •   17%

• Molecule 1: S-100P protein

4.2.11 Score per residue for model 11

• Molecule 1: S-100P protein

• Molecule 1: S-100P protein

4.2.12 Score per residue for model 12

• Molecule 1: S-100P protein
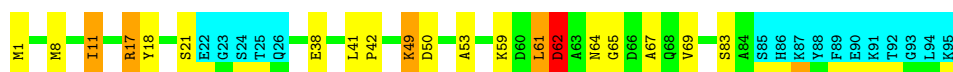
• Molecule 1: S-100P protein
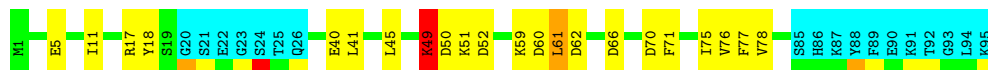
4.2.13 Score per residue for model 13

• Molecule 1: S-100P protein

• Molecule 1: S-100P protein

Chain B:

49%   25%   5%   •   19%
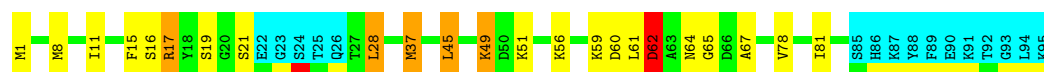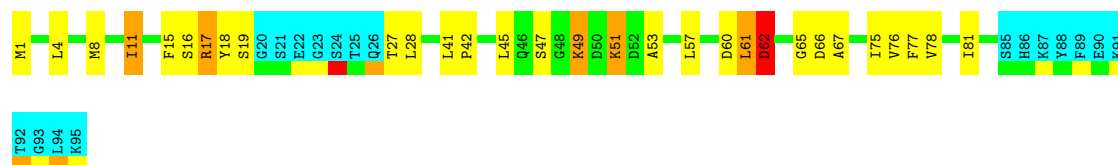
4.2.14 Score per residue for model 14

• Molecule 1: S-100P protein

Chain A:

64%   14%   5%   17%

• Molecule 1: S-100P protein

Chain B:

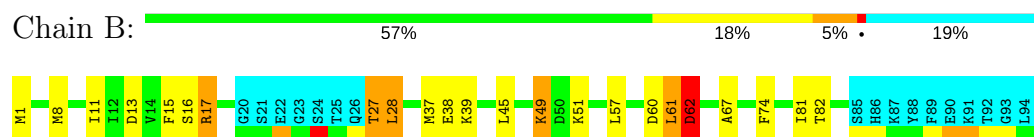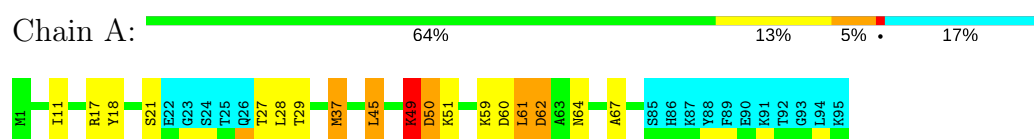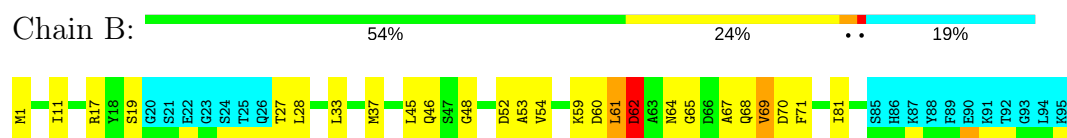58%   19%   •   •   19%

4.2.15 Score per residue for model 15

• Molecule 1: S-100P protein

Chain A:

65%   12%   •   •   17%

• Molecule 1: S-100P protein

Chain B:

62%   14%   5%   19%
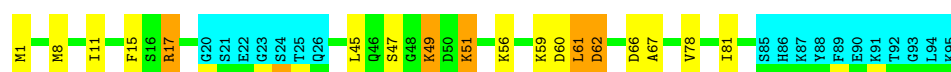
4.2.16　Score per residue for model 16

• Molecule 1: S-100P protein

Chain A:

• Molecule 1: S-100P protein

Chain B:
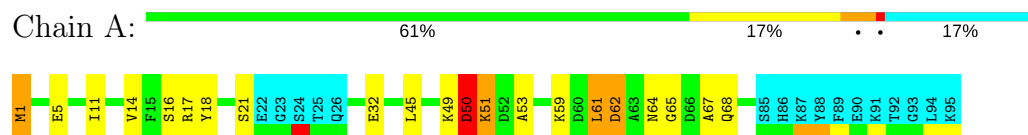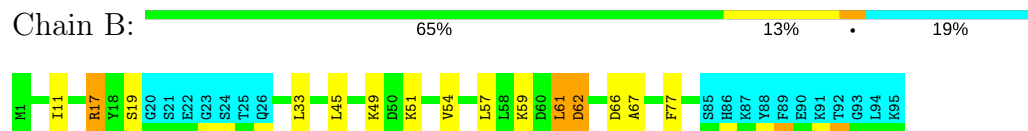
5 Refinement protocol and experimental data overview ⓘ

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

Of the 50 calculated structures, 16 were deposited, based on the following criterion: *structures with the least restraint violations,structures with the lowest energy.*

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

Software name	Classification	Version
AMBER	structure solution	6/7
DIAMD	structure solution	
DIAMD	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 ⓘ

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	0.65±0.01	0±0/605 (0.0±0.0%)	1.25±0.05	2±1/813 (0.2±0.1%)
1	B	0.65±0.01	0±0/595 (0.0±0.0%)	1.25±0.07	2±2/800 (0.3±0.2%)
All	All	0.65	0/19200 (0.0%)	1.25	67/25808 (0.3%)

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	1.8±1.3
1	B	0.0±0.0	2.3±1.3
All	All	0	66

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	17	ARG	NE-CZ-NH1	13.27	126.93	120.30	15	10
1	A	17	ARG	NE-CZ-NH1	10.17	125.39	120.30	15	12
1	B	17	ARG	NE-CZ-NH2	-9.66	115.47	120.30	15	4
1	B	18	TYR	CB-CG-CD2	-8.65	115.81	121.00	4	1
1	B	17	ARG	CD-NE-CZ	7.90	134.66	123.60	15	3
1	A	17	ARG	NE-CZ-NH2	-7.43	116.58	120.30	13	1
1	B	17	ARG	C-N-CA	6.41	137.72	121.70	4	1
1	B	50	ASP	C-N-CA	6.29	137.43	121.70	4	1
1	B	11	ILE	CA-CB-CG1	6.18	122.73	111.00	1	1
1	B	18	TYR	N-CA-CB	-6.13	99.56	110.60	4	1
1	B	62	ASP	N-CA-CB	-5.88	100.02	110.60	16	9
1	A	58	LEU	CB-CA-C	5.75	121.12	110.20	10	2
1	A	49	LYS	C-N-CA	5.68	135.89	121.70	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models Worst	Total
1	A	18	TYR	CB-CG-CD1	-5.60	117.64	121.00	3	1
1	A	62	ASP	N-CA-CB	-5.51	100.69	110.60	6	4
1	A	49	LYS	CA-CB-CG	5.49	125.47	113.40	3	1
1	B	17	ARG	NH1-CZ-NH2	-5.42	113.44	119.40	1	1
1	A	70	ASP	CB-CG-OD1	5.39	123.15	118.30	11	1
1	B	19	SER	C-N-CA	5.34	133.53	122.30	4	1
1	A	69	VAL	CA-CB-CG1	5.26	118.79	110.90	5	2
1	A	17	ARG	CA-CB-CG	5.24	124.93	113.40	8	3
1	B	8	MET	CA-CB-CG	-5.15	104.55	113.30	15	1
1	B	18	TYR	CA-CB-CG	5.12	123.14	113.40	4	1
1	A	50	ASP	C-N-CA	5.08	134.41	121.70	16	1
1	B	69	VAL	CA-CB-CG1	5.05	118.47	110.90	4	2
1	B	48	GLY	C-N-CA	5.02	134.24	121.70	6	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	B	28	LEU	Peptide	10
1	A	28	LEU	Peptide	7
1	A	18	TYR	Sidechain,Peptide	6
1	B	17	ARG	Sidechain	6
1	B	19	SER	Peptide	6
1	B	53	ALA	Peptide	4
1	A	17	ARG	Sidechain	3
1	A	38	GLU	Peptide	3
1	B	18	TYR	Sidechain	2
1	B	11	ILE	Peptide	2
1	A	11	ILE	Peptide	2
1	B	48	GLY	Peptide	2
1	A	56	LYS	Peptide	2
1	B	38	GLU	Peptide	1
1	A	52	ASP	Peptide	1
1	A	62	ASP	Sidechain	1
1	B	50	ASP	Peptide	1
1	B	13	ASP	Peptide	1
1	A	53	ALA	Peptide	1
1	B	52	ASP	Peptide	1
1	A	49	LYS	Peptide	1
1	B	44	PHE	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	48	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	598	606	606	3±1
1	B	588	598	598	4±2
All	All	18976	19264	19264	91

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:8:MET:SD	1:B:78:VAL:HG12	0.61	2.35	4	7
1:B:15:PHE:CE1	1:B:28:LEU:HD13	0.60	2.31	7	2
1:A:4:LEU:HD22	1:B:11:ILE:HG22	0.59	1.73	9	1
1:B:61:LEU:HD22	1:B:77:PHE:CG	0.57	2.34	2	5
1:B:33:LEU:HD22	1:B:54:VAL:HG13	0.54	1.80	11	2
1:B:61:LEU:H	1:B:61:LEU:HD23	0.52	1.63	6	3
1:A:13:ASP:HA	1:A:16:SER:HB3	0.52	1.81	3	1
1:A:61:LEU:HD22	1:A:77:PHE:CG	0.51	2.41	14	1
1:A:78:VAL:HG12	1:B:8:MET:SD	0.50	2.46	7	2
1:B:15:PHE:CE2	1:B:28:LEU:HD13	0.49	2.41	10	1
1:B:61:LEU:HD23	1:B:61:LEU:H	0.49	1.67	14	3
1:B:18:TYR:CG	1:B:36:LEU:HD22	0.48	2.43	2	1
1:A:82:THR:HG21	1:B:75:ILE:HG12	0.48	1.85	14	1
1:B:37:MET:SD	1:B:41:LEU:HD22	0.48	2.48	10	1
1:B:61:LEU:HD23	1:B:61:LEU:N	0.47	2.24	14	6
1:A:18:TYR:HB3	1:A:36:LEU:HD13	0.47	1.87	15	1
1:B:49:LYS:HG2	1:B:50:ASP:H	0.46	1.71	12	1
1:A:61:LEU:H	1:A:61:LEU:HD23	0.46	1.70	5	1
1:B:41:LEU:HD23	1:B:44:PHE:CD2	0.45	2.46	10	1
1:A:11:ILE:CG2	1:A:78:VAL:HG21	0.45	2.42	1	1
1:A:82:THR:HB	1:B:8:MET:SD	0.45	2.51	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:B:61:LEU:N	1:B:61:LEU:HD23	0.45	2.26	8	7
1:B:14:VAL:HG13	1:B:36:LEU:HD11	0.45	1.89	1	1
1:A:61:LEU:HD12	1:A:69:VAL:HG11	0.44	1.89	9	2
1:B:47:SER:OG	1:B:52:ASP:OD1	0.44	2.35	3	1
1:A:61:LEU:HD23	1:A:61:LEU:N	0.44	2.28	1	7
1:B:11:ILE:CG1	1:B:75:ILE:HD11	0.43	2.43	1	1
1:B:57:LEU:O	1:B:61:LEU:HD21	0.43	2.13	7	1
1:A:61:LEU:HD23	1:A:61:LEU:H	0.43	1.72	1	1
1:B:13:ASP:HA	1:B:16:SER:HB3	0.43	1.90	11	1
1:A:61:LEU:N	1:A:61:LEU:HD23	0.43	2.29	6	3
1:A:15:PHE:CE1	1:A:28:LEU:HD13	0.43	2.48	14	1
1:B:14:VAL:CG1	1:B:36:LEU:HD21	0.43	2.43	2	1
1:A:15:PHE:CE2	1:A:28:LEU:HD13	0.43	2.49	13	1
1:B:61:LEU:HD12	1:B:69:VAL:HG11	0.43	1.90	8	2
1:B:69:VAL:HG13	1:B:73:GLU:HB2	0.43	1.89	4	1
1:A:74:PHE:O	1:A:78:VAL:HG23	0.42	2.13	1	1
1:A:37:MET:CB	1:A:45:LEU:HD21	0.42	2.44	8	2
1:B:15:PHE:CE2	1:B:19:SER:HB2	0.42	2.50	14	2
1:A:57:LEU:O	1:A:61:LEU:HD21	0.41	2.15	1	1
1:A:50:ASP:CG	1:A:51:LYS:H	0.41	2.18	15	1
1:B:37:MET:SD	1:B:41:LEU:HD13	0.41	2.56	11	1
1:A:75:ILE:HG12	1:B:82:THR:HG21	0.41	1.93	7	1
1:B:41:LEU:N	1:B:42:PRO:CD	0.41	2.84	2	1
1:B:15:PHE:CD1	1:B:74:PHE:CG	0.41	3.09	7	1
1:A:49:LYS:HG2	1:A:50:ASP:H	0.40	1.76	8	1
1:A:1:MET:HA	1:A:5:GLU:HB2	0.40	1.93	16	1
1:A:49:LYS:CG	1:A:50:ASP:H	0.40	2.30	4	1
1:B:33:LEU:C	1:B:33:LEU:HD23	0.40	2.36	16	1
1:B:11:ILE:HG13	1:B:75:ILE:HD11	0.40	1.93	1	1
1:B:13:ASP:HA	1:B:16:SER:CB	0.40	2.47	7	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	78/95 (82%)	61±2 (78±3%)	12±2 (15±3%)	6±2 (8±2%)	2	15
1	B	76/95 (80%)	57±3 (75±4%)	13±2 (17±3%)	6±2 (8±3%)	2	15
All	All	2464/3040 (81%)	1882 (76%)	394 (16%)	188 (8%)	2	15

All 36 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	67	ALA	14
1	A	21	SER	14
1	A	62	ASP	13
1	A	67	ALA	13
1	B	62	ASP	12
1	B	49	LYS	11
1	A	65	GLY	10
1	A	50	ASP	9
1	B	66	ASP	8
1	A	49	LYS	8
1	B	27	THR	7
1	B	65	GLY	7
1	A	27	THR	6
1	B	51	LYS	5
1	A	51	LYS	5
1	A	53	ALA	4
1	B	42	PRO	4
1	A	48	GLY	3
1	B	19	SER	3
1	A	68	GLN	3
1	A	42	PRO	3
1	B	50	ASP	3
1	B	48	GLY	3
1	A	66	ASP	3
1	B	28	LEU	2
1	B	54	VAL	2
1	B	16	SER	2
1	B	68	GLN	2
1	B	17	ARG	2
1	B	52	ASP	1
1	B	18	TYR	1
1	B	46	GLN	1
1	B	69	VAL	1
1	A	30	LYS	1
1	B	53	ALA	1

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Mol	Chain	Res	Type	Models (Total)
1	A	69	VAL	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	65/79 (82%)	53±2 (82±3%)	12±2 (18±3%)	5	39
1	B	64/79 (81%)	52±3 (81±4%)	12±3 (19±4%)	5	37
All	All	2064/2528 (82%)	1685 (82%)	379 (18%)	5	38

All 80 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	62	ASP	16
1	A	61	LEU	16
1	B	61	LEU	16
1	B	11	ILE	15
1	B	62	ASP	15
1	A	59	LYS	14
1	B	51	LYS	13
1	A	11	ILE	13
1	A	45	LEU	13
1	B	45	LEU	12
1	A	64	ASN	12
1	B	49	LYS	12
1	A	49	LYS	12
1	B	59	LYS	11
1	A	51	LYS	10
1	B	60	ASP	8
1	A	19	SER	8
1	B	64	ASN	7
1	B	17	ARG	7
1	B	1	MET	7
1	B	81	ILE	6
1	A	37	MET	6
1	A	60	ASP	6

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Mol	Chain	Res	Type	Models (Total)
1	A	17	ARG	6
1	A	1	MET	5
1	A	28	LEU	4
1	A	16	SER	4
1	B	18	TYR	4
1	B	71	PHE	4
1	B	70	ASP	4
1	B	47	SER	4
1	B	57	LEU	4
1	B	56	LYS	4
1	A	34	LYS	4
1	A	81	ILE	4
1	A	50	ASP	4
1	A	29	THR	3
1	B	52	ASP	3
1	A	40	GLU	3
1	B	14	VAL	3
1	B	4	LEU	3
1	A	4	LEU	3
1	B	41	LEU	3
1	A	57	LEU	2
1	B	54	VAL	2
1	B	46	GLN	2
1	B	19	SER	2
1	B	16	SER	2
1	A	14	VAL	2
1	B	76	VAL	2
1	B	40	GLU	2
1	B	50	ASP	2
1	B	37	MET	2
1	B	75	ILE	2
1	B	8	MET	1
1	A	38	GLU	1
1	A	70	ASP	1
1	B	10	MET	1
1	B	15	PHE	1
1	A	41	LEU	1
1	A	33	LEU	1
1	A	47	SER	1
1	A	56	LYS	1
1	A	83	SER	1
1	B	28	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	B	39	LYS	1
1	A	54	VAL	1
1	B	34	LYS	1
1	A	39	LYS	1
1	B	2	THR	1
1	A	18	TYR	1
1	B	72	SER	1
1	A	58	LEU	1
1	B	35	VAL	1
1	B	33	LEU	1
1	A	2	THR	1
1	A	69	VAL	1
1	A	35	VAL	1
1	A	46	GLN	1
1	A	71	PHE	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 ⓘ

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