



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:06 PM BST

PDB ID : 1IRP
Title : SOLUTION STRUCTURE OF HUMAN INTERLEUKIN-1 RECEPTOR
ANTAGONIST PROTEIN
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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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

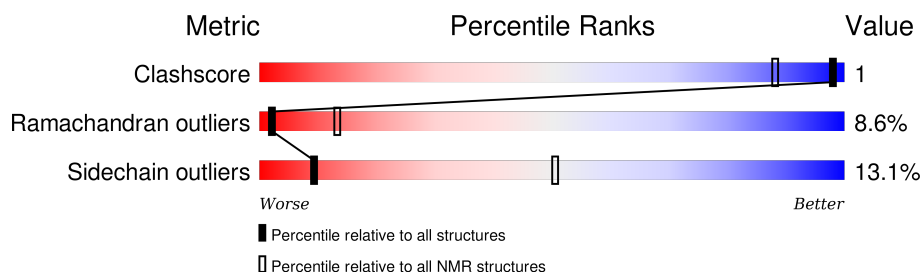
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	 75% 22% •

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)	1.49	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 [i](#)

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.

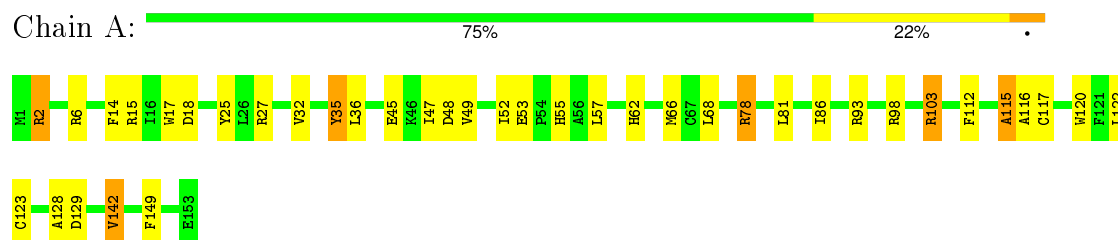
Mol	Chain	Residues	Atoms						Trace
1	A	153	Total	C	H	N	O	S	0
			2392	759	1183	208	232	10	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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

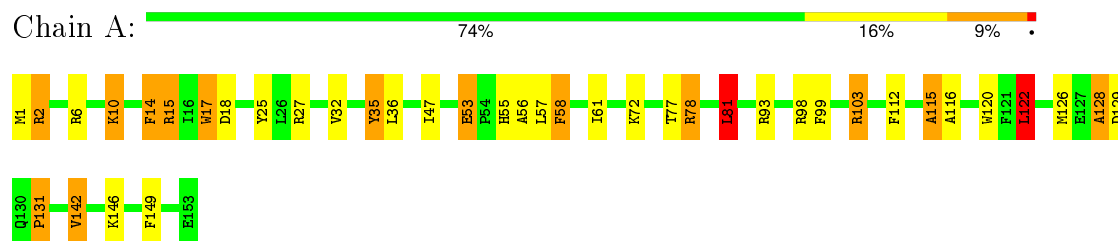


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

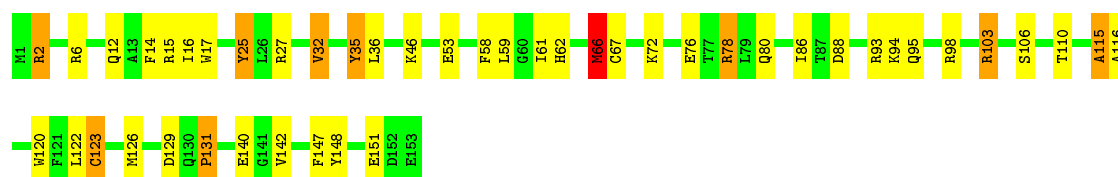
- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST



4.2.2 Score per residue for model 2

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST

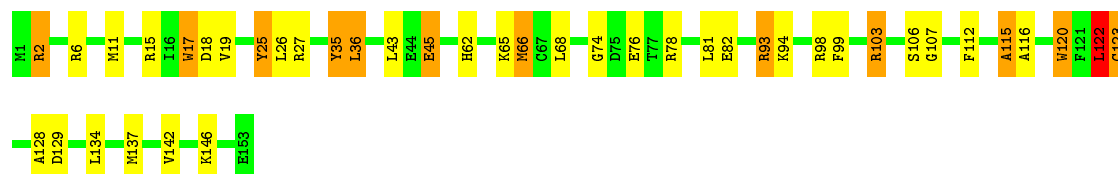




4.2.3 Score per residue for model 3

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST

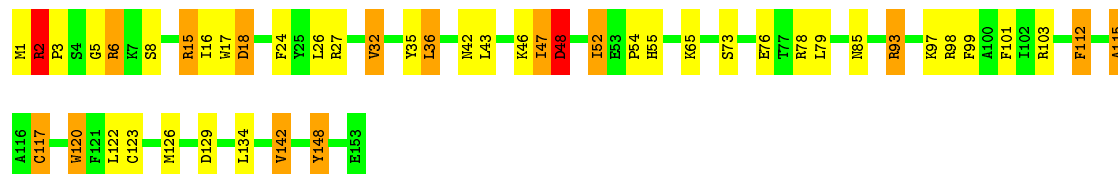
Chain A: 73% 19% 8% •



4.2.4 Score per residue for model 4

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST

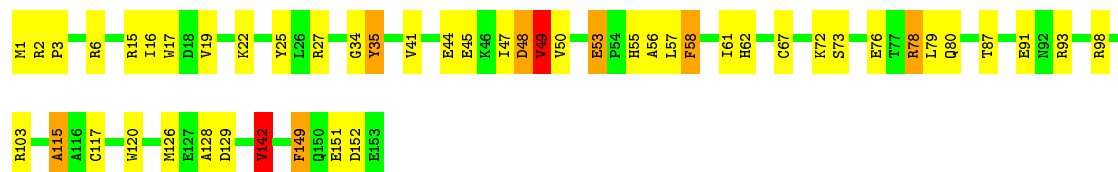
Chain A: 69% 20% 9% •



4.2.5 Score per residue for model 5

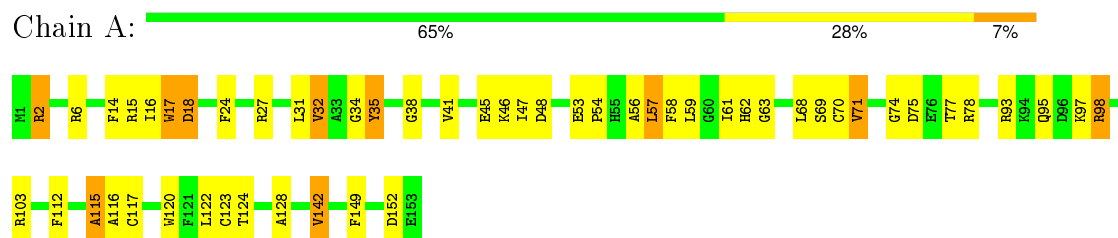
- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST

Chain A: 68% 26% 5% •



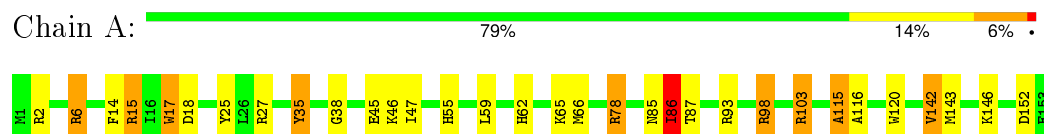
4.2.6 Score per residue for model 6

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST



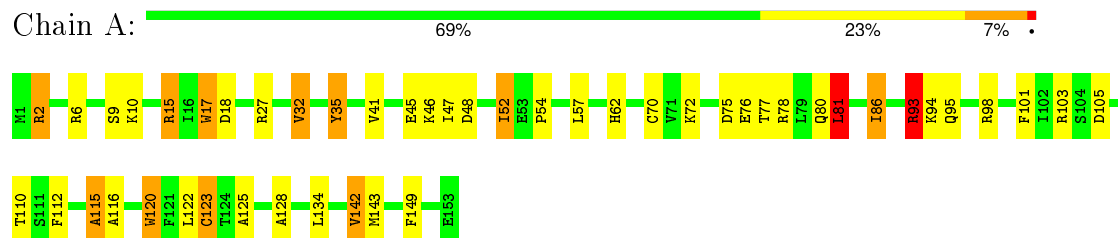
4.2.7 Score per residue for model 7

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST



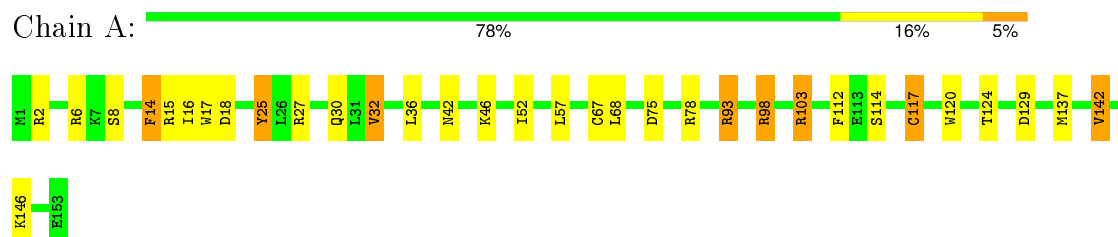
4.2.8 Score per residue for model 8

- 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

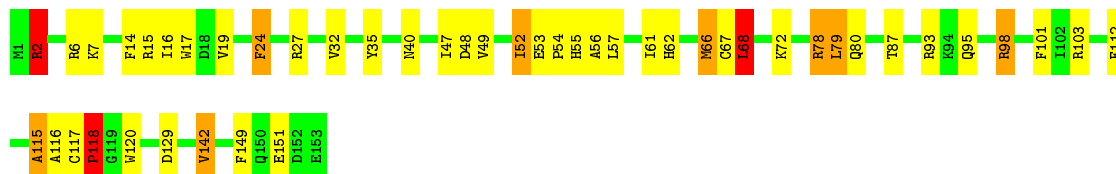
Chain A: 76% 18% 5%



4.2.12 Score per residue for model 12

- Molecule 1: INTERLEUKIN-1 RECEPTOR ANTAGONIST

Chain A: 69% 24% 5%



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. No validations of the models with respect to experimental NMR restraints is performed at this time.

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	1.25±0.01	0±0/1234 (0.0±0.0%)	1.62±0.04	25±5/1664 (1.5±0.3%)
All	All	1.25	0/14808 (0.0%)	1.62	296/19968 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.8±1.4
All	All	0	33

There are no bond-length outliers.

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	15	ARG	NE-CZ-NH1	11.80	126.20	120.30	11	12
1	A	78	ARG	NE-CZ-NH1	10.29	125.44	120.30	11	12
1	A	103	ARG	NE-CZ-NH1	10.16	125.38	120.30	12	12
1	A	27	ARG	NE-CZ-NH1	9.41	125.00	120.30	9	12
1	A	2	ARG	NE-CZ-NH1	9.37	124.98	120.30	2	12
1	A	115	ALA	CB-CA-C	9.26	123.99	110.10	2	10
1	A	25	TYR	CB-CG-CD2	-9.16	115.51	121.00	3	2
1	A	35	TYR	CB-CG-CD2	-9.01	115.60	121.00	5	7
1	A	93	ARG	NE-CZ-NH1	8.82	124.71	120.30	11	12
1	A	122	LEU	N-CA-C	8.64	134.34	111.00	1	1
1	A	103	ARG	NE-CZ-NH2	-8.37	116.11	120.30	12	4
1	A	14	PHE	CB-CG-CD2	-8.21	115.06	120.80	10	1
1	A	142	VAL	CA-CB-CG1	7.95	122.83	110.90	1	11
1	A	35	TYR	CB-CG-CD1	7.94	125.76	121.00	10	7
1	A	98	ARG	NE-CZ-NH1	7.80	124.20	120.30	10	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	128	ALA	N-CA-CB	-7.75	99.25	110.10	1	5
1	A	25	TYR	CB-CG-CD1	7.68	125.61	121.00	3	1
1	A	6	ARG	NE-CZ-NH1	7.63	124.11	120.30	12	12
1	A	78	ARG	NE-CZ-NH2	-7.61	116.50	120.30	3	4
1	A	114	SER	N-CA-CB	-7.47	99.30	110.50	11	2
1	A	15	ARG	NE-CZ-NH2	-7.46	116.57	120.30	11	7
1	A	6	ARG	NE-CZ-NH2	-6.97	116.81	120.30	12	3
1	A	148	TYR	CB-CG-CD2	-6.86	116.88	121.00	4	1
1	A	71	VAL	CA-CB-CG1	6.71	120.97	110.90	6	1
1	A	112	PHE	CB-CG-CD2	-6.66	116.14	120.80	8	7
1	A	14	PHE	CA-CB-CG	6.51	129.51	113.90	10	1
1	A	149	PHE	N-CA-CB	-6.46	98.97	110.60	6	3
1	A	117	CYS	N-CA-C	-6.46	93.57	111.00	11	2
1	A	27	ARG	NE-CZ-NH2	-6.39	117.10	120.30	12	1
1	A	69	SER	N-CA-CB	-6.30	101.05	110.50	6	2
1	A	25	TYR	CA-CB-CG	6.21	125.20	113.40	3	3
1	A	120	TRP	CD1-NE1-CE2	-6.17	103.45	109.00	1	12
1	A	98	ARG	NE-CZ-NH2	-6.11	117.25	120.30	9	2
1	A	14	PHE	N-CA-CB	-6.09	99.63	110.60	6	4
1	A	128	ALA	CB-CA-C	6.06	119.19	110.10	10	1
1	A	66	MET	N-CA-CB	6.04	121.48	110.60	2	2
1	A	118	PRO	CB-CA-C	5.92	126.81	112.00	12	1
1	A	93	ARG	NE-CZ-NH2	-5.92	117.34	120.30	4	4
1	A	122	LEU	N-CA-CB	-5.89	98.62	110.40	1	1
1	A	118	PRO	N-CA-CB	-5.88	96.13	102.60	12	1
1	A	112	PHE	CB-CG-CD1	5.87	124.91	120.80	12	4
1	A	115	ALA	N-CA-CB	5.78	118.19	110.10	4	5
1	A	117	CYS	CB-CA-C	5.77	121.95	110.40	11	3
1	A	18	ASP	CA-CB-CG	5.74	126.02	113.40	4	2
1	A	148	TYR	CB-CG-CD1	5.71	124.43	121.00	4	1
1	A	17	TRP	CD1-NE1-CE2	-5.68	103.89	109.00	7	12
1	A	131	PRO	N-CA-CB	-5.66	96.38	102.60	1	2
1	A	49	VAL	CA-CB-CG1	5.65	119.37	110.90	5	1
1	A	101	PHE	CB-CG-CD2	-5.58	116.90	120.80	4	1
1	A	58	PHE	CB-CG-CD2	-5.56	116.91	120.80	6	2
1	A	2	ARG	NE-CZ-NH2	-5.54	117.53	120.30	4	2
1	A	52	ILE	CB-CA-C	5.49	122.58	111.60	8	2
1	A	62	HIS	CG-ND1-CE1	-5.47	98.59	105.70	10	7
1	A	115	ALA	N-CA-C	-5.46	96.25	111.00	4	1
1	A	24	PHE	CB-CG-CD2	-5.46	116.98	120.80	4	3
1	A	81	LEU	CB-CA-C	5.45	120.56	110.20	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	32	VAL	CA-CB-CG2	5.42	119.03	110.90	6	6
1	A	22	LYS	CB-CA-C	5.34	121.08	110.40	5	1
1	A	55	HIS	CG-ND1-CE1	-5.30	98.81	105.70	5	7
1	A	81	LEU	CA-CB-CG	5.28	127.43	115.30	1	1
1	A	101	PHE	CB-CG-CD1	5.27	124.49	120.80	4	1
1	A	48	ASP	N-CA-CB	-5.24	101.17	110.60	4	1
1	A	142	VAL	CG1-CB-CG2	-5.23	102.53	110.90	8	2
1	A	99	PHE	CB-CG-CD2	-5.22	117.15	120.80	10	2
1	A	56	ALA	N-CA-CB	-5.21	102.80	110.10	1	2
1	A	149	PHE	CB-CG-CD1	5.20	124.44	120.80	5	1
1	A	24	PHE	CB-CG-CD1	5.18	124.43	120.80	4	1
1	A	53	GLU	CB-CA-C	5.17	120.74	110.40	5	1
1	A	48	ASP	CA-CB-CG	5.16	124.74	113.40	5	1
1	A	82	GLU	N-CA-CB	-5.13	101.36	110.60	10	2
1	A	41	VAL	CA-CB-CG2	5.12	118.58	110.90	6	1
1	A	122	LEU	CA-CB-CG	5.10	127.03	115.30	1	1
1	A	38	GLY	N-CA-C	5.10	125.84	113.10	6	1
1	A	149	PHE	CB-CG-CD2	-5.09	117.24	120.80	5	1
1	A	86	ILE	CB-CA-C	5.08	121.76	111.60	7	1
1	A	68	LEU	CB-CA-C	5.07	119.83	110.20	12	1
1	A	128	ALA	N-CA-C	5.05	124.64	111.00	11	1
1	A	88	ASP	N-CA-CB	-5.02	101.56	110.60	2	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	103	ARG	Sidechain	5
1	A	2	ARG	Sidechain	5
1	A	25	TYR	Sidechain	4
1	A	14	PHE	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	101	PHE	Sidechain	1
1	A	148	TYR	Sidechain	1
1	A	49	VAL	Mainchain	1
1	A	117	CYS	Mainchain	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	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:H	1:A:81:LEU:HD13	0.41	1.76	1	1
1:A:70:CYS:SG	1:A:77:THR:CG2	0.41	3.09	8	1
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 ⓘ

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	151/153 (99%)	105±4 (70±3%)	33±4 (22±2%)	13±4 (9±3%)	2	13
All	All	1812/1836 (99%)	1265 (70%)	391 (22%)	156 (9%)	2	13

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	117	CYS	5
1	A	36	LEU	5
1	A	137	MET	4
1	A	19	VAL	4
1	A	54	PRO	4
1	A	95	GLN	4
1	A	52	ILE	4
1	A	45	GLU	4
1	A	48	ASP	4
1	A	57	LEU	4
1	A	87	THR	3
1	A	53	GLU	3
1	A	86	ILE	3
1	A	61	ILE	3
1	A	47	ILE	3
1	A	68	LEU	3
1	A	131	PRO	2
1	A	49	VAL	2
1	A	34	GLY	2
1	A	80	GLN	2
1	A	142	VAL	2
1	A	66	MET	2
1	A	56	ALA	2
1	A	74	GLY	2
1	A	3	PRO	2
1	A	99	PHE	2
1	A	41	VAL	2
1	A	62	HIS	2
1	A	125	ALA	2
1	A	42	ASN	2
1	A	106	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	152	ASP	2
1	A	8	SER	2
1	A	98	ARG	1
1	A	67	CYS	1
1	A	50	VAL	1
1	A	75	ASP	1
1	A	127	GLU	1
1	A	107	GLY	1
1	A	63	GLY	1
1	A	40	ASN	1
1	A	38	GLY	1
1	A	59	LEU	1
1	A	7	LYS	1
1	A	85	ASN	1
1	A	135	THR	1
1	A	10	LYS	1
1	A	5	GLY	1
1	A	2	ARG	1
1	A	128	ALA	1
1	A	118	PRO	1
1	A	81	LEU	1
1	A	31	LEU	1
1	A	55	HIS	1
1	A	94	LYS	1
1	A	65	LYS	1
1	A	11	MET	1
1	A	9	SER	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	134/134 (100%)	116±4 (87±3%)	18±4 (13±3%)	9	50
All	All	1608/1608 (100%)	1397 (87%)	211 (13%)	9	50

All 71 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	142	VAL	10
1	A	35	TYR	9
1	A	18	ASP	8
1	A	32	VAL	8
1	A	46	LYS	6
1	A	16	ILE	6
1	A	76	GLU	6
1	A	72	LYS	5
1	A	17	TRP	5
1	A	81	LEU	5
1	A	146	LYS	5
1	A	78	ARG	5
1	A	47	ILE	5
1	A	120	TRP	4
1	A	2	ARG	4
1	A	36	LEU	4
1	A	126	MET	4
1	A	57	LEU	4
1	A	149	PHE	3
1	A	58	PHE	3
1	A	66	MET	3
1	A	151	GLU	3
1	A	26	LEU	3
1	A	43	LEU	3
1	A	110	THR	3
1	A	93	ARG	3
1	A	86	ILE	3
1	A	1	MET	3
1	A	122	LEU	3
1	A	61	ILE	3
1	A	45	GLU	3
1	A	25	TYR	3
1	A	94	LYS	3
1	A	65	LYS	3
1	A	14	PHE	3
1	A	79	LEU	3
1	A	134	LEU	3
1	A	98	ARG	2
1	A	80	GLN	2
1	A	73	SER	2
1	A	75	ASP	2
1	A	71	VAL	2
1	A	129	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	6	ARG	2
1	A	59	LEU	2
1	A	10	LYS	2
1	A	97	LYS	2
1	A	24	PHE	2
1	A	48	ASP	2
1	A	53	GLU	2
1	A	124	THR	2
1	A	105	ASP	2
1	A	68	LEU	2
1	A	15	ARG	2
1	A	148	TYR	1
1	A	101	PHE	1
1	A	112	PHE	1
1	A	77	THR	1
1	A	12	GLN	1
1	A	118	PRO	1
1	A	103	ARG	1
1	A	85	ASN	1
1	A	143	MET	1
1	A	140	GLU	1
1	A	49	VAL	1
1	A	42	ASN	1
1	A	30	GLN	1
1	A	91	GLU	1
1	A	152	ASP	1
1	A	27	ARG	1
1	A	44	GLU	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 carbohydrates 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