



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 07:08 PM UTC

PDB ID : 1IRP / pdb_00001irp
Title : SOLUTION STRUCTURE OF HUMAN INTERLEUKIN-1 RECEPTOR
ANTAGONIST PROTEIN
Authors : Stockman, B.J.; Scahill, T.A.; Strakalaitis, N.A.
Deposited on : 1994-10-18

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

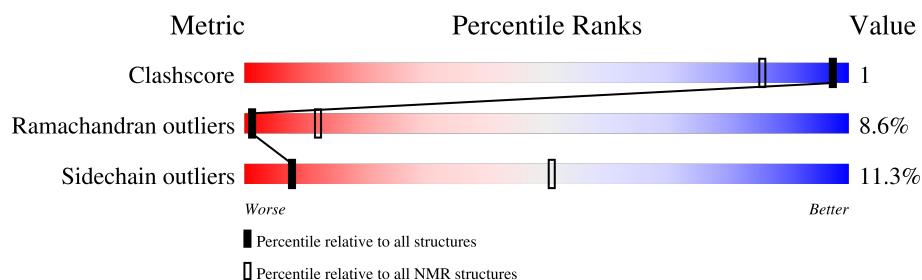
1 Overall quality at a glance

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	153	69% 29% .

2 Ensemble composition and analysis

This entry contains 12 models. Model 1 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:1-A:153 (153)	2.58	1

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, 9, 10, 11
2	6, 12

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2392 atoms, of which 1183 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called INTERLEUKIN-1 RECEPTOR ANTAGONIST.

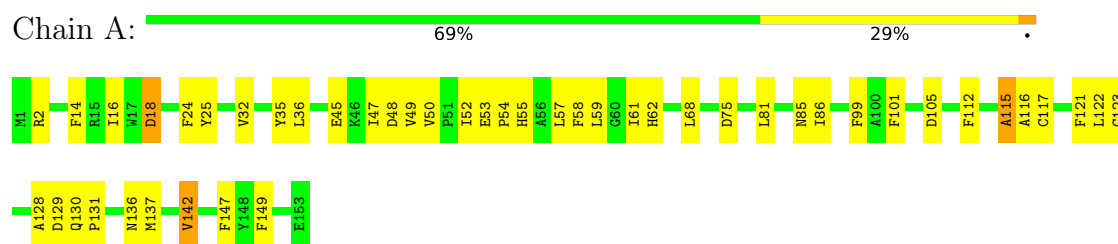
Mol	Chain	Residues	Atoms						Trace
1	A	153	Total	C	H	N	O	S	0
			2392	759	1183	208	232	10	

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: INTERLEUKIN-1 RECEPTOR ANTAGONIST

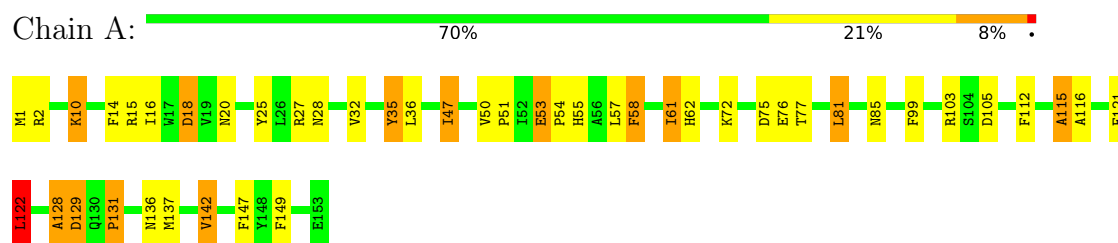


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

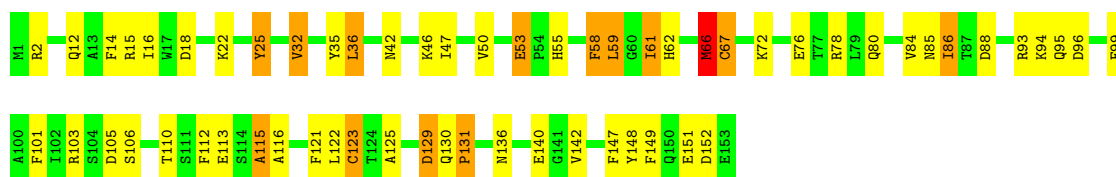
- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST



4.2.2 Score per residue for model 2

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST





4.2.3 Score per residue for model 3

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST

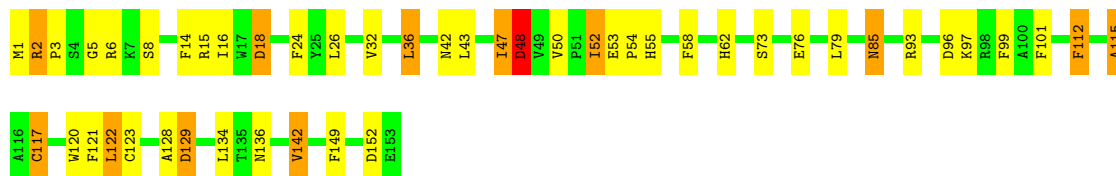
Chain A: 66% 28% 5% •



4.2.4 Score per residue for model 4

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST

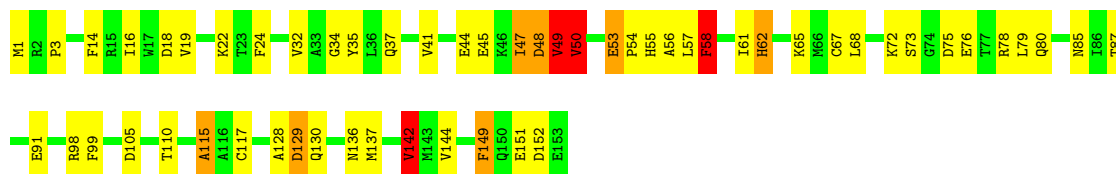
Chain A: 69% 23% 8% •



4.2.5 Score per residue for model 5

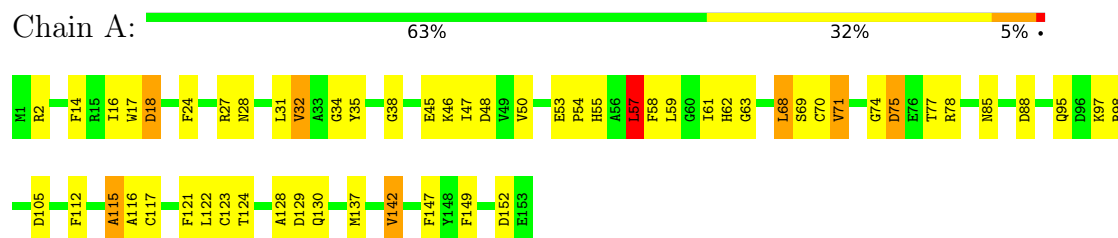
- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST

Chain A: 63% 29% 5% •



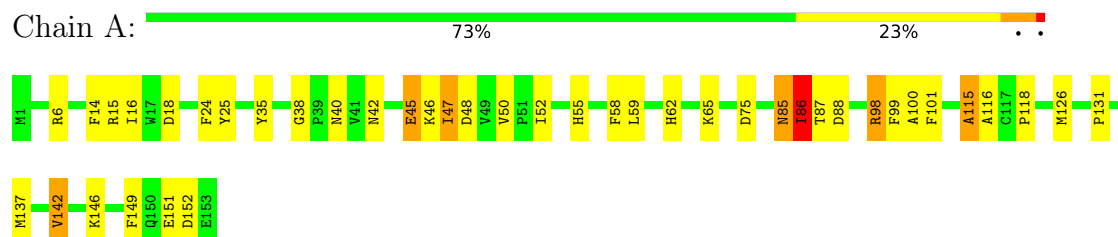
4.2.6 Score per residue for model 6

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST



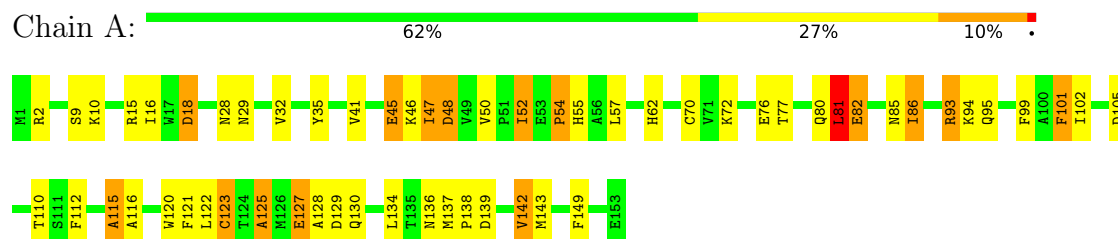
4.2.7 Score per residue for model 7

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST



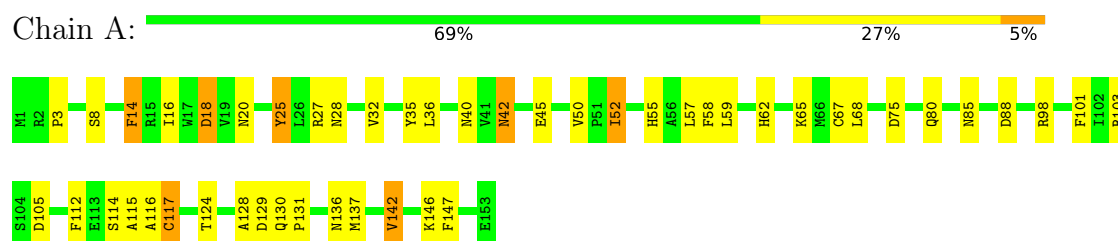
4.2.8 Score per residue for model 8

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST



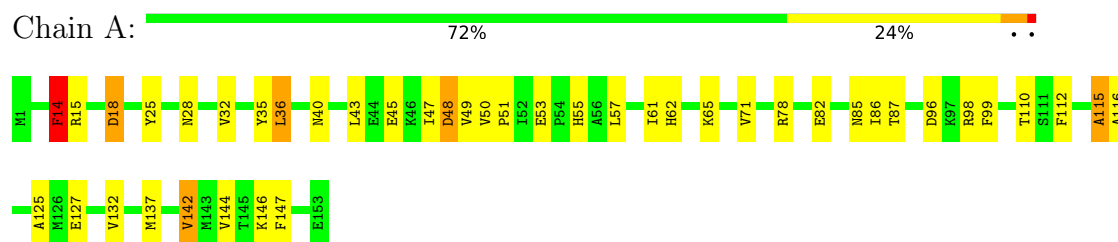
4.2.9 Score per residue for model 9

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST



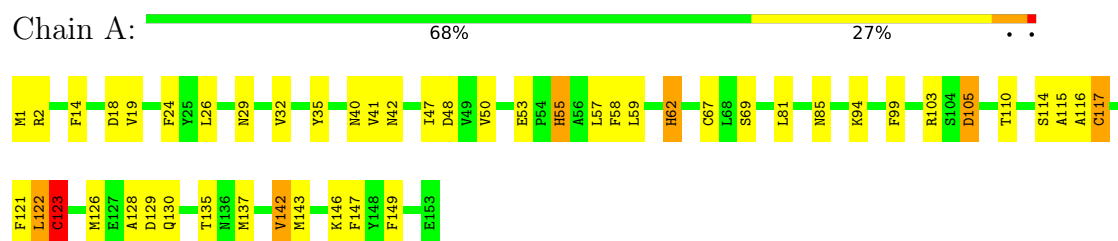
4.2.10 Score per residue for model 10

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST



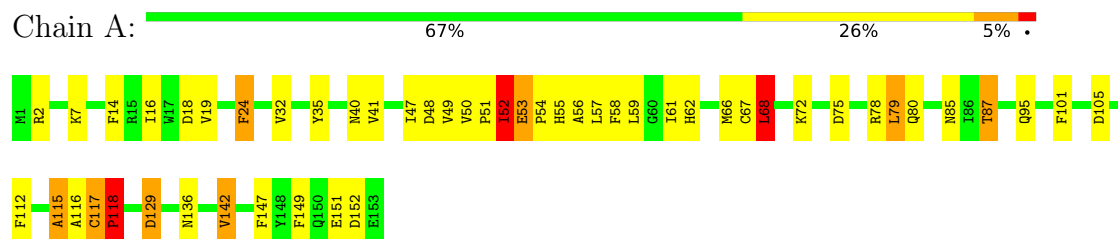
4.2.11 Score per residue for model 11

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST



4.2.12 Score per residue for model 12

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 12 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DGII	refinement	

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	1.97±0.02	9±3/1234 (0.8± 0.2%)	1.91±0.02	32±4/1664 (1.9± 0.2%)
All	All	1.97	113/14808 (0.8%)	1.91	381/19968 (1.9%)

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	2.8±1.4
All	All	0	33

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	28	ASN	CA-C	8.24	1.57	1.52	9	4
1	A	52	ILE	CA-C	7.32	1.62	1.52	12	3
1	A	53	GLU	CA-C	7.24	1.59	1.52	2	5
1	A	50	VAL	CA-C	7.06	1.57	1.52	4	11
1	A	129	ASP	CA-C	6.94	1.58	1.52	5	1
1	A	93	ARG	CA-C	6.59	1.56	1.52	2	1
1	A	130	GLN	CA-C	6.30	1.58	1.52	11	7
1	A	32	VAL	CA-C	6.25	1.58	1.52	10	2
1	A	50	VAL	N-CA	6.24	1.50	1.45	12	5
1	A	84	VAL	CA-C	6.18	1.58	1.52	2	1
1	A	137	MET	CA-C	6.15	1.58	1.52	1	5
1	A	22	LYS	CA-C	6.00	1.59	1.52	5	1
1	A	50	VAL	CA-CB	5.97	1.58	1.54	12	1
1	A	75	ASP	CA-C	5.93	1.58	1.52	5	4
1	A	47	ILE	CA-C	5.89	1.59	1.52	1	3
1	A	118	PRO	CA-C	5.70	1.58	1.52	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	68	LEU	CA-C	5.68	1.59	1.52	5	2
1	A	121	PHE	CA-C	5.67	1.59	1.52	1	1
1	A	54	PRO	CA-C	5.65	1.58	1.53	5	2
1	A	41	VAL	CA-C	5.62	1.57	1.52	12	2
1	A	127	GLU	CA-C	5.60	1.58	1.53	8	1
1	A	105	ASP	CA-C	5.59	1.60	1.52	5	1
1	A	55	HIS	ND1-CE1	5.53	1.38	1.32	5	7
1	A	122	LEU	CA-C	5.53	1.60	1.52	4	1
1	A	35	TYR	CA-C	5.52	1.59	1.52	9	1
1	A	35	TYR	CA-CB	5.50	1.58	1.53	1	1
1	A	62	HIS	ND1-CE1	5.46	1.38	1.32	3	9
1	A	6	ARG	CA-CB	5.45	1.57	1.53	7	1
1	A	51	PRO	CA-C	5.43	1.58	1.52	1	2
1	A	134	LEU	CA-C	5.41	1.59	1.52	3	1
1	A	15	ARG	CA-C	5.39	1.59	1.52	7	2
1	A	27	ARG	CA-C	5.38	1.57	1.52	6	4
1	A	117	CYS	CA-C	5.37	1.59	1.52	9	1
1	A	55	HIS	CA-C	5.34	1.59	1.52	12	1
1	A	39	PRO	CA-C	5.30	1.57	1.52	3	1
1	A	116	ALA	CA-C	5.30	1.59	1.52	11	2
1	A	16	ILE	CA-C	5.29	1.59	1.52	7	1
1	A	57	LEU	N-CA	5.29	1.53	1.46	6	1
1	A	132	VAL	CA-C	5.23	1.58	1.52	10	1
1	A	49	VAL	CA-C	5.22	1.59	1.52	5	1
1	A	86	ILE	CA-C	5.22	1.59	1.52	2	1
1	A	2	ARG	CA-C	5.21	1.59	1.52	11	1
1	A	137	MET	N-CA	5.17	1.50	1.45	1	1
1	A	144	VAL	CA-C	5.16	1.57	1.53	10	2
1	A	62	HIS	CG-CD2	5.14	1.41	1.35	3	2
1	A	123	CYS	CA-C	5.09	1.59	1.52	11	1
1	A	98	ARG	CA-C	5.05	1.59	1.52	5	1
1	A	55	HIS	CG-CD2	5.03	1.41	1.35	6	1
1	A	94	LYS	CA-C	5.02	1.58	1.53	8	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	14	PHE	CA-CB-CG	15.71	129.51	113.80	10	3
1	A	18	ASP	CA-CB-CG	13.42	126.02	112.60	4	12
1	A	48	ASP	CA-CB-CG	12.14	124.74	112.60	5	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	62	HIS	ND1-CE1-NE2	11.97	120.37	108.40	3	12
1	A	149	PHE	CA-CB-CG	11.94	125.74	113.80	5	8
1	A	55	HIS	ND1-CE1-NE2	11.89	120.29	108.40	9	12
1	A	122	LEU	N-CA-C	11.05	134.34	110.80	1	1
1	A	42	ASN	CA-CB-CG	11.01	123.61	112.60	9	3
1	A	152	ASP	CA-CB-CG	10.26	122.86	112.60	2	2
1	A	112	PHE	CA-CB-CG	9.75	123.55	113.80	8	9
1	A	147	PHE	CA-CB-CG	9.58	123.38	113.80	12	6
1	A	58	PHE	CA-CB-CG	9.49	123.29	113.80	1	10
1	A	128	ALA	N-CA-C	9.46	124.64	112.34	11	3
1	A	62	HIS	CE1-NE2-CD2	-9.40	99.60	109.00	3	12
1	A	55	HIS	CE1-NE2-CD2	-9.28	99.72	109.00	9	12
1	A	118	PRO	CB-CA-C	9.24	126.81	111.56	12	2
1	A	105	ASP	CA-CB-CG	9.14	121.74	112.60	12	7
1	A	99	PHE	CA-CB-CG	9.10	122.90	113.80	11	8
1	A	129	ASP	CA-CB-CG	8.86	121.46	112.60	5	7
1	A	85	ASN	CA-CB-CG	8.72	121.33	112.60	4	12
1	A	28	ASN	CA-CB-CG	8.43	121.03	112.60	8	2
1	A	24	PHE	CA-CB-CG	8.35	122.15	113.80	12	7
1	A	121	PHE	CA-CB-CG	8.31	122.11	113.80	11	6
1	A	136	ASN	CA-CB-CG	8.12	120.72	112.60	9	7
1	A	40	ASN	CA-CB-CG	8.04	120.64	112.60	7	4
1	A	101	PHE	CA-CB-CG	7.74	121.54	113.80	2	6
1	A	75	ASP	CA-CB-CG	7.68	120.28	112.60	1	4
1	A	114	SER	N-CA-CB	-7.65	99.30	110.70	11	2
1	A	117	CYS	N-CA-C	-7.35	93.57	109.81	11	2
1	A	125	ALA	N-CA-C	7.34	119.78	110.24	2	2
1	A	142	VAL	CA-CB-CG1	7.31	122.83	110.40	1	11
1	A	122	LEU	N-CA-CB	-7.03	98.62	110.49	1	1
1	A	14	PHE	N-CA-CB	-6.99	99.63	111.31	6	6
1	A	149	PHE	N-CA-CB	-6.92	98.97	110.39	6	5
1	A	52	ILE	CB-CA-C	6.88	122.58	111.29	8	2
1	A	115	ALA	N-CA-C	-6.83	96.25	110.80	4	12
1	A	115	ALA	CB-CA-C	6.82	123.99	110.42	2	9
1	A	126	MET	N-CA-C	6.81	120.07	111.69	11	2
1	A	118	PRO	N-CA-CB	-6.78	96.13	103.25	12	1
1	A	49	VAL	N-CA-C	6.74	117.87	108.23	10	1
1	A	121	PHE	N-CA-C	6.70	119.75	108.02	1	1
1	A	128	ALA	N-CA-CB	-6.65	99.25	110.49	1	5
1	A	142	VAL	CB-CA-C	6.64	117.36	111.71	10	2
1	A	38	GLY	N-CA-C	6.62	125.84	112.34	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	47	ILE	N-CA-CB	6.60	122.12	111.23	7	3
1	A	131	PRO	N-CA-CB	-6.55	96.38	103.25	1	5
1	A	66	MET	N-CA-CB	6.50	121.48	110.49	2	2
1	A	82	GLU	N-CA-C	6.48	117.13	108.38	8	1
1	A	29	ASN	CA-CB-CG	6.42	119.02	112.60	11	2
1	A	22	LYS	CB-CA-C	6.40	121.08	109.37	5	1
1	A	86	ILE	CB-CA-C	6.38	121.76	111.29	7	1
1	A	82	GLU	N-CA-CB	-6.33	101.46	110.58	3	2
1	A	47	ILE	CB-CA-C	6.30	120.01	110.62	5	2
1	A	62	HIS	CG-ND1-CE1	-6.30	98.59	109.30	10	12
1	A	25	TYR	CA-CB-CG	6.28	125.20	113.90	3	3
1	A	14	PHE	N-CA-C	6.27	118.38	108.79	7	2
1	A	71	VAL	CA-CB-CG1	6.21	120.97	110.40	6	1
1	A	142	VAL	N-CA-CB	-6.19	106.56	111.64	11	2
1	A	55	HIS	CG-ND1-CE1	-6.17	98.81	109.30	5	12
1	A	69	SER	N-CA-CB	-6.14	101.05	111.31	6	2
1	A	61	ILE	N-CA-CB	6.10	121.30	111.23	1	2
1	A	88	ASP	CA-CB-CG	6.00	118.60	112.60	9	1
1	A	117	CYS	CB-CA-C	5.98	121.95	110.17	11	3
1	A	62	HIS	CB-CG-CD2	-5.89	123.55	131.20	4	4
1	A	59	LEU	N-CA-C	5.83	119.07	109.85	9	2
1	A	20	ASN	CA-CB-CG	5.81	118.41	112.60	9	2
1	A	50	VAL	CA-C-O	-5.81	116.92	119.94	12	1
1	A	88	ASP	N-CA-CB	-5.81	101.56	109.98	2	3
1	A	102	ILE	N-CA-CB	5.79	117.61	111.00	8	1
1	A	59	LEU	N-CA-CB	5.79	120.27	110.49	2	1
1	A	57	LEU	N-CA-C	5.78	117.03	108.60	8	2
1	A	62	HIS	CA-CB-CG	5.75	119.55	113.80	5	3
1	A	96	ASP	N-CA-CB	-5.72	102.47	110.25	4	1
1	A	61	ILE	N-CA-C	-5.64	97.61	109.34	2	1
1	A	42	ASN	OD1-CG-ND2	-5.63	116.97	122.60	9	1
1	A	96	ASP	CA-CB-CG	5.59	118.19	112.60	4	3
1	A	53	GLU	O-C-N	-5.59	117.11	121.14	3	2
1	A	36	LEU	N-CA-CB	-5.58	101.06	110.49	3	1
1	A	76	GLU	N-CA-CB	-5.54	102.03	110.45	1	1
1	A	48	ASP	N-CA-CB	-5.52	101.17	110.49	4	2
1	A	55	HIS	CA-CB-CG	5.51	119.31	113.80	6	2
1	A	49	VAL	CB-CA-C	5.51	120.33	111.29	5	1
1	A	55	HIS	CB-CG-CD2	-5.51	124.04	131.20	1	4
1	A	122	LEU	CA-C-O	-5.50	112.65	120.51	1	1
1	A	138	PRO	N-CA-C	5.49	119.83	111.11	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	139	ASP	CA-CB-CG	5.46	118.06	112.60	8	1
1	A	113	GLU	O-C-N	-5.42	116.67	122.85	2	1
1	A	112	PHE	N-CA-C	5.39	117.18	108.34	4	1
1	A	51	PRO	N-CA-C	5.39	119.65	111.19	10	1
1	A	110	THR	N-CA-C	5.38	115.38	108.34	11	1
1	A	53	GLU	CB-CA-C	5.37	120.74	110.17	5	1
1	A	87	THR	N-CA-C	-5.35	99.40	110.80	12	1
1	A	3	PRO	N-CA-C	5.35	119.70	112.48	9	1
1	A	54	PRO	N-CA-CB	-5.34	97.64	103.25	8	1
1	A	45	GLU	N-CA-C	5.33	119.63	113.18	8	1
1	A	49	VAL	CA-CB-CG1	5.28	119.37	110.40	5	1
1	A	48	ASP	N-CA-C	5.26	117.53	109.07	7	1
1	A	80	GLN	OE1-CD-NE2	-5.22	117.38	122.60	9	1
1	A	78	ARG	N-CA-CB	-5.21	102.62	111.69	6	1
1	A	39	PRO	CB-CA-C	5.21	116.14	111.40	3	1
1	A	102	ILE	CB-CA-C	5.20	117.91	110.84	3	1
1	A	36	LEU	N-CA-C	5.18	119.47	113.20	2	1
1	A	52	ILE	O-C-N	-5.18	116.10	122.57	12	1
1	A	114	SER	N-CA-C	5.10	117.64	110.14	11	1
1	A	67	CYS	N-CA-C	5.10	117.21	108.90	2	1
1	A	81	LEU	CB-CA-C	5.09	120.56	110.42	8	1
1	A	152	ASP	N-CA-C	5.09	116.47	109.15	4	1
1	A	45	GLU	N-CA-CB	-5.08	101.90	110.49	7	1
1	A	32	VAL	CA-CB-CG2	5.08	119.03	110.40	6	2
1	A	105	ASP	N-CA-C	5.08	117.73	109.86	2	1
1	A	58	PHE	N-CA-C	5.06	116.00	108.86	1	1
1	A	100	ALA	N-CA-CB	-5.06	103.42	111.62	7	1
1	A	121	PHE	CA-C-N	5.05	131.18	121.54	1	1
1	A	121	PHE	C-N-CA	5.05	131.18	121.54	1	1
1	A	93	ARG	CA-CB-CG	5.04	124.17	114.10	3	1
1	A	130	GLN	CB-CA-C	5.03	120.07	110.17	3	1
1	A	117	CYS	CA-C-N	5.02	126.12	119.84	12	1
1	A	117	CYS	C-N-CA	5.02	126.12	119.84	12	1
1	A	50	VAL	CB-CA-C	5.02	116.09	110.52	7	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	2	ARG	Sidechain	5

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	103	ARG	Sidechain	5
1	A	14	PHE	Sidechain	4
1	A	25	TYR	Sidechain	4
1	A	15	ARG	Sidechain	3
1	A	35	TYR	Sidechain	3
1	A	93	ARG	Sidechain	2
1	A	98	ARG	Sidechain	2
1	A	148	TYR	Sidechain	1
1	A	49	VAL	Mainchain	1
1	A	78	ARG	Sidechain	1
1	A	101	PHE	Sidechain	1
1	A	117	CYS	Mainchain	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	1209	1183	1183	2±1
All	All	14508	14196	14196	18

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ILE:HG23	1:A:48:ASP:H	0.62	1.53	4	1
1:A:123:CYS:SG	1:A:143:MET:HB3	0.51	2.46	8	2
1:A:123:CYS:SG	1:A:147:PHE:CD1	0.50	3.05	2	1
1:A:66:MET:SD	1:A:79:LEU:O	0.48	2.71	12	1
1:A:1:MET:SD	1:A:67:CYS:SG	0.47	3.12	5	2
1:A:86:ILE:HG23	1:A:87:THR:H	0.46	1.70	7	1
1:A:70:CYS:SG	1:A:77:THR:HG22	0.46	2.51	8	2
1:A:52:ILE:HG22	1:A:53:GLU:H	0.43	1.74	12	1
1:A:67:CYS:SG	1:A:68:LEU:N	0.42	2.93	12	1
1:A:81:LEU:HD13	1:A:81:LEU:H	0.41	1.76	1	1
1:A:70:CYS:SG	1:A:77:THR:CG2	0.41	3.09	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:VAL:HG13	1:A:58:PHE:O	0.40	2.16	5	1
1:A:122:LEU:HD22	1:A:123:CYS:SG	0.40	2.57	3	1
1:A:66:MET:SD	1:A:67:CYS:HB2	0.40	2.56	2	1
1:A:123:CYS:SG	1:A:143:MET:CB	0.40	3.10	8	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	151/153 (99%)	105±4 (70±3%)	33±4 (22±2%)	13±4 (9±3%)	1	12
All	All	1812/1836 (99%)	1265 (70%)	391 (22%)	156 (9%)	1	12

All 63 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	115	ALA	10
1	A	116	ALA	8
1	A	122	LEU	7
1	A	129	ASP	6
1	A	123	CYS	6
1	A	36	LEU	5
1	A	117	CYS	5
1	A	57	LEU	4
1	A	95	GLN	4
1	A	19	VAL	4
1	A	45	GLU	4
1	A	137	MET	4
1	A	48	ASP	4
1	A	52	ILE	4
1	A	54	PRO	4
1	A	53	GLU	3
1	A	61	ILE	3
1	A	86	ILE	3

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Mol	Chain	Res	Type	Models (Total)
1	A	47	ILE	3
1	A	87	THR	3
1	A	68	LEU	3
1	A	99	PHE	2
1	A	131	PRO	2
1	A	66	MET	2
1	A	106	SER	2
1	A	142	VAL	2
1	A	74	GLY	2
1	A	3	PRO	2
1	A	8	SER	2
1	A	42	ASN	2
1	A	34	GLY	2
1	A	41	VAL	2
1	A	49	VAL	2
1	A	56	ALA	2
1	A	62	HIS	2
1	A	152	ASP	2
1	A	80	GLN	2
1	A	125	ALA	2
1	A	10	LYS	1
1	A	128	ALA	1
1	A	59	LEU	1
1	A	11	MET	1
1	A	65	LYS	1
1	A	107	GLY	1
1	A	2	ARG	1
1	A	5	GLY	1
1	A	50	VAL	1
1	A	31	LEU	1
1	A	63	GLY	1
1	A	75	ASP	1
1	A	98	ARG	1
1	A	38	GLY	1
1	A	85	ASN	1
1	A	9	SER	1
1	A	81	LEU	1
1	A	67	CYS	1
1	A	127	GLU	1
1	A	55	HIS	1
1	A	94	LYS	1
1	A	135	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	7	LYS	1
1	A	40	ASN	1
1	A	118	PRO	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	134/134 (100%)	119±4 (89±3%)	15±4 (11±3%)	8	51
All	All	1608/1608 (100%)	1427 (89%)	181 (11%)	8	51

All 69 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	32	VAL	10
1	A	142	VAL	10
1	A	16	ILE	8
1	A	35	TYR	7
1	A	18	ASP	6
1	A	47	ILE	5
1	A	72	LYS	5
1	A	46	LYS	5
1	A	76	GLU	5
1	A	146	LYS	5
1	A	81	LEU	4
1	A	36	LEU	4
1	A	110	THR	4
1	A	151	GLU	4
1	A	45	GLU	4
1	A	65	LYS	4
1	A	58	PHE	3
1	A	122	LEU	3
1	A	78	ARG	3
1	A	26	LEU	3
1	A	43	LEU	3
1	A	120	TRP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	134	LEU	3
1	A	79	LEU	3
1	A	57	LEU	3
1	A	59	LEU	3
1	A	61	ILE	3
1	A	86	ILE	3
1	A	1	MET	2
1	A	10	LYS	2
1	A	53	GLU	2
1	A	80	GLN	2
1	A	94	LYS	2
1	A	25	TYR	2
1	A	68	LEU	2
1	A	73	SER	2
1	A	97	LYS	2
1	A	48	ASP	2
1	A	129	ASP	2
1	A	71	VAL	2
1	A	124	THR	2
1	A	98	ARG	2
1	A	77	THR	1
1	A	12	GLN	1
1	A	22	LYS	1
1	A	140	GLU	1
1	A	2	ARG	1
1	A	6	ARG	1
1	A	15	ARG	1
1	A	85	ASN	1
1	A	112	PHE	1
1	A	37	GLN	1
1	A	44	GLU	1
1	A	49	VAL	1
1	A	50	VAL	1
1	A	91	GLU	1
1	A	149	PHE	1
1	A	17	TRP	1
1	A	152	ASP	1
1	A	82	GLU	1
1	A	93	ARG	1
1	A	101	PHE	1
1	A	127	GLU	1
1	A	42	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	75	ASP	1
1	A	14	PHE	1
1	A	105	ASP	1
1	A	24	PHE	1
1	A	118	PRO	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