



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:50 PM UTC

PDB ID : 1IDF / pdb_00001idf
Title : ISOCITRATE DEHYDROGENASE K230M MUTANT APO ENZYME
Authors : Bolduc, J.M.; Dyer, D.H.; Scott, W.G.; Singer, P.; Sweet, R.M.; Koshland Junior, D.E.; Stoddard, B.L.
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

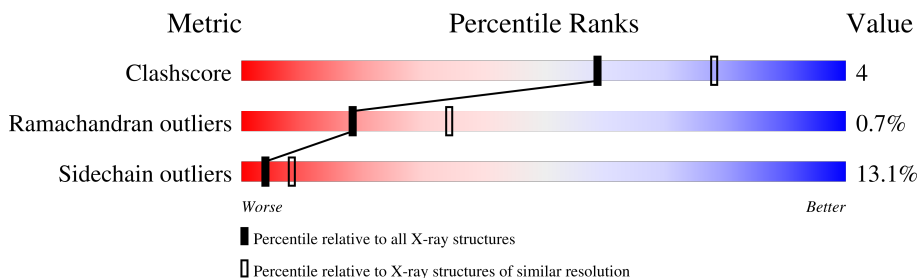
1 Overall quality at a glance

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	2034	22	537	605	19			

There is a discrepancy between the modelled and reference sequences:

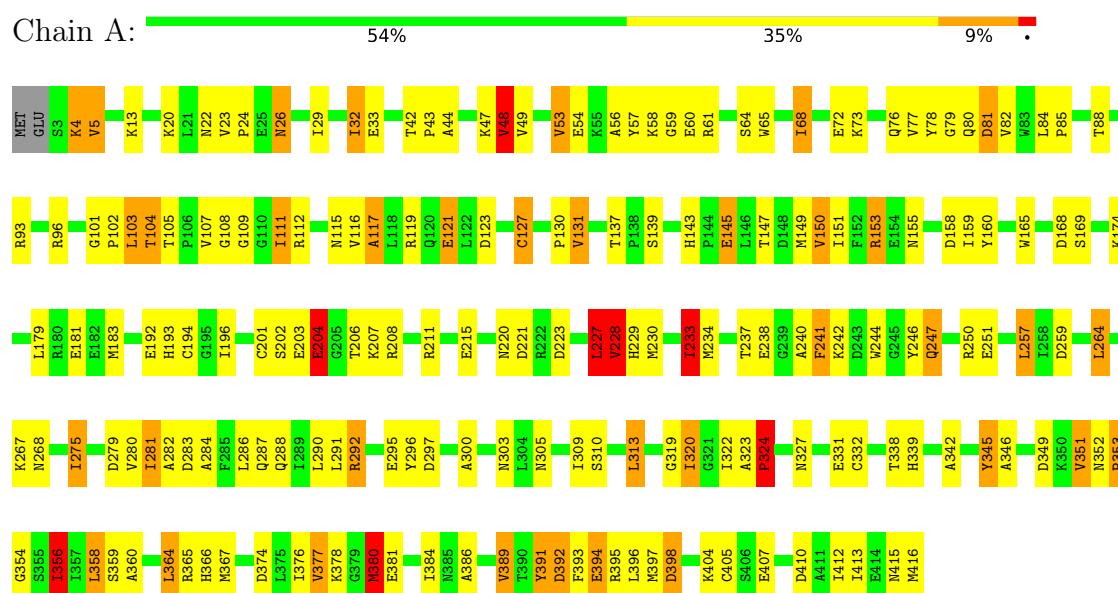
Chain	Residue	Modelled	Actual	Comment	Reference
A	230	MET	LYS	engineered mutation	UNP P08200

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}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.223 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3217	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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	1.54	28/3256 (0.9%)	2.34	193/4404 (4.4%)

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	2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	HIS	CD2-NE2	-8.93	1.28	1.37
1	A	229	HIS	CD2-NE2	-8.14	1.28	1.37
1	A	320	ILE	CA-CB	7.84	1.66	1.54
1	A	345	TYR	CA-CB	7.66	1.65	1.53
1	A	193	HIS	CD2-NE2	-7.61	1.29	1.37
1	A	48	VAL	CA-CB	7.41	1.64	1.54
1	A	339	HIS	CD2-NE2	-7.28	1.29	1.37
1	A	143	HIS	CD2-NE2	-6.94	1.30	1.37
1	A	378	LYS	CA-CB	6.68	1.63	1.53
1	A	85	PRO	CA-CB	-6.33	1.45	1.53
1	A	131	VAL	CA-CB	6.32	1.62	1.54
1	A	53	VAL	CA-CB	6.22	1.62	1.54
1	A	292	ARG	CA-CB	6.03	1.60	1.53
1	A	244	TRP	NE1-CE2	-6.03	1.30	1.37
1	A	366	HIS	CG-ND1	-6.03	1.31	1.38
1	A	193	HIS	CG-ND1	-5.89	1.31	1.38
1	A	5	VAL	CA-CB	5.69	1.61	1.54
1	A	229	HIS	CG-ND1	-5.63	1.32	1.38
1	A	4	LYS	CA-CB	5.48	1.62	1.53
1	A	391	TYR	CA-CB	5.38	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	ILE	CA-CB	5.37	1.60	1.54
1	A	24	PRO	CA-CB	-5.20	1.46	1.53
1	A	310	SER	CA-C	-5.18	1.46	1.52
1	A	275	ILE	CA-CB	5.16	1.59	1.53
1	A	305	ASN	CA-CB	-5.13	1.45	1.53
1	A	324	PRO	CA-CB	-5.12	1.46	1.53
1	A	359	SER	CA-CB	-5.07	1.45	1.53
1	A	233	ILE	CA-CB	5.02	1.60	1.54

All (193) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	ASP	CA-CB-CG	12.59	125.19	112.60
1	A	251	GLU	N-CA-C	12.35	124.29	111.07
1	A	349	ASP	CA-CB-CG	12.06	124.66	112.60
1	A	392	ASP	CA-CB-CG	11.32	123.92	112.60
1	A	259	ASP	CA-CB-CG	10.96	123.56	112.60
1	A	352	ASN	OD1-CG-ND2	-10.34	112.26	122.60
1	A	287	GLN	N-CA-CB	-10.09	95.22	110.26
1	A	107	VAL	O-C-N	9.34	133.74	122.72
1	A	22	ASN	CA-CB-CG	9.31	121.91	112.60
1	A	389	VAL	N-CA-CB	-9.30	95.89	111.23
1	A	378	LYS	N-CA-C	-8.82	101.66	111.28
1	A	82	VAL	N-CA-C	8.76	120.34	107.37
1	A	204	GLU	CB-CG-CD	8.39	126.86	112.60
1	A	397	MET	N-CA-C	8.23	120.61	108.60
1	A	327	ASN	OD1-CG-ND2	-8.06	114.54	122.60
1	A	282	ALA	N-CA-C	8.05	120.97	111.71
1	A	82	VAL	N-CA-CB	-7.92	101.69	111.67
1	A	287	GLN	CA-CB-CG	7.86	129.83	114.10
1	A	4	LYS	N-CA-C	7.81	127.44	110.80
1	A	291	LEU	N-CA-C	7.71	123.17	112.45
1	A	104	THR	O-C-N	7.67	132.83	123.16
1	A	22	ASN	OD1-CG-ND2	-7.59	115.01	122.60
1	A	241	PHE	CA-CB-CG	7.59	121.39	113.80
1	A	108	GLY	O-C-N	7.58	132.56	122.70
1	A	360	ALA	N-CA-C	-7.58	102.95	111.14
1	A	257	LEU	N-CA-C	7.53	121.32	110.24
1	A	297	ASP	CA-CB-CG	7.49	120.09	112.60
1	A	127	CYS	N-CA-C	-7.48	96.32	108.52
1	A	410	ASP	CA-CB-CG	7.38	119.98	112.60
1	A	5	VAL	N-CA-CB	7.24	118.62	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	THR	N-CA-C	7.18	122.14	113.23
1	A	49	VAL	N-CA-C	-7.17	103.79	110.53
1	A	396	LEU	N-CA-C	7.17	122.05	113.16
1	A	366	HIS	CA-CB-CG	7.17	120.97	113.80
1	A	193	HIS	CB-CG-CD2	-7.13	121.93	131.20
1	A	377	VAL	CA-C-O	-7.12	112.79	120.47
1	A	356	ILE	N-CA-C	-7.08	104.08	111.58
1	A	13	LYS	CA-CB-CG	7.05	128.21	114.10
1	A	169	SER	CA-CB-OG	7.05	125.20	111.10
1	A	230	MET	CG-SD-CE	6.98	116.25	100.90
1	A	168	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	267	LYS	CA-CB-CG	6.96	128.02	114.10
1	A	223	ASP	N-CA-C	6.92	120.94	112.23
1	A	319	GLY	CA-C-O	-6.89	108.57	120.57
1	A	112	ARG	CA-C-O	-6.86	114.08	121.56
1	A	378	LYS	CB-CG-CD	6.83	127.01	111.30
1	A	22	ASN	N-CA-C	-6.82	97.61	108.73
1	A	111	ILE	CA-CB-CG2	-6.82	98.91	110.50
1	A	283	ASP	CA-CB-CG	6.80	119.40	112.60
1	A	244	TRP	CG-CD2-CE3	6.77	140.67	133.90
1	A	376	ILE	CA-C-O	-6.75	113.93	120.95
1	A	23	VAL	N-CA-C	6.74	114.81	107.60
1	A	158	ASP	CA-CB-CG	6.74	119.34	112.60
1	A	229	HIS	O-C-N	-6.66	115.62	123.41
1	A	275	ILE	O-C-N	-6.60	115.25	122.64
1	A	153	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	A	415	ASN	OD1-CG-ND2	-6.51	116.09	122.60
1	A	339	HIS	CB-CG-ND1	6.50	132.45	122.70
1	A	398	ASP	N-CA-C	6.50	119.29	108.96
1	A	47	LYS	CA-CB-CG	6.49	127.08	114.10
1	A	394	GLU	CA-C-O	-6.49	112.14	119.79
1	A	280	VAL	CG1-CB-CG2	-6.43	96.64	110.80
1	A	194	CYS	CA-C-N	6.43	128.60	122.36
1	A	194	CYS	C-N-CA	6.43	128.60	122.36
1	A	393	PHE	CA-CB-CG	6.43	120.23	113.80
1	A	105	THR	CA-C-N	6.41	126.44	119.90
1	A	105	THR	C-N-CA	6.41	126.44	119.90
1	A	230	MET	N-CA-C	-6.40	100.69	109.71
1	A	281	ILE	N-CA-C	-6.40	100.51	109.21
1	A	108	GLY	CA-C-N	6.31	133.77	121.41
1	A	108	GLY	C-N-CA	6.31	133.77	121.41
1	A	353	PRO	CA-C-N	6.30	127.09	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	PRO	C-N-CA	6.30	127.09	120.03
1	A	339	HIS	CB-CG-CD2	-6.29	123.02	131.20
1	A	345	TYR	O-C-N	-6.29	114.77	122.25
1	A	192	GLU	N-CA-C	-6.27	100.29	110.20
1	A	395	ARG	CB-CG-CD	6.26	125.71	111.30
1	A	228	VAL	CA-C-O	6.26	127.86	120.72
1	A	364	LEU	CA-C-O	-6.26	114.25	120.82
1	A	169	SER	N-CA-C	-6.23	102.14	110.55
1	A	32	ILE	N-CA-C	-6.19	98.95	107.99
1	A	26	ASN	CA-C-N	6.18	126.10	119.85
1	A	26	ASN	C-N-CA	6.18	126.10	119.85
1	A	292	ARG	CA-C-N	6.12	125.75	119.56
1	A	292	ARG	C-N-CA	6.12	125.75	119.56
1	A	279	ASP	CA-CB-CG	6.00	118.61	112.60
1	A	123	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	305	ASN	OD1-CG-ND2	-6.00	116.60	122.60
1	A	143	HIS	CA-CB-CG	-5.97	107.83	113.80
1	A	284	ALA	N-CA-C	-5.96	104.86	111.36
1	A	150	VAL	O-C-N	-5.95	116.65	123.07
1	A	246	TYR	CA-C-N	5.94	128.56	120.54
1	A	246	TYR	C-N-CA	5.94	128.56	120.54
1	A	267	LYS	O-C-N	-5.93	115.48	122.96
1	A	268	ASN	O-C-N	-5.93	116.27	121.31
1	A	116	VAL	O-C-N	-5.90	115.22	122.18
1	A	323	ALA	CA-C-N	5.89	125.86	120.03
1	A	323	ALA	C-N-CA	5.89	125.86	120.03
1	A	352	ASN	CA-CB-CG	5.86	118.46	112.60
1	A	240	ALA	CA-C-O	-5.86	114.87	120.90
1	A	220	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	A	287	GLN	CB-CA-C	5.85	121.17	110.11
1	A	174	LYS	CB-CG-CD	5.84	124.73	111.30
1	A	247	GLN	OE1-CD-NE2	-5.84	116.76	122.60
1	A	150	VAL	CG1-CB-CG2	-5.79	98.06	110.80
1	A	23	VAL	CA-C-N	5.75	127.03	119.84
1	A	23	VAL	C-N-CA	5.75	127.03	119.84
1	A	324	PRO	N-CA-CB	-5.74	97.35	103.38
1	A	331	GLU	CA-CB-CG	5.69	125.48	114.10
1	A	165	TRP	CG-CD2-CE3	5.68	139.58	133.90
1	A	81	ASP	CA-C-N	-5.68	115.39	123.11
1	A	81	ASP	C-N-CA	-5.68	115.39	123.11
1	A	223	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	227	LEU	CA-C-O	-5.67	114.51	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	ASN	O-C-N	-5.66	116.61	123.29
1	A	259	ASP	N-CA-C	-5.65	98.76	110.80
1	A	360	ALA	CA-C-O	-5.62	114.91	120.70
1	A	244	TRP	CE2-CD2-CG	-5.62	100.46	107.20
1	A	65	TRP	CG-CD2-CE3	5.61	139.51	133.90
1	A	137	THR	N-CA-CB	-5.61	102.72	110.29
1	A	111	ILE	CA-CB-CG1	5.57	119.87	110.40
1	A	313	LEU	CA-C-N	5.56	127.73	120.28
1	A	313	LEU	C-N-CA	5.56	127.73	120.28
1	A	303	ASN	CA-CB-CG	5.51	118.11	112.60
1	A	117	ALA	CA-C-N	5.50	127.93	120.44
1	A	117	ALA	C-N-CA	5.50	127.93	120.44
1	A	42	THR	CA-C-O	-5.49	112.64	120.16
1	A	137	THR	CB-CA-C	5.49	116.60	108.87
1	A	332	CYS	N-CA-C	5.48	115.78	108.38
1	A	102	PRO	CB-CA-C	5.47	118.45	110.63
1	A	32	ILE	N-CA-CB	-5.46	104.82	111.21
1	A	76	GLN	N-CA-C	5.46	118.15	111.82
1	A	320	ILE	CA-CB-CG1	5.46	119.68	110.40
1	A	295	GLU	N-CA-C	-5.46	106.58	113.18
1	A	405	CYS	CA-C-O	-5.46	115.08	120.70
1	A	351	VAL	N-CA-CB	-5.44	102.35	111.38
1	A	73	LYS	O-C-N	-5.44	116.00	122.20
1	A	79	GLY	N-CA-C	-5.44	101.68	111.19
1	A	131	VAL	O-C-N	5.42	128.81	123.18
1	A	103	LEU	CA-C-O	5.40	126.31	120.32
1	A	386	ALA	CA-C-N	5.39	130.22	122.40
1	A	386	ALA	C-N-CA	5.39	130.22	122.40
1	A	68	ILE	O-C-N	-5.38	117.32	122.97
1	A	53	VAL	O-C-N	-5.38	115.83	122.18
1	A	201	CYS	O-C-N	-5.35	116.43	123.28
1	A	145	GLU	CA-CB-CG	5.34	124.79	114.10
1	A	143	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	A	56	ALA	N-CA-C	5.33	116.78	111.07
1	A	389	VAL	CB-CA-C	5.32	120.01	111.29
1	A	237	THR	N-CA-C	-5.32	105.00	112.12
1	A	183	MET	N-CA-C	5.31	120.42	113.30
1	A	250	ARG	CG-CD-NE	5.31	123.68	112.00
1	A	196	ILE	CA-C-N	5.30	126.50	121.46
1	A	196	ILE	C-N-CA	5.30	126.50	121.46
1	A	376	ILE	O-C-N	-5.30	116.73	121.87
1	A	238	GLU	CA-C-N	5.30	126.94	120.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	GLU	C-N-CA	5.30	126.94	120.22
1	A	211	ARG	CA-CB-CG	5.26	124.62	114.10
1	A	102	PRO	N-CA-CB	-5.25	98.06	103.15
1	A	342	ALA	O-C-N	-5.24	115.30	121.32
1	A	346	ALA	N-CA-C	5.24	117.45	110.53
1	A	111	ILE	N-CA-C	5.23	115.13	108.12
1	A	380	MET	CG-SD-CE	-5.23	89.39	100.90
1	A	139	SER	CA-C-N	5.22	124.72	119.19
1	A	139	SER	C-N-CA	5.22	124.72	119.19
1	A	137	THR	CA-CB-CG2	5.22	119.37	110.50
1	A	65	TRP	CE2-CD2-CG	-5.21	100.94	107.20
1	A	76	GLN	CA-C-O	5.19	125.94	119.97
1	A	264	LEU	O-C-N	-5.18	115.29	122.76
1	A	215	GLU	CA-CB-CG	5.16	124.42	114.10
1	A	244	TRP	CB-CG-CD1	-5.16	119.16	126.90
1	A	310	SER	CA-CB-OG	-5.15	100.79	111.10
1	A	320	ILE	CB-CG1-CD1	5.15	124.62	113.80
1	A	360	ALA	O-C-N	-5.14	116.54	122.09
1	A	381	GLU	CA-CB-CG	5.14	124.37	114.10
1	A	103	LEU	CA-CB-CG	5.13	134.26	116.30
1	A	105	THR	N-CA-CB	-5.13	101.65	110.11
1	A	352	ASN	CB-CG-ND2	5.13	124.09	116.40
1	A	365	ARG	CB-CA-C	-5.12	100.53	110.46
1	A	384	ILE	CA-C-O	-5.12	115.42	120.85
1	A	220	ASN	CA-CB-CG	5.11	117.70	112.60
1	A	101	GLY	O-C-N	-5.10	116.67	121.77
1	A	33	GLU	N-CA-C	5.09	116.83	111.28
1	A	72	GLU	N-CA-CB	-5.09	102.63	110.01
1	A	366	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	A	84	LEU	O-C-N	-5.06	117.24	121.44
1	A	181	GLU	CB-CG-CD	5.05	121.18	112.60
1	A	211	ARG	N-CA-C	-5.05	105.67	111.07
1	A	54	GLU	CA-CB-CG	5.04	124.19	114.10
1	A	159	ILE	N-CA-CB	-5.04	102.91	111.23
1	A	202	SER	N-CA-C	5.02	117.52	110.14
1	A	221	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	82	VAL	CA-CB-CG2	-5.00	101.89	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	TYR	Sidechain
1	A	345	TYR	Sidechain

5.2 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 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	3218	28	0
All	All	3195	22	3218	28	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 4.

All (28) 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:413:ILE:O	1:A:416:MET:HG2	2.01	0.60
1:A:119:ARG:HD2	1:A:155:ASN:ND2	2.18	0.59
1:A:29:ILE:HD11	1:A:367:MET:HE1	1.85	0.59
1:A:115:ASN:O	1:A:119:ARG:HG3	2.04	0.58
1:A:322:ILE:HG22	1:A:354:GLY:HA3	1.87	0.56
1:A:380:MET:HE2	1:A:412:ILE:HD11	1.87	0.56
1:A:44:ALA:O	1:A:48:VAL:HG13	2.08	0.53
1:A:207:LYS:NZ	1:A:247:GLN:HE21	2.06	0.52
1:A:206:THR:CG2	1:A:241:PHE:HD2	2.25	0.50
1:A:203:GLU:HG3	1:A:207:LYS:HE3	1.95	0.48
1:A:228:VAL:HG21	1:A:309:ILE:HD11	1.95	0.48
1:A:227:LEU:HD12	1:A:300:ALA:HB3	1.96	0.48
1:A:288:GLN:HE22	1:A:292:ARG:HD2	1.79	0.48
1:A:404:LYS:HB2	1:A:407:GLU:HG3	1.96	0.48
1:A:68:ILE:HD12	1:A:88:THR:HG23	1.97	0.46
1:A:32:ILE:HG13	1:A:68:ILE:HG13	1.99	0.45
1:A:147:THR:HG23	1:A:149:MET:HE3	2.00	0.44
1:A:204:GLU:O	1:A:208:ARG:HG2	2.17	0.44
1:A:324:PRO:HB3	1:A:358:LEU:HB3	2.00	0.43
1:A:233:ILE:HG22	1:A:234:MET:HG3	2.01	0.43
1:A:57:TYR:O	1:A:59:GLY:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:CYS:SG	1:A:153:ARG:HD3	2.59	0.43
1:A:117:ALA:O	1:A:121:GLU:HB2	2.19	0.42
1:A:353:PRO:O	1:A:356:ILE:HG22	2.19	0.41
1:A:93:ARG:O	1:A:96:ARG:HD2	2.20	0.41
1:A:130:PRO:HA	1:A:150:VAL:HA	2.02	0.41
1:A:206:THR:HG22	1:A:241:PHE:HD2	1.84	0.41
1:A:77:VAL:HG12	1:A:78:TYR:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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 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%)	383 (93%)	26 (6%)	3 (1%)	18	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	58	LYS
1	A	109	GLY

5.3.2 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 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%)	292 (87%)	44 (13%)	4 8

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	20	LYS
1	A	26	ASN
1	A	43	PRO
1	A	48	VAL
1	A	53	VAL
1	A	60	GLU
1	A	61	ARG
1	A	64	SER
1	A	80	GLN
1	A	81	ASP
1	A	103	LEU
1	A	104	THR
1	A	111	ILE
1	A	121	GLU
1	A	131	VAL
1	A	145	GLU
1	A	160	TYR
1	A	179	LEU
1	A	204	GLU
1	A	227	LEU
1	A	228	VAL
1	A	233	ILE
1	A	242	LYS
1	A	257	LEU
1	A	264	LEU
1	A	275	ILE
1	A	281	ILE
1	A	286	LEU
1	A	290	LEU
1	A	313	LEU
1	A	320	ILE
1	A	324	PRO
1	A	351	VAL
1	A	356	ILE
1	A	358	LEU
1	A	364	LEU
1	A	377	VAL

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Mol	Chain	Res	Type
1	A	380	MET
1	A	389	VAL
1	A	391	TYR
1	A	392	ASP
1	A	394	GLU
1	A	398	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	247	GLN
1	A	288	GLN
1	A	327	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.