



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:50 PM UTC

PDB ID : 9GAA / pdb_00009gaa
Title : PRECURSOR OF THE T152A MUTANT GLYCOSYLASPARAGINASE
FROM FLAVOBACTERIUM MENINGOSEPTICUM
Authors : Guo, H.-C.; Xu, Q.
Deposited on : 1999-06-15
Resolution : 2.10 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

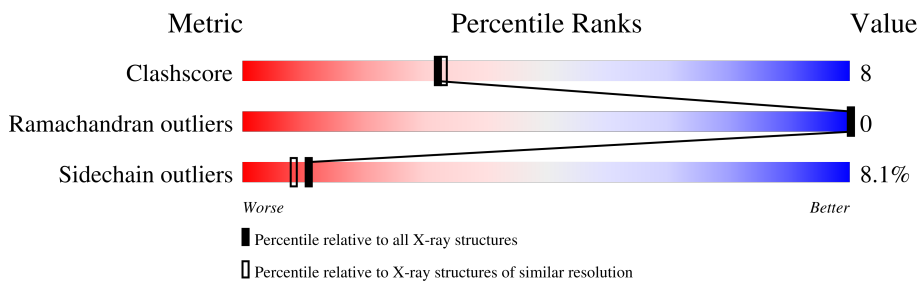
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	295	
1	C	295	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4362 atoms, of which 0 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 PROTEIN (GLYCOSYLASPARAGINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2119	1325	378	403	13			
1	C	279	Total	C	N	O	S	0	0	0
			2119	1325	378	403	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	ALA	THR	engineered mutation	UNP Q47898
C	452	ALA	THR	engineered mutation	UNP Q47898

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	61	Total	O	0	0
			61	61		
2	C	63	Total	O	0	0
			63	63		

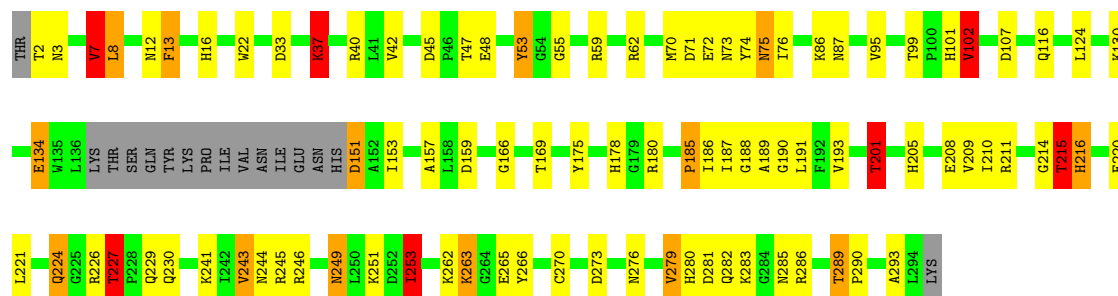
3 Residue-property plots

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.

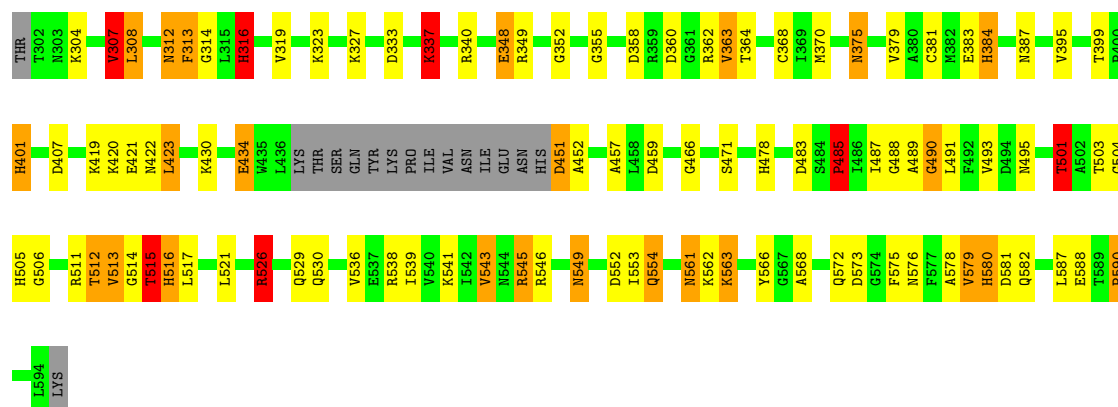
• Molecule 1: PROTEIN (GLYCOSYLASPARAGINASE)

Chain A: 



• Molecule 1: PROTEIN (GLYCOSYLASPARAGINASE)

Chain C: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.30 Å 52.80 Å 62.40 Å 80.80° 90.50° 105.10°	Depositor
Resolution (Å)	6.00 – 2.10	Depositor
% Data completeness (in resolution range)	89.8 (6.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	7.60	Depositor
Refinement program	XTALVIEW, X-PLOR 3.1	Depositor
R, R_{free}	0.232 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4362	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	1.27	14/2153 (0.7%)	2.01	78/2903 (2.7%)
1	C	1.27	19/2153 (0.9%)	1.97	76/2903 (2.6%)
All	All	1.27	33/4306 (0.8%)	1.99	154/5806 (2.7%)

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	2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	VAL	CA-CB	9.74	1.68	1.54
1	A	253	ILE	CA-CB	8.94	1.66	1.54
1	C	543	VAL	CA-CB	8.81	1.66	1.54
1	A	95	VAL	CA-CB	7.78	1.63	1.54
1	A	169	THR	CA-CB	7.70	1.67	1.53
1	C	478	HIS	CD2-NE2	-7.55	1.29	1.37
1	C	401	HIS	CD2-NE2	-7.45	1.29	1.37
1	A	187	ILE	CA-CB	7.43	1.62	1.54
1	C	379	VAL	CA-CB	7.20	1.65	1.54
1	A	216	HIS	CD2-NE2	-6.81	1.30	1.37
1	A	210	ILE	CA-CB	6.70	1.62	1.54
1	C	580	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	101	HIS	CD2-NE2	-6.26	1.30	1.37
1	C	316	HIS	CG-ND1	-6.19	1.31	1.38
1	A	178	HIS	CD2-NE2	-6.17	1.31	1.37
1	C	488	GLY	N-CA	6.16	1.54	1.45
1	A	16	HIS	CD2-NE2	-6.13	1.31	1.37
1	C	516	HIS	CD2-NE2	-5.92	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	384	HIS	CG-ND1	-5.81	1.31	1.38
1	A	280	HIS	CD2-NE2	-5.77	1.31	1.37
1	C	399	THR	CA-CB	5.69	1.61	1.54
1	C	505	HIS	CG-ND1	-5.60	1.32	1.38
1	A	153	ILE	CA-CB	5.60	1.60	1.54
1	C	316	HIS	CD2-NE2	-5.57	1.31	1.37
1	C	384	HIS	CD2-NE2	-5.51	1.31	1.37
1	C	505	HIS	CD2-NE2	-5.42	1.31	1.37
1	C	319	VAL	CA-CB	5.38	1.61	1.54
1	C	363	VAL	CA-CB	5.26	1.59	1.53
1	A	205	HIS	CD2-NE2	-5.23	1.32	1.37
1	A	209	VAL	CA-CB	5.19	1.61	1.54
1	C	513	VAL	CA-CB	5.13	1.61	1.54
1	C	485	PRO	N-CA	-5.00	1.44	1.47
1	C	395	VAL	CA-CB	5.00	1.60	1.54

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ASP	CA-CB-CG	12.90	125.50	112.60
1	A	215	THR	N-CA-CB	-11.56	92.50	110.30
1	C	316	HIS	ND1-CG-CD2	10.92	117.02	106.10
1	C	515	THR	N-CA-CB	-9.65	95.44	110.30
1	C	313	PHE	CA-CB-CG	9.42	123.22	113.80
1	C	478	HIS	CB-CG-CD2	-9.27	119.15	131.20
1	A	13	PHE	CA-CB-CG	9.25	123.05	113.80
1	C	358	ASP	CA-CB-CG	9.16	121.76	112.60
1	C	487	ILE	O-C-N	-9.08	112.48	121.83
1	A	7	VAL	CB-CA-C	-9.02	96.61	110.50
1	A	211	ARG	NE-CZ-NH2	-8.68	111.39	119.20
1	A	102	VAL	N-CA-CB	-8.57	100.55	112.12
1	A	75	ASN	OD1-CG-ND2	-8.38	114.22	122.60
1	A	53	TYR	O-C-N	-8.24	113.39	122.12
1	C	307	VAL	CB-CA-C	-8.22	97.83	110.50
1	A	102	VAL	CB-CA-C	8.16	118.64	110.65
1	C	478	HIS	CB-CG-ND1	7.95	134.62	122.70
1	C	576	ASN	CA-CB-CG	7.81	120.41	112.60
1	C	511	ARG	NE-CZ-NH2	-7.74	112.23	119.20
1	C	451	ASP	CA-C-N	7.73	134.73	122.59
1	C	451	ASP	C-N-CA	7.73	134.73	122.59
1	A	224	GLN	OE1-CD-NE2	-7.72	114.88	122.60
1	C	573	ASP	CA-CB-CG	7.62	120.22	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	HIS	CB-CG-CD2	-7.57	121.36	131.20
1	C	375	ASN	N-CA-C	-7.55	97.28	109.96
1	A	62	ARG	O-C-N	-7.48	114.82	123.27
1	C	579	VAL	CB-CA-C	-7.47	100.16	110.77
1	A	227	THR	CA-C-N	7.39	126.92	119.24
1	A	227	THR	C-N-CA	7.39	126.92	119.24
1	C	562	LYS	N-CA-C	7.26	121.24	112.38
1	A	227	THR	N-CA-CB	-7.24	99.11	110.03
1	A	262	LYS	N-CA-C	7.16	121.12	112.38
1	A	87	ASN	OD1-CG-ND2	-7.15	115.45	122.60
1	C	407	ASP	CA-CB-CG	7.12	119.72	112.60
1	A	215	THR	CB-CA-C	7.12	124.90	110.38
1	A	279	VAL	CB-CA-C	-7.06	100.75	110.77
1	C	580	HIS	CB-CG-CD2	-6.97	122.14	131.20
1	C	459	ASP	CA-CB-CG	6.95	119.55	112.60
1	C	316	HIS	CG-CD2-NE2	-6.83	100.37	107.20
1	C	312	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	A	159	ASP	CA-CB-CG	6.70	119.30	112.60
1	A	188	GLY	CA-C-O	-6.65	112.62	119.20
1	A	40	ARG	CB-CG-CD	-6.61	96.10	111.30
1	A	7	VAL	N-CA-CB	6.61	122.28	111.44
1	C	549	ASN	OD1-CG-ND2	-6.60	116.00	122.60
1	C	581	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	16	HIS	ND1-CG-CD2	6.58	112.68	106.10
1	C	401	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	A	201	THR	N-CA-CB	6.50	122.86	111.55
1	A	101	HIS	CA-CB-CG	-6.49	107.31	113.80
1	A	3	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	A	40	ARG	NE-CZ-NH2	-6.45	113.39	119.20
1	C	360	ASP	CA-CB-CG	6.43	119.03	112.60
1	C	340	ARG	NE-CZ-NH2	-6.39	113.45	119.20
1	A	178	HIS	CB-CG-CD2	-6.38	122.90	131.20
1	A	71	ASP	CA-CB-CG	6.37	118.97	112.60
1	C	488	GLY	N-CA-C	6.29	122.04	113.99
1	A	185	PRO	CB-CA-C	6.27	117.60	109.89
1	C	375	ASN	OD1-CG-ND2	-6.26	116.33	122.60
1	A	265	GLU	N-CA-C	-6.25	101.23	110.48
1	A	227	THR	CB-CA-C	6.23	119.67	109.46
1	A	59	ARG	CB-CG-CD	-6.23	96.98	111.30
1	C	495	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	A	55	GLY	N-CA-C	6.17	118.58	111.36
1	A	293	ALA	N-CA-C	6.17	119.28	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	422	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	C	387	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	A	102	VAL	N-CA-C	-6.06	107.59	113.53
1	C	485	PRO	CB-CA-C	6.04	116.57	109.92
1	A	116	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	C	340	ARG	CB-CG-CD	-6.02	97.45	111.30
1	C	348	GLU	CA-C-O	6.01	126.79	120.36
1	C	471	SER	O-C-N	-5.96	114.89	122.34
1	C	384	HIS	N-CA-C	5.93	120.46	113.23
1	C	515	THR	CB-CA-C	5.93	122.47	110.38
1	C	488	GLY	CA-C-O	5.87	126.58	119.65
1	A	55	GLY	O-C-N	-5.84	117.15	122.93
1	C	307	VAL	N-CA-CB	5.82	120.98	111.44
1	C	304	LYS	CA-C-O	-5.81	114.30	120.28
1	C	545	ARG	O-C-N	-5.79	115.45	122.22
1	C	511	ARG	CA-CB-CG	5.78	125.67	114.10
1	C	316	HIS	CG-ND1-CE1	-5.73	99.55	109.30
1	A	45	ASP	CA-C-O	5.72	123.87	119.46
1	C	536	VAL	CA-C-O	-5.72	115.00	120.95
1	C	572	GLN	CA-C-N	5.71	128.95	120.90
1	C	572	GLN	C-N-CA	5.71	128.95	120.90
1	A	276	ASN	OD1-CG-ND2	-5.68	116.92	122.60
1	A	186	ILE	N-CA-C	5.67	116.27	107.99
1	C	316	HIS	ND1-CE1-NE2	5.64	114.04	108.40
1	A	289	THR	O-C-N	5.64	127.60	121.23
1	A	72	GLU	CB-CG-CD	5.63	122.16	112.60
1	A	47	THR	N-CA-C	-5.61	106.20	113.16
1	A	221	LEU	N-CA-C	-5.61	105.17	112.23
1	C	579	VAL	N-CA-CB	5.61	118.93	111.64
1	C	314	GLY	O-C-N	-5.60	116.38	122.54
1	A	280	HIS	CB-CG-ND1	5.58	131.08	122.70
1	A	62	ARG	CA-C-O	5.57	126.50	120.43
1	A	45	ASP	CA-C-N	5.56	125.17	119.56
1	A	45	ASP	C-N-CA	5.56	125.17	119.56
1	A	107	ASP	CA-CB-CG	5.55	118.16	112.60
1	C	561	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	C	554	GLN	CA-C-O	-5.53	114.38	120.24
1	C	490	GLY	CA-C-O	5.50	125.99	119.50
1	A	37	LYS	N-CA-CB	-5.50	102.04	110.01
1	A	37	LYS	CA-CB-CG	5.48	125.07	114.10
1	A	134	GLU	CB-CG-CD	5.48	121.92	112.60
1	C	337	LYS	N-CA-CB	-5.43	102.13	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	THR	CA-C-O	-5.43	114.55	120.69
1	A	22	TRP	CE2-CD2-CG	-5.43	100.69	107.20
1	C	352	GLY	O-C-N	5.42	129.75	122.70
1	A	273	ASP	N-CA-C	5.42	117.53	110.43
1	A	186	ILE	N-CA-CB	-5.40	104.89	111.21
1	C	471	SER	N-CA-C	-5.39	106.38	113.17
1	C	511	ARG	CG-CD-NE	-5.38	100.15	112.00
1	C	576	ASN	O-C-N	-5.38	115.44	122.59
1	C	487	ILE	CA-C-O	-5.38	115.15	120.85
1	C	588	GLU	CB-CG-CD	5.37	121.72	112.60
1	A	101	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	A	229	GLN	N-CA-CB	-5.35	102.26	110.01
1	A	244	ASN	CA-CB-CG	-5.34	107.26	112.60
1	C	434	GLU	CB-CG-CD	5.28	121.57	112.60
1	C	526	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	A	16	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	C	362	ARG	O-C-N	-5.26	117.33	123.27
1	C	421	GLU	CB-CG-CD	5.25	121.52	112.60
1	C	529	GLN	N-CA-CB	-5.25	102.40	110.01
1	A	201	THR	CB-CA-C	-5.24	99.05	109.79
1	C	512	THR	O-C-N	-5.20	116.09	122.34
1	A	281	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	580	HIS	CB-CG-ND1	5.19	130.48	122.70
1	A	270	CYS	CB-CA-C	-5.18	99.31	110.45
1	A	12	ASN	CA-C-O	5.18	126.04	120.55
1	C	521	LEU	N-CA-C	-5.17	105.71	112.23
1	A	99	THR	CA-C-N	5.16	124.77	119.56
1	A	99	THR	C-N-CA	5.16	124.77	119.56
1	A	216	HIS	CB-CG-CD2	-5.16	124.50	131.20
1	A	73	ASN	CA-CB-CG	-5.14	107.46	112.60
1	A	16	HIS	CG-CD2-NE2	-5.13	102.07	107.20
1	C	487	ILE	CA-C-N	-5.13	111.92	120.74
1	C	487	ILE	C-N-CA	-5.13	111.92	120.74
1	A	253	ILE	CA-C-O	5.11	126.65	120.67
1	C	526	ARG	CB-CG-CD	5.10	123.03	111.30
1	A	285	ASN	CA-CB-CG	5.08	117.68	112.60
1	A	224	GLN	N-CA-C	-5.08	107.37	113.21
1	C	526	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	C	514	GLY	O-C-N	-5.07	117.25	122.17
1	A	224	GLN	CG-CD-NE2	5.07	124.00	116.40
1	C	312	ASN	CA-C-O	-5.05	115.19	120.55
1	A	214	GLY	N-CA-C	5.04	118.77	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	C	452	ALA	CA-C-N	-5.01	116.98	123.19
1	C	452	ALA	C-N-CA	-5.01	116.98	123.19
1	A	215	THR	OG1-CB-CG2	5.00	119.31	109.30
1	C	501	THR	N-CA-CB	5.00	120.25	111.55

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	TYR	Sidechain
1	A	74	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	2119	0	2110	33	0
1	C	2119	0	2110	43	0
2	A	61	0	0	2	0
2	C	63	0	0	1	0
All	All	4362	0	4220	68	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 8.

All (68) 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:216:HIS:HD2	1:C:516:HIS:HD2	1.15	0.95
1:A:42:VAL:HG13	1:A:48:GLU:HG2	1.53	0.90
1:A:208:GLU:HG3	1:A:253:ILE:HD13	1.65	0.77
1:C:364:THR:HG22	1:C:383:GLU:HG3	1.74	0.68
1:A:249:ASN:HD22	1:A:251:LYS:H	1.42	0.66
1:C:489:ALA:O	1:C:515:THR:HB	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:HIS:HD2	1:C:516:HIS:CD2	2.07	0.64
1:A:216:HIS:CD2	1:C:516:HIS:HD2	2.06	0.64
1:A:76:ILE:HG13	1:A:102:VAL:HG22	1.82	0.62
1:C:563:LYS:HD2	1:C:563:LYS:H	1.64	0.62
1:A:70:MET:HG2	1:A:193:VAL:HB	1.83	0.61
1:C:312:ASN:ND2	1:C:587:LEU:HD21	2.16	0.59
1:C:483:ASP:OD1	1:C:506:GLY:HA2	2.04	0.58
1:C:308:LEU:HD11	1:C:566:TYR:HB2	1.87	0.57
1:C:512:THR:HG21	1:C:539:ILE:HG12	1.87	0.56
1:A:75:ASN:ND2	1:C:546:ARG:HE	2.04	0.55
1:C:308:LEU:HD22	1:C:579:VAL:HG13	1.88	0.55
1:A:220:GLU:HG3	1:A:224:GLN:HE21	1.71	0.55
1:A:7:VAL:HG13	1:A:157:ALA:HB2	1.90	0.54
1:A:246:ARG:HH21	1:C:375:ASN:HD22	1.55	0.53
1:C:384:HIS:HB3	1:C:420:LYS:HG3	1.90	0.53
1:C:323:LYS:O	1:C:327:LYS:HG2	2.09	0.52
1:A:8:LEU:HD22	1:A:279:VAL:HG13	1.90	0.52
1:C:368:CYS:HB3	1:C:485:PRO:HA	1.90	0.52
1:A:249:ASN:ND2	1:A:251:LYS:H	2.07	0.51
1:C:307:VAL:HG23	1:C:580:HIS:HB3	1.92	0.51
1:C:307:VAL:HG13	1:C:457:ALA:HB2	1.92	0.51
1:A:8:LEU:HD11	1:A:266:TYR:HB2	1.93	0.50
1:A:130:LYS:O	1:A:134:GLU:HG3	2.10	0.50
1:A:246:ARG:HH21	1:C:375:ASN:ND2	2.09	0.50
1:A:227:THR:HB	1:A:230:GLN:CD	2.37	0.50
1:C:466:GLY:HA3	1:C:491:LEU:HD11	1.93	0.50
1:A:241:LYS:O	1:A:245:ARG:HG3	2.12	0.49
1:C:349:ARG:O	1:C:355:GLY:HA2	2.12	0.49
1:C:503:THR:HG21	1:C:575:PHE:CD1	2.48	0.49
1:C:363:VAL:HG21	1:C:423:LEU:HB2	1.94	0.49
1:A:180:ARG:HG3	1:C:401:HIS:CD2	2.48	0.48
1:C:503:THR:HG21	1:C:575:PHE:CE1	2.49	0.48
1:A:190:GLY:O	1:A:201:THR:HG22	2.14	0.48
1:A:226:ARG:HD2	2:A:618:HOH:O	2.14	0.47
1:A:189:ALA:O	1:A:215:THR:HB	2.14	0.47
1:C:490:GLY:O	1:C:501:THR:HG22	2.14	0.47
1:C:333:ASP:O	1:C:337:LYS:HB2	2.16	0.46
1:A:166:GLY:HA3	1:A:191:LEU:HD11	1.96	0.46
1:C:316:HIS:ND1	1:C:316:HIS:N	2.63	0.46
1:C:504:GLY:HA3	1:C:554:GLN:O	2.16	0.46
1:C:541:LYS:O	1:C:545:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:THR:HG23	1:A:263:LYS:HA	1.99	0.45
1:A:227:THR:HG22	1:A:230:GLN:H	1.82	0.45
1:C:526:ARG:HG2	1:C:530:GLN:HB3	1.99	0.45
1:C:364:THR:HB	1:C:381:CYS:HA	1.99	0.45
1:A:227:THR:HB	1:A:230:GLN:OE1	2.18	0.44
1:A:286:ARG:HA	2:A:690:HOH:O	2.17	0.44
1:C:561:ASN:OD1	1:C:563:LYS:HD2	2.17	0.44
1:A:75:ASN:HD22	1:C:546:ARG:HH21	1.64	0.44
1:C:568:ALA:HB3	1:C:590:PRO:HB3	2.00	0.43
1:C:430:LYS:O	1:C:434:GLU:HG3	2.19	0.42
1:A:33:ASP:O	1:A:37:LYS:HB2	2.19	0.42
1:C:517:LEU:HD21	1:C:538:ARG:HD2	2.01	0.42
1:A:246:ARG:HH11	1:A:246:ARG:HD3	1.69	0.42
1:C:312:ASN:CG	1:C:587:LEU:HD21	2.45	0.41
1:A:289:THR:HA	1:A:290:PRO:HD2	1.74	0.41
1:C:312:ASN:HB2	2:C:679:HOH:O	2.20	0.41
1:C:549:ASN:HB3	1:C:552:ASP:OD2	2.20	0.41
1:C:491:LEU:C	1:C:515:THR:HG21	2.46	0.41
1:C:308:LEU:HA	1:C:578:ALA:O	2.21	0.40
1:C:370:MET:HG2	1:C:493:VAL:HB	2.03	0.40
1:A:53:TYR:HB2	1:A:86:LYS:HG3	2.03	0.40

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	275/295 (93%)	265 (96%)	10 (4%)	0	100	100
1	C	275/295 (93%)	265 (96%)	10 (4%)	0	100	100
All	All	550/590 (93%)	530 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	221/237 (93%)	204 (92%)	17 (8%)	12	9
1	C	221/237 (93%)	202 (91%)	19 (9%)	10	7
All	All	442/474 (93%)	406 (92%)	36 (8%)	11	8

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	8	LEU
1	A	13	PHE
1	A	37	LYS
1	A	102	VAL
1	A	124	LEU
1	A	151	ASP
1	A	185	PRO
1	A	201	THR
1	A	215	THR
1	A	227	THR
1	A	243	VAL
1	A	249	ASN
1	A	253	ILE
1	A	263	LYS
1	A	282	GLN
1	A	283	LYS
1	C	307	VAL
1	C	308	LEU
1	C	313	PHE
1	C	316	HIS
1	C	337	LYS
1	C	348	GLU
1	C	419	LYS
1	C	423	LEU

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Mol	Chain	Res	Type
1	C	451	ASP
1	C	485	PRO
1	C	501	THR
1	C	513	VAL
1	C	515	THR
1	C	526	ARG
1	C	543	VAL
1	C	553	ILE
1	C	563	LYS
1	C	582	GLN
1	C	590	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	84	HIS
1	A	87	ASN
1	A	216	HIS
1	A	224	GLN
1	A	249	ASN
1	C	312	ASN
1	C	375	ASN
1	C	387	ASN
1	C	401	HIS
1	C	478	HIS
1	C	516	HIS
1	C	576	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.