



Full wwPDB NMR Structure Validation Report ⓘ

Jun 24, 2024 – 03:38 AM EDT

PDB ID : 6QH2
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 : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
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) : 2.37.1

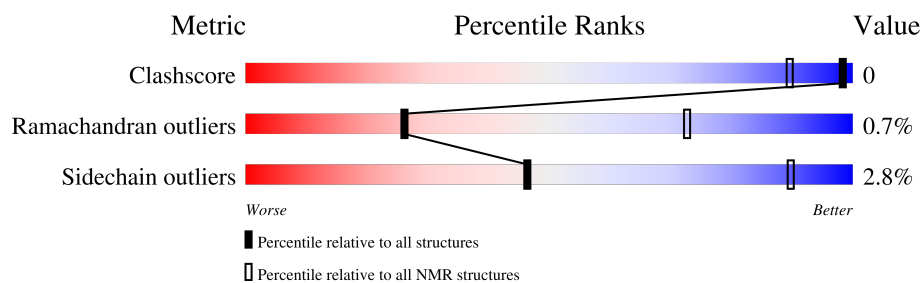
1 Overall quality at a glance

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 [i](#)

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:

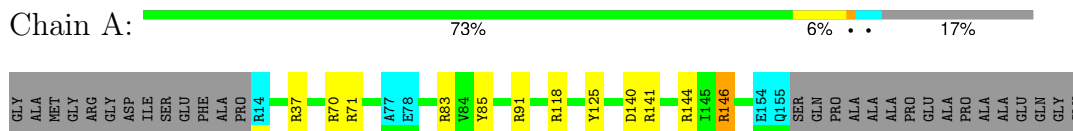
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP B6I1N9
A	2	ALA	-	expression tag	UNP B6I1N9
A	3	MET	-	expression tag	UNP B6I1N9
A	4	GLY	-	expression tag	UNP B6I1N9

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

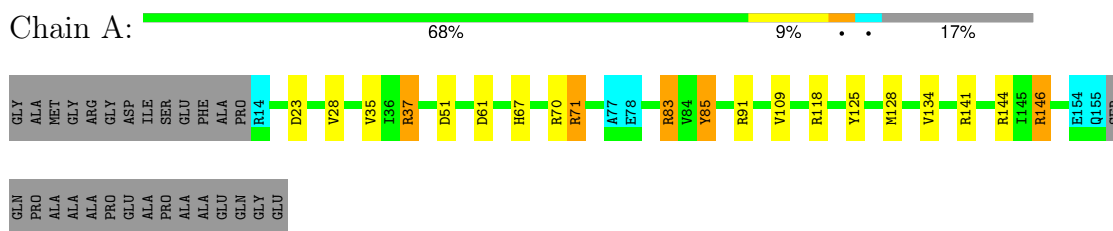


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

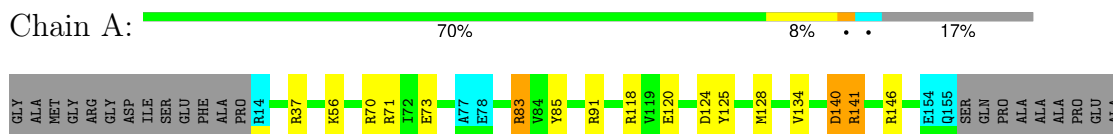
4.2.1 Score per residue for model 1

- Molecule 1: Polyribonucleotide nucleotidyltransferase



4.2.2 Score per residue for model 2

- Molecule 1: Polyribonucleotide nucleotidyltransferase



PRO
ALA
ALA
GLU
GLY
GLY
GLU

4.2.3 Score per residue for model 3

- Molecule 1: Polyribonucleotide nucleotidyltransferase

Chain A: 68% 9% 17%

GLY ALA MET GLY ARG GLY ASP ILE SER PRO PHE ALA PRO R14 D23 V35 Y36 R37 T45 R70 R71 A77 E78 R83 F95 G102 E106 R118 K121 Y125 V132 F133 V134 K135 V136 L137 D140 R141 R144 I145 R146 E154 Q155 SER

GLN PRO ALA ALA ALA PRO GLU ALA PRO GLU ALA ALA ALA GLU GLN GLY GLU

4.2.4 Score per residue for model 4

- Molecule 1: Polyribonucleotide nucleotidyltransferase

Chain A: 68% 9% 17%

GLY ALA MET GLY ARG GLY ASP ILE SER PRO PHE ALA PRO R14 T17 R37 R52 K56 A59 A65 R66 H67 R70 R71 A77 E78 R83 R91 D94 F98 K105 R118 E131 V136 D140 R144 I145 R146 E154 Q155 SER

GLN PRO ALA ALA ALA PRO GLU ALA PRO GLU ALA ALA ALA GLU GLN GLY GLU

4.2.5 Score per residue for model 5

- Molecule 1: Polyribonucleotide nucleotidyltransferase

Chain A: 70% 8% 17%

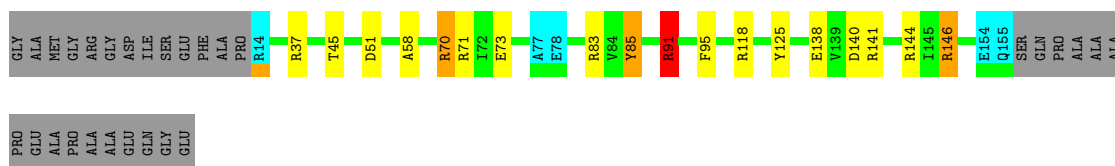
GLY ALA MET GLY ARG GLY ASP ILE SER PRO PHE ALA PRO R14 R37 R70 R71 A77 E78 I79 E80 R83 R91 F95 I111 R118 Y125 M128 R141 R144 I145 R146 E151 A152 T153 E154 Q155 SER GLN PRO ALA ALA ALA PRO GLU ALA PRO

ALA ALA GLU GLN GLY GLU

4.2.6 Score per residue for model 6

- Molecule 1: Polyribonucleotide nucleotidyltransferase

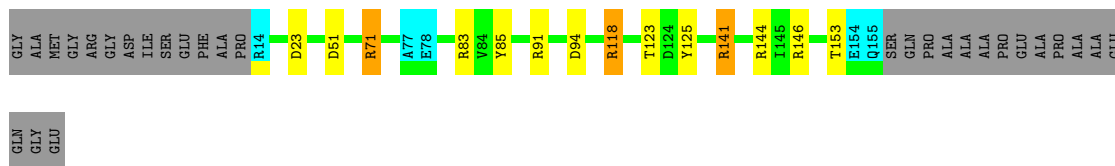
Chain A: 70% 8% 17%



4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Polyribonucleotide nucleotidyltransferase

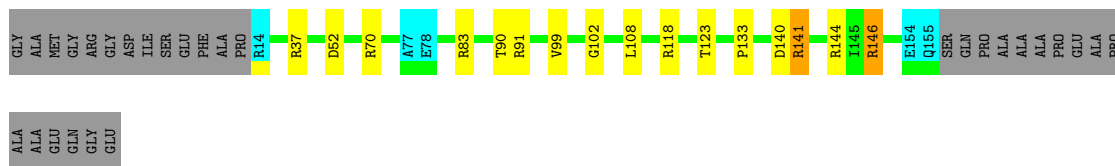
Chain A: 72% 6% 17%



4.2.8 Score per residue for model 8

- Molecule 1: Polyribonucleotide nucleotidyltransferase

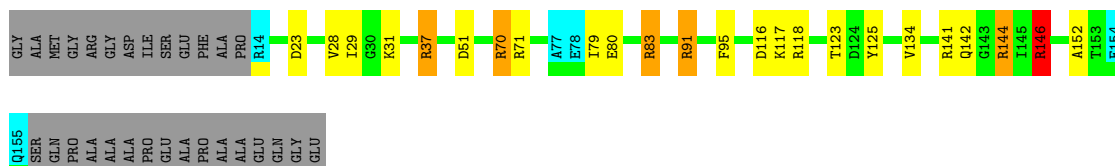
Chain A: 71% 8% 17%



4.2.9 Score per residue for model 9

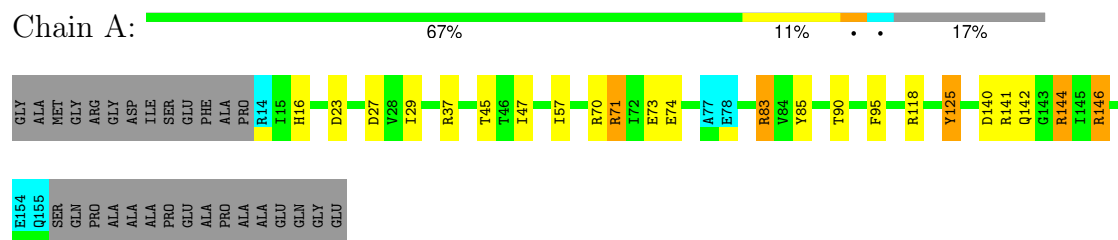
- Molecule 1: Polyribonucleotide nucleotidyltransferase

Chain A: 66% 11% 17%



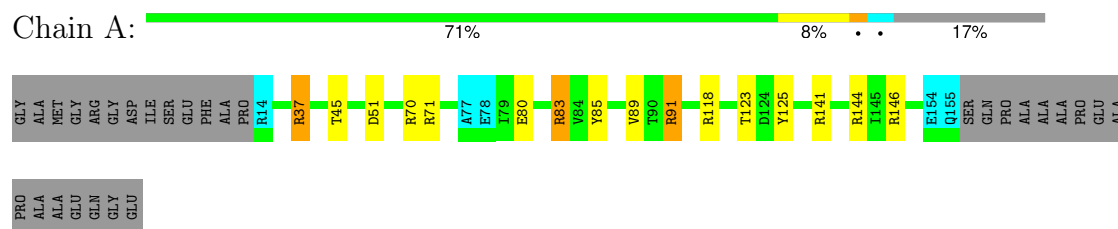
4.2.10 Score per residue for model 10

- Molecule 1: Polyribonucleotide nucleotidyltransferase



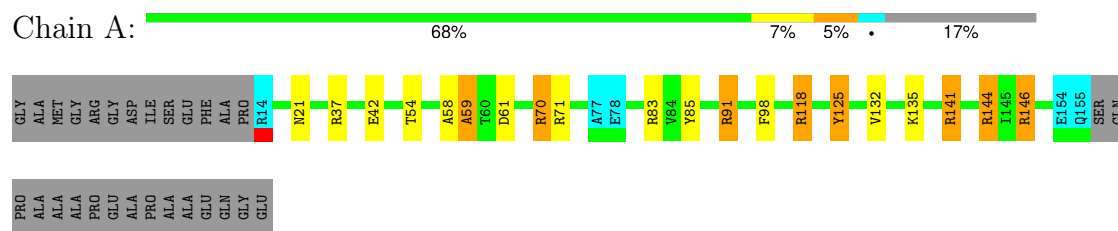
4.2.11 Score per residue for model 11

- Molecule 1: Polyribonucleotide nucleotidyltransferase



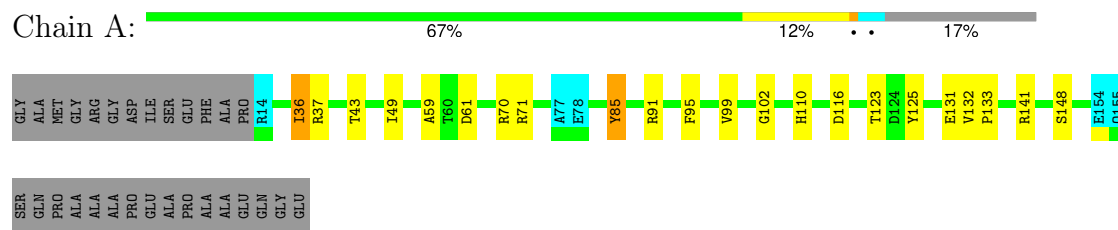
4.2.12 Score per residue for model 12

- Molecule 1: Polyribonucleotide nucleotidyltransferase



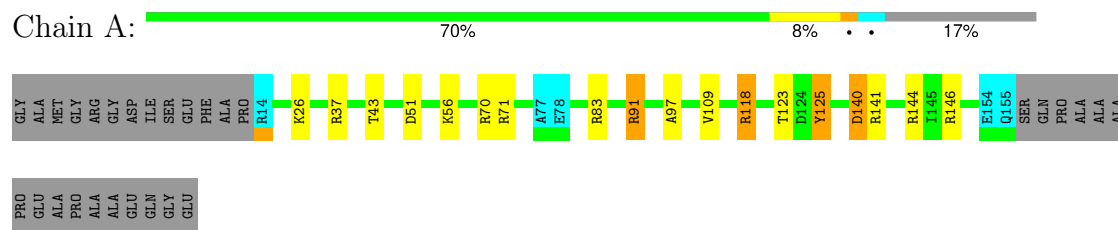
4.2.13 Score per residue for model 13

- Molecule 1: Polyribonucleotide nucleotidyltransferase



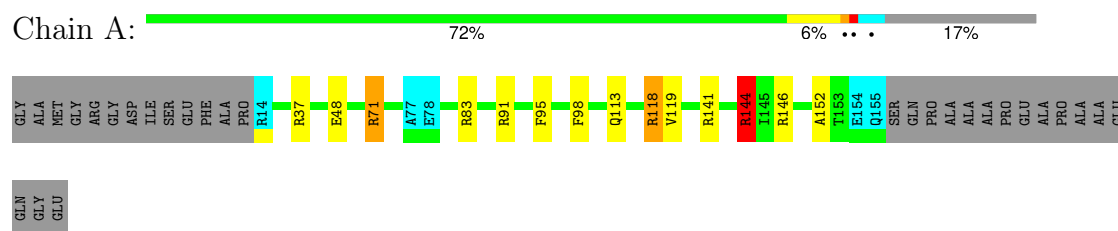
4.2.14 Score per residue for model 14

- Molecule 1: Polyribonucleotide nucleotidyltransferase



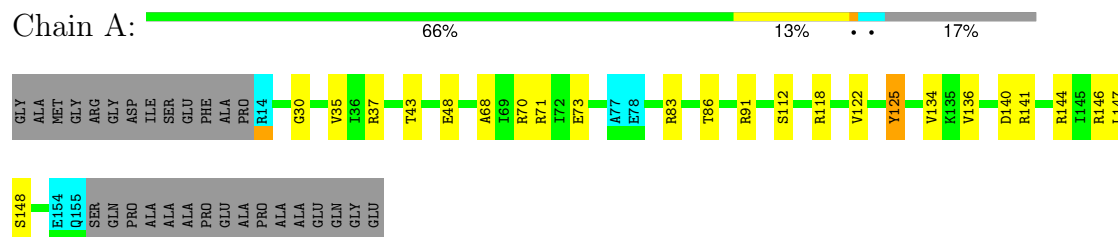
4.2.15 Score per residue for model 15

- Molecule 1: Polyribonucleotide nucleotidyltransferase



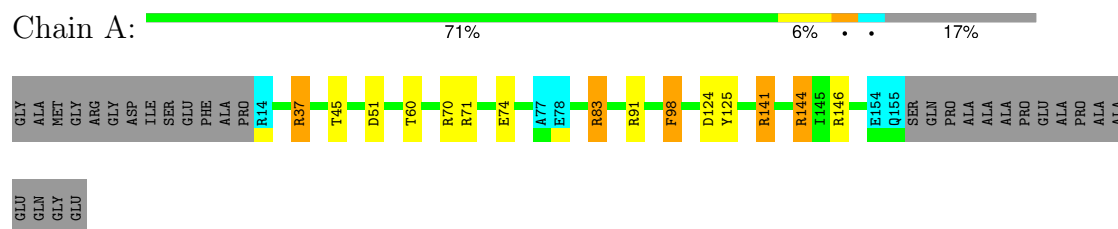
4.2.16 Score per residue for model 16

- Molecule 1: Polyribonucleotide nucleotidyltransferase



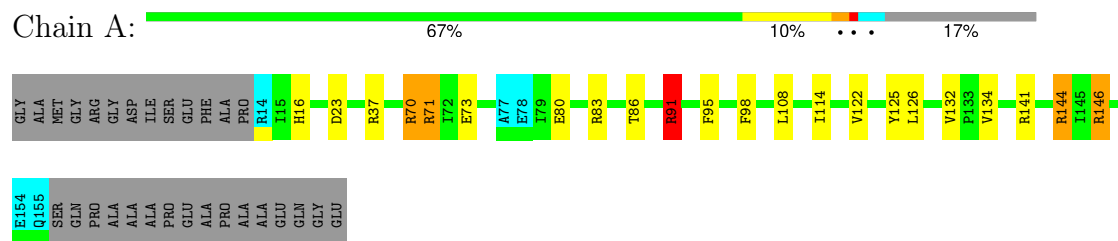
4.2.17 Score per residue for model 17

- Molecule 1: Polyribonucleotide nucleotidyltransferase



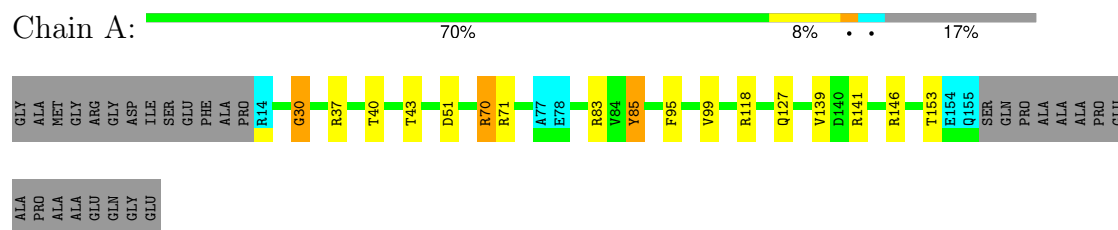
4.2.18 Score per residue for model 18

- Molecule 1: Polyribonucleotide nucleotidyltransferase



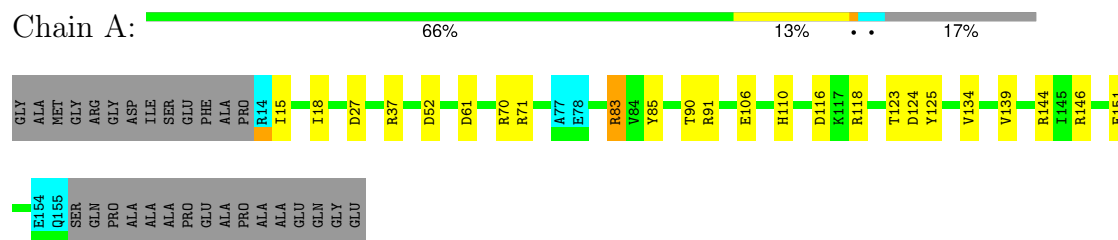
4.2.19 Score per residue for model 19

- Molecule 1: Polyribonucleotide nucleotidyltransferase



4.2.20 Score per residue for model 20

- Molecule 1: Polyribonucleotide nucleotidyltransferase



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	1.40±0.03	2±1/1060 (0.2± 0.1%)	1.74±0.09	19±3/1426 (1.3± 0.2%)
All	All	1.40	34/21200 (0.2%)	1.75	383/28520 (1.3%)

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	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	42	GLU	CG-CD	7.19	1.62	1.51	12	1
1	A	37	ARG	CZ-NH1	-6.81	1.24	1.33	2	1
1	A	131	GLU	CG-CD	6.62	1.61	1.51	4	2
1	A	144	ARG	CZ-NH2	-6.58	1.24	1.33	8	2
1	A	73	GLU	CG-CD	6.52	1.61	1.51	16	4
1	A	118	ARG	CZ-NH2	-6.31	1.24	1.33	15	2
1	A	141	ARG	CZ-NH2	-6.04	1.25	1.33	1	1
1	A	83	ARG	CD-NE	5.75	1.56	1.46	6	1
1	A	80	GLU	CB-CG	5.75	1.63	1.52	9	3
1	A	48	GLU	CB-CG	5.71	1.62	1.52	15	1
1	A	74	GLU	CD-OE2	-5.68	1.19	1.25	17	1
1	A	136	VAL	CB-CG1	5.67	1.64	1.52	4	1
1	A	83	ARG	CZ-NH2	-5.67	1.25	1.33	12	1
1	A	138	GLU	CB-CG	5.64	1.62	1.52	6	1
1	A	80	GLU	CG-CD	5.60	1.60	1.51	11	1
1	A	89	VAL	CB-CG2	5.57	1.64	1.52	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	48	GLU	CG-CD	5.46	1.60	1.51	16	1
1	A	106	GLU	CG-CD	5.43	1.60	1.51	20	1
1	A	148	SER	CA-CB	5.42	1.61	1.52	16	2
1	A	85	TYR	CE1-CZ	5.13	1.45	1.38	6	1
1	A	117	LYS	CD-CE	5.12	1.64	1.51	9	1
1	A	74	GLU	CG-CD	5.09	1.59	1.51	10	1
1	A	73	GLU	CB-CG	5.07	1.61	1.52	10	1
1	A	106	GLU	CB-CG	5.04	1.61	1.52	3	1
1	A	120	GLU	CB-CG	5.00	1.61	1.52	2	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	23.44	132.02	120.30	12	16
1	A	144	ARG	NE-CZ-NH1	21.58	131.09	120.30	9	11
1	A	71	ARG	NE-CZ-NH1	20.70	130.65	120.30	10	18
1	A	37	ARG	NE-CZ-NH2	-20.49	110.06	120.30	9	12
1	A	146	ARG	NE-CZ-NH2	-18.25	111.18	120.30	12	6
1	A	71	ARG	NE-CZ-NH2	-17.87	111.36	120.30	3	14
1	A	118	ARG	NE-CZ-NH1	17.71	129.16	120.30	7	10
1	A	144	ARG	NE-CZ-NH2	-17.53	111.53	120.30	9	14
1	A	70	ARG	NE-CZ-NH1	15.86	128.23	120.30	13	12
1	A	83	ARG	NE-CZ-NH1	15.12	127.86	120.30	8	15
1	A	141	ARG	NE-CZ-NH1	14.31	127.46	120.30	18	14
1	A	70	ARG	NE-CZ-NH2	-14.13	113.23	120.30	5	13
1	A	146	ARG	NE-CZ-NH1	14.08	127.34	120.30	12	17
1	A	83	ARG	NE-CZ-NH2	-14.03	113.28	120.30	12	10
1	A	91	ARG	NE-CZ-NH2	-12.74	113.93	120.30	15	9
1	A	91	ARG	NH1-CZ-NH2	-12.16	106.02	119.40	11	3
1	A	141	ARG	NE-CZ-NH2	-11.71	114.44	120.30	10	9
1	A	91	ARG	NE-CZ-NH1	11.44	126.02	120.30	12	12
1	A	118	ARG	NE-CZ-NH2	-10.24	115.18	120.30	19	8
1	A	144	ARG	NH1-CZ-NH2	-9.81	108.61	119.40	9	2
1	A	125	TYR	CB-CG-CD1	-9.47	115.32	121.00	2	9
1	A	95	PHE	CB-CG-CD2	-9.38	114.23	120.80	6	5
1	A	85	TYR	CB-CG-CD2	-9.37	115.38	121.00	11	5
1	A	83	ARG	NH1-CZ-NH2	-9.13	109.36	119.40	2	4
1	A	70	ARG	NH1-CZ-NH2	-9.11	109.38	119.40	9	4
1	A	71	ARG	NH1-CZ-NH2	-8.19	110.39	119.40	17	6
1	A	140	ASP	CB-CG-OD1	-8.13	110.98	118.30	4	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	85	TYR	CB-CG-CD1	-8.13	116.12	121.00	10	3
1	A	141	ARG	NH1-CZ-NH2	-8.05	110.55	119.40	16	3
1	A	37	ARG	NH1-CZ-NH2	-8.00	110.61	119.40	12	4
1	A	146	ARG	NH1-CZ-NH2	-7.97	110.63	119.40	6	7
1	A	23	ASP	CB-CG-OD2	-7.55	111.51	118.30	7	4
1	A	128	MET	CG-SD-CE	-7.41	88.35	100.20	5	2
1	A	27	ASP	CB-CG-OD2	7.39	124.95	118.30	20	1
1	A	124	ASP	CB-CG-OD1	7.28	124.85	118.30	17	1
1	A	124	ASP	CB-CG-OD2	-7.22	111.80	118.30	17	3
1	A	118	ARG	NH1-CZ-NH2	-7.17	111.51	119.40	5	4
1	A	140	ASP	CB-CG-OD2	6.98	124.58	118.30	4	2
1	A	23	ASP	CB-CG-OD1	-6.96	112.03	118.30	1	3
1	A	116	ASP	CB-CG-OD1	-6.87	112.12	118.30	13	1
1	A	125	TYR	CB-CG-CD2	-6.86	116.89	121.00	13	4
1	A	98	PHE	CB-CG-CD1	-6.83	116.02	120.80	12	3
1	A	61	ASP	CB-CG-OD1	-6.80	112.18	118.30	12	1
1	A	116	ASP	CB-CG-OD2	-6.76	112.22	118.30	9	2
1	A	28	VAL	CA-CB-CG2	-6.76	100.76	110.90	9	1
1	A	85	TYR	CG-CD2-CE2	-6.74	115.91	121.30	13	1
1	A	28	VAL	CG1-CB-CG2	-6.72	100.14	110.90	1	1
1	A	146	ARG	CG-CD-NE	-6.72	97.69	111.80	6	1
1	A	95	PHE	CB-CG-CD1	6.68	125.47	120.80	5	7
1	A	37	ARG	CG-CD-NE	-6.56	98.02	111.80	17	2
1	A	99	VAL	CA-CB-CG2	-6.53	101.10	110.90	19	2
1	A	70	ARG	CD-NE-CZ	6.45	132.63	123.60	19	1
1	A	140	ASP	CB-CA-C	6.42	123.23	110.40	2	2
1	A	59	ALA	CB-CA-C	-6.36	100.56	110.10	12	1
1	A	125	TYR	CG-CD2-CE2	-6.29	116.27	121.30	3	2
1	A	137	LEU	CB-CG-CD1	-6.22	100.42	111.00	3	1
1	A	152	ALA	N-CA-CB	-6.21	101.40	110.10	15	3
1	A	45	THR	CA-CB-CG2	-6.17	103.77	112.40	11	1
1	A	58	ALA	N-CA-CB	-6.04	101.65	110.10	12	2
1	A	98	PHE	CB-CG-CD2	-6.04	116.58	120.80	17	1
1	A	31	LYS	N-CA-CB	5.84	121.11	110.60	9	1
1	A	99	VAL	CG1-CB-CG2	-5.75	101.70	110.90	13	1
1	A	30	GLY	N-CA-C	5.75	127.47	113.10	19	1
1	A	52	ASP	CB-CG-OD1	-5.70	113.17	118.30	8	2
1	A	153	THR	CA-CB-CG2	-5.67	104.46	112.40	7	2
1	A	60	THR	CA-CB-CG2	-5.63	104.52	112.40	17	1
1	A	43	THR	CA-CB-CG2	-5.52	104.67	112.40	13	3
1	A	54	THR	CA-CB-CG2	-5.52	104.67	112.40	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	51	ASP	CB-CG-OD1	-5.51	113.34	118.30	14	1
1	A	136	VAL	CA-CB-CG2	-5.50	102.65	110.90	3	1
1	A	61	ASP	CB-CG-OD2	-5.47	113.38	118.30	1	2
1	A	79	ILE	CB-CA-C	-5.45	100.70	111.60	9	1
1	A	135	LYS	O-C-N	-5.43	114.01	122.70	12	1
1	A	146	ARG	N-CA-CB	5.40	120.32	110.60	20	1
1	A	23	ASP	N-CA-CB	-5.40	100.88	110.60	3	1
1	A	15	ILE	CA-CB-CG1	-5.37	100.80	111.00	20	1
1	A	112	SER	CB-CA-C	-5.35	99.94	110.10	16	1
1	A	123	THR	CA-CB-CG2	-5.35	104.92	112.40	14	2
1	A	94	ASP	CB-CG-OD1	-5.34	113.50	118.30	7	1
1	A	16	HIS	CA-CB-CG	-5.30	104.59	113.60	18	1
1	A	108	LEU	CB-CG-CD2	-5.30	102.00	111.00	18	1
1	A	125	TYR	CA-CB-CG	-5.29	103.34	113.40	11	1
1	A	114	ILE	O-C-N	-5.29	114.24	122.70	18	1
1	A	21	ASN	N-CA-CB	-5.27	101.12	110.60	12	1
1	A	27	ASP	CB-CG-OD1	-5.25	113.57	118.30	10	1
1	A	67	HIS	CA-CB-CG	5.25	122.52	113.60	1	1
1	A	35	VAL	CA-CB-CG2	-5.24	103.04	110.90	1	1
1	A	40	THR	CA-CB-CG2	-5.23	105.07	112.40	19	1
1	A	51	ASP	CB-CG-OD2	-5.22	113.61	118.30	6	1
1	A	45	THR	N-CA-CB	5.12	120.03	110.30	10	1
1	A	119	VAL	CG1-CB-CG2	-5.11	102.72	110.90	15	1
1	A	109	VAL	CA-CB-CG2	-5.09	103.26	110.90	1	1
1	A	122	VAL	CG1-CB-CG2	-5.08	102.78	110.90	16	1
1	A	35	VAL	CA-CB-CG1	-5.03	103.35	110.90	3	1
1	A	98	PHE	CG-CD1-CE1	-5.03	115.26	120.80	17	1
1	A	70	ARG	CG-CD-NE	-5.03	101.24	111.80	2	1
1	A	91	ARG	CG-CD-NE	-5.01	101.27	111.80	16	1
1	A	139	VAL	CA-CB-CG2	-5.01	103.38	110.90	20	1
1	A	118	ARG	CG-CD-NE	-5.00	101.29	111.80	19	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	83	ARG	Sidechain	10
1	A	125	TYR	Sidechain	8
1	A	144	ARG	Sidechain	8
1	A	146	ARG	Sidechain	8

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Mol	Chain	Res	Type	Group	Models (Total)
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	0±1
All	All	21020	22120	22120	10

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

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	137/171 (80%)	133±1 (97±1%)	3±1 (2±1%)	1±1 (1±1%)	26	73
All	All	2740/3420 (80%)	2658 (97%)	63 (2%)	19 (1%)	26	73

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
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 [i](#)

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%)	46	90
All	All	2260/2680 (84%)	2197 (97%)	63 (3%)	46	90

All 30 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	146	ARG	3
1	A	56	LYS	3
1	A	45	THR	3
1	A	90	THR	3
1	A	144	ARG	2
1	A	151	GLU	2
1	A	91	ARG	2
1	A	118	ARG	2
1	A	133	PRO	2
1	A	142	GLN	2
1	A	86	THR	2
1	A	128	MET	1
1	A	121	LYS	1
1	A	17	THR	1
1	A	67	HIS	1
1	A	94	ASP	1
1	A	153	THR	1
1	A	51	ASP	1
1	A	108	LEU	1
1	A	141	ARG	1
1	A	36	ILE	1
1	A	61	ASP	1
1	A	26	LYS	1
1	A	113	GLN	1
1	A	127	GLN	1
1	A	18	ILE	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 monosaccharides 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

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	CG	27.36	0.05	1
1	A	162	PRO	CD	50.39	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

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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	-0.38 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	128	0.06 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	126	-0.28 ± 0.10	None needed (< 0.5 ppm)
^{15}N	131	0.33 ± 0.57	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:

