



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:44 PM UTC

PDB ID : 1IDD / pdb_00001idd
Title : ISOCITRATE DEHYDROGENASE Y160F MUTANT APO ENZYME
Authors : Lee, M.E.; Dyer, D.H.; Klein, O.D.; Bolduc, J.M.; Stoddard, B.L.; Koshland Junior, D.E.
Deposited on : 1995-01-18
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp>

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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

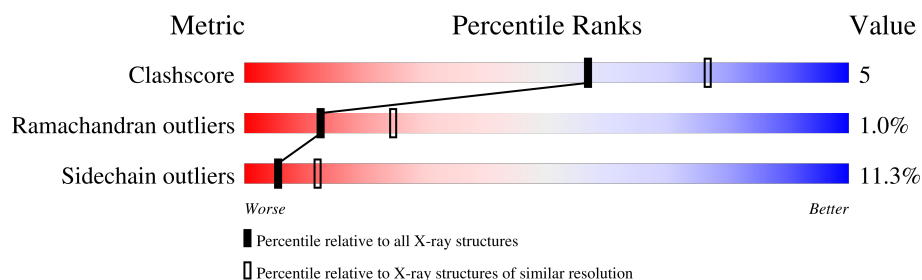
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	416	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3217 atoms, of which 22 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ISOCITRATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	414	Total	C	H	N	O	S	30	0	0
			3217	2035	22	538	604	18			

There is a discrepancy between the modelled and reference sequences:

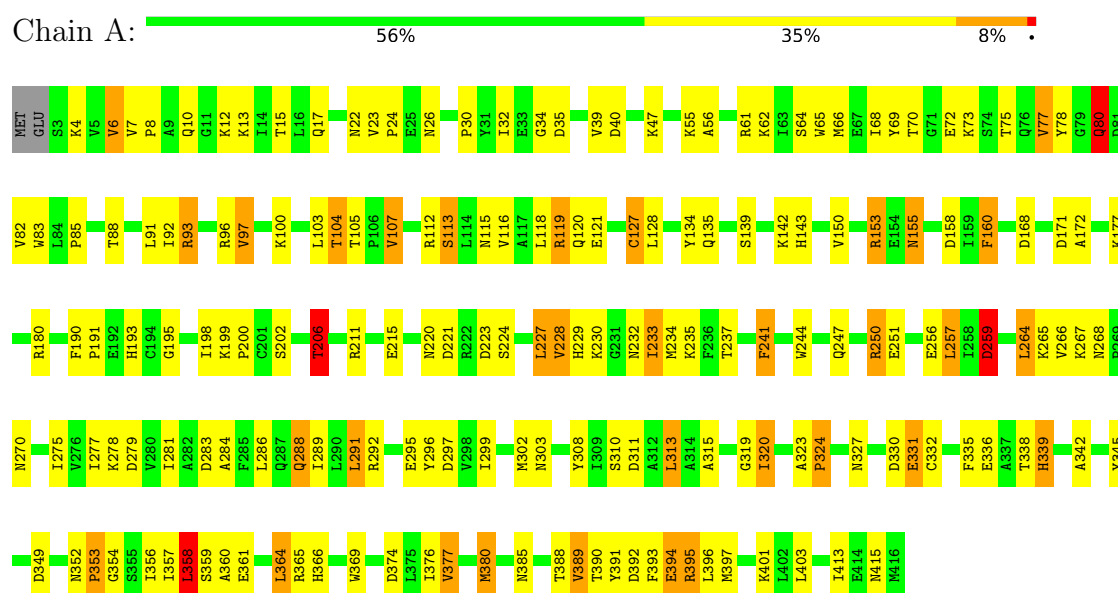
Chain	Residue	Modelled	Actual	Comment	Reference
A	160	PHE	TYR	engineered mutation	UNP P08200

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: ISOCITRATE DEHYDROGENASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.10Å 105.10Å 150.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.215 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3217	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

5 Model quality

5.1 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 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	1.75	39/3256 (1.2%)	2.50	208/4403 (4.7%)

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 outliers	#Planarity outliers
1	A	0	1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	ARG	CA-CB	20.06	1.85	1.53
1	A	119	ARG	NE-CZ	14.20	1.48	1.33
1	A	119	ARG	CB-CG	10.47	1.83	1.52
1	A	221	ASP	CA-CB	10.19	1.69	1.53
1	A	229	HIS	CD2-NE2	-9.11	1.27	1.37
1	A	119	ARG	CD-NE	8.81	1.58	1.46
1	A	395	ARG	CA-CB	8.35	1.67	1.53
1	A	391	TYR	CA-CB	8.35	1.66	1.53
1	A	339	HIS	CD2-NE2	-8.13	1.28	1.37
1	A	366	HIS	CD2-NE2	-8.09	1.28	1.37
1	A	119	ARG	CG-CD	8.02	1.76	1.52
1	A	377	VAL	CA-CB	7.88	1.65	1.54
1	A	229	HIS	CG-ND1	-7.48	1.30	1.38
1	A	395	ARG	NE-CZ	7.47	1.41	1.33
1	A	345	TYR	CA-CB	7.35	1.64	1.53
1	A	228	VAL	CA-CB	7.33	1.63	1.54
1	A	23	VAL	CA-CB	7.17	1.61	1.53
1	A	119	ARG	CA-C	6.65	1.62	1.52
1	A	310	SER	CA-CB	-6.65	1.43	1.53
1	A	193	HIS	CD2-NE2	-6.58	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	PRO	CA-CB	-6.43	1.45	1.53
1	A	320	ILE	CA-CB	6.29	1.62	1.54
1	A	139	SER	CA-CB	-6.28	1.45	1.53
1	A	143	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	353	PRO	N-CA	-6.15	1.43	1.47
1	A	275	ILE	CA-CB	6.09	1.61	1.54
1	A	118	LEU	C-N	6.09	1.41	1.33
1	A	353	PRO	CA-CB	-6.06	1.46	1.53
1	A	6	VAL	CA-CB	6.04	1.61	1.53
1	A	200	PRO	CA-CB	-5.86	1.45	1.53
1	A	7	VAL	CA-CB	5.72	1.61	1.53
1	A	369	TRP	NE1-CE2	-5.54	1.31	1.37
1	A	191	PRO	CA-CB	-5.47	1.46	1.53
1	A	244	TRP	NE1-CE2	-5.42	1.31	1.37
1	A	413	ILE	CA-CB	-5.29	1.48	1.54
1	A	206	THR	CA-CB	5.25	1.61	1.53
1	A	369	TRP	CG-CD2	-5.20	1.34	1.43
1	A	315	ALA	CA-CB	-5.11	1.45	1.53
1	A	85	PRO	CA-CB	-5.00	1.47	1.53

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ASP	CA-CB-CG	22.43	135.03	112.60
1	A	119	ARG	NE-CZ-NH1	17.52	139.02	121.50
1	A	119	ARG	NH1-CZ-NH2	-16.57	97.75	119.30
1	A	4	LYS	N-CA-C	15.26	134.36	110.70
1	A	119	ARG	CA-CB-CG	14.32	142.74	114.10
1	A	119	ARG	O-C-N	-14.12	105.11	122.20
1	A	395	ARG	CA-CB-CG	12.59	139.28	114.10
1	A	283	ASP	CA-CB-CG	12.45	125.05	112.60
1	A	119	ARG	CB-CG-CD	12.01	138.92	111.30
1	A	390	THR	N-CA-CB	-11.85	93.04	110.70
1	A	119	ARG	CD-NE-CZ	11.79	140.91	124.40
1	A	279	ASP	CA-CB-CG	11.44	124.04	112.60
1	A	119	ARG	N-CA-C	-11.13	93.11	111.37
1	A	233	ILE	N-CA-C	-11.08	102.81	112.12
1	A	349	ASP	CA-CB-CG	10.85	123.45	112.60
1	A	374	ASP	CA-CB-CG	10.81	123.41	112.60
1	A	120	GLN	N-CA-C	10.56	126.16	113.28
1	A	22	ASN	OD1-CG-ND2	-10.56	112.04	122.60
1	A	118	LEU	CA-C-O	-10.24	109.59	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ASN	CA-CB-CG	10.08	122.68	112.60
1	A	389	VAL	N-CA-CB	-9.68	95.27	111.23
1	A	303	ASN	CA-CB-CG	9.33	121.93	112.60
1	A	352	ASN	OD1-CG-ND2	-9.30	113.30	122.60
1	A	388	THR	CA-CB-OG1	-8.92	96.22	109.60
1	A	391	TYR	CA-CB-CG	8.74	129.64	113.90
1	A	332	CYS	O-C-N	-8.74	113.95	123.04
1	A	26	ASN	CA-CB-CG	8.63	121.23	112.60
1	A	364	LEU	CA-C-O	-8.49	111.91	120.82
1	A	177	LYS	N-CA-C	-8.33	101.89	110.97
1	A	223	ASP	CA-CB-CG	8.27	120.87	112.60
1	A	47	LYS	CA-C-O	-8.22	112.19	120.82
1	A	232	ASN	CA-CB-CG	8.11	120.71	112.60
1	A	10	GLN	N-CA-C	-8.10	96.86	109.25
1	A	115	ASN	CB-CG-ND2	8.09	128.53	116.40
1	A	115	ASN	OD1-CG-ND2	-7.97	114.63	122.60
1	A	56	ALA	N-CA-C	7.95	120.02	111.36
1	A	235	LYS	N-CA-C	7.94	119.94	111.28
1	A	22	ASN	CB-CG-ND2	7.93	128.29	116.40
1	A	332	CYS	N-CA-C	7.93	119.06	107.88
1	A	297	ASP	CA-CB-CG	7.85	120.45	112.60
1	A	395	ARG	CA-C-N	7.84	132.24	120.17
1	A	395	ARG	C-N-CA	7.84	132.24	120.17
1	A	119	ARG	CG-CD-NE	7.78	129.11	112.00
1	A	215	GLU	CA-CB-CG	7.75	129.60	114.10
1	A	22	ASN	CA-CB-CG	7.65	120.25	112.60
1	A	32	ILE	N-CA-C	-7.65	97.46	108.17
1	A	112	ARG	CA-C-O	-7.64	112.95	121.89
1	A	390	THR	CB-CA-C	7.57	123.83	110.36
1	A	392	ASP	N-CA-C	7.43	120.25	111.71
1	A	119	ARG	CB-CA-C	7.42	123.15	110.84
1	A	153	ARG	NE-CZ-NH2	-7.42	112.53	119.20
1	A	233	ILE	CA-C-O	-7.41	113.59	120.34
1	A	268	ASN	OD1-CG-ND2	-7.41	115.19	122.60
1	A	270	ASN	OD1-CG-ND2	-7.39	115.21	122.60
1	A	257	LEU	N-CA-C	7.30	121.28	110.48
1	A	244	TRP	CG-CD2-CE3	7.30	141.20	133.90
1	A	385	ASN	CA-CB-CG	7.29	119.89	112.60
1	A	7	VAL	CA-C-N	7.28	127.27	119.78
1	A	7	VAL	C-N-CA	7.28	127.27	119.78
1	A	365	ARG	CA-CB-CG	7.27	128.64	114.10
1	A	345	TYR	O-C-N	-7.20	113.68	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	ASN	OD1-CG-ND2	-7.19	115.41	122.60
1	A	193	HIS	CB-CG-CD2	-7.18	121.87	131.20
1	A	415	ASN	N-CA-C	7.06	121.50	113.02
1	A	241	PHE	O-C-N	-7.00	114.81	122.09
1	A	278	LYS	CA-CB-CG	6.94	127.97	114.10
1	A	104	THR	CA-C-O	6.92	128.90	120.60
1	A	265	LYS	CA-CB-CG	6.92	127.93	114.10
1	A	331	GLU	CB-CG-CD	6.91	124.35	112.60
1	A	311	ASP	N-CA-C	-6.90	103.84	111.36
1	A	190	PHE	CA-C-N	6.85	126.45	119.19
1	A	190	PHE	C-N-CA	6.85	126.45	119.19
1	A	319	GLY	CA-C-O	-6.84	108.67	120.57
1	A	120	GLN	O-C-N	-6.74	112.84	122.41
1	A	401	LYS	O-C-N	-6.73	115.66	123.27
1	A	266	VAL	CA-C-O	-6.72	113.34	120.39
1	A	220	ASN	OD1-CG-ND2	-6.70	115.90	122.60
1	A	380	MET	N-CA-C	-6.70	103.90	111.14
1	A	80	GLN	OE1-CD-NE2	-6.68	115.92	122.60
1	A	198	ILE	CB-CG1-CD1	6.67	127.82	113.80
1	A	330	ASP	CA-CB-CG	6.67	119.27	112.60
1	A	168	ASP	CA-CB-CG	6.66	119.25	112.60
1	A	292	ARG	CA-C-N	6.62	126.25	119.56
1	A	292	ARG	C-N-CA	6.62	126.25	119.56
1	A	380	MET	CG-SD-CE	-6.61	86.36	100.90
1	A	8	PRO	N-CA-C	6.58	121.68	111.21
1	A	158	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	26	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	A	93	ARG	CA-CB-CG	6.55	127.19	114.10
1	A	127	CYS	N-CA-C	-6.49	98.15	108.73
1	A	134	TYR	O-C-N	-6.43	115.11	123.02
1	A	142	LYS	CA-CB-CG	6.42	126.94	114.10
1	A	388	THR	CA-CB-CG2	6.42	121.41	110.50
1	A	195	GLY	O-C-N	-6.40	116.95	123.35
1	A	234	MET	CA-C-N	6.40	128.85	120.28
1	A	234	MET	C-N-CA	6.40	128.85	120.28
1	A	339	HIS	CB-CG-CD2	-6.37	122.92	131.20
1	A	180	ARG	CA-CB-CG	6.37	126.83	114.10
1	A	268	ASN	CB-CG-ND2	6.35	125.93	116.40
1	A	7	VAL	CB-CA-C	6.34	116.84	110.94
1	A	12	LYS	O-C-N	-6.32	114.93	123.15
1	A	281	ILE	CB-CG1-CD1	6.29	127.02	113.80
1	A	77	VAL	N-CA-CB	-6.28	100.86	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	LEU	CA-C-N	6.27	131.15	121.19
1	A	118	LEU	C-N-CA	6.27	131.15	121.19
1	A	250	ARG	CA-CB-CG	6.24	126.58	114.10
1	A	73	LYS	N-CA-CB	-6.23	100.30	110.14
1	A	327	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	A	96	ARG	CA-CB-CG	-6.20	101.69	114.10
1	A	295	GLU	CA-CB-CG	6.20	126.50	114.10
1	A	303	ASN	N-CA-C	6.17	118.00	111.28
1	A	223	ASP	N-CA-C	6.16	119.99	112.23
1	A	120	GLN	CG-CD-NE2	6.16	125.64	116.40
1	A	13	LYS	CA-C-N	6.14	128.73	120.50
1	A	13	LYS	C-N-CA	6.14	128.73	120.50
1	A	233	ILE	O-C-N	-6.13	115.72	121.97
1	A	393	PHE	N-CA-C	-6.07	106.01	113.41
1	A	311	ASP	CA-C-O	-5.98	114.08	120.42
1	A	153	ARG	NE-CZ-NH1	5.98	127.48	121.50
1	A	143	HIS	N-CA-C	5.97	119.84	108.97
1	A	80	GLN	CG-CD-NE2	5.93	125.30	116.40
1	A	339	HIS	CB-CG-ND1	5.92	131.58	122.70
1	A	376	ILE	N-CA-C	-5.90	104.76	110.72
1	A	320	ILE	CA-CB-CG1	5.90	120.43	110.40
1	A	288	GLN	CA-C-O	-5.89	113.44	120.10
1	A	107	VAL	N-CA-C	-5.88	101.21	109.21
1	A	34	GLY	N-CA-C	-5.87	105.23	112.33
1	A	237	THR	CA-C-N	5.85	128.12	120.28
1	A	237	THR	C-N-CA	5.85	128.12	120.28
1	A	247	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	A	150	VAL	CG1-CB-CG2	-5.78	98.08	110.80
1	A	291	LEU	N-CA-C	5.78	119.51	112.23
1	A	310	SER	CB-CA-C	-5.75	101.86	110.88
1	A	193	HIS	CB-CG-ND1	5.74	131.31	122.70
1	A	82	VAL	CA-C-O	5.73	127.37	120.66
1	A	308	TYR	N-CA-C	5.71	117.50	111.28
1	A	360	ALA	CA-C-O	-5.70	113.91	120.24
1	A	23	VAL	CA-C-N	5.69	126.95	119.84
1	A	23	VAL	C-N-CA	5.69	126.95	119.84
1	A	73	LYS	O-C-N	-5.67	115.73	122.20
1	A	199	LYS	CA-C-O	-5.67	114.38	119.59
1	A	267	LYS	CA-CB-CG	5.66	125.42	114.10
1	A	155	ASN	CA-CB-CG	5.66	118.26	112.60
1	A	120	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	A	40	ASP	CA-CB-CG	5.62	118.22	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	PHE	CA-CB-CG	5.62	119.42	113.80
1	A	358	LEU	N-CA-CB	-5.60	101.67	110.30
1	A	103	LEU	CA-C-O	5.58	127.30	120.60
1	A	244	TRP	CB-CG-CD1	-5.57	118.55	126.90
1	A	244	TRP	CE2-CD2-CG	-5.56	100.53	107.20
1	A	65	TRP	CG-CD2-CE3	5.53	139.43	133.90
1	A	12	LYS	CA-CB-CG	5.50	125.09	114.10
1	A	7	VAL	N-CA-CB	-5.49	104.36	110.23
1	A	385	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	A	105	THR	N-CA-CB	-5.47	103.41	110.03
1	A	17	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	A	380	MET	CA-C-O	-5.47	115.07	120.70
1	A	401	LYS	CB-CG-CD	5.46	123.86	111.30
1	A	113	SER	CA-CB-OG	5.45	121.99	111.10
1	A	389	VAL	CB-CA-C	5.44	120.22	111.29
1	A	171	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	342	ALA	N-CA-CB	-5.43	103.74	111.51
1	A	198	ILE	CG1-CB-CG2	-5.42	94.43	110.70
1	A	356	ILE	CA-C-N	5.41	128.10	120.42
1	A	356	ILE	C-N-CA	5.41	128.10	120.42
1	A	104	THR	N-CA-C	-5.41	99.87	109.06
1	A	310	SER	CA-CB-OG	-5.40	100.29	111.10
1	A	302	MET	N-CA-C	5.40	116.89	110.19
1	A	275	ILE	O-C-N	-5.39	117.05	123.03
1	A	359	SER	CA-CB-OG	-5.39	100.33	111.10
1	A	69	TYR	N-CA-C	5.36	117.63	108.90
1	A	92	ILE	CA-C-N	5.34	127.88	120.29
1	A	92	ILE	C-N-CA	5.34	127.88	120.29
1	A	342	ALA	N-CA-C	5.34	123.97	112.23
1	A	251	GLU	O-C-N	-5.32	116.56	122.09
1	A	353	PRO	CA-C-N	5.29	125.85	119.98
1	A	353	PRO	C-N-CA	5.29	125.85	119.98
1	A	256	GLU	CA-C-O	-5.29	115.25	121.44
1	A	277	ILE	CB-CG1-CD1	5.24	124.81	113.80
1	A	395	ARG	CG-CD-NE	5.24	123.53	112.00
1	A	105	THR	CA-C-O	-5.24	115.88	120.60
1	A	172	ALA	N-CA-C	5.20	116.95	111.28
1	A	275	ILE	CA-C-O	-5.17	115.04	120.57
1	A	388	THR	N-CA-CB	-5.16	102.18	110.69
1	A	292	ARG	O-C-N	-5.13	115.42	121.32
1	A	302	MET	CA-C-O	-5.13	116.62	122.01
1	A	259	ASP	CA-CB-CG	-5.13	107.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	LYS	O-C-N	-5.12	117.64	123.48
1	A	211	ARG	CA-CB-CG	5.12	124.35	114.10
1	A	323	ALA	CA-C-N	5.12	125.33	120.31
1	A	323	ALA	C-N-CA	5.12	125.33	120.31
1	A	78	TYR	N-CA-C	5.11	121.22	114.12
1	A	227	LEU	CA-C-O	-5.10	114.71	120.43
1	A	338	THR	N-CA-C	5.10	119.56	113.23
1	A	83	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	A	366	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	A	377	VAL	CA-C-O	-5.09	113.54	119.85
1	A	228	VAL	CA-C-O	5.08	126.52	120.72
1	A	259	ASP	CA-C-O	-5.08	113.24	120.51
1	A	390	THR	CA-C-O	-5.08	115.28	121.78
1	A	397	MET	CA-CB-CG	5.07	124.23	114.10
1	A	335	PHE	O-C-N	-5.04	117.29	123.19
1	A	311	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	61	ARG	CB-CG-CD	5.03	122.86	111.30
1	A	70	THR	CA-CB-OG1	-5.01	102.08	109.60
1	A	6	VAL	N-CA-C	5.01	114.98	107.51
1	A	256	GLU	O-C-N	-5.01	116.64	123.15
1	A	394	GLU	O-C-N	-5.00	116.45	122.15

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	TYR	Sidechain

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3195	22	3222	29	0
All	All	3195	22	3222	29	0

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 5.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ARG:CD	1:A:119:ARG:CG	1.76	1.61
1:A:119:ARG:CG	1:A:119:ARG:CB	1.83	1.56
1:A:119:ARG:CB	1:A:119:ARG:CA	1.85	1.52
1:A:119:ARG:HH11	1:A:153:ARG:HH22	1.31	0.76
1:A:75:THR:HB	1:A:80:GLN:HA	1.68	0.75
1:A:119:ARG:CB	1:A:119:ARG:HA	2.15	0.67
1:A:202:SER:O	1:A:206:THR:HG23	1.95	0.66
1:A:284:ALA:O	1:A:288:GLN:HG2	1.96	0.65
1:A:68:ILE:HD12	1:A:88:THR:HG23	1.81	0.62
1:A:289:ILE:HD12	1:A:313:LEU:HD13	1.82	0.61
1:A:119:ARG:CD	1:A:119:ARG:HG3	2.18	0.56
1:A:93:ARG:HH12	1:A:331:GLU:HG3	1.73	0.54
1:A:113:SER:HB3	1:A:116:VAL:HB	1.90	0.54
1:A:394:GLU:C	1:A:396:LEU:H	2.18	0.51
1:A:127:CYS:HB2	1:A:155:ASN:ND2	2.26	0.51
1:A:119:ARG:HH11	1:A:153:ARG:NH2	2.07	0.50
1:A:30:PRO:HA	1:A:66:MET:O	2.13	0.49
1:A:35:ASP:OD1	1:A:72:GLU:HB3	2.13	0.48
1:A:257:LEU:HD23	1:A:264:LEU:HD12	1.95	0.48
1:A:206:THR:HB	1:A:241:PHE:CD1	2.49	0.47
1:A:119:ARG:CG	1:A:119:ARG:HB3	2.23	0.47
1:A:119:ARG:CD	1:A:119:ARG:HG2	2.18	0.46
1:A:30:PRO:HD2	1:A:97:VAL:O	2.17	0.45
1:A:324:PRO:HB3	1:A:358:LEU:HB3	2.00	0.43
1:A:354:GLY:O	1:A:358:LEU:HB2	2.18	0.43
1:A:93:ARG:NH1	1:A:331:GLU:HG3	2.34	0.42
1:A:119:ARG:CG	1:A:119:ARG:HB2	2.23	0.42
1:A:250:ARG:HH11	1:A:250:ARG:HD2	1.73	0.41
1:A:100:LYS:HE3	1:A:336:GLU:OE1	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	412/416 (99%)	382 (93%)	26 (6%)	4 (1%)	12	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	ASP
1	A	395	ARG
1	A	80	GLN
1	A	24	PRO

5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	336/338 (99%)	298 (89%)	38 (11%)	5	12

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	15	THR
1	A	39	VAL
1	A	55	LYS
1	A	64	SER
1	A	77	VAL
1	A	80	GLN
1	A	91	LEU
1	A	97	VAL
1	A	104	THR
1	A	107	VAL
1	A	121	GLU
1	A	128	LEU
1	A	135	GLN
1	A	160	PHE

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Mol	Chain	Res	Type
1	A	206	THR
1	A	224	SER
1	A	227	LEU
1	A	228	VAL
1	A	230	LYS
1	A	233	ILE
1	A	259	ASP
1	A	264	LEU
1	A	286	LEU
1	A	291	LEU
1	A	299	ILE
1	A	313	LEU
1	A	320	ILE
1	A	339	HIS
1	A	353	PRO
1	A	357	ILE
1	A	358	LEU
1	A	361	GLU
1	A	364	LEU
1	A	377	VAL
1	A	380	MET
1	A	389	VAL
1	A	403	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	287	GLN
1	A	288	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.