



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:01 PM UTC

PDB ID : 9GAC / pdb_00009gac
Title : PRECURSOR OF THE T152C MUTANT GLYCOSYLASPARAGINASE
FROM FLAVOBACTERIUM MENINGOSEPTICUM
Authors : Guo, H.-C.; Xu, Q.
Deposited on : 1999-06-15
Resolution : 1.90 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

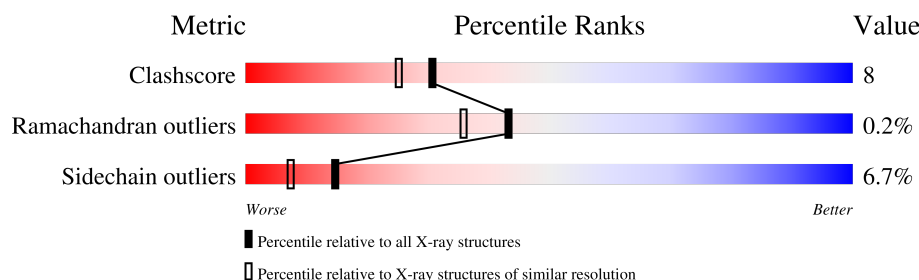
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	 61% 25% 7% • 5%
1	C	295	 67% 21% 6% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4423 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.

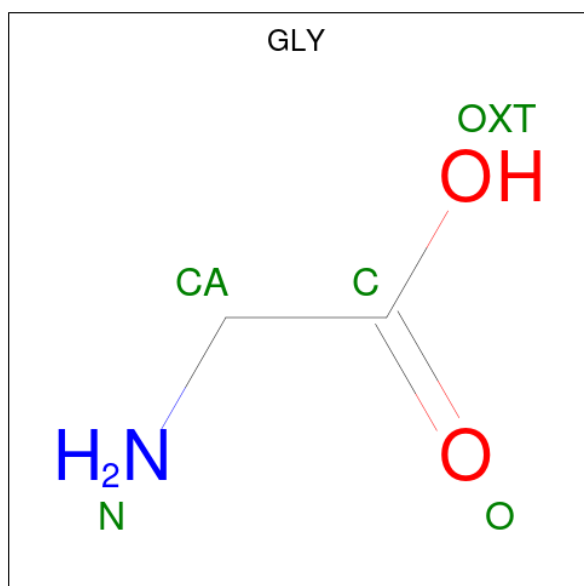
- Molecule 1 is a protein called PROTEIN (GLYCOSYLASPARAGINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2130	1331	381	404	14			
1	C	280	Total	C	N	O	S	0	0	0
			2132	1333	382	403	14			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	2	1	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 3 is water.

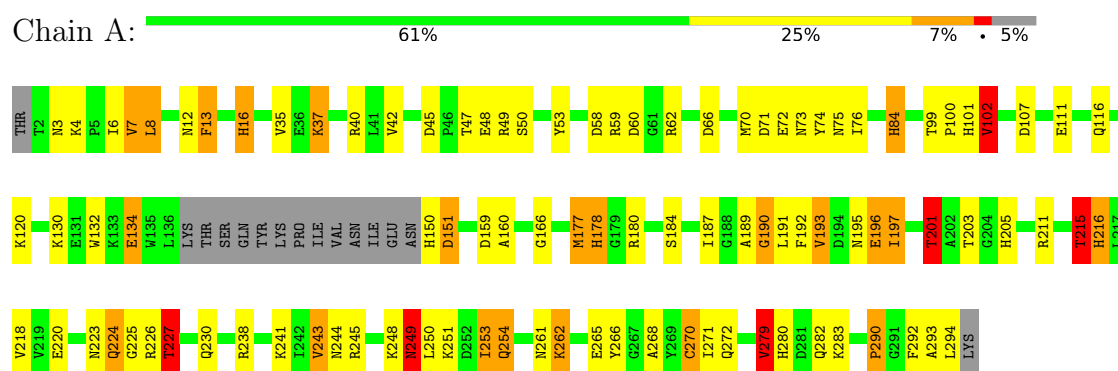
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	76	Total	O	0	0
			76	76		
3	C	75	Total	O	0	0
			75	75		

3 Residue-property plots [i](#)

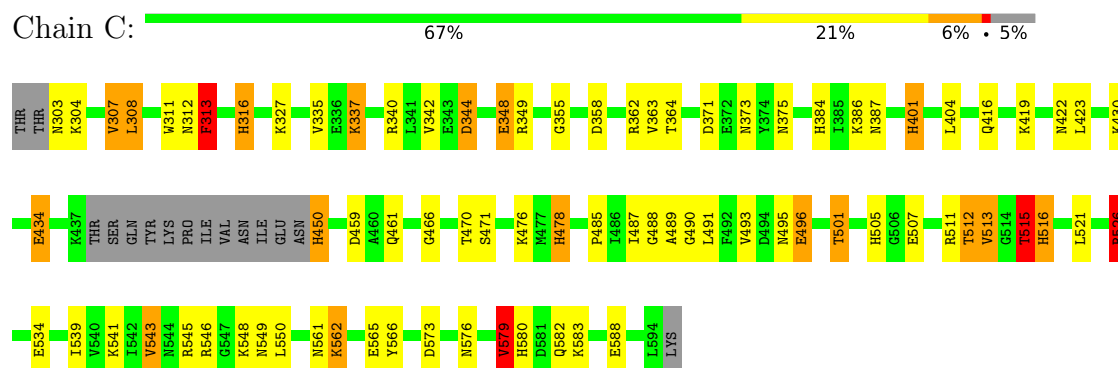
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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)



• Molecule 1: PROTEIN (GLYCOSYLASPARAGINASE)



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 – 1.90	Depositor
% Data completeness (in resolution range)	92.8 (6.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	5.60	Depositor
Refinement program	XTALVIEW, X-PLOR 3.1	Depositor
R, R_{free}	0.232 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4423	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	1.20	20/2165 (0.9%)	2.12	91/2919 (3.1%)
1	C	1.19	16/2167 (0.7%)	2.12	83/2920 (2.8%)
All	All	1.19	36/4332 (0.8%)	2.12	174/5839 (3.0%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	478	HIS	CD2-NE2	-7.72	1.29	1.37
1	A	216	HIS	CD2-NE2	-7.63	1.29	1.37
1	A	6	ILE	CA-CB	7.24	1.63	1.55
1	C	316	HIS	CD2-NE2	-7.23	1.29	1.37
1	C	513	VAL	CA-CB	7.21	1.64	1.54
1	C	384	HIS	CD2-NE2	-7.19	1.29	1.37
1	C	580	HIS	CD2-NE2	-7.17	1.29	1.37
1	C	516	HIS	CD2-NE2	-7.14	1.29	1.37
1	C	505	HIS	CD2-NE2	-6.80	1.30	1.37
1	C	401	HIS	CD2-NE2	-6.78	1.30	1.37
1	C	493	VAL	CA-CB	6.53	1.62	1.54
1	A	205	HIS	CD2-NE2	-6.51	1.30	1.37
1	C	316	HIS	CG-ND1	-6.22	1.31	1.38
1	A	178	HIS	CD2-NE2	-6.14	1.31	1.37
1	A	270	CYS	CA-CB	-6.04	1.42	1.54
1	A	16	HIS	CD2-NE2	-6.02	1.31	1.37
1	A	280	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	84	HIS	CD2-NE2	-5.91	1.31	1.37
1	A	101	HIS	CD2-NE2	-5.71	1.31	1.37
1	C	543	VAL	CA-CB	5.60	1.61	1.54
1	A	16	HIS	CG-ND1	-5.54	1.32	1.38
1	A	193	VAL	CA-CB	5.51	1.61	1.54
1	A	243	VAL	CA-CB	5.49	1.61	1.54
1	A	150	HIS	CD2-NE2	-5.41	1.31	1.37
1	A	35	VAL	CA-CB	5.40	1.61	1.54
1	C	516	HIS	CG-ND1	-5.36	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	HIS	CG-ND1	-5.35	1.32	1.38
1	C	505	HIS	CG-ND1	-5.34	1.32	1.38
1	A	205	HIS	CG-ND1	-5.33	1.32	1.38
1	C	384	HIS	CG-ND1	-5.19	1.32	1.38
1	C	488	GLY	CA-C	5.19	1.59	1.51
1	A	218	VAL	CA-CB	5.17	1.60	1.54
1	A	187	ILE	CA-CB	5.17	1.60	1.54
1	C	470	THR	CA-CB	5.07	1.62	1.53
1	A	184	SER	C-N	5.05	1.37	1.33
1	A	99	THR	CA-CB	5.03	1.60	1.54

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	THR	N-CA-CB	-13.93	88.85	110.30
1	A	211	ARG	NE-CZ-NH2	-13.48	107.07	119.20
1	C	511	ARG	NE-CZ-NH2	-13.14	107.38	119.20
1	A	40	ARG	NE-CZ-NH2	-13.03	107.47	119.20
1	C	515	THR	N-CA-CB	-12.74	90.68	110.30
1	C	303	ASN	CA-CB-CG	-11.63	100.97	112.60
1	C	340	ARG	NE-CZ-NH2	-11.63	108.73	119.20
1	C	461	GLN	OE1-CD-NE2	-11.34	111.26	122.60
1	C	576	ASN	OD1-CG-ND2	-11.26	111.34	122.60
1	A	7	VAL	CB-CA-C	-10.64	94.12	110.50
1	C	543	VAL	CG1-CB-CG2	-10.48	87.75	110.80
1	C	526	ARG	NE-CZ-NH1	10.23	131.73	121.50
1	C	434	GLU	CB-CG-CD	10.13	129.83	112.60
1	C	307	VAL	CB-CA-C	-9.97	95.15	110.50
1	C	526	ARG	NE-CZ-NH2	-9.77	110.41	119.20
1	A	134	GLU	CB-CG-CD	9.71	129.11	112.60
1	A	102	VAL	N-CA-CB	-9.43	95.68	111.23
1	C	450	HIS	CA-CB-CG	9.24	123.04	113.80
1	C	511	ARG	CA-CB-CG	9.21	132.52	114.10
1	A	53	TYR	O-C-N	-9.19	112.47	122.03
1	C	487	ILE	O-C-N	-8.89	112.67	121.83
1	A	53	TYR	CA-C-O	-8.89	111.67	121.00
1	A	150	HIS	CA-CB-CG	8.83	122.63	113.80
1	C	582	GLN	OE1-CD-NE2	-8.82	113.78	122.60
1	C	358	ASP	CA-CB-CG	8.82	121.42	112.60
1	C	478	HIS	CB-CG-CD2	-8.75	119.83	131.20
1	C	401	HIS	CB-CG-CD2	-8.54	120.11	131.20
1	A	249	ASN	OD1-CG-ND2	-8.52	114.08	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	HIS	CB-CG-CD2	-8.38	120.31	131.20
1	A	243	VAL	CG1-CB-CG2	-8.38	92.37	110.80
1	C	340	ARG	NE-CZ-NH1	8.23	129.73	121.50
1	A	215	THR	CB-CA-C	8.21	127.13	110.38
1	C	316	HIS	ND1-CG-CD2	8.13	114.23	106.10
1	A	16	HIS	ND1-CG-CD2	8.00	114.10	106.10
1	C	573	ASP	CA-CB-CG	7.99	120.59	112.60
1	A	7	VAL	N-CA-CB	7.83	124.27	111.44
1	C	541	LYS	CA-CB-CG	-7.78	98.55	114.10
1	C	312	ASN	CA-C-O	-7.76	112.33	120.55
1	A	211	ARG	CD-NE-CZ	7.75	135.25	124.40
1	A	224	GLN	OE1-CD-NE2	-7.75	114.85	122.60
1	C	579	VAL	CB-CA-C	-7.68	99.11	110.33
1	A	40	ARG	CB-CG-CD	-7.62	93.77	111.30
1	A	59	ARG	CB-CG-CD	-7.60	93.82	111.30
1	C	307	VAL	N-CA-CB	7.54	123.80	111.44
1	C	576	ASN	CB-CG-ND2	7.50	127.65	116.40
1	C	348	GLU	CA-C-O	7.44	128.42	120.46
1	A	40	ARG	NE-CZ-NH1	7.38	128.88	121.50
1	C	515	THR	CB-CA-C	7.38	125.43	110.38
1	A	244	ASN	OD1-CG-ND2	-7.37	115.23	122.60
1	A	241	LYS	CA-CB-CG	-7.35	99.39	114.10
1	C	401	HIS	CB-CG-ND1	7.29	133.64	122.70
1	A	227	THR	N-CA-CB	-7.20	97.56	110.37
1	A	66	ASP	CA-CB-CG	7.18	119.78	112.60
1	C	340	ARG	CB-CG-CD	-7.14	94.89	111.30
1	A	279	VAL	CB-CA-C	-7.13	99.92	110.33
1	A	227	THR	OG1-CB-CG2	7.08	123.46	109.30
1	A	107	ASP	CA-CB-CG	7.05	119.65	112.60
1	A	12	ASN	CA-C-O	7.01	127.98	120.55
1	C	582	GLN	CG-CD-NE2	6.95	126.83	116.40
1	C	576	ASN	CA-CB-CG	6.95	119.55	112.60
1	A	223	ASN	OD1-CG-ND2	-6.93	115.67	122.60
1	C	387	ASN	OD1-CG-ND2	-6.93	115.67	122.60
1	C	478	HIS	CB-CG-ND1	6.92	133.09	122.70
1	C	526	ARG	CD-NE-CZ	6.86	134.00	124.40
1	A	150	HIS	CB-CG-ND1	6.85	132.97	122.70
1	A	151	ASP	N-CA-C	6.84	125.37	110.80
1	A	253	ILE	N-CA-C	6.80	118.27	108.48
1	C	316	HIS	CG-CD2-NE2	-6.79	100.41	107.20
1	C	488	GLY	CA-C-O	6.76	127.63	119.65
1	A	270	CYS	CB-CA-C	-6.73	95.26	110.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	511	ARG	CD-NE-CZ	6.72	133.81	124.40
1	C	461	GLN	CG-CD-NE2	6.71	126.47	116.40
1	A	211	ARG	CA-CB-CG	6.70	127.49	114.10
1	A	47	THR	N-CA-C	-6.64	105.14	113.18
1	C	549	ASN	OD1-CG-ND2	-6.63	115.97	122.60
1	C	340	ARG	CD-NE-CZ	6.52	133.53	124.40
1	A	49	ARG	CA-C-N	6.51	133.50	121.52
1	A	49	ARG	C-N-CA	6.51	133.50	121.52
1	A	71	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	37	LYS	CB-CA-C	-6.51	99.99	110.79
1	A	73	ASN	OD1-CG-ND2	-6.50	116.10	122.60
1	C	565	GLU	CB-CG-CD	6.49	123.62	112.60
1	A	102	VAL	CB-CA-C	6.46	121.89	111.29
1	A	102	VAL	CG1-CB-CG2	6.45	125.00	110.80
1	C	562	LYS	N-CA-C	6.36	120.14	112.38
1	C	561	ASN	CA-CB-CG	6.36	118.96	112.60
1	C	384	HIS	CB-CG-CD2	-6.28	123.04	131.20
1	C	337	LYS	CB-CA-C	-6.24	100.44	110.79
1	C	580	HIS	CB-CG-CD2	-6.22	123.11	131.20
1	C	373	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	C	362	ARG	O-C-N	-6.18	116.28	123.27
1	A	226	ARG	CA-CB-CG	6.17	126.45	114.10
1	A	293	ALA	N-CA-C	6.17	118.08	111.36
1	A	224	GLN	CG-CD-NE2	6.16	125.64	116.40
1	A	261	ASN	CA-CB-CG	6.15	118.75	112.60
1	C	515	THR	OG1-CB-CG2	6.10	121.50	109.30
1	C	313	PHE	CA-CB-CG	6.10	119.90	113.80
1	C	362	ARG	NE-CZ-NH2	-6.07	113.74	119.20
1	A	201	THR	N-CA-CB	6.05	122.08	111.55
1	A	35	VAL	CA-CB-CG2	6.05	120.68	110.40
1	A	211	ARG	CG-CD-NE	-6.02	98.75	112.00
1	A	159	ASP	CA-CB-CG	6.01	118.61	112.60
1	C	327	LYS	CA-CB-CG	-6.01	102.08	114.10
1	C	583	LYS	CG-CD-CE	5.99	125.08	111.30
1	A	227	THR	CA-CB-OG1	-5.98	100.63	109.60
1	A	40	ARG	CG-CD-NE	-5.97	98.87	112.00
1	C	583	LYS	CB-CG-CD	5.96	125.02	111.30
1	A	282	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	A	283	LYS	CG-CD-CE	5.89	124.84	111.30
1	A	3	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	A	280	HIS	CB-CG-CD2	-5.86	123.58	131.20
1	A	59	ARG	NE-CZ-NH2	-5.84	113.94	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	62	ARG	O-C-N	-5.84	116.67	123.27
1	C	488	GLY	N-CA-C	5.77	121.37	113.99
1	C	304	LYS	CG-CD-CE	-5.76	98.05	111.30
1	A	35	VAL	CA-CB-CG1	-5.75	100.62	110.40
1	C	478	HIS	CA-CB-CG	-5.74	108.06	113.80
1	C	375	ASN	N-CA-C	-5.71	100.37	109.96
1	A	215	THR	OG1-CB-CG2	5.71	120.72	109.30
1	C	364	THR	N-CA-C	-5.70	99.61	108.90
1	A	40	ARG	CD-NE-CZ	5.67	132.34	124.40
1	C	344	ASP	N-CA-C	5.66	118.38	111.82
1	A	262	LYS	N-CA-C	5.65	119.28	112.38
1	C	511	ARG	CG-CD-NE	-5.65	99.57	112.00
1	A	244	ASN	CB-CG-ND2	5.60	124.80	116.40
1	A	211	ARG	NE-CZ-NH1	5.57	127.07	121.50
1	C	416	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	A	290	PRO	N-CA-C	5.54	119.25	111.33
1	A	99	THR	O-C-N	-5.53	117.24	121.55
1	A	225	GLY	CA-C-O	-5.50	112.90	119.06
1	C	579	VAL	N-CA-CB	5.45	119.48	111.52
1	C	450	HIS	O-C-N	-5.43	114.32	123.00
1	C	340	ARG	CA-CB-CG	5.42	124.95	114.10
1	A	254	GLN	CB-CG-CD	5.42	121.81	112.60
1	C	422	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	A	116	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	A	223	ASN	CA-CB-CG	5.38	117.98	112.60
1	A	187	ILE	N-CA-C	-5.35	102.61	109.30
1	A	254	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	C	358	ASP	N-CA-C	-5.35	102.97	110.35
1	C	512	THR	O-C-N	-5.34	115.94	122.34
1	A	13	PHE	CA-CB-CG	5.34	119.14	113.80
1	C	335	VAL	CA-CB-CG1	-5.33	101.34	110.40
1	A	45	ASP	N-CA-C	5.33	117.31	109.42
1	A	3	ASN	CB-CG-ND2	5.32	124.38	116.40
1	C	511	ARG	NH1-CZ-NH2	5.32	126.22	119.30
1	A	201	THR	CB-CA-C	-5.31	98.90	109.79
1	C	316	HIS	CB-CA-C	-5.31	101.82	110.85
1	A	190	GLY	O-C-N	-5.29	116.70	122.68
1	C	459	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	40	ARG	CA-CB-CG	5.27	124.65	114.10
1	C	337	LYS	N-CA-CB	5.27	117.87	110.12
1	A	282	GLN	CG-CD-NE2	5.27	124.30	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	495	ASN	CB-CG-ND2	5.25	124.27	116.40
1	A	132	TRP	CE2-CD2-CG	-5.24	100.91	107.20
1	C	583	LYS	O-C-N	-5.23	115.24	122.46
1	A	265	GLU	N-CA-C	-5.21	102.76	110.48
1	C	471	SER	O-C-N	-5.19	116.11	122.34
1	C	588	GLU	CB-CG-CD	5.18	121.41	112.60
1	A	16	HIS	CG-CD2-NE2	-5.17	102.03	107.20
1	C	476	LYS	O-C-N	-5.15	116.92	122.79
1	A	226	ARG	NE-CZ-NH2	-5.15	114.57	119.20
1	A	238	ARG	CD-NE-CZ	-5.13	117.21	124.40
1	C	505	HIS	CA-CB-CG	-5.12	108.68	113.80
1	C	562	LYS	CG-CD-CE	5.07	122.95	111.30
1	C	371	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	192	PHE	CA-CB-CG	-5.03	108.77	113.80
1	A	196	GLU	CA-CB-CG	-5.03	104.05	114.10
1	A	253	ILE	CA-C-N	-5.01	114.80	122.62
1	A	253	ILE	C-N-CA	-5.01	114.80	122.62
1	C	496	GLU	CB-CA-C	-5.01	100.99	110.01
1	A	197	ILE	CB-CG1-CD1	-5.01	103.28	113.80
1	A	211	ARG	NH1-CZ-NH2	5.00	125.81	119.30

There are no chirality outliers.

There are no planarity outliers.

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	2130	0	2117	48	0
1	C	2132	0	2123	39	0
2	A	5	0	2	0	0
2	C	5	0	2	0	0
3	A	76	0	0	0	0
3	C	75	0	0	1	0
All	All	4423	0	4244	71	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 (71) 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	1.18	0.89
1:A:249:ASN:HD22	1:A:251:LYS:H	1.34	0.75
1:A:250:LEU:HD23	1:A:294:LEU:HD13	1.74	0.70
1:A:216:HIS:CD2	1:C:516:HIS:HD2	2.08	0.68
1:C:308:LEU:HD22	1:C:579:VAL:HG13	1.76	0.67
1:A:8:LEU:HD22	1:A:279:VAL:HG13	1.76	0.67
1:A:227:THR:HG22	1:A:230:GLN:H	1.60	0.66
1:C:430:LYS:O	1:C:434:GLU:HG3	1.97	0.65
1:A:220:GLU:HG3	1:A:224:GLN:HE21	1.61	0.65
1:A:245:ARG:NH2	1:C:496:GLU:HG2	2.12	0.64
1:A:130:LYS:O	1:A:134:GLU:HG3	1.98	0.63
1:A:74:TYR:OH	1:C:545:ARG:NH2	2.32	0.63
1:A:177:MET:HE2	1:C:401:HIS:ND1	2.14	0.63
1:C:489:ALA:O	1:C:515:THR:HB	1.98	0.62
1:A:189:ALA:O	1:A:215:THR:HB	2.01	0.61
1:A:42:VAL:HG13	1:A:48:GLU:HG2	1.83	0.60
1:A:177:MET:HE3	1:C:404:LEU:HD21	1.84	0.59
1:A:75:ASN:ND2	1:C:546:ARG:HE	2.00	0.59
1:C:526:ARG:HD3	1:C:534:GLU:OE1	2.03	0.58
1:A:216:HIS:HD2	1:C:516:HIS:CD2	2.10	0.57
1:A:76:ILE:HG13	1:A:102:VAL:HG22	1.88	0.56
1:A:177:MET:CE	1:C:404:LEU:HD21	2.36	0.56
1:A:249:ASN:ND2	1:A:251:LYS:H	2.01	0.56
1:A:4:LYS:NZ	1:A:160:ALA:O	2.39	0.54
1:A:216:HIS:HE1	3:C:683:HOH:O	1.93	0.51
1:C:466:GLY:HA3	1:C:491:LEU:HD11	1.92	0.50
1:A:8:LEU:CD2	1:A:279:VAL:HG13	2.41	0.50
1:A:245:ARG:HH22	1:C:496:GLU:HG2	1.76	0.50
1:C:308:LEU:CD2	1:C:579:VAL:HG13	2.42	0.49
1:A:180:ARG:HG3	1:C:401:HIS:CD2	2.46	0.49
1:C:430:LYS:NZ	1:C:434:GLU:OE2	2.45	0.49
1:C:543:VAL:HG11	1:C:550:LEU:HD13	1.95	0.49
1:A:190:GLY:O	1:A:201:THR:HG22	2.12	0.49
1:A:70:MET:HG2	1:A:193:VAL:HB	1.96	0.48
1:A:268:ALA:HB3	1:A:290:PRO:HB3	1.94	0.48
1:A:243:VAL:HG23	1:A:248:LYS:HB2	1.96	0.47
1:C:490:GLY:O	1:C:501:THR:HG22	2.15	0.47
1:A:130:LYS:NZ	1:A:134:GLU:OE2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MET:H	1:C:401:HIS:HE1	1.63	0.46
1:A:102:VAL:HB	1:C:507:GLU:HG3	1.96	0.46
1:A:270:CYS:O	1:A:292:PHE:HA	2.15	0.46
1:C:363:VAL:HG11	1:C:423:LEU:HB2	1.98	0.46
1:C:308:LEU:HD11	1:C:566:TYR:HB2	1.97	0.46
1:C:512:THR:HG21	1:C:539:ILE:HG12	1.97	0.46
1:A:249:ASN:HD22	1:A:251:LYS:N	2.09	0.45
1:A:111:GLU:OE2	1:C:478:HIS:HD2	2.00	0.45
1:C:311:TRP:HB2	1:C:313:PHE:CE1	2.51	0.45
1:C:311:TRP:HB3	1:C:450:HIS:ND1	2.32	0.45
1:C:543:VAL:HG23	1:C:548:LYS:HB2	1.98	0.45
1:A:8:LEU:HD11	1:A:266:TYR:HB2	1.99	0.44
1:A:243:VAL:HG11	1:A:250:LEU:CD1	2.48	0.43
1:C:342:VAL:HG13	1:C:348:GLU:HG2	2.01	0.43
1:C:562:LYS:HA	1:C:562:LYS:HD2	1.70	0.43
1:A:177:MET:H	1:C:401:HIS:CE1	2.37	0.43
1:A:72:GLU:O	1:A:195:ASN:HB2	2.18	0.43
1:A:271:ILE:HG22	1:A:272:GLN:HG3	2.00	0.42
1:C:342:VAL:CG1	1:C:348:GLU:HG2	2.49	0.42
1:A:243:VAL:HG11	1:A:250:LEU:HD13	1.99	0.42
1:C:311:TRP:CE2	1:C:450:HIS:HA	2.55	0.42
1:C:344:ASP:OD1	1:C:386:LYS:HE3	2.19	0.42
1:C:491:LEU:C	1:C:515:THR:HG21	2.45	0.42
1:C:521:LEU:HB3	1:C:526:ARG:HD2	2.01	0.42
1:A:197:ILE:HD13	1:A:197:ILE:HG21	1.85	0.42
1:A:60:ASP:OD2	1:A:178:HIS:HB2	2.20	0.41
1:A:84:HIS:HB3	1:A:120:LYS:HG3	2.02	0.41
1:A:195:ASN:O	1:A:262:LYS:HD3	2.21	0.41
1:A:166:GLY:HA3	1:A:191:LEU:HD11	2.01	0.41
1:A:272:GLN:HG2	1:A:294:LEU:HD23	2.02	0.41
1:C:349:ARG:O	1:C:355:GLY:HA2	2.20	0.41
1:A:111:GLU:OE2	1:C:478:HIS:CD2	2.73	0.41
1:A:191:LEU:N	1:A:215:THR:HG21	2.35	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	276/295 (94%)	264 (96%)	11 (4%)	1 (0%)	30	22
1	C	276/295 (94%)	270 (98%)	6 (2%)	0	100	100
All	All	552/590 (94%)	534 (97%)	17 (3%)	1 (0%)	43	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ASP

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	223/238 (94%)	205 (92%)	18 (8%)	11	5
1	C	223/238 (94%)	211 (95%)	12 (5%)	20	12
All	All	446/476 (94%)	416 (93%)	30 (7%)	15	7

All (30) 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	16	HIS
1	A	37	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	50	SER
1	A	100	PRO
1	A	102	VAL
1	A	177	MET
1	A	196	GLU
1	A	201	THR
1	A	203	THR
1	A	215	THR
1	A	227	THR
1	A	249	ASN
1	A	253	ILE
1	A	254	GLN
1	A	279	VAL
1	C	307	VAL
1	C	308	LEU
1	C	313	PHE
1	C	316	HIS
1	C	337	LYS
1	C	419	LYS
1	C	485	PRO
1	C	501	THR
1	C	513	VAL
1	C	515	THR
1	C	526	ARG
1	C	579	VAL

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	87	ASN
1	A	216	HIS
1	A	224	GLN
1	A	230	GLN
1	A	249	ASN
1	C	312	ASN
1	C	375	ASN
1	C	387	ASN
1	C	422	ASN
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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLY	A	296	-	4,4,4	1.41	1 (25%)	3,4,4	1.20	0
2	GLY	C	596	-	4,4,4	1.34	1 (25%)	3,4,4	1.53	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLY	A	296	-	-	0/2/2/2	-
2	GLY	C	596	-	-	0/2/2/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	296	GLY	OXT-C	-2.68	1.21	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	596	GLY	OXT-C	-2.52	1.22	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	596	GLY	OXT-C-CA	2.03	121.44	113.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.