



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:45 AM UTC

PDB ID : 1AGX / pdb_00001agx
Title : REFINED CRYSTAL STRUCTURE OF ACINETOBACTER GLUTAMINASIFICANS GLUTAMINASE-ASPARAGINASE
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Deposited on : 1994-07-13
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

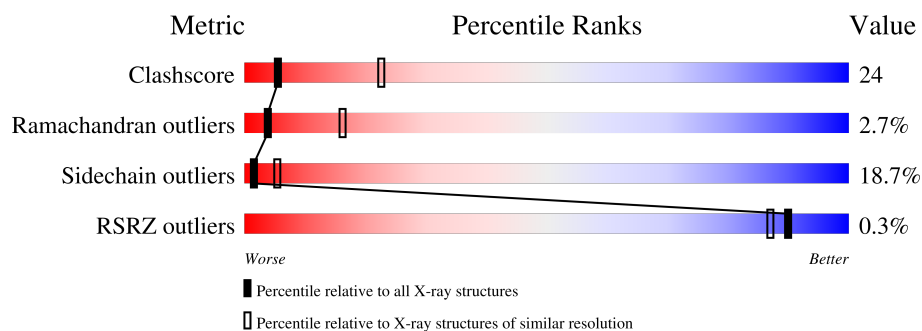
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	28% 45% 21% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2497 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.

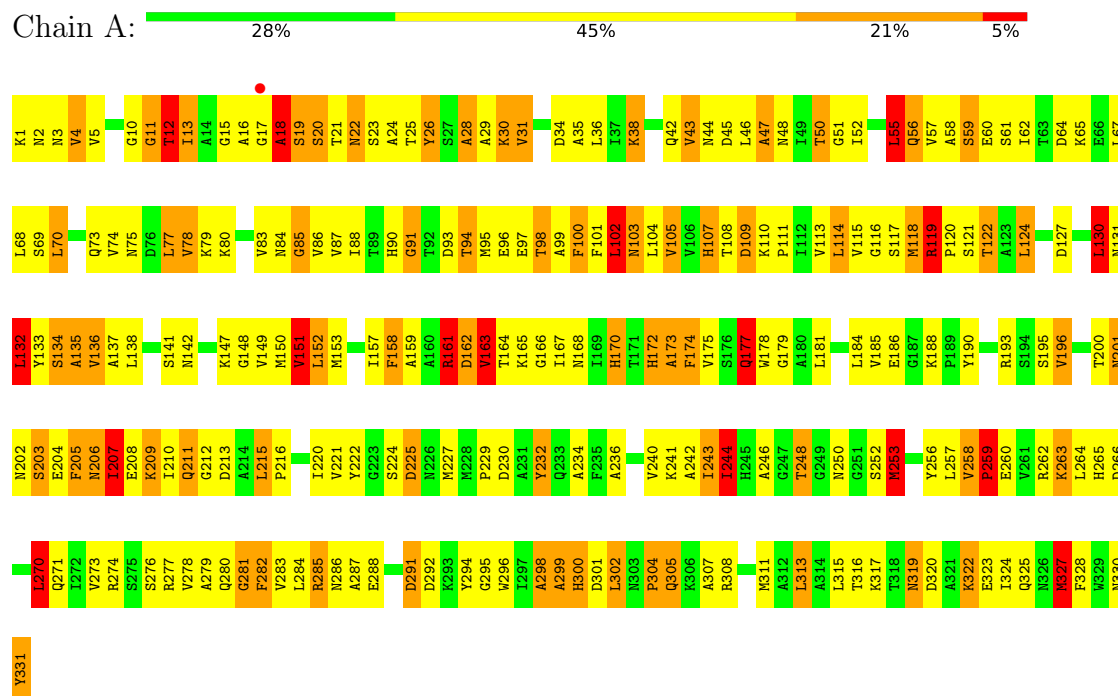
- Molecule 1 is a protein called GLUTAMINASE-ASPARAGINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	331	2497	1573	437	478	9	0	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: GLUTAMINASE-ASPARAGINASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	96.60Å 112.50Å 71.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 10.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.90) 82.0 (10.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROFFT, X-PLOR	Depositor
R, R_{free}	0.171 , (Not available) 0.160 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 53.0	EDS
L-test for twinning ¹	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2497	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.44	14/2541 (0.6%)	2.87	268/3451 (7.8%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	ILE	CA-CB	8.82	1.64	1.54
1	A	151	VAL	CA-C	6.47	1.60	1.52
1	A	195	SER	CA-C	-6.27	1.44	1.52
1	A	111	PRO	N-CA	-6.03	1.39	1.47
1	A	258	VAL	CA-CB	-5.90	1.51	1.54
1	A	225	ASP	N-CA	5.88	1.53	1.45
1	A	107	HIS	ND1-CE1	5.81	1.38	1.32
1	A	86	VAL	N-CA	5.68	1.52	1.46
1	A	114	LEU	CA-CB	-5.52	1.45	1.53
1	A	97	GLU	CA-CB	-5.47	1.44	1.53
1	A	225	ASP	C-N	-5.30	1.26	1.33
1	A	48	ASN	N-CA	5.17	1.52	1.46
1	A	56	GLN	CA-CB	-5.13	1.49	1.53
1	A	114	LEU	N-CA	5.02	1.52	1.46

All (268) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	LYS	N-CA-C	21.27	134.12	111.14
1	A	26	TYR	CA-CB-CG	19.11	148.29	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	ASP	O-C-N	13.72	136.67	122.12
1	A	102	LEU	CA-C-N	13.53	139.76	120.28
1	A	102	LEU	C-N-CA	13.53	139.76	120.28
1	A	64	ASP	CA-CB-CG	12.14	124.74	112.60
1	A	244	ILE	CB-CA-C	11.84	127.19	110.98
1	A	109	ASP	CA-CB-CG	11.69	124.29	112.60
1	A	87	VAL	CA-CB-CG1	11.39	129.76	110.40
1	A	286	ASN	CA-CB-CG	10.91	123.51	112.60
1	A	225	ASP	CB-CA-C	10.91	132.99	110.40
1	A	45	ASP	CA-CB-CG	10.69	123.29	112.60
1	A	244	ILE	CA-C-O	10.63	132.18	120.59
1	A	96	GLU	CA-C-N	10.61	134.24	120.44
1	A	96	GLU	C-N-CA	10.61	134.24	120.44
1	A	127	ASP	CA-CB-CG	10.47	123.08	112.60
1	A	56	GLN	N-CA-CB	10.37	128.73	110.79
1	A	225	ASP	CA-C-N	10.29	137.43	122.82
1	A	225	ASP	C-N-CA	10.29	137.43	122.82
1	A	291	ASP	CA-CB-CG	-10.25	102.35	112.60
1	A	56	GLN	OE1-CD-NE2	-10.14	112.46	122.60
1	A	277	ARG	NE-CZ-NH2	-9.85	110.34	119.20
1	A	172	HIS	CA-C-N	9.64	134.16	120.28
1	A	172	HIS	C-N-CA	9.64	134.16	120.28
1	A	22	ASN	CA-C-N	9.64	139.95	121.54
1	A	22	ASN	C-N-CA	9.64	139.95	121.54
1	A	302	LEU	CA-C-O	-9.38	109.95	120.54
1	A	308	ARG	N-CA-CB	9.36	123.88	109.94
1	A	161	ARG	CD-NE-CZ	9.29	137.41	124.40
1	A	307	ALA	CA-C-N	9.29	133.08	120.54
1	A	307	ALA	C-N-CA	9.29	133.08	120.54
1	A	56	GLN	CB-CG-CD	9.29	128.38	112.60
1	A	22	ASN	CA-CB-CG	9.18	121.78	112.60
1	A	323	GLU	CB-CG-CD	9.03	127.96	112.60
1	A	161	ARG	NH1-CZ-NH2	-9.00	107.61	119.30
1	A	157	ILE	CA-C-O	-8.98	110.32	120.74
1	A	202	ASN	CA-CB-CG	8.94	121.54	112.60
1	A	258	VAL	N-CA-CB	8.92	116.50	110.52
1	A	265	HIS	CA-C-N	8.88	131.99	120.44
1	A	265	HIS	C-N-CA	8.88	131.99	120.44
1	A	253	MET	O-C-N	8.85	133.74	123.29
1	A	174	PHE	O-C-N	8.80	133.50	122.93
1	A	330	ASN	OD1-CG-ND2	-8.76	113.84	122.60
1	A	136	VAL	CA-C-O	-8.72	112.20	121.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ASP	CA-CB-CG	8.63	121.23	112.60
1	A	168	ASN	N-CA-C	8.57	124.86	113.72
1	A	252	SER	N-CA-C	8.53	122.78	110.24
1	A	167	ILE	O-C-N	-8.38	114.23	123.03
1	A	93	ASP	O-C-N	8.34	130.76	122.09
1	A	320	ASP	CA-C-N	8.31	132.51	120.38
1	A	320	ASP	C-N-CA	8.31	132.51	120.38
1	A	47	ALA	CA-C-N	-8.31	111.72	122.77
1	A	47	ALA	C-N-CA	-8.31	111.72	122.77
1	A	330	ASN	N-CA-C	8.28	124.57	113.97
1	A	29	ALA	CA-C-N	8.23	131.64	120.44
1	A	29	ALA	C-N-CA	8.23	131.64	120.44
1	A	19	SER	N-CA-C	8.19	121.63	109.59
1	A	317	LYS	CA-CB-CG	8.16	130.42	114.10
1	A	188	LYS	N-CA-C	8.08	121.34	109.62
1	A	80	LYS	CA-C-O	8.08	126.95	119.76
1	A	114	LEU	N-CA-C	-8.07	96.07	109.07
1	A	131	ASN	CA-CB-CG	8.05	120.65	112.60
1	A	87	VAL	O-C-N	7.99	131.89	123.26
1	A	316	THR	N-CA-C	-7.93	103.75	113.50
1	A	270	LEU	CA-C-O	-7.92	112.48	121.19
1	A	87	VAL	CA-C-O	-7.85	112.15	120.39
1	A	173	ALA	CA-C-N	7.84	132.84	122.42
1	A	173	ALA	C-N-CA	7.84	132.84	122.42
1	A	190	TYR	CA-C-N	7.81	133.64	122.09
1	A	190	TYR	C-N-CA	7.81	133.64	122.09
1	A	292	ASP	CA-CB-CG	7.71	120.31	112.60
1	A	119	ARG	CD-NE-CZ	7.63	135.08	124.40
1	A	201	ASN	CA-CB-CG	7.60	120.20	112.60
1	A	30	LYS	CA-C-O	-7.51	112.96	120.70
1	A	4	VAL	CA-C-N	-7.50	113.89	123.19
1	A	4	VAL	C-N-CA	-7.50	113.89	123.19
1	A	220	ILE	N-CA-C	7.46	119.03	108.36
1	A	170	HIS	N-CA-CB	-7.42	99.48	110.17
1	A	93	ASP	N-CA-C	7.37	119.96	111.11
1	A	105	VAL	CA-CB-CG2	-7.37	97.87	110.40
1	A	196	VAL	CB-CA-C	7.37	122.26	112.46
1	A	311	MET	CA-C-O	-7.36	113.09	120.82
1	A	151	VAL	CA-CB-CG1	7.20	122.64	110.40
1	A	165	LYS	CA-CB-CG	-7.12	99.86	114.10
1	A	96	GLU	CA-CB-CG	7.09	128.29	114.10
1	A	165	LYS	CB-CA-C	7.08	122.20	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	THR	CA-C-O	7.01	128.90	121.33
1	A	45	ASP	N-CA-C	-7.00	104.55	113.23
1	A	151	VAL	CA-C-O	6.97	130.25	121.40
1	A	168	ASN	CB-CG-ND2	6.88	126.73	116.40
1	A	193	ARG	CB-CG-CD	6.88	127.13	111.30
1	A	279	ALA	N-CA-C	6.87	119.79	111.82
1	A	215	LEU	O-C-N	6.85	126.07	121.14
1	A	18	ALA	CA-C-N	6.84	131.09	121.24
1	A	18	ALA	C-N-CA	6.84	131.09	121.24
1	A	215	LEU	CA-C-O	-6.82	115.01	121.08
1	A	202	ASN	CA-C-N	6.82	132.63	121.86
1	A	202	ASN	C-N-CA	6.82	132.63	121.86
1	A	170	HIS	N-CA-C	6.81	120.10	110.50
1	A	274	ARG	NE-CZ-NH2	6.81	125.33	119.20
1	A	316	THR	N-CA-CB	6.80	120.53	110.53
1	A	325	GLN	CG-CD-NE2	6.80	126.60	116.40
1	A	130	LEU	N-CA-C	-6.79	103.90	111.71
1	A	225	ASP	O-C-N	-6.78	114.32	122.65
1	A	70	LEU	CA-C-N	6.70	129.56	120.38
1	A	70	LEU	C-N-CA	6.70	129.56	120.38
1	A	304	PRO	CB-CA-C	6.68	122.58	111.56
1	A	84	ASN	CA-CB-CG	6.66	119.26	112.60
1	A	205	PHE	O-C-N	6.65	130.38	122.79
1	A	68	LEU	CB-CA-C	6.61	122.86	110.63
1	A	99	ALA	N-CA-C	-6.60	104.16	111.36
1	A	323	GLU	N-CA-CB	6.59	120.49	110.28
1	A	177	GLN	N-CA-C	6.58	121.14	113.18
1	A	196	VAL	N-CA-CB	-6.57	103.62	112.22
1	A	236	ALA	CA-C-O	6.54	127.69	120.82
1	A	257	LEU	N-CA-CB	-6.54	100.92	110.47
1	A	278	VAL	CA-C-O	-6.51	112.81	120.75
1	A	243	ILE	CA-C-N	-6.50	114.58	122.90
1	A	243	ILE	C-N-CA	-6.50	114.58	122.90
1	A	291	ASP	CA-C-O	-6.50	113.61	120.63
1	A	281	GLY	N-CA-C	-6.47	101.06	112.77
1	A	225	ASP	N-CA-C	-6.46	102.19	110.53
1	A	307	ALA	CA-C-O	-6.45	113.71	120.55
1	A	162	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	178	TRP	O-C-N	6.45	130.04	122.24
1	A	85	GLY	CA-C-N	-6.43	114.18	123.06
1	A	85	GLY	C-N-CA	-6.43	114.18	123.06
1	A	283	VAL	CA-C-O	6.43	128.59	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	LYS	CA-C-N	6.42	127.87	119.84
1	A	110	LYS	C-N-CA	6.42	127.87	119.84
1	A	151	VAL	N-CA-C	-6.40	99.16	108.89
1	A	181	LEU	N-CA-C	-6.39	104.41	111.82
1	A	43	VAL	CB-CA-C	6.38	122.04	112.16
1	A	153	MET	CA-C-N	6.31	131.12	122.34
1	A	153	MET	C-N-CA	6.31	131.12	122.34
1	A	161	ARG	NE-CZ-NH1	6.30	127.80	121.50
1	A	316	THR	CA-C-O	6.30	126.07	119.14
1	A	87	VAL	CG1-CB-CG2	-6.30	96.95	110.80
1	A	174	PHE	N-CA-C	6.28	118.52	108.41
1	A	325	GLN	N-CA-C	-6.28	103.73	111.33
1	A	103	ASN	CA-C-O	6.27	127.19	120.10
1	A	175	VAL	CA-C-N	6.27	133.28	121.69
1	A	175	VAL	C-N-CA	6.27	133.28	121.69
1	A	277	ARG	NE-CZ-NH1	6.24	127.74	121.50
1	A	166	GLY	CA-C-O	-6.20	109.79	120.57
1	A	122	THR	N-CA-C	6.19	120.96	113.17
1	A	64	ASP	CA-C-O	-6.15	113.90	120.42
1	A	294	TYR	N-CA-C	6.11	120.73	113.28
1	A	147	LYS	N-CA-C	-6.10	105.88	113.38
1	A	163	VAL	O-C-N	-6.09	116.04	122.67
1	A	163	VAL	CA-C-O	6.04	127.92	121.04
1	A	65	LYS	CA-C-N	6.02	128.84	120.29
1	A	65	LYS	C-N-CA	6.02	128.84	120.29
1	A	149	VAL	CB-CA-C	6.02	120.65	111.68
1	A	213	ASP	N-CA-C	-6.00	104.81	113.21
1	A	151	VAL	CB-CA-C	6.00	120.61	110.95
1	A	207	ILE	N-CA-CB	6.00	120.91	110.65
1	A	93	ASP	CB-CG-OD1	5.98	132.15	118.40
1	A	288	GLU	CB-CG-CD	5.95	122.72	112.60
1	A	109	ASP	CA-C-N	5.95	128.94	120.49
1	A	109	ASP	C-N-CA	5.95	128.94	120.49
1	A	248	THR	CA-CB-CG2	5.95	120.61	110.50
1	A	114	LEU	CA-CB-CG	5.92	137.03	116.30
1	A	22	ASN	OD1-CG-ND2	-5.92	116.69	122.60
1	A	173	ALA	N-CA-CB	-5.91	101.11	110.22
1	A	168	ASN	CA-C-O	-5.90	112.56	119.05
1	A	135	ALA	N-CA-C	-5.88	104.95	111.36
1	A	193	ARG	CD-NE-CZ	5.86	132.61	124.40
1	A	114	LEU	O-C-N	5.83	130.17	123.29
1	A	161	ARG	N-CA-C	5.83	118.42	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	VAL	N-CA-CB	5.83	120.03	111.52
1	A	80	LYS	N-CA-C	5.82	116.98	109.65
1	A	206	ASN	N-CA-C	5.81	117.52	107.93
1	A	51	GLY	O-C-N	-5.79	119.70	123.35
1	A	151	VAL	CA-C-N	5.79	131.28	122.95
1	A	151	VAL	C-N-CA	5.79	131.28	122.95
1	A	288	GLU	CA-CB-CG	5.78	125.66	114.10
1	A	206	ASN	O-C-N	-5.75	116.13	123.26
1	A	250	ASN	CB-CA-C	5.74	118.27	111.22
1	A	213	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	220	ILE	N-CA-CB	-5.73	104.11	110.99
1	A	83	VAL	N-CA-C	-5.71	99.65	107.99
1	A	51	GLY	CA-C-O	5.71	125.72	120.81
1	A	90	HIS	N-CA-C	5.69	118.04	109.23
1	A	55	LEU	CA-CB-CG	5.66	136.10	116.30
1	A	282	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	35	ALA	CA-C-N	5.65	130.03	120.88
1	A	35	ALA	C-N-CA	5.65	130.03	120.88
1	A	331	TYR	N-CA-C	5.63	126.77	111.00
1	A	313	LEU	CA-C-N	5.63	127.76	120.44
1	A	313	LEU	C-N-CA	5.63	127.76	120.44
1	A	103	ASN	O-C-N	5.63	128.81	122.22
1	A	243	ILE	N-CA-CB	5.63	119.18	111.41
1	A	59	SER	N-CA-C	5.62	120.64	111.37
1	A	107	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	A	42	GLN	CA-C-O	5.59	126.25	119.31
1	A	230	ASP	CA-C-O	-5.59	114.95	120.82
1	A	102	LEU	O-C-N	-5.58	115.69	122.22
1	A	277	ARG	CG-CD-NE	5.57	124.26	112.00
1	A	244	ILE	CA-CB-CG2	5.54	119.91	110.50
1	A	107	HIS	CB-CG-ND1	5.52	130.98	122.70
1	A	31	VAL	N-CA-CB	-5.50	103.51	111.21
1	A	93	ASP	CA-C-O	-5.50	115.02	120.90
1	A	84	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	A	203	SER	CA-C-O	5.49	127.63	120.11
1	A	280	GLN	OE1-CD-NE2	5.49	128.09	122.60
1	A	298	ALA	N-CA-CB	5.48	118.93	110.21
1	A	59	SER	CA-C-N	5.46	128.14	120.28
1	A	59	SER	C-N-CA	5.46	128.14	120.28
1	A	12	THR	CA-C-N	5.46	127.54	120.88
1	A	12	THR	C-N-CA	5.46	127.54	120.88
1	A	110	LYS	CA-C-O	5.46	126.14	120.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	91	GLY	N-CA-C	-5.45	105.11	112.14
1	A	240	VAL	CA-C-O	5.44	129.07	121.51
1	A	107	HIS	CE1-NE2-CD2	5.43	114.43	109.00
1	A	107	HIS	ND1-CE1-NE2	-5.42	102.98	108.40
1	A	98	THR	CA-CB-OG1	-5.40	101.50	109.60
1	A	12	THR	N-CA-C	5.40	122.30	110.80
1	A	203	SER	N-CA-C	5.40	117.41	108.13
1	A	285	ARG	CA-C-N	5.37	131.79	121.54
1	A	285	ARG	C-N-CA	5.37	131.79	121.54
1	A	148	GLY	N-CA-C	-5.36	100.47	113.18
1	A	280	GLN	N-CA-C	5.36	118.45	110.14
1	A	165	LYS	CB-CG-CD	-5.36	98.97	111.30
1	A	322	LYS	CG-CD-CE	5.35	123.61	111.30
1	A	211	GLN	N-CA-C	5.34	120.81	113.97
1	A	59	SER	CA-CB-OG	-5.33	100.43	111.10
1	A	60	GLU	CA-CB-CG	5.33	124.77	114.10
1	A	205	PHE	CA-CB-CG	-5.33	108.47	113.80
1	A	300	HIS	CA-CB-CG	-5.33	108.47	113.80
1	A	60	GLU	CB-CG-CD	5.33	121.66	112.60
1	A	234	ALA	CA-C-N	5.32	127.41	120.28
1	A	234	ALA	C-N-CA	5.32	127.41	120.28
1	A	98	THR	CA-C-O	-5.29	114.95	120.55
1	A	61	SER	N-CA-C	5.28	119.36	113.02
1	A	232	TYR	CA-C-O	5.27	126.54	120.90
1	A	141	SER	N-CA-CB	5.26	117.71	109.97
1	A	325	GLN	OE1-CD-NE2	-5.25	117.34	122.60
1	A	300	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	A	124	LEU	N-CA-C	-5.24	102.64	110.23
1	A	88	ILE	CA-CB-CG1	-5.22	101.52	110.40
1	A	266	ASP	CA-C-O	5.22	126.31	120.82
1	A	47	ALA	N-CA-C	5.22	114.73	107.73
1	A	266	ASP	N-CA-C	5.21	116.65	111.07
1	A	179	GLY	CA-C-N	5.19	130.01	121.39
1	A	179	GLY	C-N-CA	5.19	130.01	121.39
1	A	256	TYR	N-CA-C	-5.19	106.45	112.89
1	A	195	SER	CA-C-O	-5.19	116.05	121.55
1	A	11	GLY	CA-C-N	5.18	131.44	121.54
1	A	11	GLY	C-N-CA	5.18	131.44	121.54
1	A	38	LYS	CG-CD-CE	5.18	123.21	111.30
1	A	319	ASN	CA-C-O	5.16	124.86	119.03
1	A	327	MET	CA-CB-CG	-5.14	103.82	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	LYS	CB-CA-C	-5.14	102.99	109.31
1	A	4	VAL	N-CA-CB	-5.13	102.66	110.86
1	A	259	PRO	CA-C-N	5.12	127.41	120.65
1	A	259	PRO	C-N-CA	5.12	127.41	120.65
1	A	158	PHE	CB-CG-CD1	-5.12	112.00	120.70
1	A	84	ASN	O-C-N	5.11	129.66	122.20
1	A	307	ALA	N-CA-C	-5.10	105.72	111.28
1	A	96	GLU	CA-C-O	-5.08	115.23	120.92
1	A	161	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	A	163	VAL	CA-CB-CG2	5.06	119.00	110.40
1	A	44	ASN	OD1-CG-ND2	5.05	127.65	122.60
1	A	132	LEU	O-C-N	5.05	127.27	122.07
1	A	174	PHE	CA-C-O	-5.03	115.19	120.58
1	A	38	LYS	CB-CG-CD	5.01	122.82	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	ARG	Sidechain
1	A	161	ARG	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	2497	0	2516	119	0
All	All	2497	0	2516	119	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 24.

All (119) 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:305:GLN:NE2	1:A:305:GLN:H	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLY:HA2	1:A:31:VAL:HG23	1.48	0.93
1:A:22:ASN:ND2	1:A:23:SER:H	1.72	0.87
1:A:305:GLN:H	1:A:305:GLN:HE21	1.18	0.87
1:A:16:ALA:HB2	1:A:121:SER:H	1.41	0.85
1:A:22:ASN:HD22	1:A:23:SER:H	1.24	0.85
1:A:242:ALA:HB2	1:A:271:GLN:HB2	1.64	0.79
1:A:101:PHE:O	1:A:105:VAL:HG22	1.85	0.77
1:A:244:ILE:HD11	1:A:304:PRO:HB3	1.66	0.76
1:A:159:ALA:O	1:A:163:VAL:HG12	1.87	0.74
1:A:264:LEU:O	1:A:270:LEU:HB2	1.93	0.69
1:A:59:SER:HB2	1:A:91:GLY:HA3	1.75	0.69
1:A:16:ALA:HB2	1:A:121:SER:N	2.07	0.68
1:A:78:VAL:HG21	1:A:108:THR:HG21	1.74	0.68
1:A:118:MET:HE3	1:A:173:ALA:HB3	1.75	0.67
1:A:222:TYR:HA	1:A:246:ALA:HB3	1.78	0.66
1:A:118:MET:CE	1:A:173:ALA:HB3	2.26	0.66
1:A:170:HIS:HB3	1:A:172:HIS:ND1	2.10	0.66
1:A:52:ILE:HD12	1:A:77:LEU:HD21	1.79	0.64
1:A:12:THR:HG22	1:A:120:PRO:HA	1.78	0.64
1:A:177:GLN:HE22	1:A:281:GLY:H	1.47	0.63
1:A:20:SER:HA	1:A:122:THR:O	1.98	0.63
1:A:170:HIS:HB3	1:A:172:HIS:CE1	2.34	0.62
1:A:4:VAL:HA	1:A:85:GLY:O	2.00	0.62
1:A:43:VAL:HG23	1:A:133:TYR:HA	1.82	0.62
1:A:243:ILE:HG12	1:A:270:LEU:HD12	1.84	0.60
1:A:10:GLY:HA2	1:A:56:GLN:NE2	2.17	0.60
1:A:59:SER:OG	1:A:94:THR:HB	2.02	0.60
1:A:2:ASN:O	1:A:47:ALA:HB1	2.01	0.59
1:A:273:VAL:CG1	1:A:299:ALA:HB2	2.33	0.59
1:A:253:MET:HG2	1:A:258:VAL:HG23	1.85	0.58
1:A:17:GLY:HA2	1:A:30:LYS:HD2	1.84	0.58
1:A:10:GLY:HA2	1:A:56:GLN:CD	2.28	0.58
1:A:16:ALA:CB	1:A:121:SER:OG	2.52	0.57
1:A:57:VAL:HG12	1:A:58:ALA:N	2.19	0.57
1:A:151:VAL:HG22	1:A:158:PHE:CD2	2.39	0.57
1:A:98:THR:HG22	1:A:102:LEU:HD22	1.87	0.57
1:A:95:MET:HE1	1:A:116:GLY:HA3	1.86	0.56
1:A:70:LEU:O	1:A:74:VAL:HG23	2.05	0.56
1:A:151:VAL:HG13	1:A:163:VAL:HG11	1.88	0.56
1:A:242:ALA:CB	1:A:271:GLN:HB2	2.36	0.56
1:A:282:PHE:HB3	1:A:301:ASP:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:O	1:A:136:VAL:HG23	2.06	0.56
1:A:327:MET:O	1:A:331:TYR:HD2	1.88	0.56
1:A:16:ALA:HB3	1:A:121:SER:OG	2.06	0.55
1:A:10:GLY:HA2	1:A:56:GLN:OE1	2.07	0.55
1:A:107:HIS:CE1	1:A:203:SER:O	2.60	0.55
1:A:206:ASN:C	1:A:206:ASN:HD22	2.14	0.55
1:A:17:GLY:CA	1:A:30:LYS:HD2	2.37	0.54
1:A:130:LEU:O	1:A:134:SER:HB2	2.08	0.53
1:A:100:PHE:O	1:A:103:ASN:HB3	2.10	0.52
1:A:221:VAL:HG11	1:A:232:TYR:CZ	2.46	0.51
1:A:13:ILE:HB	1:A:117:SER:HB2	1.92	0.51
1:A:18:ALA:HB3	1:A:25:THR:HB	1.92	0.51
1:A:107:HIS:HE1	1:A:203:SER:O	1.93	0.51
1:A:94:THR:O	1:A:94:THR:CG2	2.59	0.50
1:A:138:LEU:HD22	1:A:152:LEU:HD23	1.94	0.50
1:A:205:PHE:HA	1:A:209:LYS:HE3	1.93	0.50
1:A:107:HIS:HE1	1:A:205:PHE:O	1.93	0.49
1:A:305:GLN:HE21	1:A:305:GLN:N	1.99	0.49
1:A:109:ASP:HB3	1:A:201:ASN:HD21	1.77	0.49
1:A:13:ILE:HB	1:A:117:SER:CB	2.43	0.49
1:A:291:ASP:O	1:A:295:GLY:N	2.46	0.49
1:A:15:GLY:HA2	1:A:31:VAL:H	1.78	0.49
1:A:285:ARG:HA	1:A:298:ALA:HB2	1.94	0.48
1:A:13:ILE:C	1:A:15:GLY:H	2.21	0.48
1:A:241:LYS:HB3	1:A:315:LEU:HD13	1.95	0.48
1:A:258:VAL:HG22	1:A:296:TRP:HH2	1.78	0.48
1:A:203:SER:O	1:A:204:GLU:C	2.57	0.48
1:A:264:LEU:HA	1:A:264:LEU:HD12	1.63	0.48
1:A:57:VAL:HG12	1:A:58:ALA:O	2.13	0.47
1:A:215:LEU:HB3	1:A:216:PRO:HD2	1.95	0.47
1:A:118:MET:HB2	1:A:118:MET:HE2	1.53	0.46
1:A:151:VAL:O	1:A:158:PHE:N	2.26	0.46
1:A:105:VAL:HG22	1:A:105:VAL:H	1.44	0.46
1:A:18:ALA:HB3	1:A:25:THR:CB	2.46	0.46
1:A:75:ASN:O	1:A:79:LYS:HG3	2.16	0.46
1:A:15:GLY:CA	1:A:31:VAL:HG23	2.33	0.45
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.70	0.45
1:A:177:GLN:NE2	1:A:281:GLY:H	2.11	0.45
1:A:324:ILE:HG22	1:A:328:PHE:HE2	1.82	0.45
1:A:15:GLY:HA2	1:A:31:VAL:N	2.31	0.45
1:A:46:LEU:HD13	1:A:137:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ILE:HD12	1:A:207:ILE:N	2.32	0.45
1:A:55:LEU:HB3	1:A:57:VAL:HG23	1.99	0.45
1:A:324:ILE:HG22	1:A:328:PHE:CE2	2.51	0.45
1:A:16:ALA:HB2	1:A:121:SER:OG	2.17	0.45
1:A:282:PHE:HB2	1:A:300:HIS:C	2.42	0.45
1:A:161:ARG:HE	1:A:161:ARG:HB2	1.24	0.44
1:A:1:LYS:HD3	1:A:1:LYS:HA	1.76	0.44
1:A:5:VAL:HG13	1:A:50:THR:O	2.17	0.44
1:A:151:VAL:HG22	1:A:158:PHE:HD2	1.82	0.44
1:A:244:ILE:HD11	1:A:304:PRO:CB	2.44	0.44
1:A:207:ILE:HA	1:A:210:ILE:HD12	2.00	0.43
1:A:12:THR:HA	1:A:15:GLY:O	2.18	0.43
1:A:13:ILE:HG13	1:A:36:LEU:HD11	1.99	0.43
1:A:101:PHE:CE1	1:A:313:LEU:HD21	2.53	0.43
1:A:28:ALA:C	1:A:30:LYS:H	2.25	0.43
1:A:107:HIS:CE1	1:A:205:PHE:O	2.71	0.43
1:A:13:ILE:HD12	1:A:13:ILE:O	2.19	0.43
1:A:77:LEU:HD12	1:A:77:LEU:HA	1.88	0.43
1:A:104:LEU:HD23	1:A:313:LEU:CD1	2.49	0.43
1:A:69:SER:O	1:A:73:GLN:HG3	2.19	0.42
1:A:224:SER:O	1:A:227:MET:HG3	2.19	0.42
1:A:163:VAL:CG2	1:A:174:PHE:HD2	2.32	0.42
1:A:57:VAL:CG1	1:A:58:ALA:N	2.82	0.42
1:A:101:PHE:CE1	1:A:313:LEU:HD11	2.55	0.42
1:A:229:PRO:HB3	1:A:260:GLU:HG2	2.02	0.41
1:A:120:PRO:C	1:A:122:THR:N	2.77	0.41
1:A:113:VAL:HA	1:A:150:MET:O	2.21	0.41
1:A:46:LEU:HD23	1:A:46:LEU:HA	1.89	0.41
1:A:150:MET:HE3	1:A:150:MET:HB2	1.89	0.41
1:A:79:LYS:CE	1:A:208:GLU:OE2	2.69	0.41
1:A:118:MET:HE3	1:A:173:ALA:CB	2.47	0.41
1:A:258:VAL:HG13	1:A:262:ARG:HG3	2.02	0.41
1:A:120:PRO:O	1:A:121:SER:C	2.60	0.40
1:A:170:HIS:CB	1:A:172:HIS:CE1	3.04	0.40
1:A:115:VAL:HG21	1:A:135:ALA:HB2	2.04	0.40
1:A:259:PRO:O	1:A:263:LYS:NZ	2.42	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	329/331 (99%)	289 (88%)	31 (9%)	9 (3%)	4	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	18	ALA
1	A	200	THR
1	A	212	GLY
1	A	287	ALA
1	A	11	GLY
1	A	28	ALA
1	A	24	ALA
1	A	299	ALA

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	267/267 (100%)	217 (81%)	50 (19%)	1	5

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	12	THR

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Mol	Chain	Res	Type
1	A	13	ILE
1	A	19	SER
1	A	20	SER
1	A	21	THR
1	A	26	TYR
1	A	34	ASP
1	A	38	LYS
1	A	50	THR
1	A	55	LEU
1	A	62	ILE
1	A	77	LEU
1	A	78	VAL
1	A	94	THR
1	A	102	LEU
1	A	114	LEU
1	A	118	MET
1	A	119	ARG
1	A	124	LEU
1	A	130	LEU
1	A	132	LEU
1	A	134	SER
1	A	142	ASN
1	A	151	VAL
1	A	152	LEU
1	A	161	ARG
1	A	162	ASP
1	A	163	VAL
1	A	177	GLN
1	A	184	LEU
1	A	186	GLU
1	A	196	VAL
1	A	207	ILE
1	A	209	LYS
1	A	211	GLN
1	A	225	ASP
1	A	244	ILE
1	A	248	THR
1	A	253	MET
1	A	259	PRO
1	A	263	LYS
1	A	270	LEU
1	A	276	SER

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Mol	Chain	Res	Type
1	A	284	LEU
1	A	302	LEU
1	A	305	GLN
1	A	319	ASN
1	A	322	LYS
1	A	327	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	56	GLN
1	A	75	ASN
1	A	103	ASN
1	A	107	HIS
1	A	154	ASN
1	A	170	HIS
1	A	177	GLN
1	A	201	ASN
1	A	206	ASN
1	A	219	GLN
1	A	233	GLN
1	A	250	ASN
1	A	271	GLN
1	A	305	GLN
1	A	319	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	331/331 (100%)	-0.73	1 (0%) 90 87	2, 6, 24, 46	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	GLY	2.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.