



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 03:07 PM UTC

PDB ID : 2DEF / pdb\_00002def  
Title : PEPTIDE DEFORMYLASE CATALYTIC CORE (RESIDUES 1-147), NMR,  
20 STRUCTURES  
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Deposited on : 1997-12-15

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

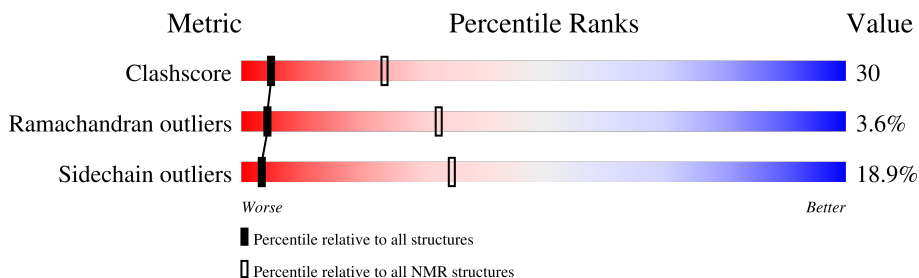
# 1 Overall quality at a glance i

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  $\geq 3$ , 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	147	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 5 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:2-A:147 (146)	0.38	5

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2339 atoms, of which 1178 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PEPTIDE DEFORMYLASE.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	146	2338	729	1178	200	225	6	0

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

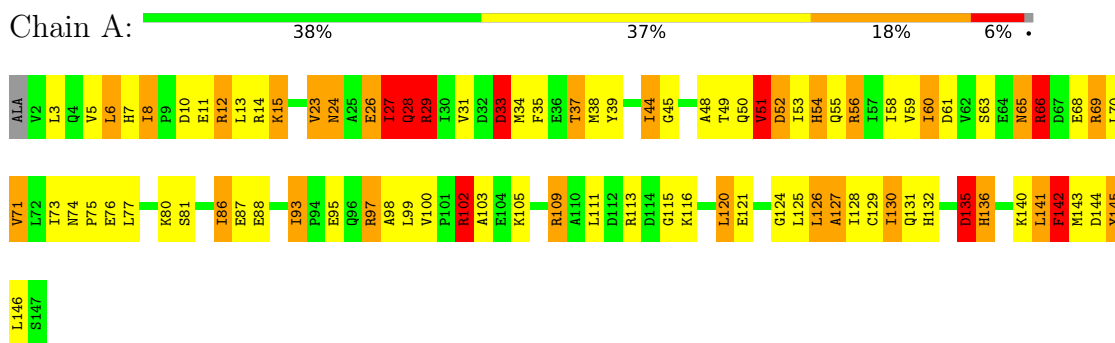
Mol	Chain	Residues	Atoms	
2	A	1	Total	Ni
			1	1

## 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: PEPTIDE DEFORMYLASE

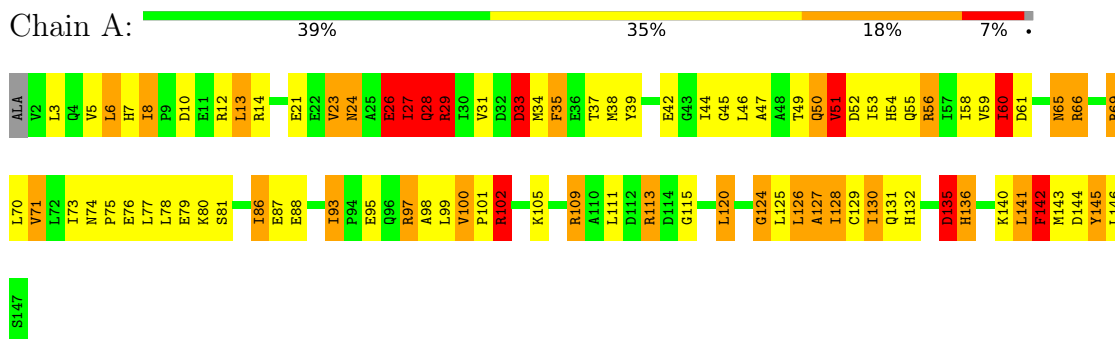


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

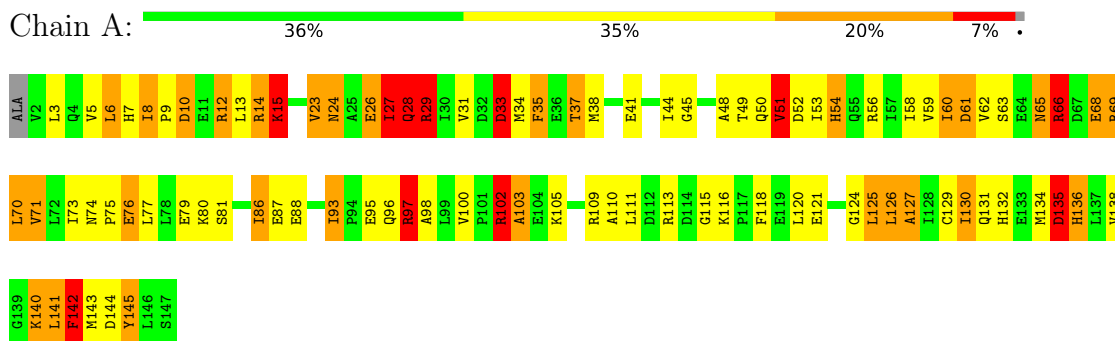
- Molecule 1: PEPTIDE DEFORMYLASE





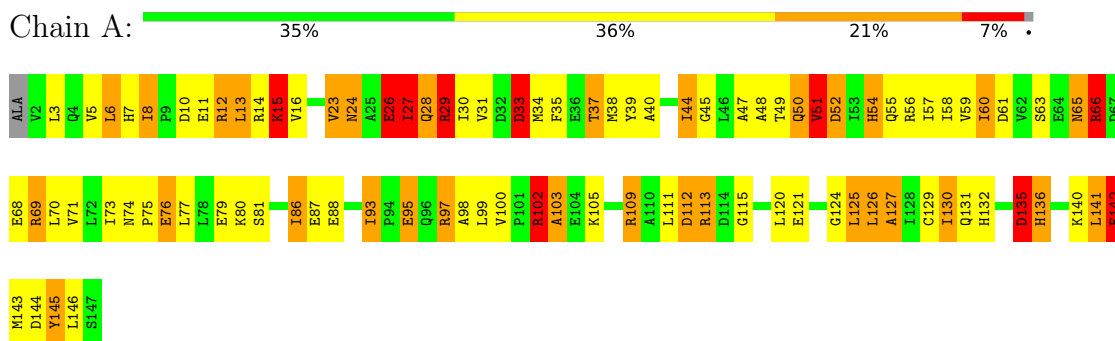
### 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: PEPTIDE DEFORMYLASE



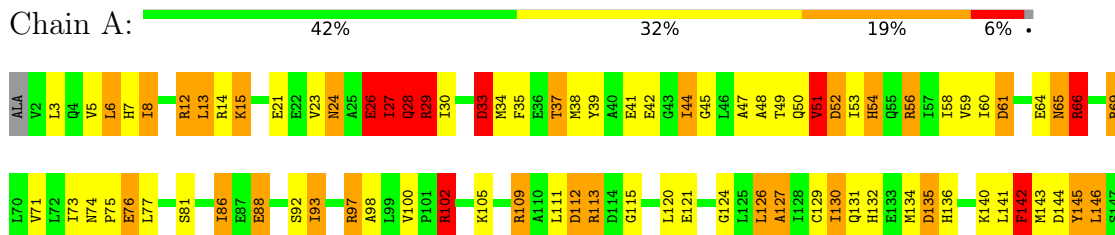
### 4.2.6 Score per residue for model 6

- Molecule 1: PEPTIDE DEFORMYLASE



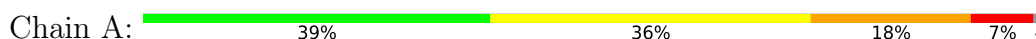
### 4.2.7 Score per residue for model 7

- Molecule 1: PEPTIDE DEFORMYLASE

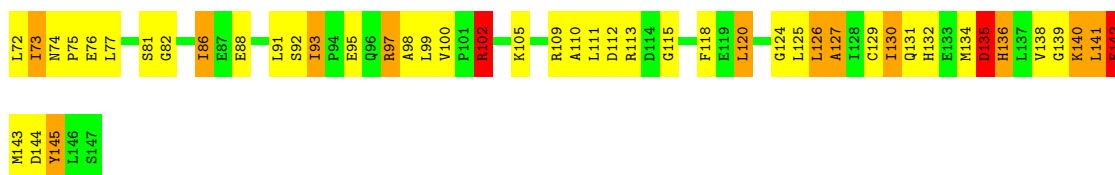


### 4.2.8 Score per residue for model 8

- Molecule 1: PEPTIDE DEFORMYLASE



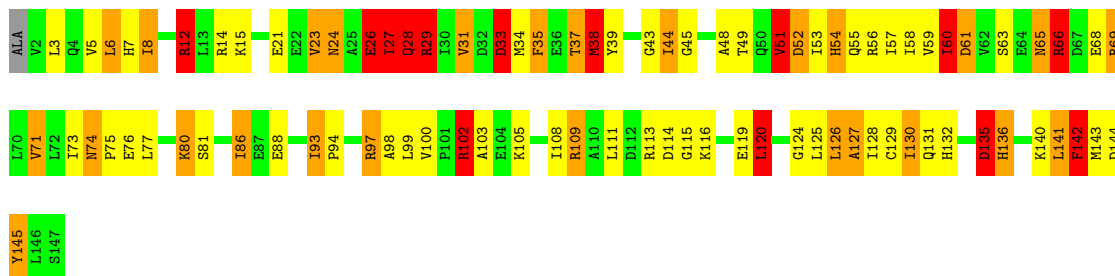




#### 4.2.12 Score per residue for model 12

- Molecule 1: PEPTIDE DEFORMYLASE

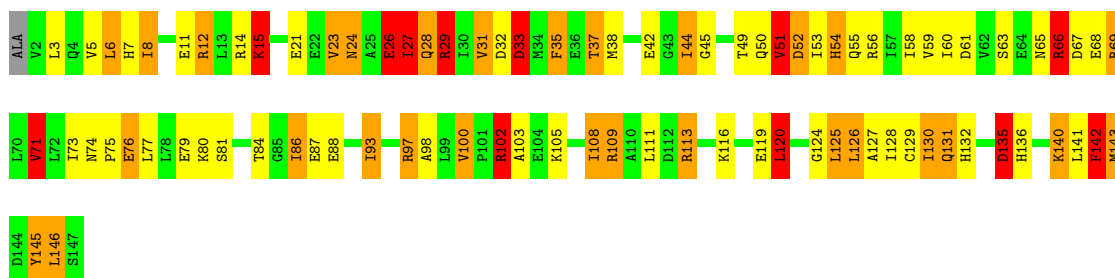
Chain A: 39% 33% 18% 10%



#### 4.2.13 Score per residue for model 13

- Molecule 1: PEPTIDE DEFORMYLASE

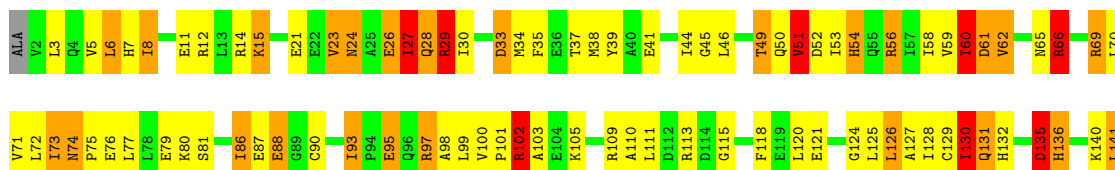
Chain A: 40% 31% 20% 8%



#### 4.2.14 Score per residue for model 14

- Molecule 1: PEPTIDE DEFORMYLASE

Chain A: 37% 38% 18% 6%





#### 4.2.15 Score per residue for model 15

- Molecule 1: PEPTIDE DEFORMYLASE

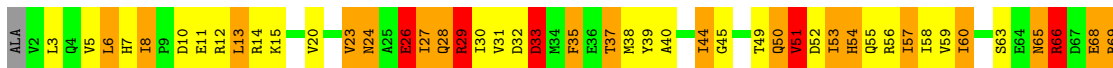
Chain A: 42% 32% 20% 5%



#### 4.2.16 Score per residue for model 16

- Molecule 1: PEPTIDE DEFORMYLASE

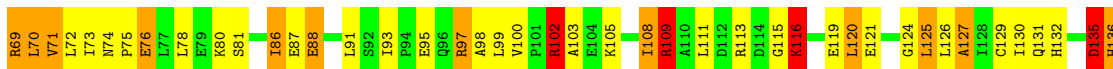
Chain A: 36% 37% 20% 7%



#### 4.2.17 Score per residue for model 17

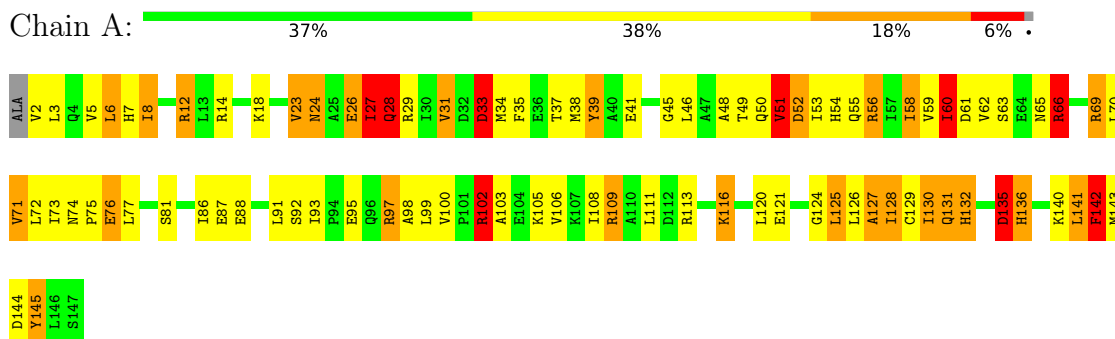
- Molecule 1: PEPTIDE DEFORMYLASE

Chain A: 34% 34% 22% 10%



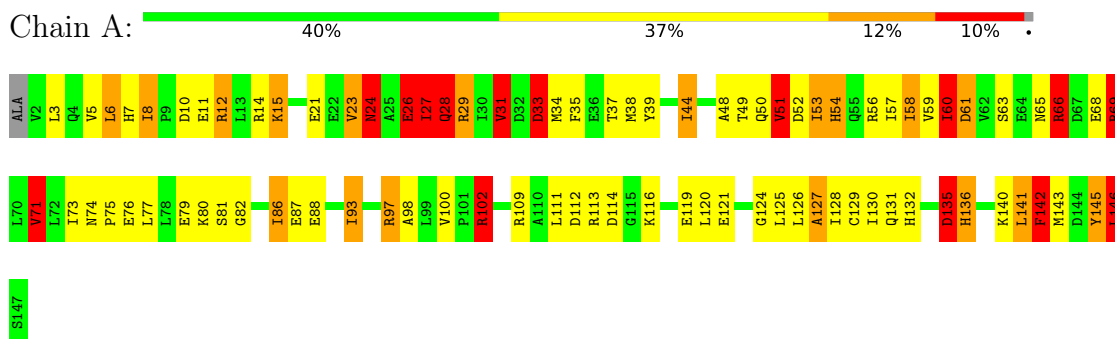
## 4.2.18 Score per residue for model 18

- Molecule 1: PEPTIDE DEFORMYLASE



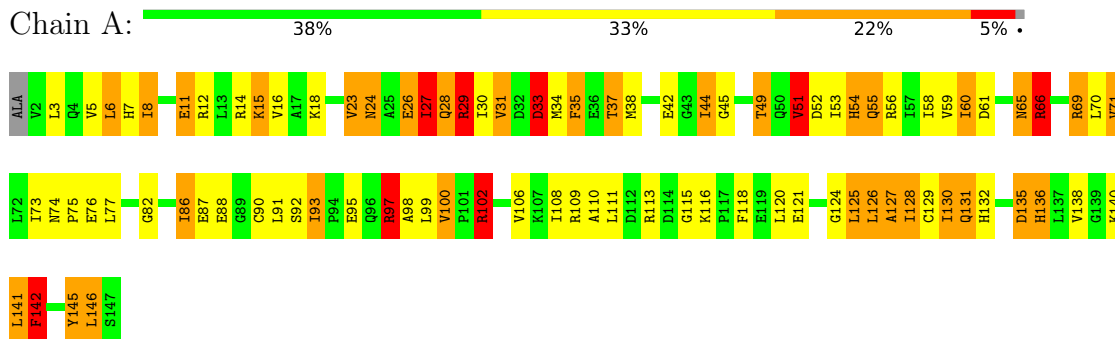
## 4.2.19 Score per residue for model 19

- Molecule 1: PEPTIDE DEFORMYLASE



## 4.2.20 Score per residue for model 20

- Molecule 1: PEPTIDE DEFORMYLASE



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY, RESTRAINED SIMULATED ANNEALING*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *LOWEST DIANA TARGET FUNCTION*.

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

Software name	Classification	Version
X-PLOR	refinement	
DIANA & X-PLOR3.1	structure solution	X-PLOR3.1

No chemical shift data was provided.

## 6 Model quality i

### 6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:  
NI

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	1.56±0.01	8±0/1174 ( 0.7± 0.0%)	2.13±0.04	42±4/1583 ( 2.6± 0.2%)
All	All	1.56	161/23480 ( 0.7%)	2.13	834/31660 ( 2.6%)

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	9.9±0.2
All	All	0	199

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	54	HIS	CG-ND1	-7.46	1.30	1.38	20	20
1	A	132	HIS	CG-ND1	-7.43	1.30	1.38	19	20
1	A	136	HIS	CG-ND1	-7.28	1.30	1.38	8	20
1	A	7	HIS	CG-ND1	-7.23	1.30	1.38	5	20
1	A	136	HIS	CD2-NE2	-6.61	1.30	1.37	3	20
1	A	54	HIS	CD2-NE2	-6.53	1.30	1.37	11	20
1	A	132	HIS	CD2-NE2	-6.29	1.30	1.37	3	20
1	A	7	HIS	CD2-NE2	-5.80	1.31	1.37	2	20
1	A	27	ILE	CA-CB	-5.03	1.48	1.54	12	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	54	HIS	CA-CB-CG	-17.26	96.54	113.80	20	20
1	A	61	ASP	CA-CB-CG	-15.10	97.50	112.60	19	9
1	A	93	ILE	N-CA-CB	-13.92	102.22	111.83	17	20
1	A	24	ASN	CA-CB-CG	-13.02	99.58	112.60	2	15
1	A	27	ILE	N-CA-C	-12.81	98.38	110.42	15	18
1	A	44	ILE	N-CA-C	-12.59	100.99	111.81	17	18
1	A	144	ASP	N-CA-C	-11.48	96.49	112.45	5	14
1	A	76	GLU	N-CA-C	-11.18	95.46	110.55	19	20
1	A	141	LEU	N-CA-C	-11.04	94.59	110.59	8	18
1	A	135	ASP	CA-CB-CG	10.88	123.48	112.60	3	2
1	A	135	ASP	N-CA-C	-10.74	99.57	111.28	6	20
1	A	132	HIS	CA-CB-CG	-10.42	103.38	113.80	3	12
1	A	51	VAL	N-CA-C	-10.18	88.16	109.34	3	20
1	A	7	HIS	CA-CB-CG	-9.91	103.89	113.80	15	10
1	A	142	PHE	N-CA-C	-9.51	102.28	112.93	18	12
1	A	102	ARG	NE-CZ-NH1	-9.47	112.03	121.50	13	4
1	A	15	LYS	N-CA-C	-9.36	97.03	110.59	11	12
1	A	33	ASP	CA-CB-CG	9.17	121.77	112.60	4	20
1	A	142	PHE	CA-CB-CG	9.01	122.81	113.80	1	16
1	A	116	LYS	N-CA-C	-8.98	97.56	110.40	10	11
1	A	49	THR	N-CA-C	-8.92	102.12	113.72	17	20
1	A	74	ASN	CA-CB-CG	-8.59	104.02	112.60	16	20
1	A	126	LEU	N-CA-C	-8.37	102.16	111.28	2	16
1	A	125	LEU	N-CA-C	8.23	121.85	111.24	8	7
1	A	87	GLU	N-CA-C	-8.11	97.46	109.62	13	13
1	A	55	GLN	N-CA-C	-8.10	97.68	109.18	18	10
1	A	24	ASN	N-CA-CB	-8.04	96.90	110.49	12	15
1	A	26	GLU	N-CA-C	-8.02	103.63	113.41	6	20
1	A	140	LYS	N-CA-C	-7.84	97.11	109.50	11	3
1	A	120	LEU	N-CA-CB	-7.68	97.92	110.43	13	4
1	A	28	GLN	N-CA-C	-7.56	102.18	111.33	16	13
1	A	146	LEU	N-CA-C	-7.55	103.06	112.72	1	7
1	A	111	LEU	N-CA-C	-7.43	98.00	109.52	1	20
1	A	141	LEU	CA-C-N	-7.43	110.93	122.08	19	18
1	A	141	LEU	C-N-CA	-7.43	110.93	122.08	19	18
1	A	143	MET	N-CA-C	-7.41	102.50	112.94	13	4
1	A	65	ASN	N-CA-C	7.39	118.96	108.54	1	14
1	A	42	GLU	CA-CB-CG	-7.25	99.60	114.10	1	1
1	A	35	PHE	CA-CB-CG	-7.22	106.58	113.80	17	4
1	A	144	ASP	CA-CB-CG	-7.19	105.41	112.60	1	3
1	A	138	VAL	N-CA-C	-7.16	103.20	111.00	11	4
1	A	127	ALA	N-CA-C	-7.11	102.34	111.02	6	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	66	ARG	N-CA-CB	-7.01	101.05	111.71	15	18
1	A	120	LEU	N-CA-C	6.99	120.07	108.96	9	5
1	A	99	LEU	N-CA-C	-6.83	98.91	108.54	8	11
1	A	70	LEU	N-CA-C	6.71	120.45	110.52	15	2
1	A	100	VAL	CG1-CB-CG2	-6.64	96.19	110.80	3	3
1	A	38	MET	CA-CB-CG	-6.61	100.88	114.10	17	3
1	A	37	THR	CA-CB-OG1	-6.54	99.78	109.60	9	20
1	A	103	ALA	N-CA-C	-6.49	100.37	110.17	18	6
1	A	29	ARG	N-CA-CB	-6.40	100.74	110.01	4	16
1	A	35	PHE	N-CA-C	-6.36	104.27	111.14	10	6
1	A	131	GLN	CB-CG-CD	-6.28	101.93	112.60	13	3
1	A	101	PRO	O-C-N	6.26	127.18	122.73	1	3
1	A	114	ASP	CA-CB-CG	-6.26	106.34	112.60	19	6
1	A	71	VAL	N-CA-CB	-6.21	101.26	111.45	13	7
1	A	41	GLU	CA-C-O	6.18	121.53	117.94	15	3
1	A	61	ASP	CB-CA-C	-6.12	103.68	111.70	15	1
1	A	10	ASP	CA-CB-CG	-6.11	106.50	112.60	3	1
1	A	141	LEU	CA-C-O	-6.08	114.77	121.89	19	1
1	A	66	ARG	N-CA-C	-6.07	103.04	111.30	13	4
1	A	24	ASN	N-CA-C	6.01	115.95	108.19	19	1
1	A	102	ARG	NE-CZ-NH2	6.00	124.60	119.20	13	3
1	A	88	GLU	N-CA-C	5.96	118.47	109.41	3	5
1	A	52	ASP	N-CA-C	-5.83	98.37	110.80	8	8
1	A	39	TYR	N-CA-C	-5.75	105.93	113.12	18	1
1	A	136	HIS	CA-CB-CG	-5.74	108.06	113.80	12	3
1	A	131	GLN	CA-CB-CG	-5.73	102.64	114.10	2	4
1	A	23	VAL	CA-CB-CG1	5.70	120.08	110.40	13	14
1	A	26	GLU	CA-C-O	5.65	125.02	118.97	15	1
1	A	101	PRO	N-CA-C	-5.62	100.99	110.21	3	2
1	A	64	GLU	N-CA-C	5.62	118.25	111.40	17	3
1	A	62	VAL	N-CA-C	5.61	117.50	112.17	14	2
1	A	128	ILE	N-CA-C	5.59	115.79	110.42	1	1
1	A	27	ILE	N-CA-CB	-5.59	104.33	110.65	15	1
1	A	82	GLY	N-CA-C	-5.59	105.64	112.68	11	1
1	A	142	PHE	CB-CG-CD2	-5.58	111.21	120.70	3	3
1	A	53	ILE	CB-CA-C	-5.56	106.52	111.74	19	1
1	A	60	ILE	CB-CG1-CD1	-5.54	102.17	113.80	18	9
1	A	57	ILE	CB-CA-C	-5.53	103.31	110.84	16	1
1	A	67	ASP	N-CA-CB	-5.51	101.90	110.39	13	1
1	A	63	SER	CA-CB-OG	-5.49	100.11	111.10	8	2
1	A	136	HIS	CE1-NE2-CD2	-5.49	103.51	109.00	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	HIS	CE1-NE2-CD2	-5.48	103.52	109.00	6	2
1	A	20	VAL	N-CA-CB	-5.47	106.11	112.34	4	8
1	A	128	ILE	CB-CA-C	-5.45	105.00	111.97	18	3
1	A	132	HIS	CE1-NE2-CD2	-5.43	103.56	109.00	8	2
1	A	132	HIS	N-CA-CB	-5.41	102.01	109.91	8	1
1	A	130	ILE	CA-CB-CG2	5.40	119.68	110.50	9	1
1	A	61	ASP	CA-C-N	-5.37	114.69	122.69	15	3
1	A	61	ASP	C-N-CA	-5.37	114.69	122.69	15	3
1	A	102	ARG	N-CA-C	-5.36	99.38	110.80	17	3
1	A	50	GLN	N-CA-C	-5.36	106.91	113.50	2	2
1	A	42	GLU	CA-C-N	-5.36	118.48	122.18	15	4
1	A	42	GLU	C-N-CA	-5.36	118.48	122.18	15	4
1	A	127	ALA	CA-C-N	-5.32	113.85	120.56	20	3
1	A	127	ALA	C-N-CA	-5.32	113.85	120.56	20	3
1	A	92	SER	CA-CB-OG	-5.32	100.45	111.10	7	3
1	A	29	ARG	N-CA-C	-5.30	105.61	111.71	19	1
1	A	68	GLU	N-CA-CB	-5.29	101.69	110.47	11	2
1	A	51	VAL	CG1-CB-CG2	-5.28	99.18	110.80	14	10
1	A	109	ARG	N-CA-C	-5.28	99.68	108.34	17	1
1	A	80	LYS	N-CA-CB	-5.28	102.93	112.27	5	4
1	A	50	GLN	CA-CB-CG	-5.26	103.57	114.10	5	5
1	A	15	LYS	N-CA-CB	-5.24	102.46	110.42	6	1
1	A	108	ILE	CB-CA-C	-5.24	104.58	111.70	20	5
1	A	23	VAL	CB-CA-C	-5.23	104.02	111.34	19	1
1	A	23	VAL	O-C-N	5.22	128.40	122.92	19	1
1	A	16	VAL	N-CA-CB	-5.19	106.16	112.07	17	1
1	A	102	ARG	NH1-CZ-NH2	5.18	126.03	119.30	1	1
1	A	52	ASP	CA-CB-CG	-5.18	107.42	112.60	2	2
1	A	142	PHE	CB-CG-CD1	5.15	129.46	120.70	1	1
1	A	31	VAL	N-CA-C	5.14	116.48	110.62	19	1
1	A	90	CYS	CA-CB-SG	5.13	126.20	114.40	14	3
1	A	109	ARG	CB-CA-C	5.12	118.35	110.62	2	2
1	A	120	LEU	CB-CA-C	5.12	118.19	109.75	2	1
1	A	100	VAL	N-CA-C	5.09	119.88	108.88	3	1
1	A	100	VAL	N-CA-CB	-5.09	104.08	111.21	16	3
1	A	56	ARG	CA-C-N	-5.09	116.88	123.19	14	1
1	A	56	ARG	C-N-CA	-5.09	116.88	123.19	14	1
1	A	16	VAL	N-CA-C	5.08	115.41	107.99	20	1
1	A	33	ASP	N-CA-C	-5.07	105.88	111.71	15	1
1	A	55	GLN	CA-CB-CG	-5.07	103.95	114.10	16	1
1	A	47	ALA	N-CA-C	-5.07	102.29	110.14	7	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	130	ILE	N-CA-CB	-5.05	104.11	110.57	14	1
1	A	29	ARG	CB-CA-C	5.04	118.79	110.88	4	1
1	A	138	VAL	CA-C-N	-5.03	117.44	123.08	10	2
1	A	138	VAL	C-N-CA	-5.03	117.44	123.08	10	2
1	A	30	ILE	N-CA-C	-5.01	105.71	110.42	7	1
1	A	27	ILE	O-C-N	5.00	127.29	121.94	15	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	12	ARG	Sidechain	20
1	A	14	ARG	Sidechain	20
1	A	29	ARG	Sidechain	20
1	A	56	ARG	Sidechain	20
1	A	66	ARG	Sidechain	20
1	A	69	ARG	Sidechain	20
1	A	97	ARG	Sidechain	20
1	A	102	ARG	Sidechain	20
1	A	109	ARG	Sidechain	20
1	A	113	ARG	Sidechain	19

## 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	1160	1178	1177	70±7
All	All	23220	23560	23540	1390

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 30.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:PHE:CE2	1:A:69:ARG:HB3	0.77	2.15	1	17
1:A:100:VAL:CG2	1:A:145:TYR:CD1	0.77	2.68	3	2
1:A:100:VAL:HG11	1:A:102:ARG:CZ	0.75	2.11	3	18
1:A:35:PHE:CZ	1:A:69:ARG:HB3	0.69	2.22	14	14
1:A:100:VAL:CG2	1:A:146:LEU:HD21	0.67	2.20	13	5
1:A:38:MET:SD	1:A:59:VAL:HG23	0.66	2.31	15	17
1:A:98:ALA:HB3	1:A:142:PHE:CE2	0.64	2.28	13	17
1:A:100:VAL:CG2	1:A:146:LEU:HD11	0.63	2.24	17	3
1:A:142:PHE:O	1:A:146:LEU:HD13	0.63	1.93	16	4
1:A:35:PHE:CE1	1:A:59:VAL:HB	0.62	2.29	7	20
1:A:27:ILE:HG22	1:A:113:ARG:HH12	0.62	1.54	19	1
1:A:31:VAL:HG21	1:A:113:ARG:NH2	0.62	2.09	19	1
1:A:60:ILE:HG12	1:A:129:CYS:SG	0.62	2.34	3	18
1:A:145:TYR:C	1:A:146:LEU:HD22	0.62	2.19	20	5
1:A:142:PHE:O	1:A:146:LEU:HD23	0.61	1.95	13	5
1:A:39:TYR:CE2	1:A:66:ARG:HD2	0.60	2.31	11	3
1:A:100:VAL:HG11	1:A:102:ARG:NH2	0.60	2.11	3	3
1:A:26:GLU:HG3	1:A:27:ILE:N	0.60	2.11	13	4
1:A:23:VAL:HG12	1:A:24:ASN:H	0.59	1.55	15	18
1:A:60:ILE:HG21	1:A:126:LEU:CD1	0.59	2.28	19	4
1:A:13:LEU:CD2	1:A:50:GLN:HA	0.58	2.28	3	5
1:A:39:TYR:CD1	1:A:66:ARG:HG3	0.58	2.32	19	1
1:A:146:LEU:HD22	1:A:146:LEU:N	0.58	2.14	7	5
1:A:45:GLY:HA3	1:A:129:CYS:SG	0.58	2.39	8	18
1:A:100:VAL:HG13	1:A:145:TYR:CD2	0.58	2.34	8	14
1:A:31:VAL:HG21	1:A:113:ARG:CZ	0.58	2.28	19	2
1:A:135:ASP:HB3	1:A:140:LYS:CG	0.57	2.29	17	19
1:A:24:ASN:ND2	1:A:27:ILE:H	0.57	1.97	13	5
1:A:15:LYS:HD3	1:A:54:HIS:NE2	0.57	2.14	11	3
1:A:29:ARG:HD3	1:A:29:ARG:C	0.57	2.24	3	8
1:A:100:VAL:CG1	1:A:102:ARG:CZ	0.57	2.82	7	19
1:A:136:HIS:CE1	1:A:141:LEU:HA	0.56	2.35	6	17
1:A:100:VAL:HG21	1:A:146:LEU:HD21	0.56	1.76	19	5
1:A:102:ARG:NH2	1:A:132:HIS:HD1	0.56	1.97	3	1
1:A:113:ARG:HE	1:A:113:ARG:N	0.56	1.97	13	1
1:A:24:ASN:N	1:A:24:ASN:ND2	0.56	2.50	19	4
1:A:8:ILE:H	1:A:8:ILE:CD1	0.56	2.14	18	19
1:A:15:LYS:HD2	1:A:54:HIS:NE2	0.56	2.16	9	9
1:A:23:VAL:HG12	1:A:24:ASN:N	0.56	2.15	10	20
1:A:51:VAL:HG23	1:A:52:ASP:H	0.55	1.60	14	20
1:A:15:LYS:HG2	1:A:16:VAL:N	0.55	2.16	15	2
1:A:38:MET:HE3	1:A:61:ASP:CG	0.55	2.26	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:ILE:C	1:A:75:PRO:HD3	0.55	2.27	20	16
1:A:24:ASN:ND2	1:A:24:ASN:N	0.55	2.51	13	2
1:A:23:VAL:HB	1:A:115:GLY:HA3	0.55	1.79	12	4
1:A:88:GLU:C	1:A:97:ARG:HG3	0.55	2.27	9	12
1:A:23:VAL:CG1	1:A:24:ASN:N	0.55	2.70	12	20
1:A:90:CYS:SG	1:A:91:LEU:N	0.54	2.79	3	1
1:A:66:ARG:HE	1:A:66:ARG:H	0.54	1.43	9	1
1:A:142:PHE:O	1:A:146:LEU:CD2	0.54	2.55	20	6
1:A:65:ASN:O	1:A:66:ARG:C	0.54	2.51	1	20
1:A:72:LEU:HD12	1:A:130:ILE:HD11	0.54	1.79	18	1
1:A:38:MET:SD	1:A:44:ILE:O	0.53	2.65	19	10
1:A:71:VAL:CG1	1:A:113:ARG:HE	0.53	2.16	19	1
1:A:74:ASN:N	1:A:75:PRO:CD	0.53	2.71	2	4
1:A:14:ARG:N	1:A:14:ARG:CD	0.53	2.71	17	4
1:A:24:ASN:N	1:A:24:ASN:HD22	0.53	2.01	13	5
1:A:31:VAL:HG23	1:A:57:ILE:CG2	0.53	2.33	19	1
1:A:102:ARG:HB3	1:A:128:ILE:HD12	0.53	1.81	14	8
1:A:8:ILE:HG13	1:A:143:MET:HE1	0.53	1.79	11	4
1:A:100:VAL:HG22	1:A:145:TYR:CD1	0.53	2.37	3	2
1:A:27:ILE:HD13	1:A:57:ILE:CD1	0.53	2.34	12	2
1:A:126:LEU:O	1:A:127:ALA:C	0.52	2.52	9	19
1:A:102:ARG:NH1	1:A:145:TYR:CE1	0.52	2.77	3	1
1:A:24:ASN:H	1:A:24:ASN:HD22	0.52	1.46	15	5
1:A:86:ILE:HD12	1:A:86:ILE:O	0.52	2.05	14	10
1:A:5:VAL:C	1:A:6:LEU:HD23	0.52	2.30	2	20
1:A:142:PHE:O	1:A:142:PHE:CG	0.52	2.63	20	6
1:A:88:GLU:C	1:A:97:ARG:HG2	0.52	2.30	1	7
1:A:39:TYR:CE2	1:A:66:ARG:HG3	0.51	2.40	1	1
1:A:124:GLY:O	1:A:128:ILE:HG12	0.51	2.05	1	1
1:A:24:ASN:H	1:A:24:ASN:ND2	0.51	2.03	5	4
1:A:73:ILE:CG1	1:A:113:ARG:NH2	0.51	2.73	13	1
1:A:39:TYR:OH	1:A:69:ARG:NE	0.51	2.44	19	1
1:A:35:PHE:CZ	1:A:59:VAL:HB	0.51	2.41	13	15
1:A:39:TYR:CE2	1:A:66:ARG:HD3	0.51	2.40	7	3
1:A:88:GLU:C	1:A:97:ARG:CG	0.51	2.83	3	2
1:A:10:ASP:CG	1:A:11:GLU:N	0.51	2.68	16	1
1:A:8:ILE:H	1:A:8:ILE:HD13	0.51	1.65	18	15
1:A:113:ARG:CA	1:A:113:ARG:NE	0.51	2.74	13	1
1:A:66:ARG:H	1:A:66:ARG:NE	0.51	2.04	9	1
1:A:72:LEU:CD1	1:A:130:ILE:HD11	0.50	2.36	14	2
1:A:23:VAL:HB	1:A:115:GLY:CA	0.50	2.36	16	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:LEU:C	1:A:143:MET:H	0.50	2.13	17	11
1:A:49:THR:HG21	1:A:136:HIS:HB3	0.50	1.83	8	5
1:A:60:ILE:HB	1:A:70:LEU:HB2	0.50	1.81	8	11
1:A:145:TYR:C	1:A:146:LEU:HD12	0.50	2.31	16	2
1:A:146:LEU:N	1:A:146:LEU:CD2	0.50	2.75	20	3
1:A:60:ILE:HG21	1:A:126:LEU:HD13	0.50	1.83	1	2
1:A:34:MET:SD	1:A:48:ALA:HB2	0.49	2.47	18	11
1:A:13:LEU:C	1:A:14:ARG:HD3	0.49	2.32	17	3
1:A:8:ILE:HA	1:A:9:PRO:C	0.49	2.30	5	2
1:A:130:ILE:HD11	1:A:134:MET:SD	0.49	2.47	11	6
1:A:31:VAL:CG2	1:A:113:ARG:CZ	0.49	2.89	13	2
1:A:100:VAL:HG21	1:A:142:PHE:HB2	0.49	1.82	3	1
1:A:27:ILE:O	1:A:28:GLN:C	0.49	2.55	11	9
1:A:86:ILE:HG13	1:A:128:ILE:HG21	0.49	1.83	18	2
1:A:28:GLN:CD	1:A:28:GLN:C	0.49	2.81	4	15
1:A:14:ARG:N	1:A:14:ARG:HD3	0.49	2.22	17	2
1:A:63:SER:CB	1:A:68:GLU:H	0.49	2.20	13	1
1:A:135:ASP:HB3	1:A:140:LYS:HG2	0.49	1.84	8	7
1:A:110:ALA:HB3	1:A:118:PHE:CZ	0.49	2.43	10	6
1:A:27:ILE:C	1:A:29:ARG:N	0.49	2.64	16	3
1:A:91:LEU:N	1:A:91:LEU:HD22	0.49	2.23	17	1
1:A:23:VAL:CG1	1:A:24:ASN:H	0.49	2.20	16	20
1:A:14:ARG:HD3	1:A:14:ARG:N	0.49	2.22	5	1
1:A:100:VAL:HG21	1:A:146:LEU:HD11	0.49	1.83	17	2
1:A:71:VAL:CG2	1:A:113:ARG:HE	0.49	2.20	19	1
1:A:3:LEU:HD12	1:A:3:LEU:N	0.49	2.23	18	20
1:A:8:ILE:CD1	1:A:8:ILE:N	0.48	2.76	7	19
1:A:34:MET:SD	1:A:57:ILE:HG22	0.48	2.48	6	4
1:A:100:VAL:CG1	1:A:145:TYR:CD2	0.48	2.96	15	13
1:A:86:ILE:H	1:A:86:ILE:HD13	0.48	1.68	15	10
1:A:100:VAL:HG23	1:A:146:LEU:HD21	0.48	1.83	3	1
1:A:81:SER:OG	1:A:105:LYS:HB2	0.48	2.08	9	16
1:A:45:GLY:CA	1:A:129:CYS:SG	0.48	3.02	5	14
1:A:63:SER:HB3	1:A:68:GLU:HB3	0.48	1.86	3	2
1:A:28:GLN:C	1:A:28:GLN:CD	0.48	2.81	11	5
1:A:102:ARG:HH22	1:A:142:PHE:CB	0.48	2.22	1	2
1:A:142:PHE:O	1:A:146:LEU:CD1	0.48	2.61	17	5
1:A:38:MET:SD	1:A:43:GLY:O	0.48	2.72	8	3
1:A:28:GLN:HG3	1:A:29:ARG:N	0.48	2.24	1	8
1:A:37:THR:O	1:A:38:MET:C	0.48	2.56	12	15
1:A:39:TYR:CE2	1:A:66:ARG:HG2	0.48	2.44	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:ASN:ND2	1:A:24:ASN:H	0.48	2.05	13	1
1:A:113:ARG:NE	1:A:113:ARG:HA	0.48	2.23	13	1
1:A:21:GLU:CD	1:A:21:GLU:N	0.48	2.71	14	6
1:A:3:LEU:HD11	1:A:33:ASP:HB2	0.47	1.85	3	18
1:A:8:ILE:CD1	1:A:8:ILE:H	0.47	2.22	7	1
1:A:27:ILE:HG22	1:A:28:GLN:N	0.47	2.23	12	1
1:A:6:LEU:HD23	1:A:6:LEU:N	0.47	2.23	3	20
1:A:79:GLU:CD	1:A:80:LYS:N	0.47	2.72	13	4
1:A:58:ILE:HD11	1:A:130:ILE:HD12	0.47	1.87	18	1
1:A:136:HIS:CE1	1:A:141:LEU:HD23	0.47	2.44	11	11
1:A:28:GLN:HA	1:A:113:ARG:HH11	0.47	1.69	19	1
1:A:35:PHE:CD2	1:A:39:TYR:CE1	0.47	3.03	17	2
1:A:60:ILE:HG21	1:A:126:LEU:HD21	0.47	1.87	2	3
1:A:8:ILE:N	1:A:8:ILE:HD13	0.47	2.24	17	5
1:A:27:ILE:HG22	1:A:113:ARG:NH1	0.47	2.25	13	2
1:A:113:ARG:NH1	1:A:113:ARG:HA	0.47	2.25	19	1
1:A:73:ILE:CD1	1:A:73:ILE:N	0.47	2.78	11	4
1:A:76:GLU:CG	1:A:109:ARG:HG2	0.47	2.40	17	2
1:A:8:ILE:HG13	1:A:143:MET:SD	0.47	2.50	13	2
1:A:102:ARG:HB3	1:A:128:ILE:CD1	0.47	2.40	1	9
1:A:79:GLU:HG2	1:A:80:LYS:N	0.47	2.25	14	2
1:A:60:ILE:CG1	1:A:129:CYS:SG	0.46	3.04	19	2
1:A:87:GLU:HG2	1:A:99:LEU:HD23	0.46	1.87	4	1
1:A:34:MET:O	1:A:35:PHE:C	0.46	2.58	17	2
1:A:132:HIS:CD2	1:A:132:HIS:C	0.46	2.92	3	1
1:A:142:PHE:C	1:A:146:LEU:HD23	0.46	2.35	7	2
1:A:38:MET:SD	1:A:46:LEU:N	0.46	2.89	1	4
1:A:100:VAL:HG11	1:A:102:ARG:NH1	0.46	2.26	8	8
1:A:27:ILE:O	1:A:30:ILE:N	0.46	2.49	4	6
1:A:84:THR:CG2	1:A:128:ILE:HD11	0.46	2.41	9	2
1:A:95:GLU:CD	1:A:95:GLU:C	0.46	2.83	16	3
1:A:121:GLU:H	1:A:121:GLU:CD	0.46	2.18	6	2
1:A:35:PHE:CE2	1:A:69:ARG:CB	0.46	2.95	1	3
1:A:27:ILE:HD11	1:A:55:GLN:NE2	0.46	2.25	11	4
1:A:23:VAL:CG1	1:A:27:ILE:HB	0.46	2.41	16	2
1:A:39:TYR:HE2	1:A:66:ARG:HG3	0.46	1.71	1	1
1:A:60:ILE:HG21	1:A:126:LEU:CD2	0.46	2.41	9	4
1:A:130:ILE:O	1:A:131:GLN:C	0.46	2.58	16	20
1:A:100:VAL:CG2	1:A:146:LEU:CD2	0.46	2.94	2	1
1:A:31:VAL:HG11	1:A:113:ARG:HD2	0.46	1.86	13	1
1:A:76:GLU:HG3	1:A:109:ARG:CG	0.46	2.41	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:TYR:CE2	1:A:61:ASP:CG	0.46	2.94	15	2
1:A:63:SER:HB3	1:A:68:GLU:CB	0.45	2.41	16	8
1:A:24:ASN:ND2	1:A:27:ILE:HB	0.45	2.26	13	3
1:A:141:LEU:C	1:A:143:MET:N	0.45	2.73	17	6
1:A:142:PHE:O	1:A:145:TYR:CD2	0.45	2.69	10	5
1:A:39:TYR:CZ	1:A:61:ASP:CG	0.45	2.94	14	2
1:A:38:MET:HE3	1:A:61:ASP:OD2	0.45	2.12	15	1
1:A:145:TYR:CD1	1:A:145:TYR:N	0.45	2.84	18	3
1:A:44:ILE:HG13	1:A:129:CYS:SG	0.45	2.51	20	1
1:A:26:GLU:HG2	1:A:27:ILE:N	0.45	2.26	17	8
1:A:26:GLU:HG2	1:A:27:ILE:HD12	0.45	1.87	7	4
1:A:12:ARG:NE	1:A:54:HIS:NE2	0.45	2.64	3	4
1:A:39:TYR:CD2	1:A:66:ARG:HD2	0.45	2.47	16	3
1:A:27:ILE:HD11	1:A:55:GLN:HE21	0.45	1.72	6	3
1:A:23:VAL:HG13	1:A:27:ILE:HG21	0.45	1.88	19	2
1:A:34:MET:HE1	1:A:58:ILE:HA	0.45	1.89	18	2
1:A:60:ILE:HG21	1:A:126:LEU:HD12	0.45	1.87	19	1
1:A:121:GLU:N	1:A:121:GLU:CD	0.45	2.75	19	3
1:A:53:ILE:CG2	1:A:54:HIS:N	0.45	2.80	16	4
1:A:98:ALA:CB	1:A:146:LEU:HD22	0.45	2.40	2	1
1:A:31:VAL:HG12	1:A:32:ASP:N	0.45	2.23	13	3
1:A:146:LEU:CD1	1:A:146:LEU:N	0.45	2.80	17	2
1:A:3:LEU:HD11	1:A:33:ASP:CB	0.44	2.42	11	20
1:A:121:GLU:CD	1:A:121:GLU:C	0.44	2.85	20	5
1:A:39:TYR:CZ	1:A:66:ARG:HD3	0.44	2.47	9	1
1:A:73:ILE:HG12	1:A:113:ARG:HH22	0.44	1.72	19	1
1:A:100:VAL:CG1	1:A:145:TYR:CD1	0.44	3.00	2	2
1:A:100:VAL:HG13	1:A:145:TYR:CD1	0.44	2.47	2	2
1:A:100:VAL:CG1	1:A:102:ARG:NH1	0.44	2.81	13	1
1:A:38:MET:HE1	1:A:60:ILE:C	0.44	2.37	14	2
1:A:110:ALA:HB3	1:A:118:PHE:CE2	0.44	2.48	16	5
1:A:125:LEU:H	1:A:125:LEU:CD2	0.44	2.26	13	2
1:A:63:SER:HB3	1:A:68:GLU:HB2	0.44	1.89	4	2
1:A:14:ARG:NH2	1:A:14:ARG:HB2	0.44	2.28	17	1
1:A:56:ARG:O	1:A:73:ILE:O	0.44	2.36	11	8
1:A:68:GLU:CD	1:A:70:LEU:HD23	0.44	2.38	4	3
1:A:53:ILE:HG22	1:A:54:HIS:N	0.44	2.28	19	4
1:A:76:GLU:HG3	1:A:109:ARG:HG2	0.44	1.88	15	2
1:A:27:ILE:HD11	1:A:55:GLN:HE22	0.44	1.73	17	1
1:A:112:ASP:CG	1:A:113:ARG:N	0.44	2.76	7	4
1:A:10:ASP:CG	1:A:11:GLU:H	0.44	2.21	16	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:VAL:CG2	1:A:113:ARG:NH2	0.44	2.81	19	1
1:A:35:PHE:CD1	1:A:39:TYR:CE1	0.44	3.06	9	1
1:A:76:GLU:HG2	1:A:109:ARG:HG2	0.44	1.89	17	1
1:A:116:LYS:HZ3	1:A:116:LYS:HA	0.44	1.73	17	1
1:A:8:ILE:HD13	1:A:8:ILE:N	0.43	2.28	19	14
1:A:103:ALA:N	1:A:131:GLN:HE22	0.43	2.11	4	1
1:A:100:VAL:HG12	1:A:102:ARG:CZ	0.43	2.42	7	2
1:A:56:ARG:HB3	1:A:73:ILE:O	0.43	2.12	8	1
1:A:23:VAL:HG13	1:A:27:ILE:CB	0.43	2.43	5	3
1:A:11:GLU:O	1:A:15:LYS:N	0.43	2.51	9	5
1:A:108:ILE:O	1:A:119:GLU:HA	0.43	2.13	13	4
1:A:103:ALA:HB3	1:A:131:GLN:NE2	0.43	2.28	5	6
1:A:73:ILE:HG22	1:A:74:ASN:ND2	0.43	2.28	12	2
1:A:35:PHE:CD2	1:A:69:ARG:CZ	0.43	3.01	10	1
1:A:73:ILE:HG12	1:A:113:ARG:NH2	0.43	2.28	13	1
1:A:125:LEU:HD22	1:A:125:LEU:N	0.43	2.28	8	4
1:A:52:ASP:O	1:A:53:ILE:HG13	0.43	2.13	8	3
1:A:14:ARG:HA	1:A:139:GLY:CA	0.43	2.44	11	1
1:A:72:LEU:CD2	1:A:130:ILE:HG13	0.43	2.43	11	1
1:A:44:ILE:HG13	1:A:45:GLY:N	0.43	2.28	17	2
1:A:142:PHE:HA	1:A:145:TYR:CE2	0.43	2.48	20	2
1:A:14:ARG:HH11	1:A:141:LEU:H	0.43	1.56	15	1
1:A:24:ASN:HD22	1:A:24:ASN:C	0.43	2.21	5	2
1:A:31:VAL:CG1	1:A:71:VAL:CG2	0.43	2.97	16	3
1:A:127:ALA:O	1:A:130:ILE:CG2	0.43	2.67	6	6
1:A:35:PHE:CD1	1:A:39:TYR:CZ	0.43	3.06	19	2
1:A:88:GLU:HA	1:A:97:ARG:HD2	0.43	1.91	9	2
1:A:19:PRO:HA	1:A:56:ARG:CG	0.43	2.44	4	1
1:A:76:GLU:HG2	1:A:109:ARG:CG	0.43	2.44	4	2
1:A:39:TYR:OH	1:A:69:ARG:HG2	0.43	2.14	8	3
1:A:18:LYS:CG	1:A:54:HIS:O	0.43	2.67	17	1
1:A:31:VAL:HG11	1:A:71:VAL:HG21	0.43	1.91	20	6
1:A:56:ARG:C	1:A:57:ILE:HG13	0.42	2.38	3	1
1:A:94:PRO:HG2	1:A:143:MET:SD	0.42	2.54	3	1
1:A:23:VAL:HG13	1:A:27:ILE:CG1	0.42	2.44	4	2
1:A:26:GLU:C	1:A:29:ARG:HB3	0.42	2.39	16	1
1:A:90:CYS:HB3	1:A:93:ILE:CG1	0.42	2.43	3	2
1:A:11:GLU:CD	1:A:11:GLU:N	0.42	2.76	20	2
1:A:145:TYR:C	1:A:146:LEU:HD23	0.42	2.39	2	1
1:A:120:LEU:C	1:A:120:LEU:HD23	0.42	2.39	3	1
1:A:27:ILE:CD1	1:A:55:GLN:HE22	0.42	2.28	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:GLU:CD	1:A:121:GLU:N	0.42	2.78	6	1
1:A:80:LYS:HA	1:A:105:LYS:O	0.42	2.14	17	3
1:A:24:ASN:HD21	1:A:27:ILE:CG1	0.42	2.27	15	1
1:A:39:TYR:CE2	1:A:61:ASP:OD2	0.42	2.72	15	1
1:A:32:ASP:C	1:A:34:MET:N	0.42	2.75	17	1
1:A:38:MET:SD	1:A:45:GLY:HA2	0.42	2.55	1	1
1:A:15:LYS:CD	1:A:54:HIS:NE2	0.42	2.82	7	2
1:A:120:LEU:HD22	1:A:120:LEU:C	0.42	2.40	12	2
1:A:38:MET:CE	1:A:59:VAL:HG23	0.42	2.45	15	1
1:A:125:LEU:O	1:A:126:LEU:C	0.42	2.58	1	4
1:A:112:ASP:O	1:A:113:ARG:C	0.42	2.61	19	1
1:A:11:GLU:CD	1:A:11:GLU:H	0.42	2.22	20	1
1:A:91:LEU:O	1:A:92:SER:C	0.42	2.62	20	6
1:A:28:GLN:CG	1:A:29:ARG:N	0.42	2.83	13	1
1:A:35:PHE:O	1:A:39:TYR:N	0.42	2.52	14	1
1:A:23:VAL:CG1	1:A:27:ILE:HG21	0.42	2.44	16	1
1:A:102:ARG:HH12	1:A:142:PHE:CB	0.42	2.28	17	1
1:A:128:ILE:O	1:A:129:CYS:C	0.42	2.62	20	4
1:A:98:ALA:HB1	1:A:100:VAL:HG23	0.42	1.91	12	3
1:A:86:ILE:HD11	1:A:102:ARG:NH1	0.42	2.30	14	1
1:A:86:ILE:CG1	1:A:128:ILE:HG21	0.42	2.45	3	2
1:A:121:GLU:CD	1:A:121:GLU:H	0.42	2.23	16	1
1:A:132:HIS:CE1	1:A:142:PHE:CG	0.42	3.07	18	1
1:A:15:LYS:NZ	1:A:54:HIS:CD2	0.41	2.88	17	1
1:A:119:GLU:N	1:A:119:GLU:CD	0.41	2.78	19	1
1:A:10:ASP:H	1:A:14:ARG:NH1	0.41	2.13	5	1
1:A:51:VAL:HG23	1:A:52:ASP:N	0.41	2.30	14	1
1:A:35:PHE:HB3	1:A:39:TYR:CE2	0.41	2.50	19	1
1:A:70:LEU:N	1:A:70:LEU:CD2	0.41	2.83	11	2
1:A:71:VAL:HG11	1:A:113:ARG:NE	0.41	2.30	13	1
1:A:60:ILE:HD13	1:A:126:LEU:HD11	0.41	1.91	18	1
1:A:103:ALA:C	1:A:131:GLN:HE22	0.41	2.23	17	1
1:A:73:ILE:O	1:A:75:PRO:CD	0.41	2.69	3	3
1:A:126:LEU:C	1:A:126:LEU:HD13	0.41	2.40	8	1
1:A:35:PHE:HD1	1:A:39:TYR:CE1	0.41	2.34	9	1
1:A:99:LEU:HD22	1:A:99:LEU:HA	0.41	1.73	4	1
1:A:35:PHE:HE2	1:A:69:ARG:CB	0.41	2.27	15	1
1:A:31:VAL:HG11	1:A:71:VAL:CG2	0.41	2.45	19	1
1:A:15:LYS:HG3	1:A:54:HIS:CE1	0.41	2.50	6	1
1:A:125:LEU:HD12	1:A:125:LEU:H	0.41	1.75	9	1
1:A:14:ARG:HE	1:A:141:LEU:CD1	0.41	2.28	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:LEU:C	1:A:126:LEU:HD23	0.41	2.40	14	1
1:A:23:VAL:CG1	1:A:27:ILE:CB	0.41	2.98	15	1
1:A:38:MET:CE	1:A:61:ASP:CG	0.41	2.94	15	1
1:A:108:ILE:HD11	1:A:120:LEU:HD12	0.41	1.93	2	1
1:A:127:ALA:O	1:A:131:GLN:HG3	0.41	2.16	4	1
1:A:15:LYS:HE2	1:A:16:VAL:C	0.41	2.41	6	1
1:A:73:ILE:C	1:A:75:PRO:CD	0.41	2.94	13	2
1:A:14:ARG:HB2	1:A:14:ARG:CZ	0.41	2.46	17	1
1:A:142:PHE:O	1:A:142:PHE:CD1	0.41	2.74	20	1
1:A:86:ILE:HG23	1:A:128:ILE:HG13	0.40	1.93	2	1
1:A:130:ILE:HG23	1:A:131:GLN:H	0.40	1.76	3	1
1:A:119:GLU:CD	1:A:119:GLU:N	0.40	2.80	12	1
1:A:13:LEU:HB2	1:A:14:ARG:NE	0.40	2.31	3	1
1:A:88:GLU:HA	1:A:97:ARG:HD3	0.40	1.92	3	1
1:A:76:GLU:CD	1:A:76:GLU:C	0.40	2.88	6	1
1:A:144:ASP:C	1:A:146:LEU:H	0.40	2.25	7	1
1:A:113:ARG:N	1:A:113:ARG:NE	0.40	2.68	13	1
1:A:102:ARG:HH22	1:A:132:HIS:HD1	0.40	1.59	3	1
1:A:134:MET:O	1:A:135:ASP:C	0.40	2.65	5	1
1:A:27:ILE:HG21	1:A:73:ILE:CD1	0.40	2.46	12	1
1:A:60:ILE:CB	1:A:70:LEU:HB2	0.40	2.47	18	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	144/147 (98%)	105±3 (73±2%)	33±3 (23±2%)	5±1 (4±1%)	4	32
All	All	2880/2940 (98%)	2109 (73%)	668 (23%)	103 (4%)	4	32

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	51	VAL	20

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Mol	Chain	Res	Type	Models (Total)
1	A	124	GLY	20
1	A	93	ILE	18
1	A	95	GLU	15
1	A	125	LEU	12
1	A	40	ALA	4
1	A	82	GLY	4
1	A	41	GLU	3
1	A	103	ALA	3
1	A	113	ARG	2
1	A	94	PRO	2

### 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	128/128 (100%)	104±3 (81±2%)	24±3 (19±2%)	3	35
All	All	2560/2560 (100%)	2077 (81%)	483 (19%)	3	35

All 61 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	6	LEU	20
1	A	8	ILE	20
1	A	27	ILE	20
1	A	58	ILE	20
1	A	102	ARG	20
1	A	142	PHE	20
1	A	145	TYR	20
1	A	28	GLN	19
1	A	33	ASP	19
1	A	77	LEU	19
1	A	60	ILE	18
1	A	71	VAL	18
1	A	86	ILE	18
1	A	120	LEU	18
1	A	130	ILE	17

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Mol	Chain	Res	Type	Models (Total)
1	A	26	GLU	16
1	A	135	ASP	16
1	A	53	ILE	14
1	A	61	ASP	13
1	A	31	VAL	12
1	A	12	ARG	12
1	A	29	ARG	9
1	A	146	LEU	7
1	A	13	LEU	6
1	A	10	ASP	5
1	A	112	ASP	5
1	A	121	GLU	5
1	A	24	ASN	5
1	A	50	GLN	4
1	A	106	VAL	4
1	A	73	ILE	4
1	A	15	LYS	4
1	A	18	LYS	4
1	A	78	LEU	3
1	A	79	GLU	3
1	A	62	VAL	3
1	A	70	LEU	3
1	A	42	GLU	3
1	A	38	MET	3
1	A	34	MET	3
1	A	109	ARG	2
1	A	55	GLN	2
1	A	68	GLU	2
1	A	96	GLN	2
1	A	97	ARG	2
1	A	66	ARG	2
1	A	81	SER	2
1	A	140	LYS	2
1	A	14	ARG	2
1	A	116	LYS	2
1	A	100	VAL	1
1	A	87	GLU	1
1	A	76	GLU	1
1	A	52	ASP	1
1	A	95	GLU	1
1	A	99	LEU	1
1	A	54	HIS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	72	LEU	1
1	A	2	VAL	1
1	A	69	ARG	1
1	A	11	GLU	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

### 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