



Full wwPDB NMR Structure Validation Report ⓘ

Mar 24, 2026 – 11:42 AM UTC

PDB ID : 2GFU / pdb_00002gfu
Title : NMR solution structure of the PWWP domain of Mismatch repair protein hMSH6
Authors : Laguri, C.; Friedrich, N.; Axt, M.; Gilquin, B.; Zinn-Justin, S.; Couprie, J.
Deposited on : 2006-03-23

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

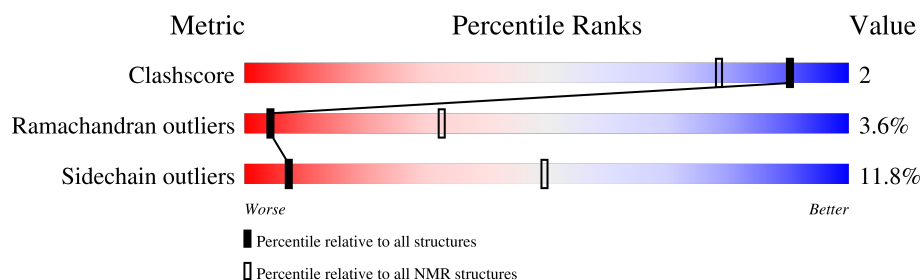
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	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	134	50% 28% • 19%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 11 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:88-A:195 (108)	0.92	11

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 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2126 atoms, of which 1059 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA mismatch repair protein MSH6.

Mol	Chain	Residues	Atoms						Trace
1	A	134	Total	C	H	N	O	S	0
			2126	679	1059	192	194	2	

There are 3 discrepancies between the modelled and reference sequences:

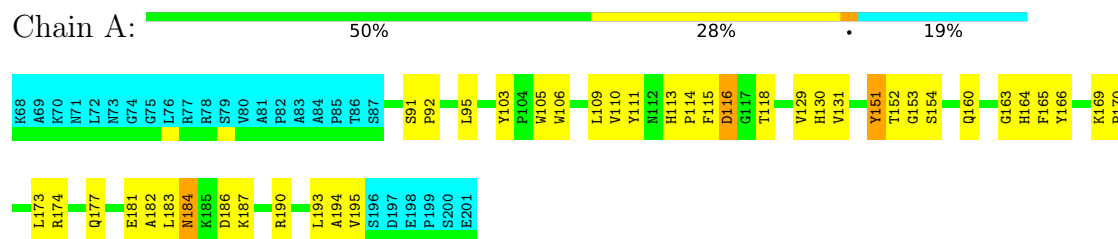
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	SER	CYS	engineered mutation	UNP P52701
A	108	SER	CYS	engineered mutation	UNP P52701
A	196	SER	CYS	engineered mutation	UNP P52701

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: DNA mismatch repair protein MSH6

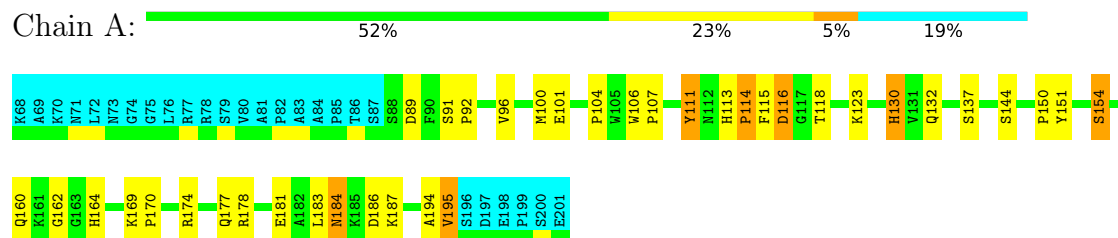


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

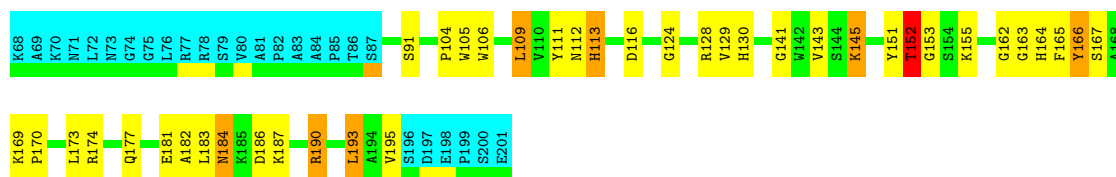
- Molecule 1: DNA mismatch repair protein MSH6



4.2.2 Score per residue for model 2

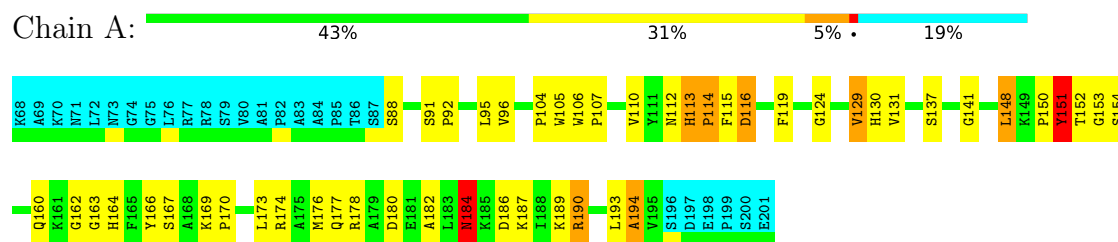
- Molecule 1: DNA mismatch repair protein MSH6





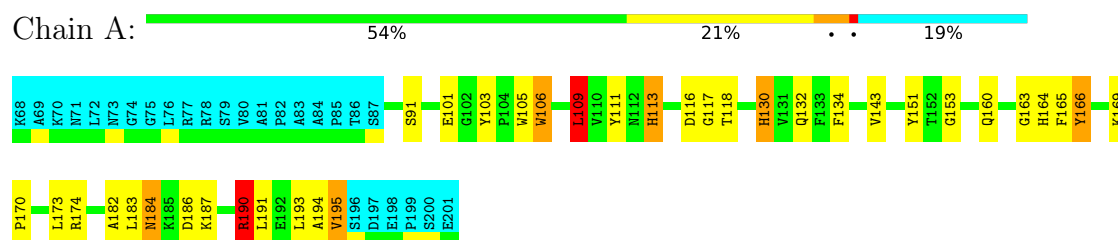
4.2.3 Score per residue for model 3

- Molecule 1: DNA mismatch repair protein MSH6



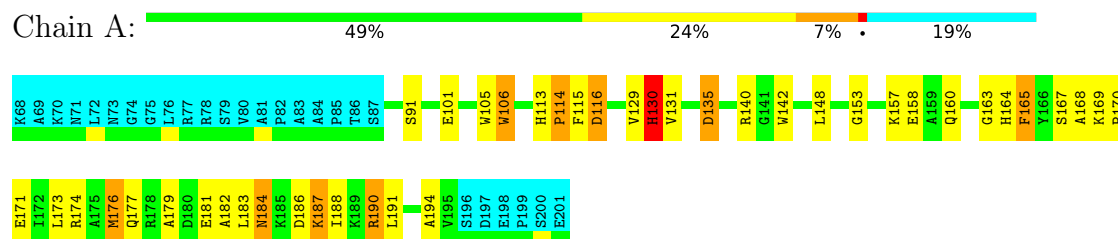
4.2.4 Score per residue for model 4

- Molecule 1: DNA mismatch repair protein MSH6



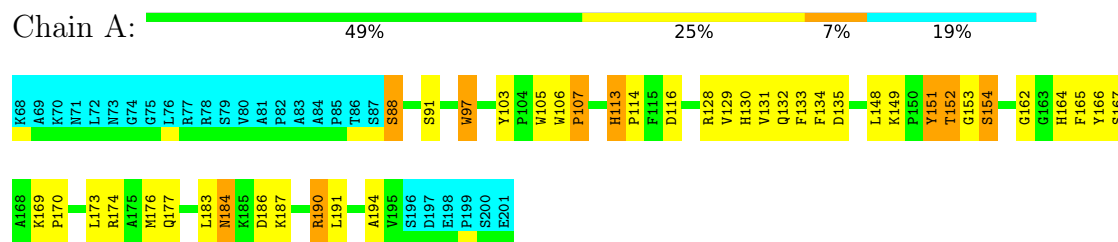
4.2.5 Score per residue for model 5

- Molecule 1: DNA mismatch repair protein MSH6



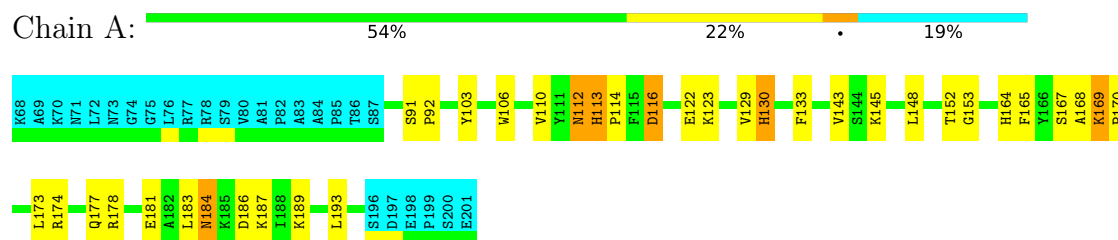
4.2.6 Score per residue for model 6

- Molecule 1: DNA mismatch repair protein MSH6



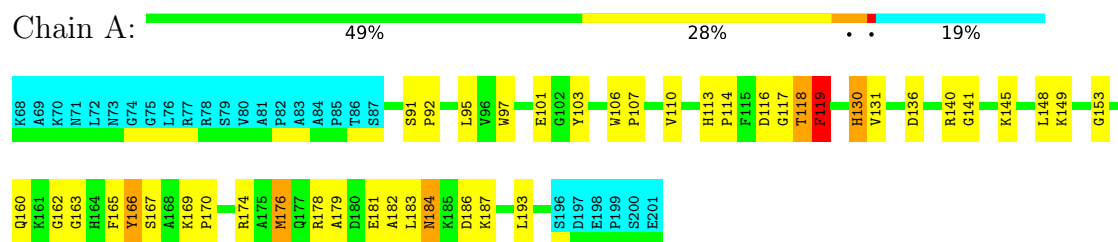
4.2.7 Score per residue for model 7

- Molecule 1: DNA mismatch repair protein MSH6



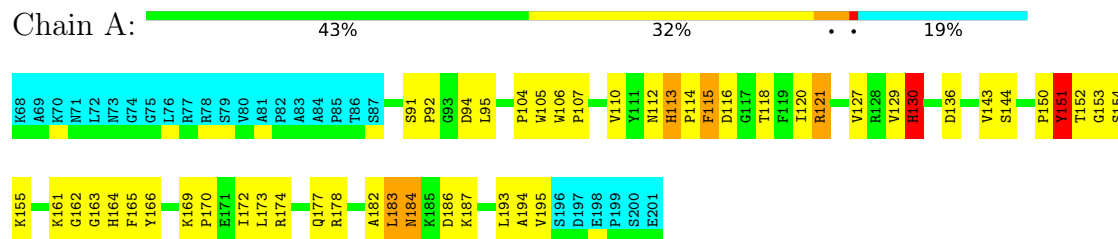
4.2.8 Score per residue for model 8

- Molecule 1: DNA mismatch repair protein MSH6



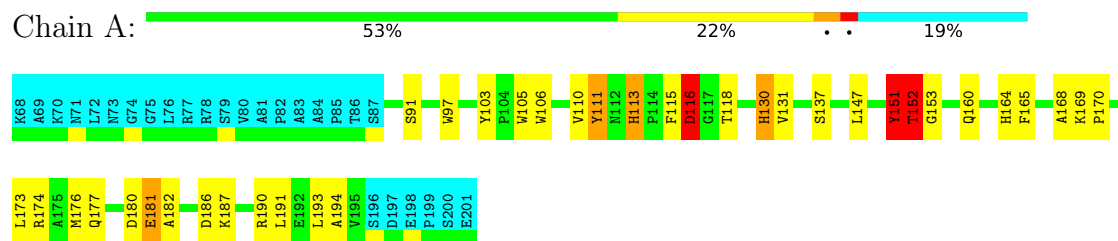
4.2.9 Score per residue for model 9

- Molecule 1: DNA mismatch repair protein MSH6



4.2.10 Score per residue for model 10

- Molecule 1: DNA mismatch repair protein MSH6



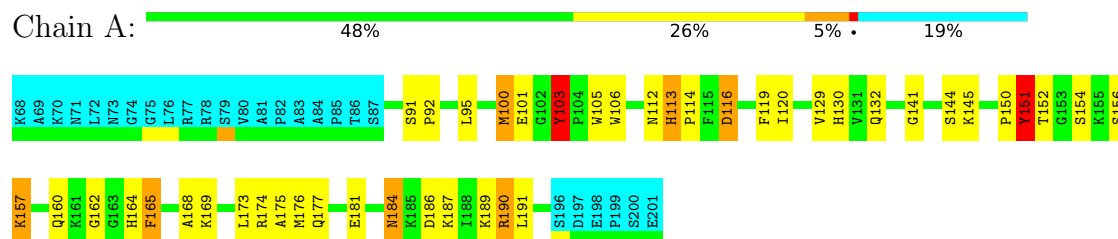
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: DNA mismatch repair protein MSH6



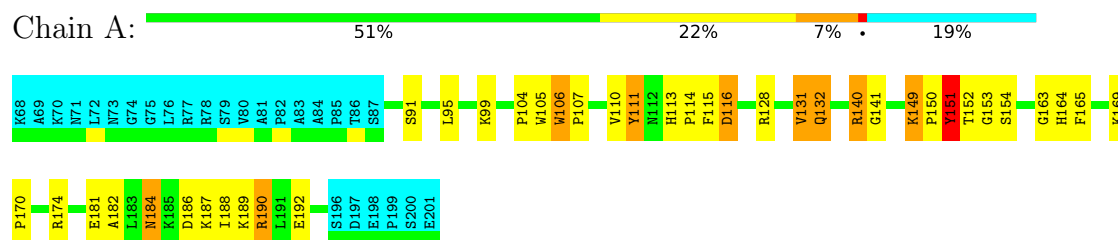
4.2.12 Score per residue for model 12

- Molecule 1: DNA mismatch repair protein MSH6



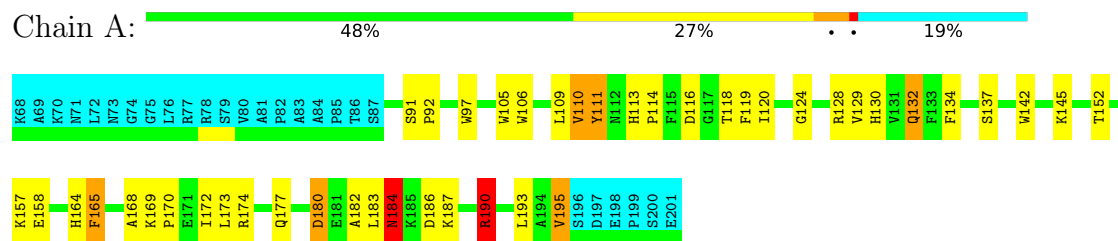
4.2.13 Score per residue for model 13

- Molecule 1: DNA mismatch repair protein MSH6



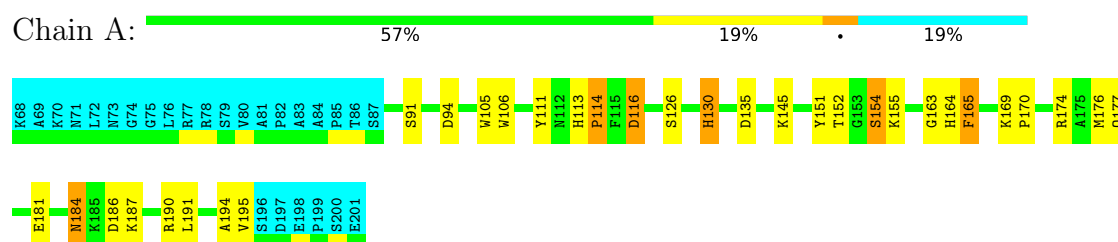
4.2.14 Score per residue for model 14

- Molecule 1: DNA mismatch repair protein MSH6



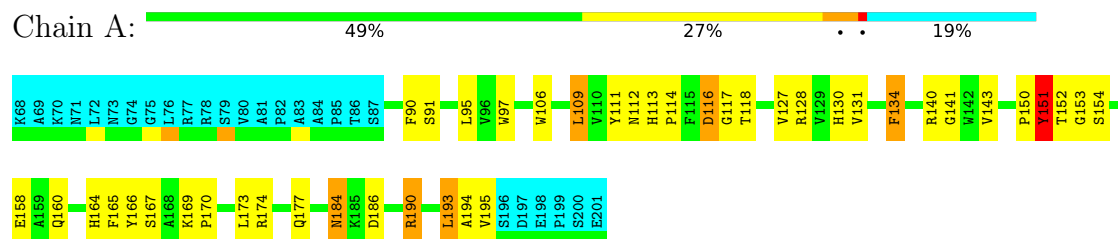
4.2.15 Score per residue for model 15

- Molecule 1: DNA mismatch repair protein MSH6



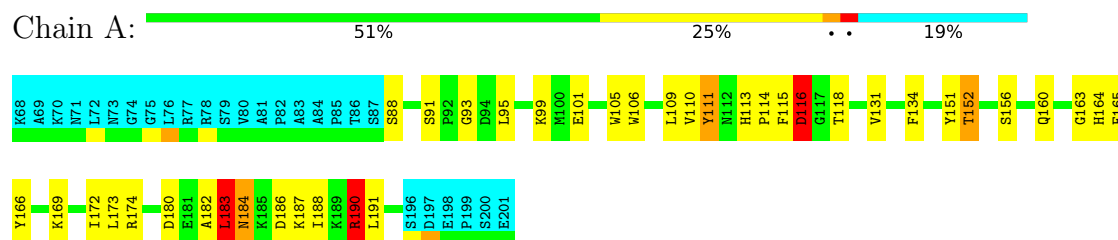
4.2.16 Score per residue for model 16

- Molecule 1: DNA mismatch repair protein MSH6



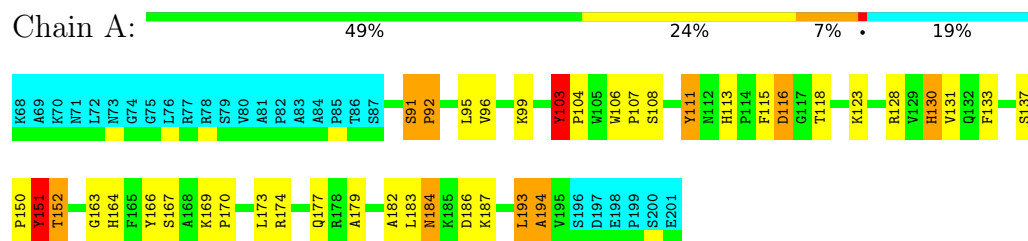
4.2.17 Score per residue for model 17

- Molecule 1: DNA mismatch repair protein MSH6



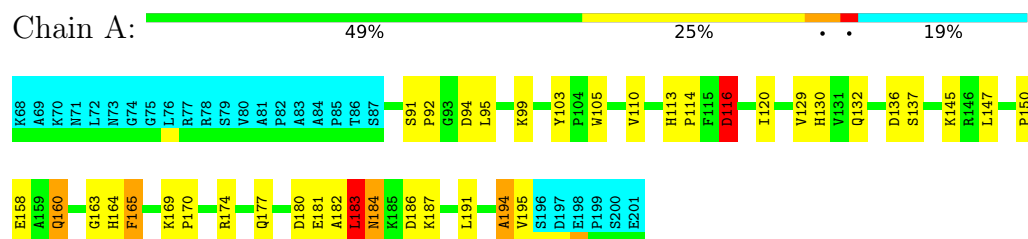
4.2.18 Score per residue for model 18

- Molecule 1: DNA mismatch repair protein MSH6



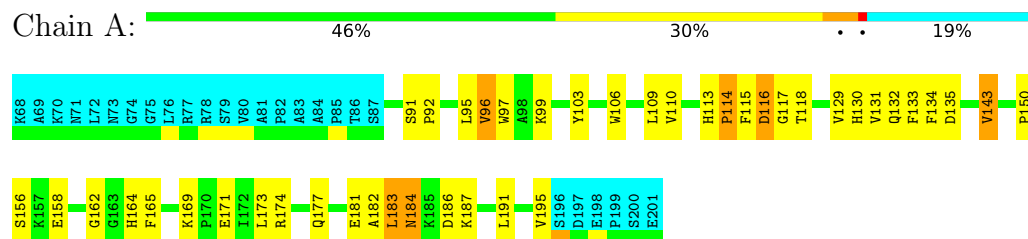
4.2.19 Score per residue for model 19

- Molecule 1: DNA mismatch repair protein MSH6



4.2.20 Score per residue for model 20

- Molecule 1: DNA mismatch repair protein MSH6



5 Refinement protocol and experimental data overview

Of the 1000 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
INCA	structure solution	1.0
INCA	refinement	1.0

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.34±0.03	1±0/910 (0.1± 0.0%)	2.19±0.05	52±8/1228 (4.2± 0.7%)
All	All	1.34	24/18200 (0.1%)	2.19	1038/24560 (4.2%)

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	1.5±1.4
All	All	0	30

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	131	VAL	CA-C	-6.45	1.47	1.52	20	1
1	A	116	ASP	CG-OD1	5.94	1.36	1.25	10	14
1	A	106	TRP	CA-C	5.85	1.57	1.52	6	1
1	A	116	ASP	CG-OD2	5.82	1.36	1.25	17	6
1	A	130	HIS	ND1-CE1	5.38	1.38	1.32	9	1
1	A	106	TRP	C-N	5.24	1.39	1.33	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	186	ASP	CA-C-N	11.63	136.32	120.38	11	20
1	A	186	ASP	C-N-CA	11.63	136.32	120.38	11	20
1	A	162	GLY	CA-C-N	10.96	130.76	120.34	12	9
1	A	162	GLY	C-N-CA	10.96	130.76	120.34	12	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	130	HIS	CA-CB-CG	10.88	124.67	113.80	5	6
1	A	184	ASN	CA-CB-CG	10.76	123.36	112.60	18	19
1	A	182	ALA	CA-C-N	9.60	132.92	120.44	9	6
1	A	182	ALA	C-N-CA	9.60	132.92	120.44	9	6
1	A	177	GLN	CA-C-N	9.52	132.82	120.44	9	15
1	A	177	GLN	C-N-CA	9.52	132.82	120.44	9	15
1	A	141	GLY	N-CA-C	-9.41	97.85	110.74	13	8
1	A	151	TYR	CA-C-N	8.91	138.56	121.54	18	9
1	A	151	TYR	C-N-CA	8.91	138.56	121.54	18	9
1	A	91	SER	CB-CA-C	8.89	122.46	109.48	12	11
1	A	164	HIS	N-CA-C	8.87	120.95	111.28	16	18
1	A	114	PRO	CA-C-N	8.85	134.75	120.60	19	11
1	A	114	PRO	C-N-CA	8.85	134.75	120.60	19	11
1	A	156	SER	CA-C-N	8.67	134.59	120.63	12	4
1	A	156	SER	C-N-CA	8.67	134.59	120.63	12	4
1	A	115	PHE	CA-C-N	8.67	134.22	121.31	20	5
1	A	115	PHE	C-N-CA	8.67	134.22	121.31	20	5
1	A	113	HIS	CA-C-N	8.41	130.36	119.84	1	13
1	A	113	HIS	C-N-CA	8.41	130.36	119.84	1	13
1	A	154	SER	CA-C-N	8.14	135.38	121.14	6	3
1	A	154	SER	C-N-CA	8.14	135.38	121.14	6	3
1	A	128	ARG	CA-C-N	8.03	133.02	122.51	13	6
1	A	128	ARG	C-N-CA	8.03	133.02	122.51	13	6
1	A	163	GLY	CA-C-N	7.95	130.93	120.28	8	10
1	A	163	GLY	C-N-CA	7.95	130.93	120.28	8	10
1	A	169	LYS	N-CA-C	-7.90	98.21	110.14	1	10
1	A	165	PHE	CA-CB-CG	7.87	121.67	113.80	4	8
1	A	174	ARG	CA-C-N	7.86	131.59	120.28	20	20
1	A	174	ARG	C-N-CA	7.86	131.59	120.28	20	20
1	A	153	GLY	CA-C-N	7.85	133.26	120.63	6	10
1	A	153	GLY	C-N-CA	7.85	133.26	120.63	6	10
1	A	97	TRP	N-CA-C	-7.81	95.80	108.52	16	6
1	A	106	TRP	N-CA-C	7.80	123.89	107.91	6	14
1	A	91	SER	CA-C-N	7.77	127.83	119.90	18	19
1	A	91	SER	C-N-CA	7.77	127.83	119.90	18	19
1	A	191	LEU	CA-C-N	7.74	130.65	120.28	5	9
1	A	191	LEU	C-N-CA	7.74	130.65	120.28	5	9
1	A	94	ASP	CA-CB-CG	7.74	120.33	112.60	15	1
1	A	170	PRO	CA-C-N	7.72	131.25	120.29	8	17
1	A	170	PRO	C-N-CA	7.72	131.25	120.29	8	17
1	A	113	HIS	CA-CB-CG	7.69	121.49	113.80	4	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	169	LYS	CA-C-N	7.63	127.68	119.28	16	19
1	A	169	LYS	C-N-CA	7.63	127.68	119.28	16	19
1	A	116	ASP	N-CA-C	7.52	120.88	110.35	20	7
1	A	106	TRP	CB-CG-CD2	-7.46	116.35	126.80	7	14
1	A	112	ASN	CA-C-N	7.42	132.90	121.03	2	5
1	A	112	ASN	C-N-CA	7.42	132.90	121.03	2	5
1	A	152	THR	N-CA-C	-7.38	95.07	110.80	10	2
1	A	135	ASP	CA-CB-CG	7.32	119.92	112.60	11	3
1	A	180	ASP	CA-CB-CG	7.23	119.83	112.60	10	1
1	A	176	MET	N-CA-CB	7.22	121.47	110.28	8	5
1	A	118	THR	N-CA-C	-7.21	96.52	108.34	18	10
1	A	187	LYS	CA-C-N	7.17	130.64	120.53	13	17
1	A	187	LYS	C-N-CA	7.17	130.64	120.53	13	17
1	A	194	ALA	CA-C-N	7.17	134.87	121.97	19	2
1	A	194	ALA	C-N-CA	7.17	134.87	121.97	19	2
1	A	91	SER	CA-C-O	-7.12	114.74	121.08	12	5
1	A	173	LEU	CA-C-N	7.06	129.74	120.28	17	14
1	A	173	LEU	C-N-CA	7.06	129.74	120.28	17	14
1	A	110	VAL	CB-CA-C	7.02	119.61	110.91	20	1
1	A	117	GLY	CA-C-N	7.00	132.86	123.00	16	4
1	A	117	GLY	C-N-CA	7.00	132.86	123.00	16	4
1	A	157	LYS	N-CA-C	6.93	121.35	112.34	11	4
1	A	92	PRO	N-CA-C	6.92	122.08	111.15	14	10
1	A	190	ARG	CA-CB-CG	6.88	127.87	114.10	4	2
1	A	190	ARG	CB-CA-C	6.86	122.51	110.85	4	1
1	A	182	ALA	N-CA-C	6.81	120.07	111.69	3	7
1	A	123	LYS	N-CA-C	6.80	120.24	110.24	7	1
1	A	107	PRO	CA-C-N	6.76	133.20	122.59	6	8
1	A	107	PRO	C-N-CA	6.76	133.20	122.59	6	8
1	A	131	VAL	N-CA-CB	6.75	120.08	112.32	20	1
1	A	106	TRP	CA-C-N	6.68	127.08	119.93	20	10
1	A	106	TRP	C-N-CA	6.68	127.08	119.93	20	10
1	A	95	LEU	N-CA-CB	6.63	121.46	110.52	18	5
1	A	145	LYS	CA-C-N	6.62	131.78	120.72	8	1
1	A	145	LYS	C-N-CA	6.62	131.78	120.72	8	1
1	A	136	ASP	CA-C-N	6.61	127.97	119.78	8	3
1	A	136	ASP	C-N-CA	6.61	127.97	119.78	8	3
1	A	113	HIS	CA-C-O	-6.57	113.80	120.96	17	9
1	A	135	ASP	CA-C-O	6.57	121.75	117.94	20	2
1	A	167	SER	N-CA-C	-6.56	98.17	108.14	3	6
1	A	104	PRO	CA-C-N	6.53	130.68	121.02	9	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	104	PRO	C-N-CA	6.53	130.68	121.02	9	7
1	A	195	VAL	CB-CA-C	6.52	121.98	111.29	1	2
1	A	129	VAL	N-CA-C	-6.52	98.24	108.86	5	3
1	A	103	TYR	CB-CA-C	6.51	118.98	109.48	12	1
1	A	111	TYR	N-CA-C	6.51	120.07	109.59	4	2
1	A	173	LEU	N-CA-CB	6.47	119.39	110.01	17	6
1	A	180	ASP	N-CA-CB	6.45	119.36	110.01	19	2
1	A	193	LEU	CA-C-N	6.42	133.81	121.54	18	7
1	A	193	LEU	C-N-CA	6.42	133.81	121.54	18	7
1	A	193	LEU	N-CA-C	-6.38	105.14	113.12	2	3
1	A	96	VAL	O-C-N	-6.38	115.97	123.05	1	2
1	A	142	TRP	CA-C-N	6.37	129.09	122.27	14	1
1	A	142	TRP	C-N-CA	6.37	129.09	122.27	14	1
1	A	183	LEU	N-CA-CB	-6.37	100.76	110.12	20	5
1	A	179	ALA	CA-C-N	6.36	128.81	120.28	18	3
1	A	179	ALA	C-N-CA	6.36	128.81	120.28	18	3
1	A	194	ALA	N-CA-C	6.32	117.92	108.31	5	3
1	A	165	PHE	CA-C-N	6.31	133.59	121.54	4	3
1	A	165	PHE	C-N-CA	6.31	133.59	121.54	4	3
1	A	106	TRP	CB-CG-CD1	6.27	136.31	126.90	7	7
1	A	140	ARG	CA-C-N	6.23	129.01	120.72	13	3
1	A	140	ARG	C-N-CA	6.23	129.01	120.72	13	3
1	A	143	VAL	N-CA-CB	-6.21	100.20	112.24	20	1
1	A	88	SER	N-CA-CB	6.20	120.97	110.49	6	1
1	A	150	PRO	CA-C-N	6.18	133.35	121.54	12	9
1	A	150	PRO	C-N-CA	6.18	133.35	121.54	12	9
1	A	180	ASP	CA-C-N	6.18	128.88	120.54	17	1
1	A	180	ASP	C-N-CA	6.18	128.88	120.54	17	1
1	A	103	TYR	CA-C-N	6.16	126.12	120.21	7	8
1	A	103	TYR	C-N-CA	6.16	126.12	120.21	7	8
1	A	164	HIS	CA-CB-CG	6.16	119.95	113.80	5	3
1	A	96	VAL	CA-CB-CG1	6.13	120.82	110.40	20	1
1	A	172	ILE	CA-C-N	6.09	128.36	120.44	9	2
1	A	172	ILE	C-N-CA	6.09	128.36	120.44	9	2
1	A	173	LEU	CB-CA-C	-6.07	101.36	110.88	17	2
1	A	151	TYR	N-CA-C	6.05	123.69	110.80	19	7
1	A	154	SER	N-CA-C	6.04	120.20	112.34	20	6
1	A	163	GLY	N-CA-C	6.02	121.13	112.82	18	5
1	A	190	ARG	N-CA-C	5.98	119.04	111.69	2	1
1	A	109	LEU	CD1-CG-CD2	-5.97	97.66	110.80	17	3
1	A	187	LYS	CB-CA-C	5.96	122.02	110.46	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	95	LEU	N-CA-C	-5.95	100.00	109.76	13	4
1	A	183	LEU	CA-C-N	5.95	129.36	120.31	17	1
1	A	183	LEU	C-N-CA	5.95	129.36	120.31	17	1
1	A	105	TRP	CB-CG-CD2	-5.95	118.47	126.80	4	8
1	A	115	PHE	N-CA-C	-5.93	105.86	112.57	3	4
1	A	169	LYS	CA-C-O	-5.93	113.85	119.55	6	3
1	A	89	ASP	CA-CB-CG	5.92	118.52	112.60	1	1
1	A	188	ILE	CA-C-N	5.87	128.15	120.28	5	1
1	A	188	ILE	C-N-CA	5.87	128.15	120.28	5	1
1	A	131	VAL	CA-CB-CG1	5.87	120.38	110.40	18	1
1	A	122	GLU	CA-C-N	5.83	129.39	121.05	7	1
1	A	122	GLU	C-N-CA	5.83	129.39	121.05	7	1
1	A	110	VAL	N-CA-CB	5.78	117.43	110.95	7	5
1	A	119	PHE	CB-CA-C	5.75	119.38	109.15	8	1
1	A	116	ASP	N-CA-CB	5.72	118.41	110.17	7	3
1	A	145	LYS	N-CA-C	5.70	119.85	113.01	7	2
1	A	121	ARG	N-CA-C	-5.69	99.13	108.41	9	1
1	A	166	TYR	N-CA-C	5.65	118.60	107.98	9	4
1	A	89	ASP	N-CA-C	5.63	117.83	108.20	11	1
1	A	103	TYR	CA-CB-CG	5.63	124.03	113.90	18	2
1	A	176	MET	CA-C-N	5.60	128.05	120.44	11	3
1	A	176	MET	C-N-CA	5.60	128.05	120.44	11	3
1	A	195	VAL	CA-C-N	5.60	130.06	120.71	14	2
1	A	195	VAL	C-N-CA	5.60	130.06	120.71	14	2
1	A	160	GLN	CB-CA-C	5.58	119.76	109.71	19	1
1	A	184	ASN	CB-CA-C	5.58	120.43	109.72	19	6
1	A	153	GLY	N-CA-C	5.57	121.92	112.22	13	1
1	A	132	GLN	CA-C-N	5.55	130.01	122.19	14	3
1	A	132	GLN	C-N-CA	5.55	130.01	122.19	14	3
1	A	169	LYS	CB-CA-C	5.53	117.19	108.84	14	3
1	A	166	TYR	CA-C-N	5.52	132.36	122.09	3	6
1	A	166	TYR	C-N-CA	5.52	132.36	122.09	3	6
1	A	90	PHE	CA-CB-CG	-5.52	108.28	113.80	16	1
1	A	192	GLU	CA-C-N	5.49	131.39	122.67	13	1
1	A	192	GLU	C-N-CA	5.49	131.39	122.67	13	1
1	A	159	ALA	CA-C-N	5.48	132.01	121.54	11	1
1	A	159	ALA	C-N-CA	5.48	132.01	121.54	11	1
1	A	149	LYS	CA-C-N	5.47	125.67	120.31	6	1
1	A	149	LYS	C-N-CA	5.47	125.67	120.31	6	1
1	A	144	SER	CA-C-N	5.41	128.28	120.38	1	1
1	A	144	SER	C-N-CA	5.41	128.28	120.38	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	168	ALA	CA-C-O	5.40	126.53	120.92	10	4
1	A	126	SER	CA-C-N	5.39	129.23	122.43	15	1
1	A	126	SER	C-N-CA	5.39	129.23	122.43	15	1
1	A	190	ARG	CA-C-N	5.37	129.69	120.72	5	3
1	A	190	ARG	C-N-CA	5.37	129.69	120.72	5	3
1	A	190	ARG	CB-CG-CD	5.35	123.61	111.30	4	1
1	A	171	GLU	CA-C-N	5.31	127.36	120.56	20	2
1	A	171	GLU	C-N-CA	5.31	127.36	120.56	20	2
1	A	100	MET	CA-C-N	5.30	131.67	121.54	1	1
1	A	100	MET	C-N-CA	5.30	131.67	121.54	1	1
1	A	137	SER	N-CA-C	5.26	119.40	112.35	19	1
1	A	91	SER	O-C-N	-5.23	117.37	121.14	4	1
1	A	190	ARG	N-CA-CB	5.20	117.94	110.20	14	1
1	A	135	ASP	N-CA-C	5.19	113.03	108.78	6	1
1	A	106	TRP	CG-CD2-CE3	-5.18	128.72	133.90	7	1
1	A	113	HIS	N-CA-C	5.17	117.64	110.20	2	3
1	A	111	TYR	CA-C-N	5.13	129.25	122.42	14	2
1	A	111	TYR	C-N-CA	5.13	129.25	122.42	14	2
1	A	137	SER	O-C-N	-5.12	115.43	121.32	1	3
1	A	168	ALA	CA-C-N	5.12	132.84	122.70	5	1
1	A	168	ALA	C-N-CA	5.12	132.84	122.70	5	1
1	A	113	HIS	CE1-NE2-CD2	-5.10	103.90	109.00	9	3
1	A	106	TRP	CE2-CD2-CE3	5.07	123.87	118.80	7	1
1	A	144	SER	N-CA-C	-5.07	100.46	108.73	9	2
1	A	130	HIS	CB-CG-CD2	-5.07	124.61	131.20	5	1
1	A	195	VAL	N-CA-CB	5.07	119.59	111.23	4	1
1	A	160	GLN	CA-CB-CG	5.05	124.21	114.10	19	1
1	A	114	PRO	N-CA-C	5.04	122.85	112.47	20	2
1	A	130	HIS	CB-CG-ND1	5.04	130.25	122.70	5	1
1	A	181	GLU	N-CA-C	5.02	116.84	111.36	10	1
1	A	175	ALA	CA-C-N	5.00	127.92	120.31	12	1
1	A	175	ALA	C-N-CA	5.00	127.92	120.31	12	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	151	TYR	Sidechain	6
1	A	111	TYR	Sidechain	5
1	A	190	ARG	Sidechain	4

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	134	PHE	Sidechain	4
1	A	130	HIS	Sidechain	3
1	A	152	THR	Peptide	2
1	A	106	TRP	Peptide	2
1	A	103	TYR	Sidechain	2
1	A	166	TYR	Sidechain	1
1	A	133	PHE	Sidechain	1

6.2 Too-close contacts [i](#)

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	882	874	874	3±2
All	All	17640	17480	17480	59

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:109:LEU:HD11	1:A:190:ARG:HE	0.74	1.42	11	1
1:A:96:VAL:HG21	1:A:148:LEU:HD13	0.65	1.69	3	1
1:A:152:THR:HA	1:A:183:LEU:HD13	0.61	1.70	18	3
1:A:120:ILE:HG22	1:A:129:VAL:HG12	0.60	1.71	19	4
1:A:113:HIS:CD2	1:A:130:HIS:CD2	0.57	2.92	12	5
1:A:105:TRP:CD2	1:A:165:PHE:HB3	0.56	2.35	2	4
1:A:129:VAL:HG22	1:A:145:LYS:HB2	0.55	1.78	2	1
1:A:130:HIS:CD2	1:A:142:TRP:CZ2	0.54	2.96	5	1
1:A:113:HIS:CD2	1:A:130:HIS:CG	0.53	2.96	16	1
1:A:152:THR:HA	1:A:183:LEU:HD11	0.51	1.83	17	1
1:A:109:LEU:CD1	1:A:190:ARG:HE	0.51	2.18	11	1
1:A:95:LEU:CD2	1:A:190:ARG:HE	0.49	2.19	12	1
1:A:149:LYS:HB2	1:A:149:LYS:HZ2	0.48	1.68	13	1
1:A:119:PHE:HA	1:A:130:HIS:CE1	0.48	2.43	8	2
1:A:113:HIS:CG	1:A:130:HIS:CD2	0.47	3.02	2	2
1:A:109:LEU:HD21	1:A:190:ARG:CZ	0.47	2.38	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:VAL:HG11	1:A:145:LYS:HD3	0.46	1.87	12	3
1:A:109:LEU:HD22	1:A:190:ARG:HE	0.46	1.71	14	1
1:A:93:GLY:HA2	1:A:190:ARG:CZ	0.45	2.42	17	1
1:A:151:TYR:CE2	1:A:153:GLY:HA2	0.44	2.47	10	1
1:A:106:TRP:CZ3	1:A:172:ILE:HD13	0.44	2.47	14	2
1:A:97:TRP:CZ3	1:A:107:PRO:HG3	0.44	2.48	6	1
1:A:180:ASP:O	1:A:184:ASN:HB3	0.43	2.13	14	2
1:A:99:LYS:O	1:A:147:LEU:HD13	0.43	2.13	19	1
1:A:95:LEU:HD22	1:A:190:ARG:HE	0.43	1.74	12	1
1:A:99:LYS:O	1:A:147:LEU:HD22	0.43	2.14	19	1
1:A:109:LEU:HD22	1:A:190:ARG:HB2	0.42	1.91	2	2
1:A:119:PHE:HB2	1:A:130:HIS:CE1	0.42	2.49	3	1
1:A:152:THR:HA	1:A:183:LEU:HD21	0.42	1.90	19	1
1:A:106:TRP:CZ2	1:A:135:ASP:HB3	0.41	2.50	11	2
1:A:113:HIS:CD2	1:A:115:PHE:CZ	0.41	3.09	9	1
1:A:111:TYR:O	1:A:130:HIS:CD2	0.41	2.73	1	1
1:A:182:ALA:HB1	1:A:190:ARG:HB3	0.41	1.93	13	1
1:A:182:ALA:HB1	1:A:190:ARG:HG2	0.41	1.92	2	1
1:A:100:MET:N	1:A:103:TYR:CE1	0.41	2.88	12	1
1:A:130:HIS:CG	1:A:140:ARG:HH22	0.41	2.33	5	1
1:A:109:LEU:HB2	1:A:134:PHE:CZ	0.40	2.51	16	1
1:A:110:VAL:HG23	1:A:131:VAL:HG12	0.40	1.94	13	1
1:A:129:VAL:O	1:A:143:VAL:HG12	0.40	2.16	20	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	108/134 (81%)	93±2 (86±2%)	12±3 (11±3%)	4±1 (4±1%)	4	32
All	All	2160/2680 (81%)	1852 (86%)	230 (11%)	78 (4%)	4	32

All 16 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	152	THR	13
1	A	114	PRO	9
1	A	151	TYR	9
1	A	194	ALA	9
1	A	101	GLU	6
1	A	195	VAL	5
1	A	116	ASP	5
1	A	154	SER	4
1	A	124	GLY	4
1	A	134	PHE	3
1	A	167	SER	2
1	A	153	GLY	2
1	A	166	TYR	2
1	A	88	SER	2
1	A	157	LYS	2
1	A	119	PHE	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	93/113 (82%)	82±2 (88±2%)	11±2 (12±2%)	7	49
All	All	1860/2260 (82%)	1640 (88%)	220 (12%)	7	49

All 56 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	184	ASN	19
1	A	116	ASP	13
1	A	181	GLU	12
1	A	160	GLN	11
1	A	190	ARG	11
1	A	183	LEU	10
1	A	151	TYR	10
1	A	130	HIS	8
1	A	131	VAL	8
1	A	111	TYR	7

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Mol	Chain	Res	Type	Models (Total)
1	A	132	GLN	7
1	A	165	PHE	7
1	A	178	ARG	6
1	A	143	VAL	5
1	A	148	LEU	5
1	A	158	GLU	5
1	A	193	LEU	4
1	A	110	VAL	4
1	A	189	LYS	4
1	A	99	LYS	4
1	A	145	LYS	3
1	A	155	LYS	3
1	A	195	VAL	3
1	A	109	LEU	3
1	A	133	PHE	3
1	A	123	LYS	2
1	A	129	VAL	2
1	A	176	MET	2
1	A	187	LYS	2
1	A	112	ASN	2
1	A	118	THR	2
1	A	149	LYS	2
1	A	94	ASP	2
1	A	127	VAL	2
1	A	137	SER	2
1	A	96	VAL	2
1	A	103	TYR	2
1	A	105	TRP	2
1	A	188	ILE	2
1	A	166	TYR	1
1	A	88	SER	1
1	A	95	LEU	1
1	A	113	HIS	1
1	A	169	LYS	1
1	A	119	PHE	1
1	A	115	PHE	1
1	A	121	ARG	1
1	A	161	LYS	1
1	A	147	LEU	1
1	A	152	THR	1
1	A	100	MET	1
1	A	140	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	154	SER	1
1	A	91	SER	1
1	A	92	PRO	1
1	A	108	SER	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

No chemical shift data were provided