



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 09:48 AM UTC

PDB ID : 6QH2 / pdb_00006qh2
BMRB ID : 34352
Title : Solution NMR ensemble for a chimeric KH-S1 domain construct of exosomal polynucleotide phosphrylase at 298K compiled using the CoMAND method
Authors : ElGamacy, M.; Truffault, V.; Zhu, H.; Coles, M.
Deposited on : 2019-01-14

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

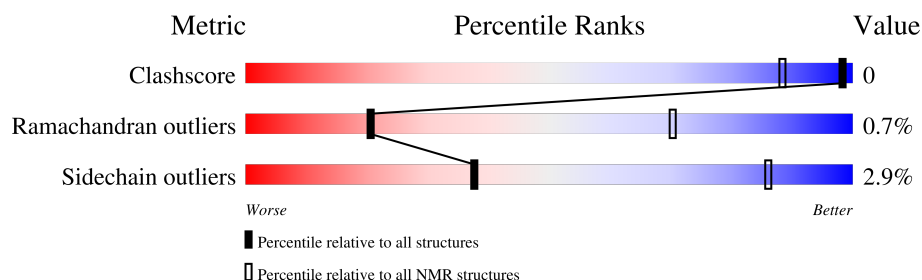
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 74%.

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	171	

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:15-A:76 (62)	0.97	18
2	A:79-A:153 (75)	0.89	7

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 6 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2238 atoms, of which 1144 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Polyribonucleotide nucleotidyltransferase.

Mol	Chain	Residues	Atoms						Trace
1	A	142	Total	C	H	N	O	S	0
			2238	683	1144	197	213	1	

There are 4 discrepancies between the modelled and reference sequences:

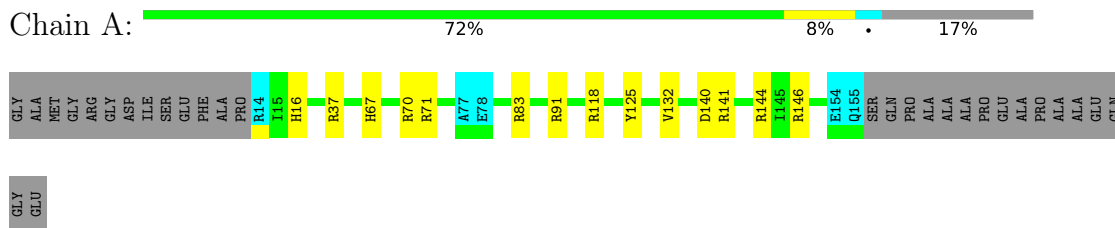
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP B6I1N9
A	2	ALA	-	expression tag	UNP B6I1N9
A	3	MET	-	expression tag	UNP B6I1N9
A	4	GLY	-	expression tag	UNP B6I1N9

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: Polyribonucleotide nucleotidyltransferase

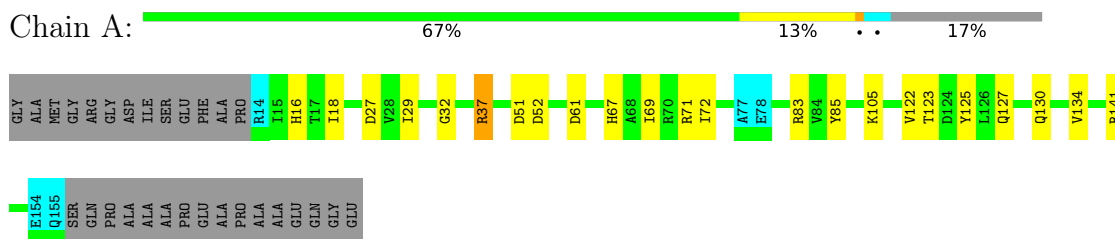


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

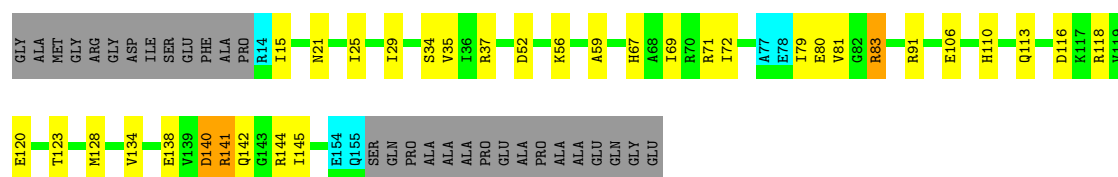
- Molecule 1: Polyribonucleotide nucleotidyltransferase



4.2.2 Score per residue for model 2

- Molecule 1: Polyribonucleotide nucleotidyltransferase

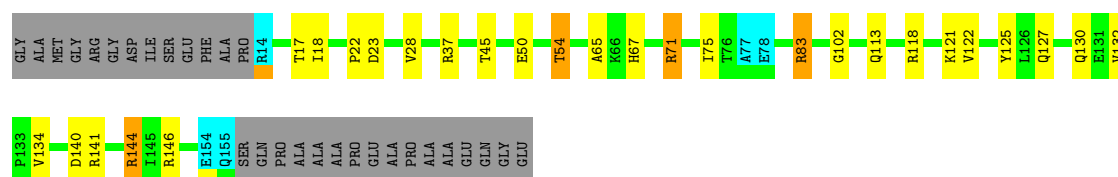




4.2.3 Score per residue for model 3

- Molecule 1: Polyribonucleotide nucleotidyltransferase

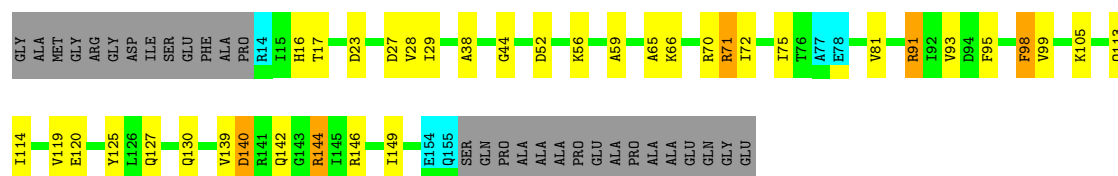
Chain A: 64% 14% 17%



4.2.4 Score per residue for model 4

- Molecule 1: Polyribonucleotide nucleotidyltransferase

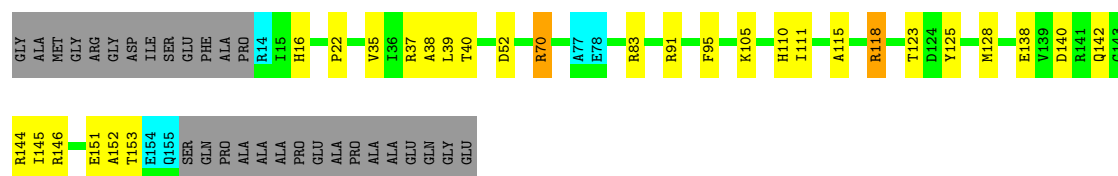
Chain A: 58% 19% 17%



4.2.5 Score per residue for model 5

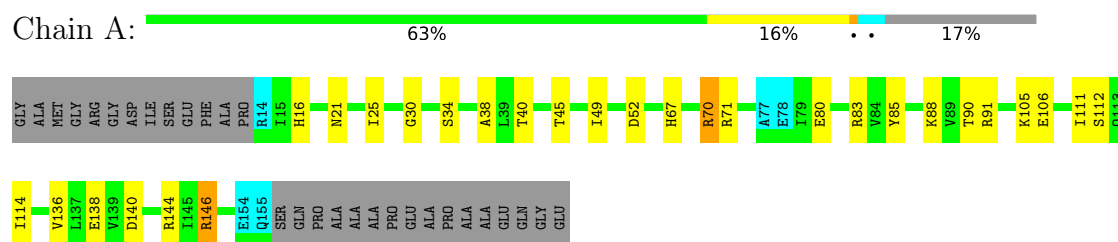
- Molecule 1: Polyribonucleotide nucleotidyltransferase

Chain A: 63% 16% 17%



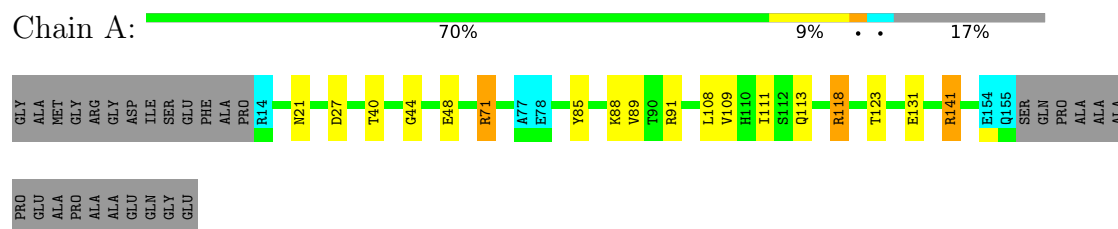
4.2.6 Score per residue for model 6

- Molecule 1: Polyribonucleotide nucleotidyltransferase



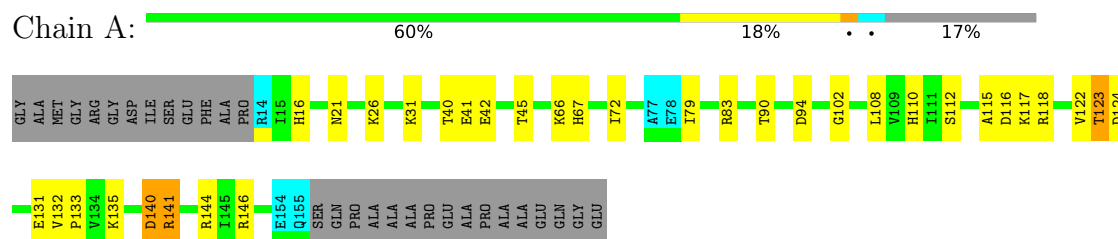
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Polyribonucleotide nucleotidyltransferase



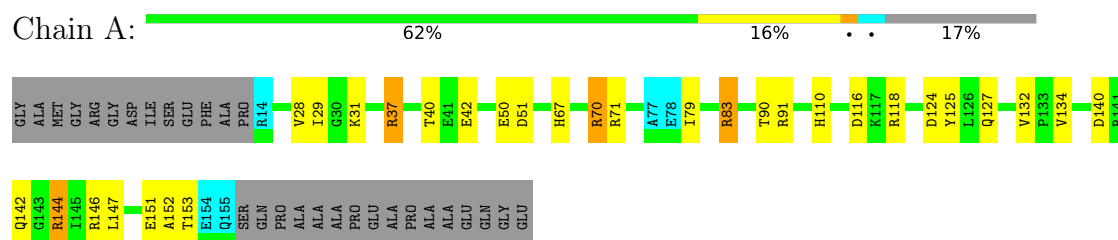
4.2.8 Score per residue for model 8

- Molecule 1: Polyribonucleotide nucleotidyltransferase



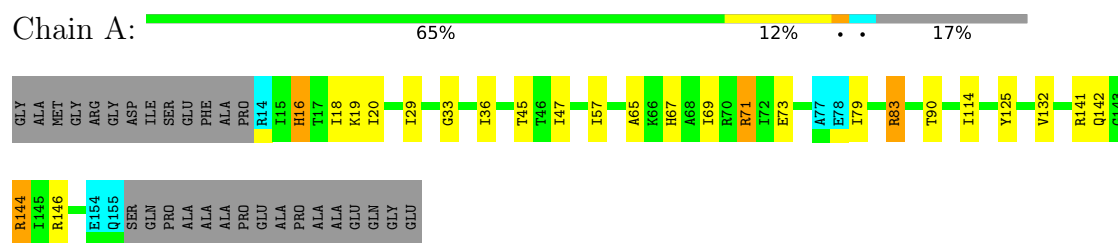
4.2.9 Score per residue for model 9

- Molecule 1: Polyribonucleotide nucleotidyltransferase

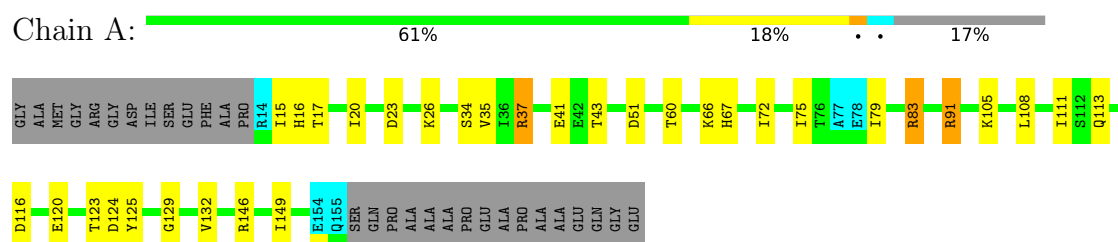


4.2.10 Score per residue for model 10

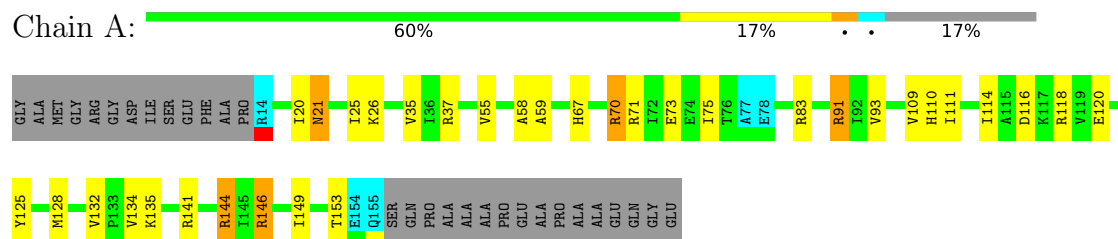
- Molecule 1: Polyribonucleotide nucleotidyltransferase



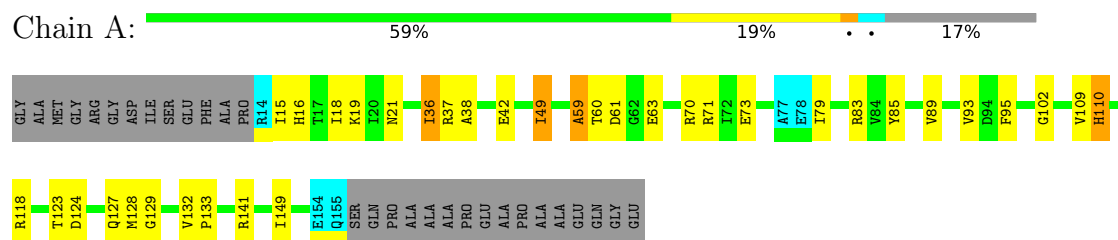
- Molecule 1: Polyribonucleotide nucleotidyltransferase



- Molecule 1: Polyribonucleotide nucleotidyltransferase

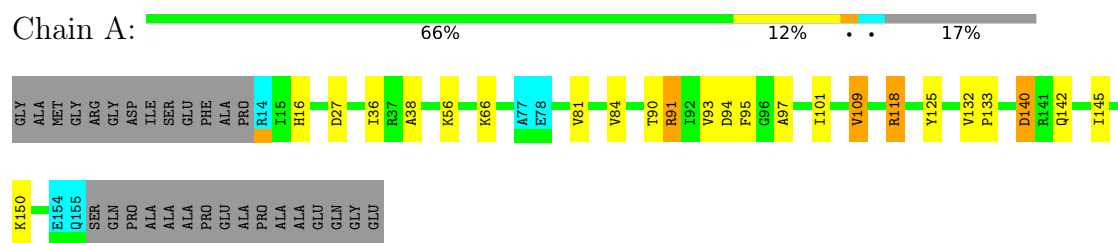


- Molecule 1: Polyribonucleotide nucleotidyltransferase



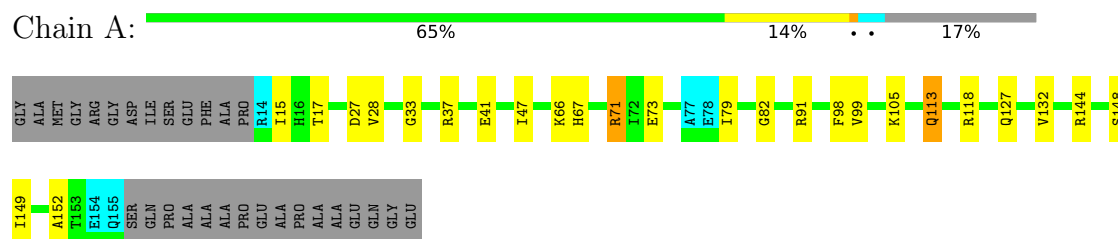
4.2.14 Score per residue for model 14

- Molecule 1: Polyribonucleotide nucleotidyltransferase



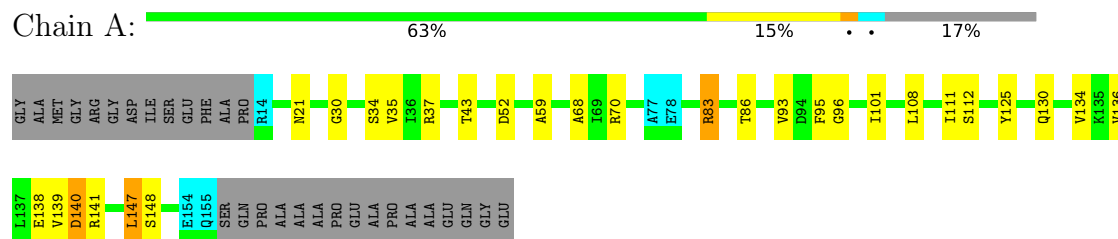
4.2.15 Score per residue for model 15

- Molecule 1: Polyribonucleotide nucleotidyltransferase



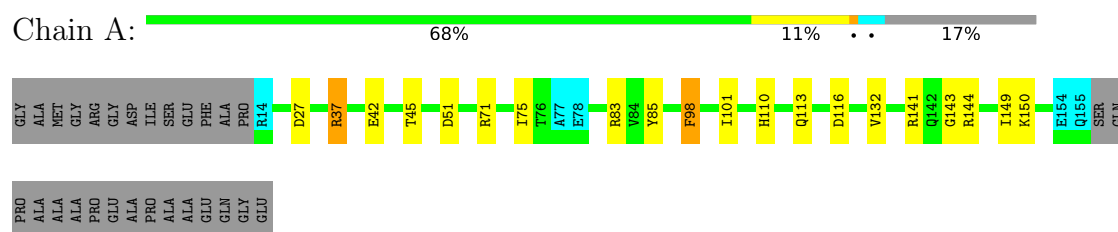
4.2.16 Score per residue for model 16

- Molecule 1: Polyribonucleotide nucleotidyltransferase



4.2.17 Score per residue for model 17

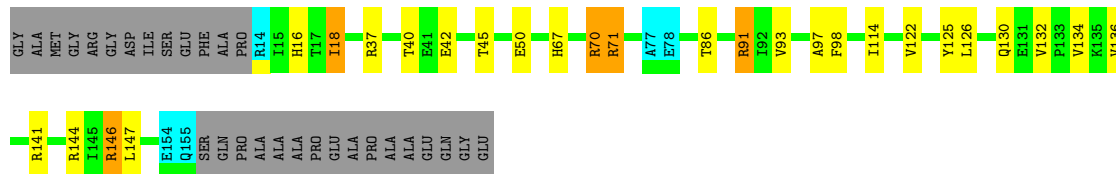
- Molecule 1: Polyribonucleotide nucleotidyltransferase



4.2.18 Score per residue for model 18

- Molecule 1: Polyribonucleotide nucleotidyltransferase

Chain A:  64% 13% 17%



4.2.19 Score per residue for model 19

- Molecule 1: Polyribonucleotide nucleotidyltransferase

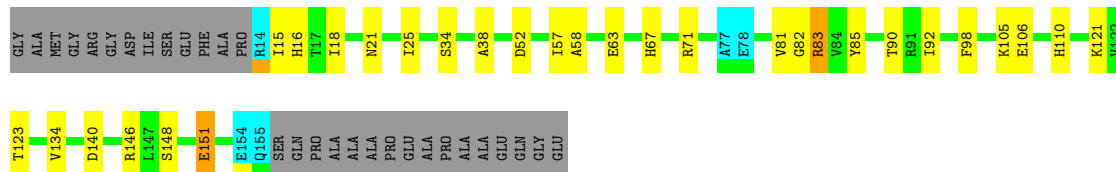
Chain A:  64% 15% 17%



4.2.20 Score per residue for model 20

- Molecule 1: Polyribonucleotide nucleotidyltransferase

Chain A:  63% 16% 17%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *R-factor based frame picking*.

Of the 10000 calculated structures, 20 were deposited, based on the following criterion: *back calculated data agree with experimental NOESY spectrum*.

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

Software name	Classification	Version
Shine	structure calculation	
Rosetta	structure calculation	3.6
NAMD	refinement	2.12
CoMAND	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1440
Number of shifts mapped to atoms	1423
Number of unparsed shifts	0
Number of shifts with mapping errors	17
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

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	1.77±0.05	7±2/1060 (0.6± 0.2%)	1.93±0.04	22±5/1426 (1.5± 0.4%)
All	All	1.77	136/21200 (0.6%)	1.93	441/28520 (1.5%)

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	3.8±1.7
All	All	0	76

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	132	VAL	CA-C	9.11	1.59	1.52	15	3
1	A	16	HIS	ND1-CE1	7.50	1.40	1.32	5	2
1	A	110	HIS	CG-CD2	7.35	1.44	1.35	12	2
1	A	83	ARG	CD-NE	7.13	1.56	1.46	6	2
1	A	132	VAL	CA-CB	7.05	1.63	1.54	11	1
1	A	93	VAL	N-CA	6.95	1.54	1.46	16	1
1	A	144	ARG	CZ-NH2	-6.89	1.24	1.33	8	2
1	A	138	GLU	N-CA	6.78	1.53	1.46	16	2
1	A	81	VAL	N-CA	6.71	1.54	1.46	14	1
1	A	118	ARG	CZ-NH2	-6.62	1.24	1.33	15	2
1	A	136	VAL	CA-CB	-6.60	1.46	1.54	19	1
1	A	93	VAL	CA-C	-6.56	1.47	1.52	18	3
1	A	47	ILE	N-CA	6.51	1.53	1.46	19	1
1	A	30	GLY	CA-C	6.44	1.58	1.52	6	1
1	A	73	GLU	N-CA	6.41	1.54	1.46	10	1
1	A	21	ASN	CA-C	6.37	1.60	1.52	2	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	141	ARG	CZ-NH2	-6.35	1.25	1.33	1	1
1	A	31	LYS	N-CA	6.22	1.54	1.46	8	1
1	A	124	ASP	N-CA	6.20	1.54	1.46	11	1
1	A	132	VAL	N-CA	-6.20	1.40	1.46	17	1
1	A	28	VAL	N-CA	6.18	1.53	1.46	3	1
1	A	26	LYS	N-CA	-6.12	1.39	1.46	8	1
1	A	37	ARG	CZ-NH1	-6.11	1.24	1.32	2	1
1	A	144	ARG	CA-CB	6.11	1.63	1.53	4	2
1	A	132	VAL	C-O	6.06	1.29	1.23	8	1
1	A	67	HIS	CG-CD2	6.00	1.42	1.35	10	2
1	A	43	THR	C-N	5.99	1.39	1.33	11	1
1	A	17	THR	N-CA	5.98	1.53	1.45	11	1
1	A	83	ARG	CZ-NH2	-5.97	1.25	1.33	12	1
1	A	146	ARG	N-CA	5.96	1.53	1.46	11	2
1	A	110	HIS	ND1-CE1	5.94	1.38	1.32	13	1
1	A	140	ASP	CA-CB	5.93	1.63	1.53	8	2
1	A	95	PHE	N-CA	5.93	1.53	1.46	19	2
1	A	60	THR	N-CA	5.92	1.53	1.45	11	1
1	A	118	ARG	CD-NE	5.85	1.54	1.46	13	1
1	A	27	ASP	CA-CB	5.83	1.62	1.53	1	1
1	A	82	GLY	N-CA	5.81	1.53	1.45	20	1
1	A	144	ARG	CA-C	5.78	1.59	1.52	2	1
1	A	92	ILE	N-CA	5.76	1.53	1.46	20	1
1	A	67	HIS	N-CA	5.74	1.53	1.46	6	2
1	A	108	LEU	CA-CB	5.72	1.60	1.53	11	1
1	A	132	VAL	C-N	-5.72	1.28	1.33	14	2
1	A	112	SER	N-CA	5.71	1.53	1.46	6	1
1	A	136	VAL	CA-C	5.71	1.59	1.52	18	1
1	A	81	VAL	CA-C	5.70	1.59	1.52	4	2
1	A	122	VAL	N-CA	-5.68	1.38	1.46	3	1
1	A	72	ILE	CA-C	5.68	1.59	1.52	4	2
1	A	106	GLU	N-CA	5.66	1.53	1.46	2	1
1	A	141	ARG	CA-C	5.65	1.60	1.52	8	1
1	A	105	LYS	CA-CB	5.64	1.60	1.53	1	1
1	A	121	LYS	N-CA	5.63	1.53	1.45	20	1
1	A	130	GLN	CA-C	5.61	1.60	1.52	4	1
1	A	148	SER	N-CA	5.59	1.53	1.46	20	2
1	A	16	HIS	CA-C	5.56	1.59	1.52	11	1
1	A	114	ILE	C-N	5.56	1.40	1.33	12	1
1	A	19	LYS	C-N	5.55	1.40	1.33	10	1
1	A	131	GLU	C-N	5.53	1.38	1.33	7	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	70	ARG	CA-CB	5.53	1.62	1.53	5	1
1	A	91	ARG	CD-NE	5.53	1.53	1.46	5	1
1	A	50	GLU	N-CA	5.53	1.52	1.45	18	1
1	A	75	ILE	N-CA	5.53	1.53	1.46	11	1
1	A	130	GLN	CA-CB	5.52	1.61	1.53	1	1
1	A	67	HIS	ND1-CE1	5.51	1.38	1.32	11	3
1	A	106	GLU	CA-CB	5.51	1.63	1.53	20	1
1	A	66	LYS	N-CA	5.50	1.53	1.46	4	1
1	A	58	ALA	C-N	5.48	1.40	1.33	20	1
1	A	71	ARG	CD-NE	5.47	1.53	1.46	9	1
1	A	89	VAL	CA-C	5.47	1.59	1.52	13	1
1	A	151	GLU	CA-C	5.47	1.59	1.52	9	1
1	A	44	GLY	C-N	5.46	1.40	1.33	4	2
1	A	144	ARG	C-N	5.45	1.40	1.33	12	1
1	A	48	GLU	N-CA	5.45	1.52	1.45	7	1
1	A	109	VAL	CA-CB	5.45	1.60	1.53	7	1
1	A	89	VAL	N-CA	5.45	1.52	1.46	7	1
1	A	128	MET	CA-C	5.43	1.59	1.52	13	1
1	A	147	LEU	N-CA	5.41	1.52	1.45	9	1
1	A	20	ILE	N-CA	5.40	1.52	1.46	11	1
1	A	39	LEU	CA-CB	5.40	1.62	1.53	5	1
1	A	20	ILE	CA-C	5.38	1.59	1.52	10	1
1	A	84	VAL	C-N	5.35	1.40	1.33	19	1
1	A	92	ILE	C-N	5.34	1.40	1.33	20	1
1	A	16	HIS	CG-ND1	5.33	1.44	1.38	8	1
1	A	37	ARG	NE-CZ	5.33	1.39	1.33	19	1
1	A	91	ARG	CZ-NH2	-5.30	1.26	1.33	7	1
1	A	42	GLU	CA-C	-5.29	1.46	1.52	9	1
1	A	22	PRO	N-CA	5.29	1.54	1.47	5	2
1	A	69	ILE	CA-CB	5.27	1.60	1.54	10	1
1	A	45	THR	C-N	5.27	1.40	1.33	8	1
1	A	109	VAL	CA-C	5.26	1.58	1.52	12	2
1	A	97	ALA	CA-C	5.25	1.59	1.52	18	1
1	A	58	ALA	CA-C	5.25	1.59	1.52	20	1
1	A	113	GLN	CA-CB	5.21	1.60	1.53	4	1
1	A	101	ILE	CB-CG1	5.18	1.63	1.53	16	1
1	A	40	THR	N-CA	5.17	1.52	1.46	6	1
1	A	108	LEU	C-N	5.17	1.40	1.33	7	1
1	A	90	THR	N-CA	5.15	1.52	1.45	9	1
1	A	15	ILE	CA-CB	5.13	1.59	1.54	13	1
1	A	80	GLU	CA-CB	5.12	1.61	1.53	2	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	59	ALA	CA-C	5.11	1.58	1.52	2	1
1	A	105	LYS	N-CA	5.09	1.51	1.45	6	1
1	A	148	SER	CA-C	5.08	1.58	1.52	16	1
1	A	37	ARG	CZ-NH2	-5.08	1.26	1.33	5	1
1	A	113	GLN	C-N	5.08	1.38	1.33	17	1
1	A	110	HIS	C-O	-5.08	1.17	1.23	19	1
1	A	70	ARG	NE-CZ	5.07	1.38	1.33	6	1
1	A	135	LYS	N-CA	5.05	1.52	1.46	8	1
1	A	116	ASP	N-CA	5.05	1.52	1.46	8	1
1	A	114	ILE	CA-C	5.04	1.59	1.52	18	1
1	A	126	LEU	N-CA	5.03	1.52	1.46	19	1
1	A	63	GLU	CA-C	5.02	1.59	1.52	20	1
1	A	140	ASP	C-N	5.01	1.40	1.34	9	1

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	37	ARG	NE-CZ-NH1	10.52	132.02	121.50	12	5
1	A	91	ARG	NH1-CZ-NH2	-10.21	106.02	119.30	11	3
1	A	37	ARG	NE-CZ-NH2	-10.16	110.06	119.20	9	2
1	A	140	ASP	CA-CB-CG	9.97	122.57	112.60	4	3
1	A	149	ILE	N-CA-C	-9.93	103.02	111.56	12	4
1	A	144	ARG	NE-CZ-NH1	9.59	131.09	121.50	9	2
1	A	130	GLN	OE1-CD-NE2	-9.56	113.04	122.60	18	2
1	A	16	HIS	CA-CB-CG	-9.21	104.59	113.80	18	4
1	A	71	ARG	NE-CZ-NH1	9.15	130.65	121.50	10	6
1	A	98	PHE	CA-CB-CG	-9.12	104.68	113.80	20	4
1	A	146	ARG	NE-CZ-NH2	-8.91	111.18	119.20	12	2
1	A	67	HIS	CA-CB-CG	8.72	122.52	113.80	1	4
1	A	71	ARG	NE-CZ-NH2	-8.71	111.36	119.20	3	9
1	A	144	ARG	NE-CZ-NH2	-8.52	111.53	119.20	9	2
1	A	79	ILE	CB-CA-C	-8.48	100.70	110.96	9	1
1	A	113	GLN	OE1-CD-NE2	-8.33	114.27	122.60	7	5
1	A	144	ARG	NH1-CZ-NH2	-8.22	108.61	119.30	9	1
1	A	139	VAL	CB-CA-C	8.15	120.14	111.09	16	1
1	A	140	ASP	CB-CA-C	8.14	123.23	109.72	2	2
1	A	111	ILE	N-CA-C	8.04	118.82	110.62	7	5
1	A	21	ASN	OD1-CG-ND2	-7.91	114.69	122.60	8	1
1	A	34	SER	N-CA-C	7.90	119.97	111.36	11	5
1	A	135	LYS	O-C-N	-7.87	114.01	123.29	12	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	110	HIS	CA-CB-CG	7.72	121.53	113.80	8	4
1	A	67	HIS	CE1-NE2-CD2	-7.69	101.31	109.00	18	4
1	A	118	ARG	NE-CZ-NH1	7.66	129.16	121.50	7	3
1	A	83	ARG	NH1-CZ-NH2	-7.65	109.36	119.30	2	3
1	A	70	ARG	NH1-CZ-NH2	-7.63	109.38	119.30	9	3
1	A	41	GLU	N-CA-C	7.60	119.57	111.28	15	1
1	A	114	ILE	CB-CA-C	-7.50	102.10	111.92	19	4
1	A	114	ILE	O-C-N	-7.37	114.24	121.83	18	1
1	A	61	ASP	CA-C-N	7.36	128.28	120.03	1	2
1	A	61	ASP	C-N-CA	7.36	128.28	120.03	1	2
1	A	81	VAL	CA-C-O	7.35	129.01	120.71	2	1
1	A	21	ASN	CA-CB-CG	7.28	119.88	112.60	13	3
1	A	67	HIS	CB-CG-CD2	7.12	140.46	131.20	10	2
1	A	84	VAL	N-CA-C	7.11	118.18	109.30	14	1
1	A	22	PRO	CA-C-N	7.04	129.71	120.28	3	1
1	A	22	PRO	C-N-CA	7.04	129.71	120.28	3	1
1	A	95	PHE	CA-CB-CG	7.02	120.82	113.80	5	4
1	A	36	ILE	CA-C-O	-7.01	113.66	120.95	14	1
1	A	105	LYS	N-CA-C	6.93	120.43	110.24	15	4
1	A	116	ASP	CA-CB-CG	6.88	119.48	112.60	2	2
1	A	132	VAL	N-CA-CB	-6.86	104.27	111.61	17	2
1	A	149	ILE	CA-C-N	6.86	129.36	120.44	17	1
1	A	149	ILE	C-N-CA	6.86	129.36	120.44	17	1
1	A	71	ARG	NH1-CZ-NH2	-6.85	110.39	119.30	17	4
1	A	70	ARG	NE-CZ-NH2	6.83	125.35	119.20	9	4
1	A	60	THR	O-C-N	6.82	129.92	122.15	19	1
1	A	141	ARG	NH1-CZ-NH2	-6.73	110.55	119.30	16	2
1	A	70	ARG	NE-CZ-NH1	6.73	128.23	121.50	13	2
1	A	37	ARG	NH1-CZ-NH2	-6.69	110.61	119.30	12	1
1	A	146	ARG	NH1-CZ-NH2	-6.67	110.63	119.30	6	2
1	A	110	HIS	CE1-NE2-CD2	-6.66	102.34	109.00	9	2
1	A	79	ILE	CA-C-O	6.66	128.36	121.23	13	2
1	A	94	ASP	N-CA-C	6.63	119.35	111.33	8	1
1	A	83	ARG	NE-CZ-NH2	-6.57	113.28	119.20	12	3
1	A	17	THR	CA-C-N	6.57	129.47	122.11	3	1
1	A	17	THR	C-N-CA	6.57	129.47	122.11	3	1
1	A	139	VAL	N-CA-C	-6.55	98.94	108.11	4	1
1	A	146	ARG	CG-CD-NE	-6.51	97.69	112.00	6	1
1	A	116	ASP	N-CA-C	-6.46	105.70	113.97	11	1
1	A	142	GLN	CA-C-O	6.46	127.09	119.28	14	1
1	A	52	ASP	CA-CB-CG	6.46	119.06	112.60	6	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	139	VAL	N-CA-CB	-6.45	104.67	112.35	16	1
1	A	123	THR	CA-C-O	-6.43	111.47	119.38	5	2
1	A	17	THR	CA-C-O	6.41	128.50	121.06	15	1
1	A	27	ASP	O-C-N	6.40	128.66	122.07	15	1
1	A	40	THR	N-CA-C	6.38	118.24	111.28	9	1
1	A	23	ASP	CA-CB-CG	-6.38	106.22	112.60	11	2
1	A	83	ARG	NE-CZ-NH1	6.36	127.86	121.50	8	3
1	A	37	ARG	CG-CD-NE	-6.36	98.02	112.00	17	2
1	A	65	ALA	N-CA-C	6.34	118.20	111.28	10	1
1	A	67	HIS	CG-CD2-NE2	6.33	113.53	107.20	18	2
1	A	91	ARG	NE-CZ-NH2	6.32	124.89	119.20	2	5
1	A	26	LYS	O-C-N	6.31	128.81	122.12	19	1
1	A	81	VAL	O-C-N	-6.29	115.75	122.61	20	1
1	A	29	ILE	CA-C-O	-6.29	112.92	120.78	2	1
1	A	23	ASP	N-CA-CB	-6.29	100.88	110.12	3	1
1	A	152	ALA	N-CA-CB	-6.24	101.40	110.70	15	3
1	A	38	ALA	N-CA-C	6.22	118.06	111.28	6	5
1	A	73	GLU	N-CA-CB	6.20	119.23	110.12	13	1
1	A	151	GLU	N-CA-CB	6.19	119.31	110.16	20	1
1	A	120	GLU	O-C-N	6.17	128.75	122.09	2	1
1	A	124	ASP	CA-CB-CG	6.15	118.75	112.60	8	2
1	A	114	ILE	CA-C-O	6.14	127.14	120.69	4	1
1	A	109	VAL	O-C-N	-6.14	115.88	122.45	14	1
1	A	142	GLN	OE1-CD-NE2	-6.13	116.47	122.60	2	2
1	A	120	GLU	N-CA-C	-6.12	106.36	113.88	12	2
1	A	72	ILE	N-CA-C	6.09	116.83	110.62	1	1
1	A	146	ARG	N-CA-CB	6.07	120.32	110.43	20	1
1	A	31	LYS	N-CA-CB	6.06	121.11	111.91	9	1
1	A	30	GLY	N-CA-C	6.03	127.47	113.18	19	1
1	A	150	LYS	N-CA-C	6.03	117.52	111.07	17	2
1	A	153	THR	CA-C-N	6.02	130.68	122.19	12	2
1	A	153	THR	C-N-CA	6.02	130.68	122.19	12	2
1	A	79	ILE	N-CA-CB	-6.00	102.09	110.13	8	3
1	A	118	ARG	NH1-CZ-NH2	-5.99	111.51	119.30	5	4
1	A	58	ALA	N-CA-CB	-5.96	101.65	110.53	12	1
1	A	134	VAL	N-CA-CB	5.96	119.63	111.41	12	1
1	A	141	ARG	NE-CZ-NH1	5.96	127.46	121.50	18	4
1	A	115	ALA	CA-C-N	5.95	128.74	120.29	5	2
1	A	115	ALA	C-N-CA	5.95	128.74	120.29	5	2
1	A	93	VAL	CA-C-N	5.94	128.72	120.29	13	1
1	A	93	VAL	C-N-CA	5.94	128.72	120.29	13	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	37	ARG	CA-C-N	5.93	128.15	120.44	15	2
1	A	37	ARG	C-N-CA	5.93	128.15	120.44	15	2
1	A	40	THR	CA-C-O	-5.91	114.28	120.55	7	2
1	A	35	VAL	N-CA-C	5.91	116.69	110.72	2	2
1	A	21	ASN	O-C-N	-5.90	116.87	121.47	16	1
1	A	20	ILE	CA-C-O	-5.89	115.48	121.67	11	1
1	A	89	VAL	CA-C-O	-5.89	114.93	121.23	19	1
1	A	35	VAL	O-C-N	5.88	127.68	121.91	5	2
1	A	67	HIS	ND1-CE1-NE2	5.88	114.28	108.40	18	2
1	A	99	VAL	O-C-N	5.88	129.43	123.20	15	1
1	A	70	ARG	CD-NE-CZ	5.88	132.63	124.40	19	1
1	A	42	GLU	CA-C-O	-5.87	114.66	120.70	17	1
1	A	125	TYR	CA-CB-CG	-5.86	103.34	113.90	11	2
1	A	69	ILE	N-CA-C	5.86	117.30	110.62	19	1
1	A	142	GLN	N-CA-C	-5.85	104.28	112.12	5	1
1	A	21	ASN	CA-C-O	-5.85	114.25	119.75	8	2
1	A	69	ILE	O-C-N	-5.85	116.20	121.87	1	1
1	A	146	ARG	NE-CZ-NH1	5.84	127.34	121.50	12	1
1	A	28	VAL	N-CA-C	5.83	116.02	110.42	15	2
1	A	120	GLU	CB-CG-CD	-5.83	102.69	112.60	11	1
1	A	42	GLU	N-CA-C	5.83	117.63	111.28	8	2
1	A	20	ILE	CA-C-N	5.81	128.47	120.39	12	1
1	A	20	ILE	C-N-CA	5.81	128.47	120.39	12	1
1	A	41	GLU	N-CA-CB	5.81	118.76	110.16	11	1
1	A	18	ILE	O-C-N	-5.81	116.61	123.00	13	1
1	A	90	THR	N-CA-C	-5.80	106.84	114.04	20	1
1	A	98	PHE	N-CA-CB	5.77	118.90	109.95	20	2
1	A	129	GLY	CA-C-O	5.77	125.39	119.10	11	1
1	A	112	SER	N-CA-C	5.77	118.34	111.71	8	1
1	A	33	GLY	N-CA-C	-5.77	107.30	115.43	10	1
1	A	75	ILE	N-CA-C	5.76	117.19	110.62	17	3
1	A	18	ILE	CB-CA-C	5.76	118.74	110.33	18	1
1	A	18	ILE	N-CA-C	-5.75	99.48	108.86	1	1
1	A	125	TYR	N-CA-CB	-5.74	102.69	110.67	19	2
1	A	79	ILE	N-CA-C	5.73	116.46	109.30	2	2
1	A	131	GLU	N-CA-C	5.71	118.62	110.10	8	1
1	A	15	ILE	N-CA-C	5.71	116.44	109.30	15	1
1	A	128	MET	CG-SD-CE	-5.71	88.35	100.90	5	2
1	A	29	ILE	O-C-N	5.70	129.52	122.05	4	1
1	A	109	VAL	CB-CA-C	-5.70	103.33	111.31	7	1
1	A	52	ASP	CA-C-O	5.69	126.32	119.43	2	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	45	THR	CA-CB-OG1	5.69	118.14	109.60	18	1
1	A	27	ASP	CA-CB-CG	-5.68	106.92	112.60	7	2
1	A	118	ARG	N-CA-C	5.68	118.07	110.35	15	1
1	A	21	ASN	CB-CG-ND2	5.67	124.91	116.40	7	1
1	A	28	VAL	CA-CB-CG2	-5.67	100.76	110.40	9	1
1	A	67	HIS	N-CA-C	5.67	117.46	111.28	2	1
1	A	110	HIS	CG-CD2-NE2	5.66	112.86	107.20	9	1
1	A	15	ILE	CA-CB-CG1	-5.65	100.80	110.40	20	1
1	A	138	GLU	CB-CG-CD	-5.64	103.01	112.60	6	1
1	A	21	ASN	N-CA-CB	-5.64	101.12	109.98	12	1
1	A	70	ARG	CA-C-N	5.64	127.84	120.28	16	1
1	A	70	ARG	C-N-CA	5.64	127.84	120.28	16	1
1	A	80	GLU	N-CA-C	5.63	117.87	109.25	6	1
1	A	55	VAL	N-CA-C	5.63	116.33	108.89	12	1
1	A	63	GLU	N-CA-C	5.62	117.49	111.36	13	1
1	A	73	GLU	CA-C-N	5.62	127.75	120.44	15	2
1	A	73	GLU	C-N-CA	5.62	127.75	120.44	15	2
1	A	16	HIS	CE1-NE2-CD2	-5.61	103.39	109.00	11	5
1	A	67	HIS	CB-CA-C	-5.61	102.07	110.88	20	1
1	A	122	VAL	CA-C-N	5.60	128.06	120.38	8	2
1	A	122	VAL	C-N-CA	5.60	128.06	120.38	8	2
1	A	36	ILE	N-CA-CB	5.59	118.15	110.54	10	1
1	A	96	GLY	N-CA-C	5.59	117.71	110.45	16	1
1	A	32	GLY	O-C-N	5.58	127.65	122.57	1	1
1	A	110	HIS	ND1-CE1-NE2	5.58	113.98	108.40	2	1
1	A	52	ASP	N-CA-C	-5.53	105.15	112.94	16	1
1	A	66	LYS	CB-CA-C	-5.53	101.29	110.68	8	1
1	A	25	ILE	CA-C-N	5.52	127.67	120.28	6	1
1	A	25	ILE	C-N-CA	5.52	127.67	120.28	6	1
1	A	147	LEU	CA-C-O	5.51	127.98	121.36	16	1
1	A	127	GLN	OE1-CD-NE2	-5.51	117.09	122.60	9	3
1	A	130	GLN	CA-C-O	5.51	127.15	120.81	3	1
1	A	29	ILE	CA-CB-CG2	5.51	119.86	110.50	1	1
1	A	52	ASP	CB-CA-C	5.50	120.20	111.51	1	1
1	A	21	ASN	CB-CA-C	5.50	118.21	109.52	12	1
1	A	129	GLY	N-CA-C	-5.50	108.06	115.21	13	1
1	A	16	HIS	CG-CD2-NE2	5.50	112.70	107.20	10	1
1	A	18	ILE	N-CA-CB	5.48	120.00	110.96	3	1
1	A	114	ILE	N-CA-C	-5.48	106.46	111.67	4	2
1	A	99	VAL	CA-CB-CG2	-5.47	101.10	110.40	19	1
1	A	130	GLN	N-CA-C	5.47	117.62	109.25	16	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	15	ILE	CB-CA-C	-5.46	103.73	111.21	2	1
1	A	59	ALA	N-CA-C	5.46	117.38	108.76	16	2
1	A	142	GLN	N-CA-CB	-5.45	102.38	110.61	4	1
1	A	50	GLU	CA-C-N	5.43	131.92	121.54	9	1
1	A	50	GLU	C-N-CA	5.43	131.92	121.54	9	1
1	A	138	GLU	N-CA-CB	-5.43	103.31	111.56	2	1
1	A	133	PRO	N-CA-C	5.43	119.03	110.50	14	1
1	A	21	ASN	N-CA-C	5.43	117.42	109.71	6	1
1	A	123	THR	CA-CB-OG1	5.42	117.73	109.60	1	1
1	A	21	ASN	CA-C-N	5.41	125.89	120.04	2	1
1	A	21	ASN	C-N-CA	5.41	125.89	120.04	2	1
1	A	141	ARG	N-CA-C	5.40	118.66	111.75	7	1
1	A	40	THR	N-CA-CB	5.40	118.06	110.12	5	1
1	A	80	GLU	CB-CA-C	-5.39	101.45	110.29	6	1
1	A	70	ARG	N-CA-C	5.38	117.22	111.36	12	2
1	A	106	GLU	CA-C-N	5.37	127.25	122.47	6	1
1	A	106	GLU	C-N-CA	5.37	127.25	122.47	6	1
1	A	144	ARG	CB-CA-C	5.36	118.58	109.84	3	1
1	A	26	LYS	N-CA-C	5.36	117.81	111.33	11	1
1	A	72	ILE	CA-C-O	-5.36	115.49	121.17	11	1
1	A	85	TYR	O-C-N	-5.35	116.94	122.94	17	1
1	A	25	ILE	N-CA-C	-5.35	105.06	112.50	20	1
1	A	123	THR	CA-C-N	5.34	128.43	120.31	2	1
1	A	123	THR	C-N-CA	5.34	128.43	120.31	2	1
1	A	143	GLY	N-CA-C	5.34	122.72	115.30	17	1
1	A	49	ILE	CB-CA-C	5.34	117.38	110.12	13	1
1	A	57	ILE	N-CA-CB	-5.34	104.56	111.82	20	1
1	A	50	GLU	CA-C-O	-5.33	115.34	121.47	3	1
1	A	145	ILE	N-CA-CB	5.32	116.33	110.53	14	1
1	A	127	GLN	CG-CD-NE2	5.30	124.35	116.40	15	2
1	A	140	ASP	N-CA-C	5.29	116.91	110.41	16	1
1	A	133	PRO	CB-CA-C	-5.29	105.80	111.56	14	1
1	A	141	ARG	NE-CZ-NH2	-5.28	114.44	119.20	10	1
1	A	128	MET	CA-C-N	5.28	129.96	120.77	12	1
1	A	128	MET	C-N-CA	5.28	129.96	120.77	12	1
1	A	116	ASP	O-C-N	5.28	128.16	122.15	12	1
1	A	124	ASP	O-C-N	5.27	128.16	122.15	9	1
1	A	19	LYS	CA-C-N	5.25	128.41	122.48	13	1
1	A	19	LYS	C-N-CA	5.25	128.41	122.48	13	1
1	A	73	GLU	N-CA-C	5.25	116.68	111.07	12	1
1	A	69	ILE	N-CA-CB	-5.25	103.41	110.54	2	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	110	HIS	N-CA-C	5.24	117.48	110.35	19	1
1	A	61	ASP	CB-CA-C	5.24	118.35	109.50	19	1
1	A	16	HIS	CB-CG-CD2	5.22	137.99	131.20	4	1
1	A	70	ARG	O-C-N	-5.22	116.20	122.15	6	1
1	A	66	LYS	N-CA-C	5.22	116.66	111.07	15	1
1	A	83	ARG	CA-C-O	-5.21	115.13	121.28	13	1
1	A	82	GLY	CA-C-O	-5.20	113.86	119.27	15	1
1	A	65	ALA	CA-C-N	5.19	127.24	120.28	3	1
1	A	65	ALA	C-N-CA	5.19	127.24	120.28	3	1
1	A	38	ALA	CA-C-N	5.19	129.38	120.71	5	1
1	A	38	ALA	C-N-CA	5.19	129.38	120.71	5	1
1	A	144	ARG	CD-NE-CZ	-5.19	117.14	124.40	10	1
1	A	40	THR	O-C-N	-5.17	116.50	122.09	8	1
1	A	147	LEU	N-CA-C	5.17	117.25	109.23	18	1
1	A	71	ARG	CA-C-N	5.16	127.07	120.56	19	1
1	A	71	ARG	C-N-CA	5.16	127.07	120.56	19	1
1	A	66	LYS	CA-C-O	-5.16	115.08	120.55	11	2
1	A	54	THR	OG1-CB-CG2	-5.15	98.99	109.30	3	1
1	A	27	ASP	CA-C-O	-5.15	114.05	119.97	17	2
1	A	94	ASP	CA-CB-CG	-5.15	107.45	112.60	14	1
1	A	38	ALA	O-C-N	5.15	128.24	122.22	5	1
1	A	119	VAL	N-CA-C	5.14	114.67	107.37	4	1
1	A	113	GLN	CG-CD-NE2	5.14	124.11	116.40	7	1
1	A	16	HIS	ND1-CE1-NE2	5.13	113.53	108.40	8	1
1	A	117	LYS	N-CA-CB	5.13	117.51	109.97	8	1
1	A	88	LYS	N-CA-CB	-5.12	101.93	110.83	7	1
1	A	93	VAL	O-C-N	-5.11	117.27	122.95	4	1
1	A	127	GLN	CB-CG-CD	5.11	121.28	112.60	3	1
1	A	33	GLY	CA-C-N	5.10	127.11	120.28	15	1
1	A	33	GLY	C-N-CA	5.10	127.11	120.28	15	1
1	A	52	ASP	N-CA-CB	-5.09	102.95	110.53	4	1
1	A	111	ILE	O-C-N	5.09	126.80	121.87	7	1
1	A	42	GLU	O-C-N	5.09	127.58	122.09	9	1
1	A	83	ARG	N-CA-CB	5.08	118.17	110.45	10	1
1	A	60	THR	N-CA-C	-5.08	107.03	113.43	13	1
1	A	133	PRO	N-CA-CB	-5.08	99.24	103.30	14	1
1	A	49	ILE	O-C-N	-5.08	117.40	123.04	6	1
1	A	140	ASP	N-CA-CB	-5.06	102.07	111.13	5	1
1	A	67	HIS	CB-CG-ND1	-5.06	115.12	122.70	10	1
1	A	25	ILE	CB-CA-C	-5.05	105.50	111.97	2	1
1	A	132	VAL	CB-CA-C	5.05	115.78	110.37	17	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	136	VAL	CA-C-N	5.05	127.05	120.28	6	1
1	A	136	VAL	C-N-CA	5.05	127.05	120.28	6	1
1	A	116	ASP	N-CA-CB	-5.05	102.45	110.28	17	1
1	A	50	GLU	N-CA-C	5.05	117.05	110.53	18	1
1	A	88	LYS	CB-CA-C	5.04	118.82	109.70	6	1
1	A	149	ILE	O-C-N	5.03	127.02	121.83	11	1
1	A	112	SER	CB-CA-C	-5.02	99.94	110.17	16	1
1	A	41	GLU	CA-C-N	5.01	126.99	120.28	8	1
1	A	41	GLU	C-N-CA	5.01	126.99	120.28	8	1
1	A	45	THR	N-CA-CB	5.01	120.03	111.66	10	1
1	A	108	LEU	CA-C-O	-5.01	115.29	120.70	16	1
1	A	41	GLU	CA-CB-CG	-5.01	104.08	114.10	19	1
1	A	47	ILE	O-C-N	-5.01	117.66	123.07	15	1
1	A	145	ILE	O-C-N	5.00	128.58	123.03	2	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	83	ARG	Sidechain	10
1	A	125	TYR	Sidechain	8
1	A	144	ARG	Sidechain	8
1	A	146	ARG	Sidechain	8
1	A	71	ARG	Sidechain	7
1	A	85	TYR	Sidechain	6
1	A	70	ARG	Sidechain	6
1	A	118	ARG	Sidechain	5
1	A	141	ARG	Sidechain	5
1	A	37	ARG	Sidechain	4
1	A	91	ARG	Sidechain	4
1	A	98	PHE	Sidechain	2
1	A	110	HIS	Sidechain	2
1	A	16	HIS	Sidechain	1

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1051	1106	1106	1±1
All	All	21020	22120	22120	11

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:ILE:HD11	1:A:49:ILE:HG22	0.58	1.75	13	1
1:A:43:THR:HG21	1:A:68:ALA:HA	0.47	1.85	16	1
1:A:47:ILE:HG23	1:A:57:ILE:HD13	0.46	1.88	10	1
1:A:30:GLY:HA3	1:A:35:VAL:H	0.46	1.69	16	1
1:A:122:VAL:HG12	1:A:126:LEU:HD12	0.45	1.89	18	1
1:A:136:VAL:HG22	1:A:147:LEU:HD23	0.45	1.89	16	1
1:A:59:ALA:CB	1:A:65:ALA:HB2	0.43	2.43	4	1
1:A:29:ILE:O	1:A:29:ILE:HG22	0.43	2.13	10	2
1:A:97:ALA:O	1:A:109:VAL:N	0.41	2.53	14	1
1:A:42:GLU:CD	1:A:71:ARG:HE	0.40	2.24	18	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	137/171 (80%)	133±1 (97±1%)	3±1 (2±1%)	1±1 (1±1%)	20	70
All	All	2740/3420 (80%)	2658 (97%)	63 (2%)	19 (1%)	20	70

All 10 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	51	ASP	5
1	A	102	GLY	3
1	A	91	ARG	3
1	A	59	ALA	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	105	LYS	1
1	A	111	ILE	1
1	A	145	ILE	1
1	A	30	GLY	1
1	A	139	VAL	1
1	A	52	ASP	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	113/134 (84%)	110±1 (97±1%)	3±1 (3±1%)	38	86
All	All	2260/2680 (84%)	2195 (97%)	65 (3%)	38	86

All 33 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	134	VAL	7
1	A	140	ASP	6
1	A	123	THR	5
1	A	132	VAL	4
1	A	90	THR	4
1	A	56	LYS	3
1	A	45	THR	3
1	A	18	ILE	3
1	A	151	GLU	2
1	A	133	PRO	2
1	A	142	GLN	2
1	A	101	ILE	2
1	A	86	THR	2
1	A	72	ILE	1
1	A	54	THR	1
1	A	121	LYS	1
1	A	17	THR	1
1	A	99	VAL	1
1	A	153	THR	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	118	ARG	1
1	A	108	LEU	1
1	A	141	ARG	1
1	A	15	ILE	1
1	A	21	ASN	1
1	A	25	ILE	1
1	A	26	LYS	1
1	A	75	ILE	1
1	A	91	ARG	1
1	A	36	ILE	1
1	A	109	VAL	1
1	A	113	GLN	1
1	A	149	ILE	1
1	A	127	GLN	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

The completeness of assignment taking into account all chemical shift lists is 74% for the well-defined parts and 73% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *kh-s1_bmr_bBA780W.str*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1440
Number of shifts mapped to atoms	1423
Number of unparsed shifts	0
Number of shifts with mapping errors	17
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 17 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	162	PRO	CA	63.02	0.05	1
1	A	162	PRO	CB	31.95	0.05	1
1	A	162	PRO	CD	50.39	0.05	1
1	A	162	PRO	CG	27.36	0.05	1
1	A	163	GLU	H	8.4	0.02	1
1	A	163	GLU	C	175.84	0.05	1
1	A	163	GLU	CA	56.32	0.05	1
1	A	163	GLU	CB	30.55	0.05	1
1	A	163	GLU	CG	36.33	0.05	1
1	A	163	GLU	N	120.93	0.05	1
1	A	164	ALA	H	8.27	0.02	1
1	A	164	ALA	HB1	1.4	0.02	1
1	A	164	ALA	HB2	1.4	0.02	1
1	A	164	ALA	HB3	1.4	0.02	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	164	ALA	CA	50.39	0.05	1
1	A	164	ALA	CB	18.28	0.05	1
1	A	164	ALA	N	126.39	0.05	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	143	-0.39 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	128	0.07 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	126	-0.28 ± 0.15	None needed (< 0.5 ppm)
^{15}N	131	0.33 ± 0.39	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 74%, i.e. 1396 atoms were assigned a chemical shift out of a possible 1888. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	658/696 (95%)	274/287 (95%)	258/274 (94%)	126/135 (93%)
Sidechain	730/1133 (64%)	416/736 (57%)	312/352 (89%)	2/45 (4%)
Aromatic	8/59 (14%)	4/30 (13%)	4/26 (15%)	0/3 (0%)
Overall	1396/1888 (74%)	694/1053 (66%)	574/652 (88%)	128/183 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 1423 atoms were assigned a chemical shift out of a possible 1959. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	674/721 (93%)	280/297 (94%)	265/284 (93%)	129/140 (92%)
Sidechain	741/1179 (63%)	419/764 (55%)	320/366 (87%)	2/49 (4%)
Aromatic	8/59 (14%)	4/30 (13%)	4/26 (15%)	0/3 (0%)
Overall	1423/1959 (73%)	703/1091 (64%)	589/676 (87%)	131/192 (68%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

