



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 02:50 PM UTC

PDB ID : 1CO1 / pdb_00001co1
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Deposited on : 1999-05-31

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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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

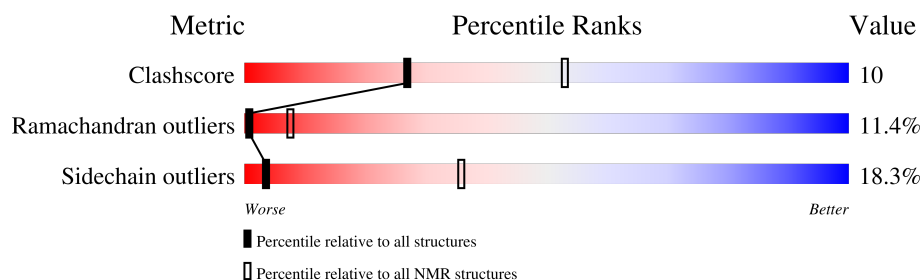
1 Overall quality at a glance

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	115	46% 49% . .

2 Ensemble composition and analysis

This entry contains 10 models. Model 10 is the overall representative, medoid model (most similar to other models).

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:21-A:132 (112)	2.46	10

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, 7, 8, 10
2	6, 9

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1788 atoms, of which 896 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CORE BINDING FACTOR ALPHA.

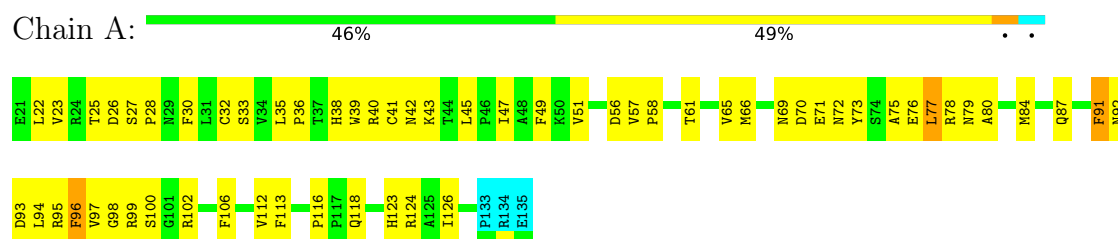
Mol	Chain	Residues	Atoms						Trace
1	A	115	Total	C	H	N	O	S	0
			1788	561	896	162	165	4	

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: CORE BINDING FACTOR ALPHA

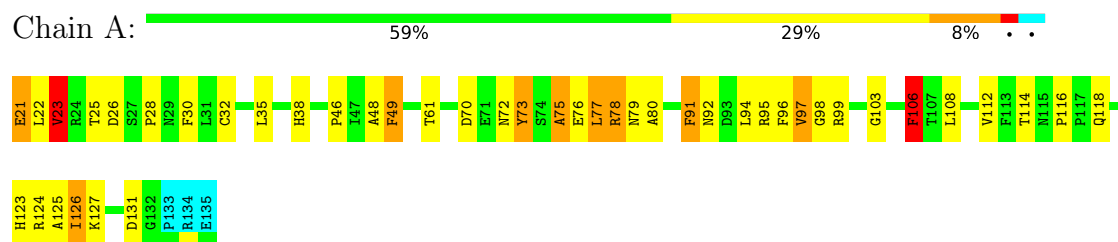


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

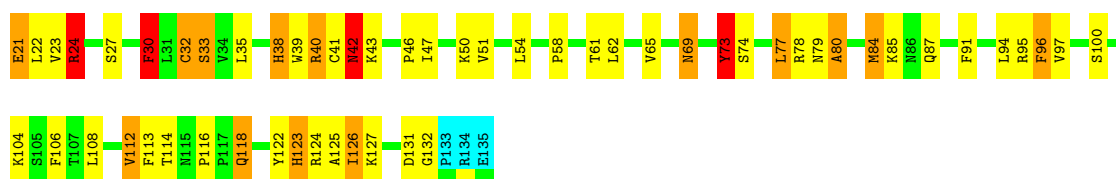
• Molecule 1: CORE BINDING FACTOR ALPHA



4.2.2 Score per residue for model 2

• Molecule 1: CORE BINDING FACTOR ALPHA

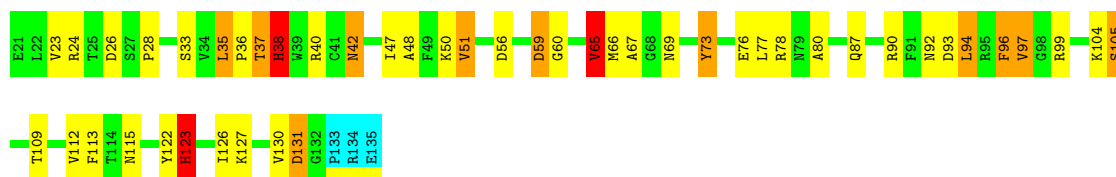




4.2.3 Score per residue for model 3

- Molecule 1: CORE BINDING FACTOR ALPHA

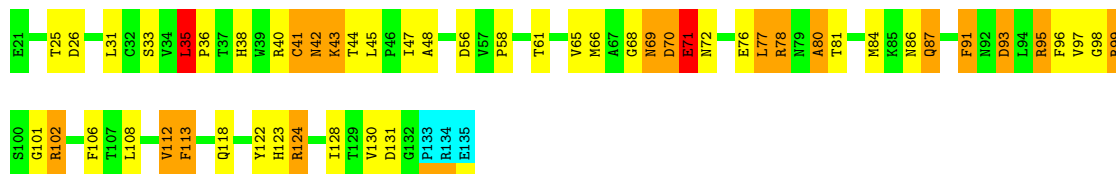
Chain A: 57% 29% 10% . .



4.2.4 Score per residue for model 4

- Molecule 1: CORE BINDING FACTOR ALPHA

Chain A: 51% 30% 15% . .



4.2.5 Score per residue for model 5

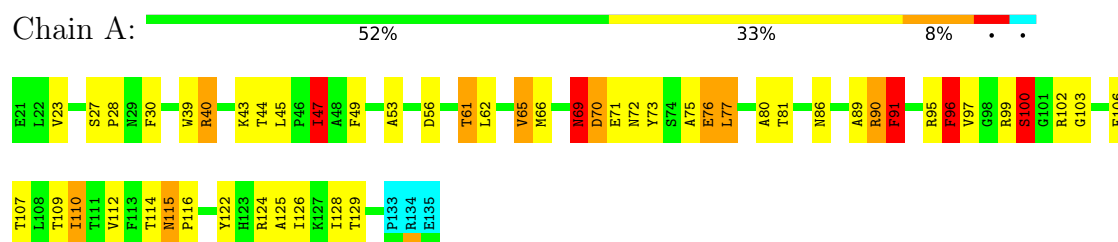
- Molecule 1: CORE BINDING FACTOR ALPHA

Chain A: 48% 37% 10% . .



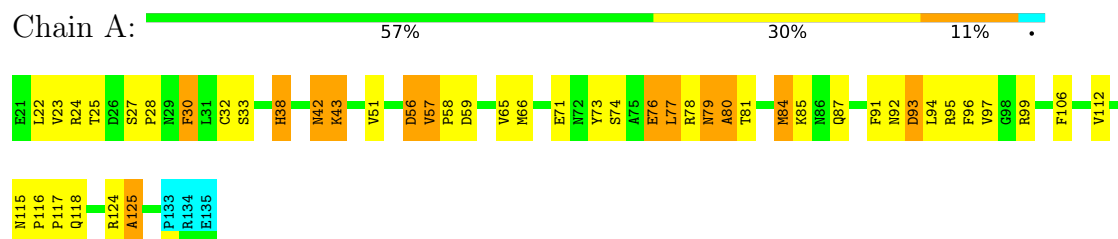
4.2.6 Score per residue for model 6

- Molecule 1: CORE BINDING FACTOR ALPHA



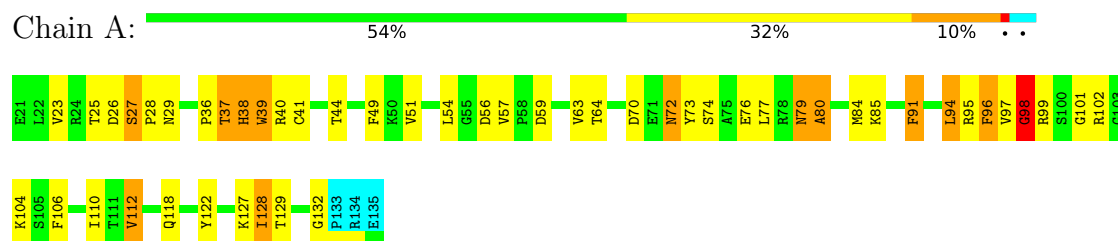
4.2.7 Score per residue for model 7

- Molecule 1: CORE BINDING FACTOR ALPHA



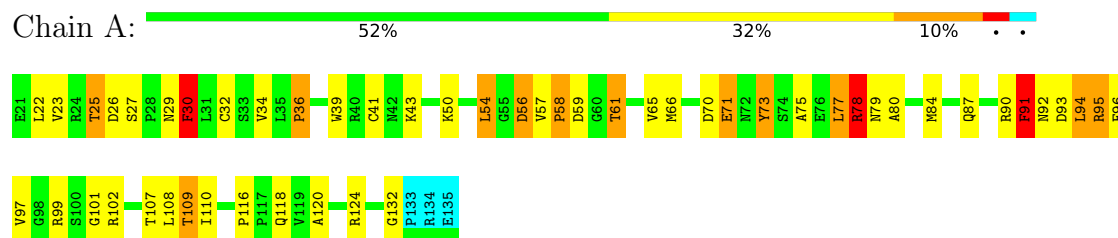
4.2.8 Score per residue for model 8

- Molecule 1: CORE BINDING FACTOR ALPHA



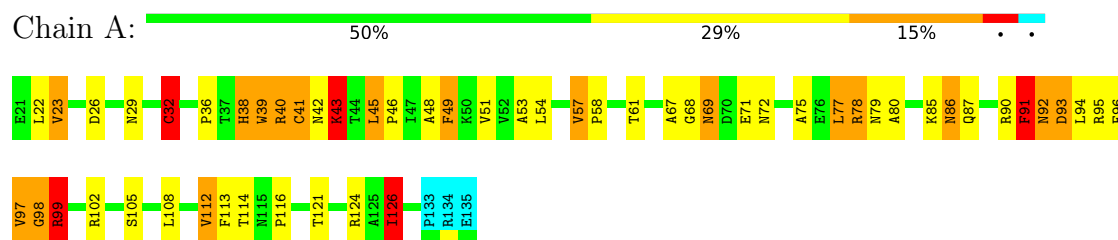
4.2.9 Score per residue for model 9

- Molecule 1: CORE BINDING FACTOR ALPHA



4.2.10 Score per residue for model 10 (medoid)

• Molecule 1: CORE BINDING FACTOR ALPHA



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 10 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
OPAL	refinement	2.6

No chemical shift data was provided.

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	1.21±0.02	0±0/882 (0.0± 0.0%)	1.99±0.05	26±7/1203 (2.1± 0.6%)
All	All	1.21	2/8820 (0.0%)	1.99	256/12030 (2.1%)

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	0.4±0.7
All	All	0	4

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	116	PRO	CA-C	5.06	1.56	1.52	7	2

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	96	PHE	CA-CB-CG	11.86	125.66	113.80	3	10
1	A	32	CYS	N-CA-C	9.82	122.94	108.60	10	1
1	A	38	HIS	CA-CB-CG	9.03	122.83	113.80	8	5
1	A	91	PHE	CA-CB-CG	8.37	122.17	113.80	6	7
1	A	130	VAL	CA-C-N	8.30	131.75	120.38	3	3
1	A	130	VAL	C-N-CA	8.30	131.75	120.38	3	3
1	A	30	PHE	CA-CB-CG	8.16	121.97	113.80	2	3
1	A	72	ASN	CA-CB-CG	7.89	120.49	112.60	5	1
1	A	97	VAL	CA-C-N	7.87	128.85	120.03	7	6
1	A	97	VAL	C-N-CA	7.87	128.85	120.03	7	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	113	PHE	CA-CB-CG	7.86	121.66	113.80	4	4
1	A	27	SER	N-CA-C	7.71	115.16	108.22	2	1
1	A	42	ASN	CA-CB-CG	7.64	120.24	112.60	7	2
1	A	86	ASN	CA-CB-CG	7.40	120.00	112.60	5	1
1	A	43	LYS	CA-C-N	7.12	130.04	120.65	7	3
1	A	43	LYS	C-N-CA	7.12	130.04	120.65	7	3
1	A	112	VAL	CA-C-N	7.04	134.98	121.54	4	4
1	A	112	VAL	C-N-CA	7.04	134.98	121.54	4	4
1	A	131	ASP	CA-CB-CG	7.01	119.61	112.60	3	1
1	A	98	GLY	N-CA-C	6.95	126.50	115.66	5	1
1	A	99	ARG	CA-C-N	6.95	134.81	121.54	6	4
1	A	99	ARG	C-N-CA	6.95	134.81	121.54	6	4
1	A	80	ALA	CA-C-N	6.93	132.70	122.86	7	2
1	A	80	ALA	C-N-CA	6.93	132.70	122.86	7	2
1	A	95	ARG	CD-NE-CZ	6.83	133.96	124.40	5	1
1	A	92	ASN	CA-CB-CG	6.81	119.41	112.60	10	1
1	A	98	GLY	CA-C-N	6.80	134.53	121.54	4	2
1	A	98	GLY	C-N-CA	6.80	134.53	121.54	4	2
1	A	92	ASN	CA-C-N	6.55	131.82	120.68	1	2
1	A	92	ASN	C-N-CA	6.55	131.82	120.68	1	2
1	A	123	HIS	CA-C-N	6.51	131.98	122.41	2	2
1	A	123	HIS	C-N-CA	6.51	131.98	122.41	2	2
1	A	46	PRO	CA-C-N	6.48	132.43	122.25	2	2
1	A	46	PRO	C-N-CA	6.48	132.43	122.25	2	2
1	A	65	VAL	CA-CB-CG2	6.43	121.34	110.40	6	1
1	A	106	PHE	CA-CB-CG	6.36	120.16	113.80	7	3
1	A	69	ASN	CA-C-N	6.28	129.01	120.54	3	4
1	A	69	ASN	C-N-CA	6.28	129.01	120.54	3	4
1	A	28	PRO	CA-C-N	6.21	133.39	121.54	5	5
1	A	28	PRO	C-N-CA	6.21	133.39	121.54	5	5
1	A	89	ALA	CA-C-N	6.06	132.03	122.21	6	1
1	A	89	ALA	C-N-CA	6.06	132.03	122.21	6	1
1	A	93	ASP	CA-C-N	6.06	133.11	121.54	4	3
1	A	93	ASP	C-N-CA	6.06	133.11	121.54	4	3
1	A	86	ASN	CA-C-N	6.06	133.11	121.54	5	2
1	A	86	ASN	C-N-CA	6.06	133.11	121.54	5	2
1	A	25	THR	CA-C-N	6.02	133.03	121.54	9	2
1	A	25	THR	C-N-CA	6.02	133.03	121.54	9	2
1	A	45	LEU	N-CA-C	6.00	113.41	108.07	10	1
1	A	72	ASN	CA-C-N	5.91	132.82	121.54	8	1
1	A	72	ASN	C-N-CA	5.91	132.82	121.54	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	38	HIS	CB-CG-CD2	-5.90	123.53	131.20	4	4
1	A	70	ASP	CA-C-N	5.87	132.75	121.54	4	3
1	A	70	ASP	C-N-CA	5.87	132.75	121.54	4	3
1	A	42	ASN	CA-C-N	5.86	132.74	121.54	10	4
1	A	42	ASN	C-N-CA	5.86	132.74	121.54	10	4
1	A	123	HIS	CA-CB-CG	5.85	119.65	113.80	4	2
1	A	33	SER	CA-C-N	5.81	132.43	121.97	4	4
1	A	33	SER	C-N-CA	5.81	132.43	121.97	4	4
1	A	70	ASP	CA-CB-CG	5.80	118.40	112.60	8	2
1	A	41	CYS	CA-C-N	5.73	132.48	121.54	4	1
1	A	41	CYS	C-N-CA	5.73	132.48	121.54	4	1
1	A	67	ALA	CA-C-N	5.72	128.64	121.83	10	1
1	A	67	ALA	C-N-CA	5.72	128.64	121.83	10	1
1	A	42	ASN	OD1-CG-ND2	-5.70	116.90	122.60	2	2
1	A	95	ARG	NH1-CZ-NH2	-5.68	111.91	119.30	9	1
1	A	49	PHE	CA-CB-CG	5.66	119.46	113.80	10	4
1	A	24	ARG	NH1-CZ-NH2	-5.63	111.98	119.30	7	1
1	A	68	GLY	CA-C-N	5.62	132.28	121.54	10	2
1	A	68	GLY	C-N-CA	5.62	132.28	121.54	10	2
1	A	37	THR	CA-C-N	5.58	132.20	121.54	3	1
1	A	37	THR	C-N-CA	5.58	132.20	121.54	3	1
1	A	23	VAL	CA-CB-CG2	5.57	119.86	110.40	1	1
1	A	79	ASN	CA-CB-CG	5.57	118.17	112.60	7	3
1	A	73	TYR	CA-C-N	5.53	132.11	121.54	2	3
1	A	73	TYR	C-N-CA	5.53	132.11	121.54	2	3
1	A	100	SER	N-CA-C	5.49	122.50	110.80	6	1
1	A	125	ALA	CA-C-N	5.49	131.85	121.97	6	3
1	A	125	ALA	C-N-CA	5.49	131.85	121.97	6	3
1	A	36	PRO	CA-C-N	5.44	130.13	122.46	5	1
1	A	36	PRO	C-N-CA	5.44	130.13	122.46	5	1
1	A	109	THR	N-CA-C	5.40	117.62	109.41	3	1
1	A	86	ASN	OD1-CG-ND2	-5.37	117.23	122.60	6	1
1	A	26	ASP	CA-CB-CG	5.36	117.96	112.60	1	1
1	A	91	PHE	CA-C-N	5.36	131.77	121.54	5	1
1	A	91	PHE	C-N-CA	5.36	131.77	121.54	5	1
1	A	104	LYS	CA-C-N	5.35	130.32	122.77	2	1
1	A	104	LYS	C-N-CA	5.35	130.32	122.77	2	1
1	A	124	ARG	N-CA-C	5.35	117.86	111.71	4	1
1	A	115	ASN	CA-C-N	5.34	125.88	120.38	6	1
1	A	115	ASN	C-N-CA	5.34	125.88	120.38	6	1
1	A	65	VAL	CA-CB-CG1	5.34	119.47	110.40	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	75	ALA	N-CA-C	5.33	120.97	113.56	10	1
1	A	21	GLU	CA-C-N	5.31	131.34	122.20	1	2
1	A	21	GLU	C-N-CA	5.31	131.34	122.20	1	2
1	A	92	ASN	OD1-CG-ND2	-5.30	117.30	122.60	9	1
1	A	72	ASN	CB-CA-C	5.28	120.94	110.42	5	1
1	A	76	GLU	N-CA-C	5.27	117.13	110.33	3	1
1	A	51	VAL	CB-CA-C	5.21	117.46	110.42	3	1
1	A	118	GLN	OE1-CD-NE2	-5.21	117.39	122.60	5	1
1	A	23	VAL	CA-C-N	5.21	128.61	120.75	10	1
1	A	23	VAL	C-N-CA	5.21	128.61	120.75	10	1
1	A	75	ALA	CA-C-N	5.20	131.47	121.54	1	1
1	A	75	ALA	C-N-CA	5.20	131.47	121.54	1	1
1	A	71	GLU	CA-C-N	5.20	131.47	121.54	10	2
1	A	71	GLU	C-N-CA	5.20	131.47	121.54	10	2
1	A	39	TRP	N-CA-C	5.20	116.19	108.60	2	1
1	A	56	ASP	CA-C-N	5.17	131.69	122.13	9	1
1	A	56	ASP	C-N-CA	5.17	131.69	122.13	9	1
1	A	94	LEU	N-CA-C	5.14	117.89	110.28	10	1
1	A	102	ARG	CD-NE-CZ	5.13	131.58	124.40	4	1
1	A	32	CYS	CA-C-N	5.13	131.12	123.23	9	1
1	A	32	CYS	C-N-CA	5.13	131.12	123.23	9	1
1	A	126	ILE	CA-C-N	5.11	130.81	122.07	10	1
1	A	126	ILE	C-N-CA	5.11	130.81	122.07	10	1
1	A	66	MET	N-CA-C	5.09	116.73	109.14	3	1
1	A	132	GLY	CA-C-N	5.07	124.56	119.19	8	1
1	A	132	GLY	C-N-CA	5.07	124.56	119.19	8	1
1	A	35	LEU	CA-C-N	5.07	125.00	119.78	4	1
1	A	35	LEU	C-N-CA	5.07	125.00	119.78	4	1
1	A	81	THR	CA-CB-CG2	5.06	119.10	110.50	6	1
1	A	91	PHE	N-CA-C	5.05	115.81	108.14	1	1
1	A	101	GLY	CA-C-N	5.04	129.21	121.19	5	1
1	A	101	GLY	C-N-CA	5.04	129.21	121.19	5	1
1	A	39	TRP	CA-CB-CG	5.04	123.18	113.60	10	1
1	A	61	THR	CA-CB-CG2	5.01	119.01	110.50	9	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	24	ARG	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	73	TYR	Sidechain	1
1	A	122	TYR	Sidechain	1
1	A	78	ARG	Sidechain	1

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	864	870	871	17±5
All	All	8640	8700	8710	171

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:LEU:HB2	1:A:80:ALA:HB3	0.97	1.31	5	7
1:A:67:ALA:HB1	1:A:105:SER:HB2	0.82	1.52	3	1
1:A:80:ALA:HA	1:A:94:LEU:HB2	0.77	1.57	8	4
1:A:65:VAL:HG22	1:A:80:ALA:HB1	0.76	1.57	6	2
1:A:43:LYS:H	1:A:95:ARG:HG2	0.74	1.41	5	1
1:A:108:LEU:HB3	1:A:122:TYR:HB2	0.71	1.61	2	1
1:A:122:TYR:CE1	1:A:124:ARG:HB2	0.71	2.20	4	2
1:A:80:ALA:HB2	1:A:95:ARG:H	0.68	1.48	9	1
1:A:35:LEU:HB2	1:A:36:PRO:HD2	0.67	1.67	3	1
1:A:38:HIS:HB2	1:A:127:LYS:O	0.67	1.88	3	1
1:A:78:ARG:O	1:A:95:ARG:HB2	0.66	1.89	2	4
1:A:106:PHE:CE1	1:A:108:LEU:HB2	0.66	2.26	1	1
1:A:66:MET:HG2	1:A:77:LEU:HB3	0.63	1.71	5	1
1:A:25:THR:H	1:A:30:PHE:HB2	0.63	1.54	9	1
1:A:67:ALA:HB2	1:A:97:VAL:HG12	0.62	1.70	3	1
1:A:114:THR:HG23	1:A:116:PRO:HD2	0.62	1.72	10	3
1:A:30:PHE:CE1	1:A:53:ALA:HB2	0.62	2.29	6	1
1:A:65:VAL:CG2	1:A:80:ALA:HB1	0.61	2.25	9	1
1:A:61:THR:CG2	1:A:84:MET:HB2	0.61	2.26	2	1
1:A:39:TRP:HB2	1:A:132:GLY:HA2	0.61	1.73	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:PRO:HB3	1:A:41:CYS:HB2	0.60	1.73	9	1
1:A:77:LEU:HB2	1:A:80:ALA:CB	0.60	2.20	5	1
1:A:87:GLN:HG2	1:A:110:ILE:HG12	0.59	1.74	9	1
1:A:27:SER:HB2	1:A:30:PHE:CE2	0.59	2.32	7	1
1:A:48:ALA:HA	1:A:92:ASN:HB2	0.59	1.74	3	1
1:A:109:THR:HG21	1:A:120:ALA:C	0.59	2.21	9	1
1:A:76:GLU:HB2	1:A:100:SER:HB2	0.59	1.72	6	1
1:A:36:PRO:HB2	1:A:38:HIS:CD2	0.58	2.33	10	1
1:A:57:VAL:HG22	1:A:58:PRO:HD2	0.58	1.75	10	1
1:A:77:LEU:HD23	1:A:80:ALA:N	0.58	2.13	10	1
1:A:87:GLN:CG	1:A:110:ILE:HG12	0.58	2.28	9	1
1:A:26:ASP:HB2	1:A:121:THR:O	0.58	1.99	10	1
1:A:32:CYS:HB2	1:A:51:VAL:HA	0.57	1.74	2	1
1:A:78:ARG:HB2	1:A:95:ARG:HD3	0.57	1.76	7	1
1:A:61:THR:HB	1:A:84:MET:HB2	0.57	1.76	4	1
1:A:80:ALA:HB2	1:A:95:ARG:N	0.57	2.14	9	6
1:A:67:ALA:HB1	1:A:105:SER:CB	0.56	2.27	3	1
1:A:35:LEU:HG	1:A:36:PRO:HD2	0.56	1.76	4	1
1:A:30:PHE:CD1	1:A:53:ALA:HB2	0.56	2.36	6	1
1:A:66:MET:HG2	1:A:74:SER:HB2	0.56	1.77	7	1
1:A:23:VAL:HG23	1:A:32:CYS:HB2	0.56	1.77	1	1
1:A:77:LEU:HB2	1:A:95:ARG:O	0.56	2.01	4	5
1:A:65:VAL:HG13	1:A:80:ALA:HB1	0.55	1.77	5	2
1:A:85:LYS:N	1:A:85:LYS:HD2	0.55	2.17	2	1
1:A:39:TRP:HB2	1:A:129:THR:HB	0.55	1.77	8	1
1:A:57:VAL:HA	1:A:87:GLN:HG2	0.55	1.79	7	1
1:A:77:LEU:HD23	1:A:80:ALA:H	0.54	1.61	10	1
1:A:69:ASN:OD1	1:A:73:TYR:HB2	0.54	2.03	2	1
1:A:58:PRO:HG2	1:A:114:THR:HG21	0.54	1.80	2	1
1:A:112:VAL:HG12	1:A:118:GLN:H	0.54	1.63	8	2
1:A:45:LEU:HD23	1:A:46:PRO:HD2	0.54	1.80	5	1
1:A:40:ARG:HG2	1:A:97:VAL:O	0.54	2.02	6	1
1:A:92:ASN:O	1:A:93:ASP:HB2	0.53	2.04	7	1
1:A:23:VAL:HB	1:A:32:CYS:HB2	0.53	1.79	7	1
1:A:65:VAL:CG1	1:A:80:ALA:HB1	0.53	2.33	5	1
1:A:95:ARG:HD2	1:A:98:GLY:HA3	0.53	1.80	8	1
1:A:40:ARG:CD	1:A:100:SER:HB2	0.53	2.34	2	1
1:A:63:VAL:HG12	1:A:110:ILE:HG12	0.52	1.80	8	1
1:A:72:ASN:ND2	1:A:73:TYR:H	0.52	2.02	5	1
1:A:37:THR:O	1:A:106:PHE:HB2	0.52	2.05	8	1
1:A:79:ASN:ND2	1:A:95:ARG:HH21	0.52	2.03	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:MET:HB2	1:A:107:THR:HG23	0.51	1.82	6	1
1:A:70:ASP:HB2	1:A:106:PHE:CD1	0.51	2.41	6	1
1:A:65:VAL:HG23	1:A:96:PHE:HB3	0.51	1.82	6	1
1:A:33:SER:HB2	1:A:50:LYS:HB2	0.51	1.82	3	1
1:A:112:VAL:CG1	1:A:118:GLN:H	0.51	2.19	2	3
1:A:40:ARG:HD2	1:A:100:SER:HB2	0.51	1.82	2	1
1:A:75:ALA:O	1:A:76:GLU:HB2	0.50	2.05	5	1
1:A:43:LYS:HB2	1:A:95:ARG:HB2	0.50	1.82	7	1
1:A:67:ALA:HB2	1:A:97:VAL:CG1	0.50	2.36	3	1
1:A:77:LEU:HB3	1:A:80:ALA:HB2	0.50	1.82	8	1
1:A:122:TYR:HE1	1:A:124:ARG:HB2	0.50	1.62	4	1
1:A:27:SER:OG	1:A:28:PRO:HD2	0.50	2.06	8	1
1:A:33:SER:HB2	1:A:50:LYS:CG	0.50	2.37	2	1
1:A:65:VAL:HG22	1:A:80:ALA:CB	0.49	2.34	6	1
1:A:24:ARG:HB2	1:A:30:PHE:CG	0.49	2.43	2	1
1:A:108:LEU:CB	1:A:122:TYR:HB2	0.49	2.34	2	1
1:A:79:ASN:HD22	1:A:95:ARG:HH21	0.49	1.50	9	1
1:A:57:VAL:HG13	1:A:58:PRO:HD2	0.49	1.84	9	1
1:A:76:GLU:CB	1:A:100:SER:HB2	0.49	2.37	6	1
1:A:114:THR:HG22	1:A:116:PRO:HD2	0.49	1.84	5	2
1:A:51:VAL:HG22	1:A:87:GLN:HG2	0.49	1.83	3	1
1:A:38:HIS:HB2	1:A:128:ILE:HB	0.49	1.85	8	1
1:A:112:VAL:CG1	1:A:114:THR:HG22	0.48	2.38	10	1
1:A:77:LEU:CB	1:A:80:ALA:HB3	0.48	2.39	2	2
1:A:25:THR:OG1	1:A:27:SER:HB2	0.48	2.08	8	1
1:A:86:ASN:O	1:A:87:GLN:HG2	0.48	2.09	10	1
1:A:45:LEU:HB2	1:A:46:PRO:HD2	0.48	1.85	10	1
1:A:33:SER:HB2	1:A:50:LYS:HG2	0.47	1.85	2	1
1:A:79:ASN:C	1:A:81:THR:H	0.47	2.17	7	1
1:A:77:LEU:O	1:A:78:ARG:HD2	0.47	2.10	4	1
1:A:25:THR:HA	1:A:122:TYR:HB2	0.46	1.87	4	1
1:A:43:LYS:HD2	1:A:43:LYS:C	0.46	2.35	10	1
1:A:40:ARG:HB2	1:A:101:GLY:O	0.46	2.10	8	1
1:A:62:LEU:O	1:A:110:ILE:HG12	0.46	2.11	6	1
1:A:42:ASN:HB2	1:A:96:PHE:H	0.46	1.71	2	1
1:A:77:LEU:CG	1:A:80:ALA:HB3	0.46	2.41	9	1
1:A:40:ARG:HD2	1:A:40:ARG:C	0.45	2.36	10	1
1:A:70:ASP:O	1:A:71:GLU:HB2	0.45	2.11	4	1
1:A:78:ARG:NH1	1:A:99:ARG:HB2	0.45	2.26	10	1
1:A:84:MET:C	1:A:85:LYS:HD2	0.45	2.36	8	1
1:A:41:CYS:HB2	1:A:98:GLY:C	0.45	2.37	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:PRO:HB2	1:A:96:PHE:CZ	0.45	2.46	8	1
1:A:77:LEU:HD12	1:A:80:ALA:HB3	0.45	1.88	6	1
1:A:90:ARG:O	1:A:91:PHE:HB2	0.45	2.12	10	3
1:A:66:MET:HB2	1:A:107:THR:HB	0.45	1.87	9	1
1:A:43:LYS:O	1:A:95:ARG:HG2	0.44	2.12	2	1
1:A:40:ARG:HB2	1:A:97:VAL:O	0.44	2.11	5	1
1:A:116:PRO:HB2	1:A:118:GLN:HE22	0.44	1.71	5	1
1:A:25:THR:HG22	1:A:30:PHE:HB2	0.44	1.88	1	1
1:A:61:THR:HG23	1:A:84:MET:HB2	0.44	1.88	2	1
1:A:77:LEU:C	1:A:78:ARG:HD2	0.44	2.38	2	1
1:A:42:ASN:C	1:A:95:ARG:HD2	0.44	2.38	7	1
1:A:32:CYS:CB	1:A:51:VAL:HA	0.44	2.42	10	1
1:A:103:GLY:C	1:A:127:LYS:HE2	0.44	2.38	1	1
1:A:58:PRO:HB2	1:A:112:VAL:CG1	0.44	2.43	4	1
1:A:58:PRO:HD2	1:A:87:GLN:HB3	0.44	1.90	5	1
1:A:78:ARG:HB2	1:A:95:ARG:CD	0.43	2.43	4	1
1:A:77:LEU:HD22	1:A:77:LEU:C	0.43	2.38	10	1
1:A:29:ASN:HB3	1:A:54:LEU:HB2	0.43	1.91	9	1
1:A:47:ILE:HG12	1:A:49:PHE:CZ	0.43	2.49	6	1
1:A:53:ALA:HB3	1:A:87:GLN:HB2	0.43	1.90	10	1
1:A:56:ASP:OD1	1:A:58:PRO:HD2	0.43	2.14	7	1
1:A:105:SER:HB2	1:A:126:ILE:HG13	0.43	1.89	10	1
1:A:77:LEU:HG	1:A:80:ALA:HB3	0.43	1.90	9	1
1:A:87:GLN:HG2	1:A:110:ILE:CG1	0.42	2.44	9	1
1:A:35:LEU:CB	1:A:36:PRO:HD2	0.42	2.42	3	1
1:A:95:ARG:HD2	1:A:98:GLY:CA	0.42	2.45	8	1
1:A:34:VAL:HG22	1:A:36:PRO:HD2	0.42	1.90	9	1
1:A:49:PHE:CE2	1:A:94:LEU:HB2	0.42	2.50	1	1
1:A:57:VAL:H	1:A:58:PRO:HD2	0.42	1.75	7	1
1:A:71:GLU:HG2	1:A:73:TYR:HB3	0.42	1.91	7	1
1:A:71:GLU:OE1	1:A:72:ASN:HB2	0.42	2.15	6	1
1:A:23:VAL:CG2	1:A:32:CYS:HB2	0.41	2.43	1	1
1:A:122:TYR:O	1:A:123:HIS:HB2	0.41	2.15	3	1
1:A:69:ASN:HB2	1:A:97:VAL:HG23	0.41	1.93	4	1
1:A:27:SER:N	1:A:28:PRO:CD	0.40	2.84	5	1
1:A:80:ALA:CB	1:A:95:ARG:H	0.40	2.26	9	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	111/115 (97%)	73±5 (66±5%)	25±4 (23±4%)	13±4 (11±3%)	1	7
All	All	1110/1150 (97%)	731 (66%)	253 (23%)	126 (11%)	1	7

All 51 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	23	VAL	8
1	A	73	TYR	6
1	A	72	ASN	5
1	A	76	GLU	5
1	A	126	ILE	5
1	A	91	PHE	5
1	A	38	HIS	4
1	A	48	ALA	4
1	A	61	THR	4
1	A	41	CYS	4
1	A	59	ASP	4
1	A	93	ASP	4
1	A	75	ALA	3
1	A	98	GLY	3
1	A	69	ASN	3
1	A	99	ARG	3
1	A	102	ARG	3
1	A	27	SER	3
1	A	80	ALA	2
1	A	125	ALA	2
1	A	132	GLY	2
1	A	42	ASN	2
1	A	44	THR	2
1	A	47	ILE	2
1	A	87	GLN	2
1	A	101	GLY	2
1	A	29	ASN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	43	LYS	2
1	A	92	ASN	2
1	A	100	SER	2
1	A	103	GLY	2
1	A	109	THR	2
1	A	57	VAL	2
1	A	26	ASP	2
1	A	97	VAL	2
1	A	124	ARG	1
1	A	74	SER	1
1	A	123	HIS	1
1	A	37	THR	1
1	A	60	GLY	1
1	A	71	GLU	1
1	A	113	PHE	1
1	A	25	THR	1
1	A	85	LYS	1
1	A	94	LEU	1
1	A	56	ASP	1
1	A	84	MET	1
1	A	117	PRO	1
1	A	79	ASN	1
1	A	36	PRO	1
1	A	58	PRO	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	95/98 (97%)	78±4 (82±4%)	17±4 (18±4%)	3	36
All	All	950/980 (97%)	776 (82%)	174 (18%)	3	36

All 72 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	77	LEU	8

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Mol	Chain	Res	Type	Models (Total)
1	A	22	LEU	6
1	A	78	ARG	6
1	A	56	ASP	5
1	A	99	ARG	5
1	A	35	LEU	4
1	A	118	GLN	4
1	A	131	ASP	4
1	A	40	ARG	4
1	A	54	LEU	4
1	A	65	VAL	4
1	A	94	LEU	4
1	A	124	ARG	4
1	A	115	ASN	4
1	A	43	LYS	4
1	A	128	ILE	4
1	A	39	TRP	4
1	A	91	PHE	3
1	A	112	VAL	3
1	A	126	ILE	3
1	A	47	ILE	3
1	A	84	MET	3
1	A	87	GLN	3
1	A	104	LYS	3
1	A	45	LEU	3
1	A	108	LEU	3
1	A	51	VAL	3
1	A	102	ARG	3
1	A	21	GLU	2
1	A	79	ASN	2
1	A	97	VAL	2
1	A	106	PHE	2
1	A	24	ARG	2
1	A	30	PHE	2
1	A	32	CYS	2
1	A	42	ASN	2
1	A	127	LYS	2
1	A	26	ASP	2
1	A	90	ARG	2
1	A	96	PHE	2
1	A	105	SER	2
1	A	71	GLU	2
1	A	76	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	95	ARG	2
1	A	44	THR	2
1	A	61	THR	2
1	A	85	LYS	2
1	A	62	LEU	1
1	A	113	PHE	1
1	A	59	ASP	1
1	A	123	HIS	1
1	A	31	LEU	1
1	A	66	MET	1
1	A	81	THR	1
1	A	86	ASN	1
1	A	72	ASN	1
1	A	69	ASN	1
1	A	100	SER	1
1	A	110	ILE	1
1	A	129	THR	1
1	A	38	HIS	1
1	A	27	SER	1
1	A	37	THR	1
1	A	64	THR	1
1	A	74	SER	1
1	A	50	LYS	1
1	A	70	ASP	1
1	A	73	TYR	1
1	A	29	ASN	1
1	A	49	PHE	1
1	A	57	VAL	1
1	A	93	ASP	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 oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided