



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:29 PM UTC

PDB ID : 2G4A / pdb_00002g4a
Title : Solution structure of a Bromodomain from RING3 protein
Authors : Huang, H.; Wu, J.; Shi, Y.
Deposited on : 2006-02-21

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

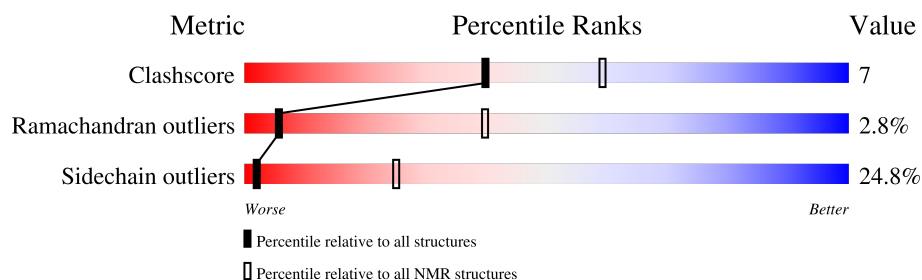
1 Overall quality at a glance

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	116	61% 32% 7%

2 Ensemble composition and analysis

This entry contains 21 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:108 (108)	0.73	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 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 5, 7, 9, 10, 11, 13, 14, 15, 17, 18, 20
2	4, 12, 16, 21
3	8, 19
Single-model clusters	6

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1787 atoms, of which 888 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bromodomain-containing protein 2.

Mol	Chain	Residues	Atoms						Trace
1	A	108	Total	C	H	N	O	S	0
			1787	576	888	157	159	7	

There are 9 discrepancies between the modelled and reference sequences:

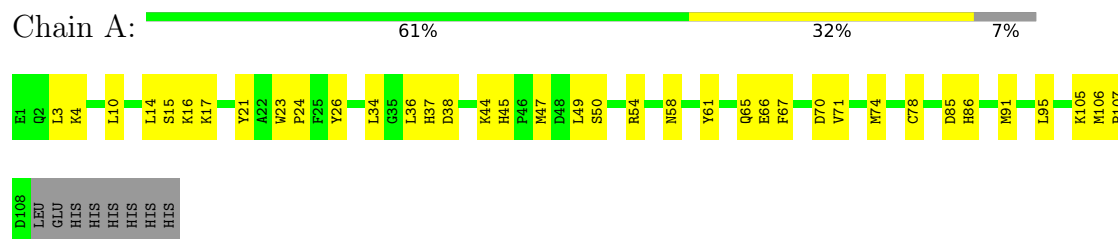
Chain	Residue	Modelled	Actual	Comment	Reference
A	8	VAL	GLY	SEE REMARK 999	UNP P25440
A	109	LEU	-	expression tag	UNP P25440
A	110	GLU	-	expression tag	UNP P25440
A	111	HIS	-	expression tag	UNP P25440
A	112	HIS	-	expression tag	UNP P25440
A	113	HIS	-	expression tag	UNP P25440
A	114	HIS	-	expression tag	UNP P25440
A	115	HIS	-	expression tag	UNP P25440
A	116	HIS	-	expression tag	UNP P25440

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: Bromodomain-containing protein 2

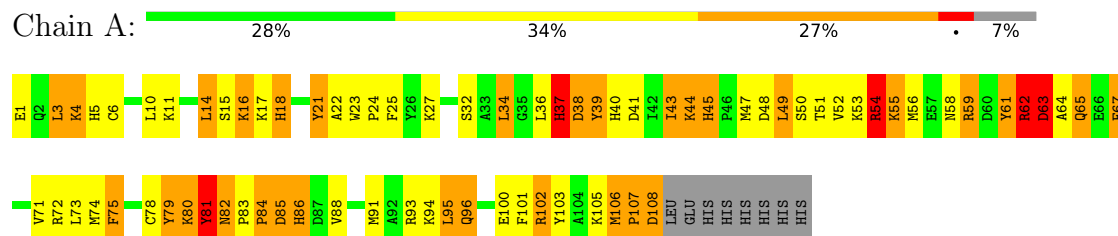


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

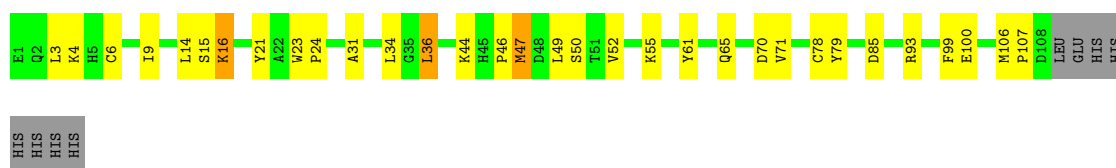
- Molecule 1: Bromodomain-containing protein 2



4.2.2 Score per residue for model 2

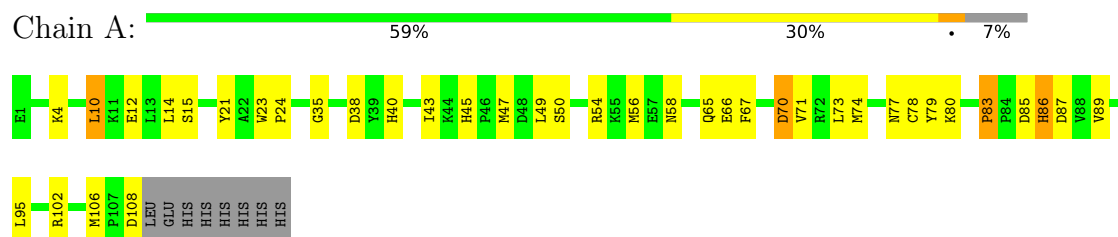
- Molecule 1: Bromodomain-containing protein 2





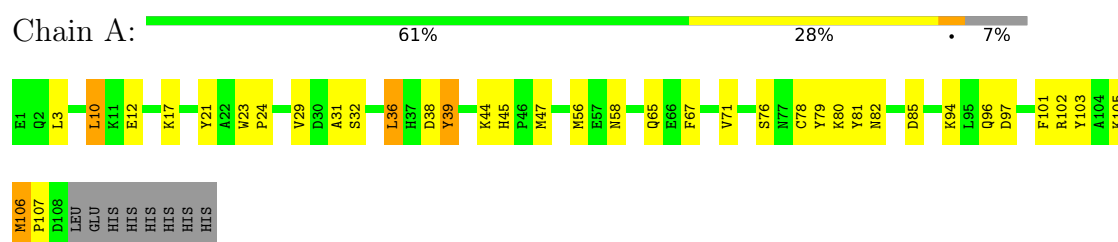
4.2.3 Score per residue for model 3

- Molecule 1: Bromodomain-containing protein 2



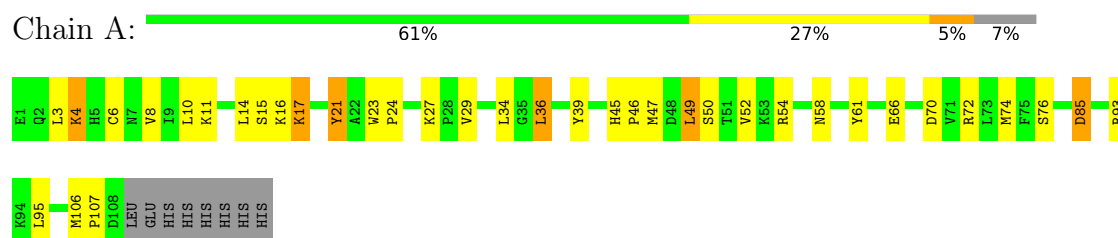
4.2.4 Score per residue for model 4

- Molecule 1: Bromodomain-containing protein 2



4.2.5 Score per residue for model 5

- Molecule 1: Bromodomain-containing protein 2

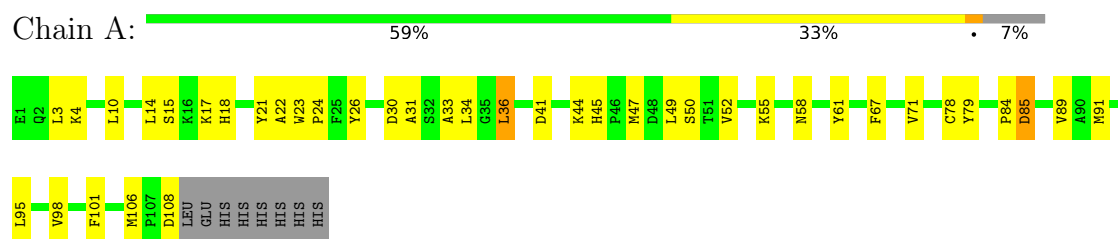


4.2.6 Score per residue for model 6

- Molecule 1: Bromodomain-containing protein 2

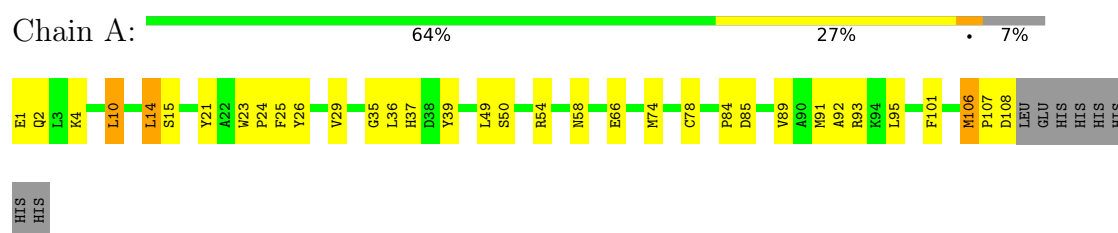
4.2.10 Score per residue for model 10

- Molecule 1: Bromodomain-containing protein 2



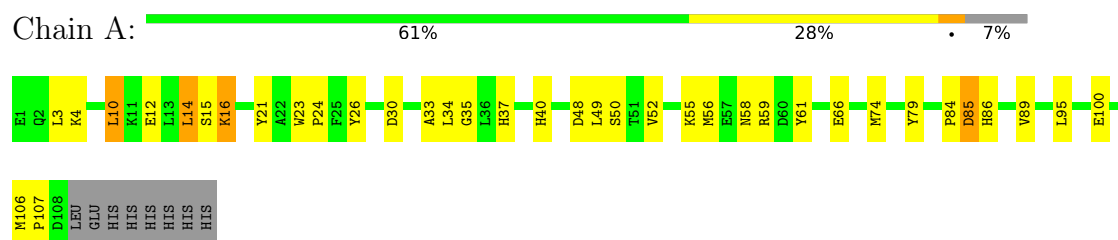
4.2.11 Score per residue for model 11

- Molecule 1: Bromodomain-containing protein 2



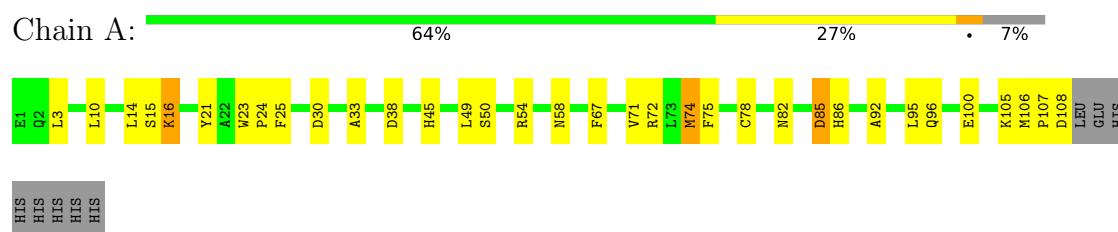
4.2.12 Score per residue for model 12

- Molecule 1: Bromodomain-containing protein 2



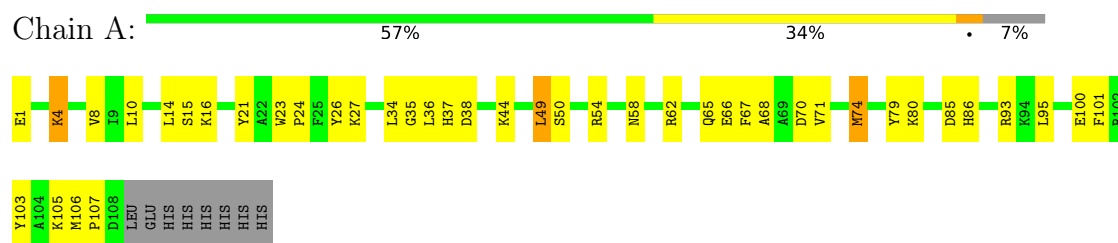
4.2.13 Score per residue for model 13

- Molecule 1: Bromodomain-containing protein 2



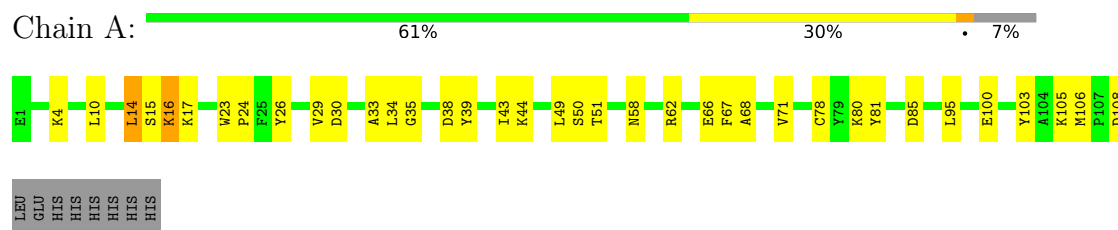
4.2.14 Score per residue for model 14

- Molecule 1: Bromodomain-containing protein 2



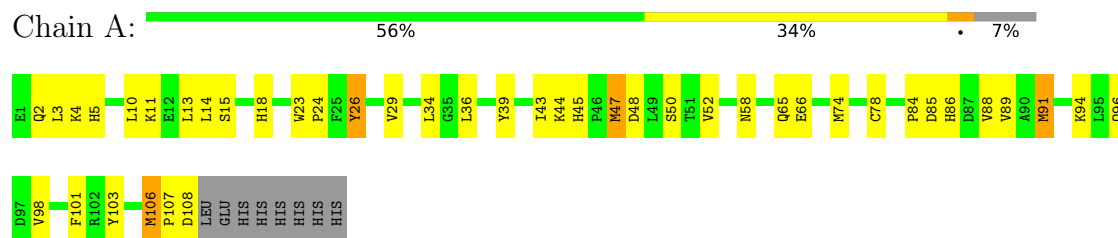
4.2.15 Score per residue for model 15

- Molecule 1: Bromodomain-containing protein 2



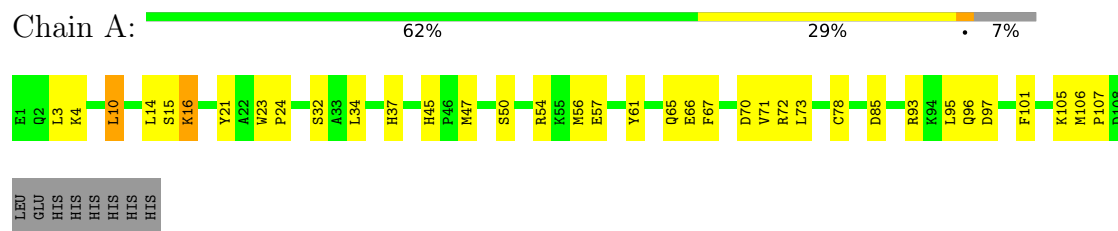
4.2.16 Score per residue for model 16

- Molecule 1: Bromodomain-containing protein 2



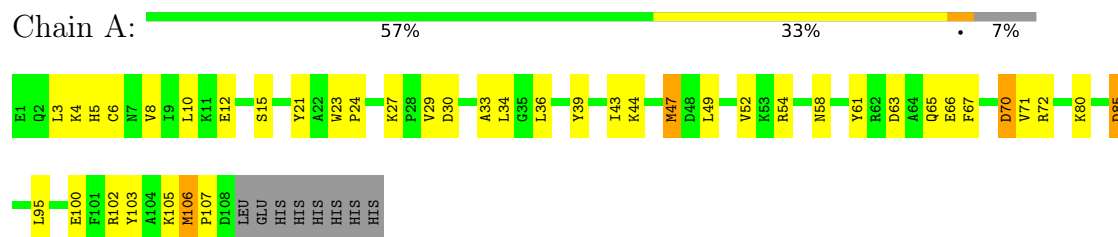
4.2.17 Score per residue for model 17

- Molecule 1: Bromodomain-containing protein 2



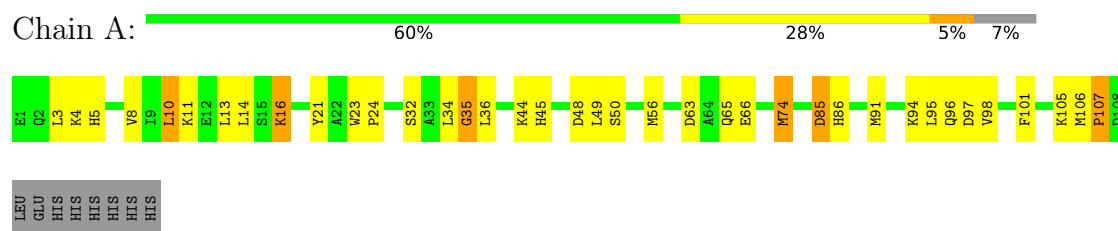
4.2.18 Score per residue for model 18

- Molecule 1: Bromodomain-containing protein 2



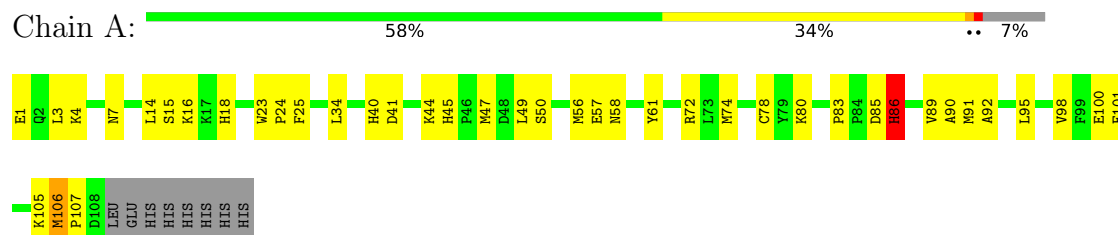
4.2.19 Score per residue for model 19

- Molecule 1: Bromodomain-containing protein 2



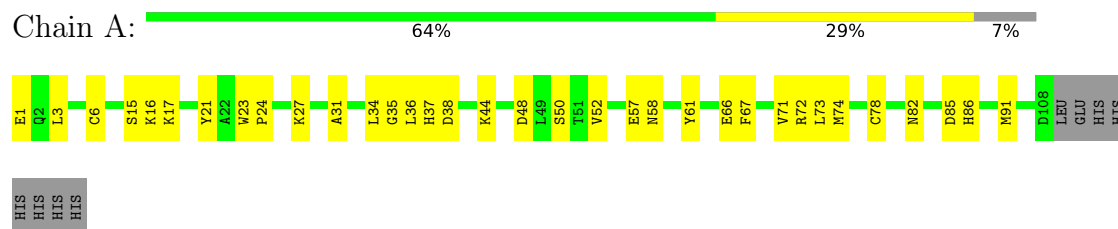
4.2.20 Score per residue for model 20

- Molecule 1: Bromodomain-containing protein 2



4.2.21 Score per residue for model 21

- Molecule 1: Bromodomain-containing protein 2



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry simulated annealing molecular dynamics torsion angle dynamics*.

Of the 200 calculated structures, 21 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

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	0.51±0.76	7±29/924 (0.7± 3.2%)	0.69±0.31	2±10/1246 (0.2± 0.8%)
All	All	0.91	138/19404 (0.7%)	0.76	46/26166 (0.2%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.3±1.3
All	All	0	6

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	108	ASP	CA-C	-21.20	1.08	1.52	1	1
1	A	37	HIS	CB-CG	-19.53	1.22	1.50	1	1
1	A	62	ARG	CD-NE	-19.46	1.19	1.46	1	1
1	A	107	PRO	CA-C	-18.34	1.30	1.52	1	1
1	A	102	ARG	NE-CZ	-16.27	1.15	1.33	1	1
1	A	93	ARG	CZ-NH2	-15.79	1.12	1.33	1	1
1	A	59	ARG	CZ-NH2	-15.75	1.12	1.33	1	1
1	A	37	HIS	CG-CD2	-15.62	1.18	1.35	1	1
1	A	72	ARG	CZ-NH2	-15.31	1.13	1.33	1	1
1	A	72	ARG	NE-CZ	-15.28	1.16	1.33	1	1
1	A	72	ARG	CD-NE	-14.13	1.26	1.46	1	1
1	A	27	LYS	CA-CB	-14.04	1.30	1.53	1	1
1	A	93	ARG	NE-CZ	-13.38	1.18	1.33	1	1
1	A	93	ARG	CD-NE	-13.14	1.27	1.46	1	1
1	A	18	HIS	CG-CD2	-12.54	1.22	1.35	1	1
1	A	45	HIS	CB-CG	-12.05	1.33	1.50	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	18	HIS	CD2-NE2	12.02	1.51	1.37	1	1
1	A	37	HIS	ND1-CE1	-11.92	1.20	1.32	1	1
1	A	54	ARG	CD-NE	-11.83	1.29	1.46	1	1
1	A	59	ARG	CD-NE	-11.79	1.29	1.46	1	1
1	A	54	ARG	CZ-NH2	-11.68	1.18	1.33	1	1
1	A	59	ARG	NE-CZ	-11.61	1.20	1.33	1	1
1	A	86	HIS	CG-ND1	-11.46	1.25	1.38	1	1
1	A	45	HIS	CG-CD2	-11.36	1.23	1.35	1	1
1	A	105	LYS	CD-CE	-10.74	1.20	1.52	1	1
1	A	5	HIS	CG-ND1	-10.66	1.26	1.38	1	1
1	A	102	ARG	CZ-NH2	-10.43	1.19	1.33	1	1
1	A	102	ARG	CG-CD	-9.72	1.23	1.52	1	1
1	A	37	HIS	CE1-NE2	-9.63	1.23	1.32	1	1
1	A	86	HIS	CB-CG	-9.49	1.36	1.50	1	1
1	A	61	TYR	C-N	-9.48	1.20	1.33	1	1
1	A	5	HIS	CB-CG	-9.44	1.36	1.50	1	1
1	A	27	LYS	CD-CE	-9.15	1.25	1.52	1	1
1	A	105	LYS	CG-CD	-9.12	1.25	1.52	1	1
1	A	37	HIS	CG-ND1	-9.08	1.28	1.38	1	1
1	A	86	HIS	CE1-NE2	-9.04	1.23	1.32	1	1
1	A	86	HIS	ND1-CE1	-9.01	1.23	1.32	1	1
1	A	18	HIS	CE1-NE2	-8.97	1.23	1.32	1	1
1	A	18	HIS	CG-ND1	-8.90	1.28	1.38	1	1
1	A	27	LYS	CB-CG	-8.87	1.25	1.52	1	1
1	A	108	ASP	N-CA	-8.82	1.29	1.46	1	1
1	A	5	HIS	CE1-NE2	-8.78	1.23	1.32	1	1
1	A	93	ARG	CG-CD	-8.75	1.26	1.52	1	1
1	A	45	HIS	CE1-NE2	-8.75	1.23	1.32	1	1
1	A	54	ARG	NE-CZ	-8.73	1.23	1.33	1	1
1	A	80	LYS	CG-CD	-8.65	1.26	1.52	1	1
1	A	45	HIS	CG-ND1	-8.59	1.28	1.38	1	1
1	A	105	LYS	CE-NZ	-8.30	1.24	1.49	1	1
1	A	17	LYS	CB-CG	-8.23	1.27	1.52	1	1
1	A	61	TYR	CG-CD2	-8.16	1.22	1.39	1	1
1	A	45	HIS	CD2-NE2	-8.11	1.28	1.37	1	1
1	A	62	ARG	CG-CD	-8.08	1.28	1.52	1	1
1	A	80	LYS	CD-CE	-7.96	1.28	1.52	1	1
1	A	59	ARG	CG-CD	-7.95	1.28	1.52	1	1
1	A	82	ASN	CG-ND2	-7.72	1.17	1.33	1	1
1	A	27	LYS	CG-CD	-7.67	1.29	1.52	1	1
1	A	86	HIS	CD2-NE2	-7.66	1.29	1.37	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	54	ARG	CZ-NH1	-7.59	1.22	1.32	1	1
1	A	16	LYS	CD-CE	-7.43	1.30	1.52	1	1
1	A	96	GLN	CD-NE2	-7.41	1.17	1.33	1	1
1	A	1	GLU	CB-CG	-7.37	1.30	1.52	1	1
1	A	45	HIS	ND1-CE1	-7.34	1.25	1.32	1	1
1	A	4	LYS	CD-CE	-7.30	1.30	1.52	1	1
1	A	5	HIS	ND1-CE1	-7.24	1.25	1.32	1	1
1	A	62	ARG	CA-CB	-7.24	1.41	1.53	1	1
1	A	1	GLU	CA-CB	-7.23	1.39	1.53	1	1
1	A	72	ARG	CG-CD	-7.22	1.30	1.52	1	1
1	A	34	LEU	CA-C	-7.20	1.44	1.52	1	1
1	A	108	ASP	CA-CB	-7.07	1.39	1.53	1	1
1	A	44	LYS	CG-CD	-6.94	1.31	1.52	1	1
1	A	5	HIS	CD2-NE2	-6.85	1.30	1.37	1	1
1	A	105	LYS	CA-CB	-6.84	1.41	1.53	1	1
1	A	102	ARG	CZ-NH1	-6.75	1.23	1.32	1	1
1	A	62	ARG	CB-CG	-6.68	1.32	1.52	1	1
1	A	21	TYR	CE1-CZ	-6.68	1.22	1.38	1	1
1	A	4	LYS	CG-CD	-6.66	1.32	1.52	1	1
1	A	17	LYS	CE-NZ	-6.65	1.29	1.49	1	1
1	A	81	TYR	CE1-CZ	-6.63	1.22	1.38	1	1
1	A	5	HIS	CG-CD2	-6.54	1.28	1.35	1	1
1	A	80	LYS	CB-CG	-6.54	1.32	1.52	1	1
1	A	44	LYS	CD-CE	-6.50	1.32	1.52	1	1
1	A	16	LYS	CB-CG	-6.50	1.32	1.52	1	1
1	A	4	LYS	CB-CG	-6.48	1.33	1.52	1	1
1	A	61	TYR	CE1-CZ	-6.38	1.23	1.38	1	1
1	A	86	HIS	CG-CD2	-6.27	1.28	1.35	1	1
1	A	39	TYR	CG-CD1	-6.25	1.26	1.39	1	1
1	A	34	LEU	CB-CG	-6.24	1.41	1.53	1	1
1	A	16	LYS	CE-NZ	-6.14	1.30	1.49	1	1
1	A	84	PRO	N-CA	-6.12	1.39	1.47	1	1
1	A	107	PRO	N-CA	-6.10	1.40	1.47	1	1
1	A	79	TYR	CG-CD2	-6.07	1.26	1.39	1	1
1	A	4	LYS	CE-NZ	-6.06	1.31	1.49	1	1
1	A	27	LYS	CE-NZ	-6.05	1.31	1.49	1	1
1	A	3	LEU	CG-CD2	-6.04	1.32	1.52	1	1
1	A	16	LYS	CA-CB	-6.04	1.43	1.53	1	1
1	A	79	TYR	CE1-CZ	-6.03	1.23	1.38	1	1
1	A	44	LYS	CE-NZ	-6.00	1.31	1.49	1	1
1	A	27	LYS	CA-C	-6.00	1.46	1.53	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	40	HIS	CE1-NE2	-5.97	1.26	1.32	1	1
1	A	61	TYR	CG-CD1	-5.93	1.26	1.39	1	1
1	A	39	TYR	CE2-CZ	-5.92	1.24	1.38	1	1
1	A	1	GLU	CG-CD	-5.92	1.37	1.52	1	1
1	A	17	LYS	CD-CE	-5.89	1.34	1.52	1	1
1	A	65	GLN	CD-NE2	-5.86	1.21	1.33	1	1
1	A	100	GLU	CB-CG	-5.83	1.34	1.52	1	1
1	A	54	ARG	CG-CD	-5.79	1.35	1.52	1	1
1	A	83	PRO	CA-CB	-5.73	1.46	1.54	1	1
1	A	53	LYS	CG-CD	-5.72	1.35	1.52	1	1
1	A	72	ARG	CB-CG	-5.71	1.35	1.52	1	1
1	A	16	LYS	C-N	-5.70	1.26	1.33	1	1
1	A	21	TYR	CG-CD2	-5.69	1.27	1.39	1	1
1	A	4	LYS	CA-CB	-5.64	1.44	1.53	1	1
1	A	14	LEU	CB-CG	-5.64	1.42	1.53	1	1
1	A	25	PHE	CG-CD2	-5.60	1.27	1.38	1	1
1	A	102	ARG	CD-NE	-5.55	1.38	1.46	1	1
1	A	102	ARG	CB-CG	-5.50	1.35	1.52	1	1
1	A	82	ASN	CA-C	-5.48	1.47	1.52	1	1
1	A	61	TYR	CB-CG	-5.46	1.39	1.51	1	1
1	A	37	HIS	CA-CB	-5.46	1.44	1.53	1	1
1	A	61	TYR	CE2-CZ	-5.41	1.25	1.38	1	1
1	A	107	PRO	CA-CB	-5.33	1.46	1.53	1	1
1	A	11	LYS	CD-CE	-5.28	1.36	1.52	1	1
1	A	34	LEU	CG-CD1	-5.26	1.35	1.52	1	1
1	A	17	LYS	CG-CD	-5.26	1.36	1.52	1	1
1	A	63	ASP	N-CA	-5.25	1.39	1.46	1	1
1	A	62	ARG	NE-CZ	-5.25	1.27	1.33	1	1
1	A	80	LYS	CE-NZ	-5.24	1.33	1.49	1	1
1	A	82	ASN	CB-CG	-5.14	1.39	1.52	1	1
1	A	100	GLU	CG-CD	-5.14	1.39	1.52	1	1
1	A	67	PHE	CG-CD1	-5.11	1.28	1.38	1	1
1	A	3	LEU	CG-CD1	-5.10	1.35	1.52	1	1
1	A	94	LYS	CE-NZ	-5.08	1.34	1.49	1	1
1	A	75	PHE	CE2-CZ	-5.05	1.23	1.38	1	1
1	A	81	TYR	CB-CG	-5.02	1.40	1.51	1	1
1	A	103	TYR	CE2-CZ	-5.02	1.26	1.38	1	1
1	A	83	PRO	CA-C	-5.01	1.47	1.52	1	1
1	A	21	TYR	CG-CD1	-5.01	1.28	1.39	1	1
1	A	62	ARG	CZ-NH2	-5.01	1.26	1.33	1	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	62	ARG	NE-CZ-NH2	-15.79	104.99	119.20	1	1
1	A	75	PHE	CG-CD2-CE2	-14.49	96.07	120.70	1	1
1	A	75	PHE	CD1-CE1-CZ	-14.42	94.05	120.00	1	1
1	A	54	ARG	NE-CZ-NH1	-11.60	109.90	121.50	1	1
1	A	105	LYS	CB-CG-CD	-11.30	85.31	111.30	1	1
1	A	61	TYR	CB-CA-C	-10.29	96.83	111.14	1	1
1	A	93	ARG	CD-NE-CZ	-9.99	110.41	124.40	1	1
1	A	17	LYS	CG-CD-CE	-9.13	90.30	111.30	1	1
1	A	59	ARG	CD-NE-CZ	-8.83	112.04	124.40	1	1
1	A	54	ARG	CB-CG-CD	-8.49	91.78	111.30	1	1
1	A	27	LYS	CB-CA-C	-8.15	96.15	109.27	1	1
1	A	75	PHE	CG-CD1-CE1	8.13	134.53	120.70	1	1
1	A	105	LYS	CG-CD-CE	8.13	129.99	111.30	1	1
1	A	75	PHE	CZ-CE2-CD2	7.98	134.36	120.00	1	1
1	A	54	ARG	NE-CZ-NH2	-7.83	112.16	119.20	1	1
1	A	16	LYS	CB-CG-CD	-7.72	93.55	111.30	1	1
1	A	75	PHE	CE1-CZ-CE2	7.53	133.56	120.00	1	1
1	A	100	GLU	CA-CB-CG	-7.35	99.41	114.10	1	1
1	A	107	PRO	N-CA-C	-7.34	99.55	111.15	1	1
1	A	1	GLU	CA-CB-CG	-7.33	99.45	114.10	1	1
1	A	27	LYS	CB-CG-CD	-6.97	95.26	111.30	1	1
1	A	72	ARG	CD-NE-CZ	-6.92	114.71	124.40	1	1
1	A	36	LEU	CD1-CG-CD2	-6.52	96.46	110.80	1	1
1	A	14	LEU	CD1-CG-CD2	-6.27	97.00	110.80	1	1
1	A	37	HIS	CA-CB-CG	-6.25	107.55	113.80	1	1
1	A	80	LYS	CA-CB-CG	-6.25	101.61	114.10	1	1
1	A	80	LYS	CB-CG-CD	6.19	125.54	111.30	1	1
1	A	16	LYS	CG-CD-CE	-6.08	97.32	111.30	1	1
1	A	54	ARG	CD-NE-CZ	6.08	132.91	124.40	1	1
1	A	102	ARG	CG-CD-NE	-5.99	98.83	112.00	1	1
1	A	54	ARG	CG-CD-NE	5.90	124.98	112.00	1	1
1	A	102	ARG	CD-NE-CZ	-5.90	116.14	124.40	1	1
1	A	75	PHE	CD1-CG-CD2	5.88	127.41	118.60	1	1
1	A	53	LYS	CG-CD-CE	-5.84	97.86	111.30	1	1
1	A	17	LYS	CA-CB-CG	-5.74	102.62	114.10	1	1
1	A	82	ASN	CA-CB-CG	-5.61	106.99	112.60	1	1
1	A	38	ASP	CA-CB-CG	5.59	118.19	112.60	1	1
1	A	107	PRO	O-C-N	5.58	129.97	122.89	1	1
1	A	105	LYS	CD-CE-NZ	5.56	129.69	111.90	1	1
1	A	4	LYS	CA-CB-CG	-5.56	102.99	114.10	1	1
1	A	49	LEU	CD1-CG-CD2	-5.51	98.67	110.80	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	107	PRO	N-CA-CB	5.45	108.05	103.25	1	1
1	A	93	ARG	CB-CG-CD	-5.42	98.83	111.30	1	1
1	A	34	LEU	CD1-CG-CD2	-5.39	98.94	110.80	1	1
1	A	88	VAL	CG1-CB-CG2	-5.35	99.03	110.80	1	1
1	A	27	LYS	CG-CD-CE	-5.33	99.05	111.30	1	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	18	HIS	Sidechain	1
1	A	37	HIS	Sidechain	1
1	A	54	ARG	Sidechain	1
1	A	59	ARG	Sidechain	1
1	A	62	ARG	Sidechain	1
1	A	81	TYR	Sidechain	1

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	899	888	882	13±7
All	All	18879	18648	18522	264

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:TYR:O	1:A:63:ASP:N	0.84	2.10	1	1
1:A:107:PRO:C	1:A:108:ASP:O	0.83	2.12	1	1
1:A:107:PRO:O	1:A:108:ASP:O	0.79	1.99	1	1
1:A:64:ALA:HB1	1:A:106:MET:HE1	0.78	1.55	1	1
1:A:25:PHE:CZ	1:A:92:ALA:HB2	0.75	2.15	20	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ALA:HB1	1:A:36:LEU:O	0.69	1.87	9	5
1:A:21:TYR:HB2	1:A:95:LEU:CD1	0.67	2.19	1	1
1:A:49:LEU:HD12	1:A:74:MET:HE1	0.66	1.67	5	3
1:A:23:TRP:CG	1:A:24:PRO:HD3	0.64	2.28	1	21
1:A:18:HIS:CE1	1:A:98:VAL:HG21	0.63	2.28	20	2
1:A:47:MET:HE1	1:A:52:VAL:HG22	0.63	1.70	18	1
1:A:29:VAL:HG11	1:A:39:TYR:CE2	0.63	2.29	4	3
1:A:10:LEU:HD22	1:A:56:MET:SD	0.63	2.34	9	5
1:A:10:LEU:HD13	1:A:56:MET:SD	0.63	2.33	19	1
1:A:29:VAL:HG21	1:A:39:TYR:CE1	0.62	2.28	8	2
1:A:83:PRO:O	1:A:89:VAL:HG21	0.62	1.95	20	2
1:A:25:PHE:HB3	1:A:74:MET:HE1	0.62	1.71	13	1
1:A:71:VAL:HG21	1:A:99:PHE:CZ	0.61	2.30	7	1
1:A:64:ALA:CB	1:A:106:MET:HE1	0.61	2.24	1	1
1:A:21:TYR:CB	1:A:95:LEU:HD11	0.59	2.28	14	3
1:A:30:ASP:HB3	1:A:33:ALA:HB3	0.59	1.74	18	6
1:A:6:CYS:HA	1:A:9:ILE:HD12	0.59	1.74	2	1
1:A:52:VAL:HG13	1:A:61:TYR:OH	0.59	1.98	18	8
1:A:23:TRP:N	1:A:24:PRO:HD2	0.58	2.14	13	11
1:A:106:MET:N	1:A:107:PRO:CD	0.58	2.67	6	9
1:A:51:THR:O	1:A:55:LYS:HD2	0.58	1.99	1	1
1:A:67:PHE:O	1:A:71:VAL:HG23	0.57	1.99	18	12
1:A:84:PRO:HA	1:A:89:VAL:HG21	0.56	1.77	12	2
1:A:23:TRP:N	1:A:24:PRO:CD	0.56	2.67	1	21
1:A:10:LEU:HD13	1:A:56:MET:HE3	0.56	1.77	3	1
1:A:75:PHE:CD1	1:A:92:ALA:HB1	0.55	2.35	13	1
1:A:10:LEU:HA	1:A:13:LEU:HD12	0.55	1.76	19	1
1:A:38:ASP:O	1:A:42:ILE:HD12	0.55	2.02	6	1
1:A:21:TYR:CB	1:A:95:LEU:CD1	0.55	2.85	1	1
1:A:84:PRO:HA	1:A:89:VAL:HG11	0.55	1.76	7	5
1:A:35:GLY:C	1:A:36:LEU:HD22	0.54	2.28	19	1
1:A:21:TYR:HB2	1:A:95:LEU:HD11	0.53	1.79	1	2
1:A:18:HIS:NE2	1:A:98:VAL:HG21	0.53	2.18	16	1
1:A:14:LEU:HD12	1:A:26:TYR:HE2	0.53	1.63	16	1
1:A:24:PRO:HG3	1:A:91:MET:HE2	0.53	1.78	16	1
1:A:81:TYR:CD1	1:A:82:ASN:OD1	0.53	2.62	1	1
1:A:106:MET:N	1:A:107:PRO:HD2	0.53	2.19	1	9
1:A:14:LEU:O	1:A:14:LEU:HD23	0.53	2.04	3	2
1:A:14:LEU:HD11	1:A:26:TYR:OH	0.53	2.02	9	2
1:A:14:LEU:HD12	1:A:26:TYR:CE2	0.53	2.39	16	1
1:A:21:TYR:C	1:A:24:PRO:HD2	0.52	2.29	14	16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LEU:HD21	1:A:53:LYS:HD3	0.52	1.80	9	1
1:A:43:ILE:HG21	1:A:77:ASN:ND2	0.52	2.20	3	1
1:A:18:HIS:NE2	1:A:98:VAL:HG11	0.52	2.19	10	1
1:A:47:MET:CE	1:A:52:VAL:HG22	0.52	2.35	18	1
1:A:13:LEU:HD23	1:A:18:HIS:CB	0.51	2.35	9	1
1:A:54:ARG:HH11	1:A:54:ARG:HG3	0.51	1.66	1	1
1:A:29:VAL:HG11	1:A:39:TYR:CD2	0.51	2.41	11	2
1:A:39:TYR:CD2	1:A:81:TYR:CE2	0.51	2.98	1	1
1:A:4:LYS:O	1:A:8:VAL:HG23	0.51	2.06	7	5
1:A:29:VAL:HG13	1:A:29:VAL:O	0.51	2.04	15	1
1:A:54:ARG:HH11	1:A:54:ARG:CG	0.51	2.19	1	1
1:A:61:TYR:CE2	1:A:67:PHE:HA	0.51	2.41	1	1
1:A:3:LEU:HD21	1:A:61:TYR:O	0.50	2.07	17	1
1:A:29:VAL:HG11	1:A:39:TYR:CD1	0.50	2.42	5	1
1:A:84:PRO:O	1:A:85:ASP:HB2	0.50	2.07	1	1
1:A:71:VAL:HG12	1:A:75:PHE:CD2	0.49	2.41	1	1
1:A:106:MET:O	1:A:107:PRO:C	0.49	2.53	1	1
1:A:39:TYR:CD1	1:A:43:ILE:HD12	0.49	2.43	18	1
1:A:91:MET:O	1:A:95:LEU:HD12	0.49	2.07	7	1
1:A:18:HIS:CE1	1:A:98:VAL:HG11	0.49	2.42	9	1
1:A:39:TYR:CE1	1:A:43:ILE:HD12	0.49	2.43	18	1
1:A:71:VAL:O	1:A:75:PHE:HD2	0.48	1.91	1	1
1:A:21:TYR:CG	1:A:95:LEU:HD11	0.48	2.43	3	1
1:A:54:ARG:CG	1:A:54:ARG:NH1	0.48	2.74	1	1
1:A:56:MET:HE3	1:A:61:TYR:OH	0.48	2.09	20	1
1:A:30:ASP:CB	1:A:33:ALA:HB3	0.48	2.38	15	1
1:A:21:TYR:HB3	1:A:95:LEU:HD11	0.48	1.86	14	1
1:A:94:LYS:O	1:A:98:VAL:HG23	0.47	2.09	19	1
1:A:48:ASP:O	1:A:52:VAL:HG23	0.47	2.09	12	5
1:A:48:ASP:HA	1:A:74:MET:HE2	0.47	1.85	19	1
1:A:10:LEU:CD1	1:A:14:LEU:HD12	0.47	2.40	11	1
1:A:106:MET:CB	1:A:107:PRO:CD	0.46	2.93	1	1
1:A:47:MET:HE1	1:A:70:ASP:HB3	0.46	1.87	3	1
1:A:68:ALA:HB2	1:A:103:TYR:CE1	0.46	2.45	15	2
1:A:71:VAL:O	1:A:75:PHE:CD2	0.46	2.68	1	1
1:A:22:ALA:O	1:A:26:TYR:HB2	0.46	2.11	6	3
1:A:43:ILE:O	1:A:44:LYS:CB	0.46	2.64	1	1
1:A:49:LEU:CD1	1:A:74:MET:HE1	0.45	2.38	5	1
1:A:23:TRP:CD1	1:A:24:PRO:HD3	0.45	2.46	1	3
1:A:16:LYS:O	1:A:17:LYS:HB2	0.45	2.11	5	1
1:A:34:LEU:HD23	1:A:36:LEU:HD13	0.45	1.88	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:LYS:HB3	1:A:61:TYR:CE1	0.44	2.47	1	1
1:A:106:MET:C	1:A:107:PRO:O	0.44	2.54	1	1
1:A:106:MET:CB	1:A:107:PRO:HD3	0.44	2.43	1	1
1:A:21:TYR:CD1	1:A:91:MET:HG2	0.44	2.48	1	2
1:A:43:ILE:HD11	1:A:81:TYR:HB2	0.44	1.88	15	1
1:A:47:MET:HG3	1:A:73:LEU:HD22	0.43	1.90	7	1
1:A:23:TRP:CD2	1:A:24:PRO:HD3	0.43	2.48	1	4
1:A:47:MET:HE1	1:A:55:LYS:HE3	0.43	1.91	10	1
1:A:10:LEU:HD12	1:A:14:LEU:HD12	0.43	1.90	11	1
1:A:14:LEU:HD21	1:A:26:TYR:OH	0.43	2.14	12	2
1:A:21:TYR:CB	1:A:95:LEU:HD12	0.42	2.44	1	1
1:A:2:GLN:HB3	1:A:106:MET:HE1	0.42	1.89	16	1
1:A:86:HIS:CD2	1:A:88:VAL:HG23	0.42	2.50	16	1
1:A:103:TYR:O	1:A:107:PRO:HD3	0.42	2.14	16	1
1:A:21:TYR:HB2	1:A:95:LEU:HD13	0.42	1.90	12	1
1:A:10:LEU:HD22	1:A:56:MET:HE2	0.42	1.92	17	1
1:A:55:LYS:CB	1:A:61:TYR:CE1	0.41	3.02	1	1
1:A:29:VAL:HG21	1:A:39:TYR:CZ	0.41	2.49	8	1
1:A:47:MET:HE2	1:A:47:MET:HA	0.41	1.92	16	1
1:A:56:MET:HE2	1:A:67:PHE:CE1	0.41	2.51	7	1
1:A:47:MET:HE3	1:A:70:ASP:OD1	0.41	2.16	2	1
1:A:71:VAL:HG21	1:A:99:PHE:CE1	0.41	2.51	2	1
1:A:83:PRO:HB2	1:A:86:HIS:HB2	0.41	1.92	3	1
1:A:47:MET:HE3	1:A:70:ASP:HB3	0.41	1.91	18	1
1:A:36:LEU:HD21	1:A:81:TYR:OH	0.40	2.16	4	1
1:A:22:ALA:C	1:A:24:PRO:HD2	0.40	2.41	1	1
1:A:86:HIS:O	1:A:90:ALA:HB2	0.40	2.15	20	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	106/116 (91%)	94±2 (89±2%)	9±2 (8±2%)	3±1 (3±1%)	6	40
All	All	2226/2436 (91%)	1975 (89%)	189 (8%)	62 (3%)	6	40

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	85	ASP	19
1	A	15	SER	14
1	A	16	LYS	12
1	A	35	GLY	8
1	A	46	PRO	3
1	A	62	ARG	1
1	A	83	PRO	1
1	A	30	ASP	1
1	A	43	ILE	1
1	A	107	PRO	1
1	A	86	HIS	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	96/104 (92%)	72±4 (75±4%)	24±4 (25±4%)	2	25
All	All	2016/2184 (92%)	1516 (75%)	500 (25%)	2	25

All 67 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	50	SER	19
1	A	49	LEU	16
1	A	58	ASN	16
1	A	10	LEU	16
1	A	78	CYS	15
1	A	3	LEU	14
1	A	4	LYS	14
1	A	44	LYS	14
1	A	14	LEU	13
1	A	34	LEU	13
1	A	66	GLU	13
1	A	65	GLN	12
1	A	74	MET	12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	45	HIS	11
1	A	106	MET	11
1	A	105	LYS	11
1	A	47	MET	10
1	A	86	HIS	10
1	A	95	LEU	10
1	A	101	PHE	10
1	A	85	ASP	10
1	A	37	HIS	9
1	A	38	ASP	9
1	A	54	ARG	9
1	A	80	LYS	9
1	A	17	LYS	9
1	A	91	MET	9
1	A	16	LYS	8
1	A	36	LEU	8
1	A	100	GLU	8
1	A	70	ASP	8
1	A	108	ASP	8
1	A	79	TYR	7
1	A	96	GLN	7
1	A	93	ARG	7
1	A	27	LYS	7
1	A	72	ARG	7
1	A	102	ARG	6
1	A	1	GLU	6
1	A	57	GLU	6
1	A	32	SER	5
1	A	62	ARG	5
1	A	103	TYR	5
1	A	11	LYS	5
1	A	5	HIS	5
1	A	6	CYS	4
1	A	41	ASP	4
1	A	55	LYS	4
1	A	73	LEU	4
1	A	12	GLU	4
1	A	40	HIS	4
1	A	97	ASP	4
1	A	26	TYR	4
1	A	63	ASP	3
1	A	76	SER	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	82	ASN	3
1	A	21	TYR	3
1	A	87	ASP	2
1	A	94	LYS	2
1	A	7	ASN	2
1	A	15	SER	2
1	A	43	ILE	1
1	A	39	TYR	1
1	A	2	GLN	1
1	A	59	ARG	1
1	A	51	THR	1
1	A	13	LEU	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	61:TYR	C	62:ARG	N	1.20

7 Chemical shift validation

No chemical shift data were provided