



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:49 AM EDT

PDB ID : 2V36 / pdb_00002v36
Title : Crystal structure of gamma-glutamyl transferase from Bacillus subtilis
Authors : Sharath, B.; Prabhune, A.A.; Suresh, C.G.; Wilkinson, A.J.; Brannigan, J.A.
Deposited on : 2007-06-13
Resolution : 1.85 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

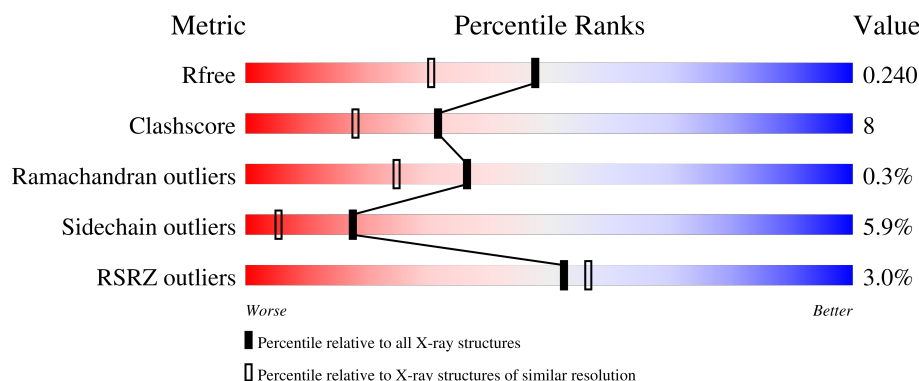
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	376	5% 71% 19% 5% 5%
1	C	376	2% 74% 16% • 5%
2	B	193	% 72% 13% 5% • 9%
2	D	193	% 70% 19% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8372 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 GAMMA-GLUTAMYLTRANSPEPTIDASE LARGE CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2693	1719	445	519	10			
1	C	357	Total	C	N	O	S	0	0	0
			2670	1702	440	518	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	PRO	LEU	conflict	UNP P54422
C	302	PRO	LEU	conflict	UNP P54422

- Molecule 2 is a protein called GAMMA-GLUTAMYLTRANSPEPTIDASE SMALL CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1297	822	213	258	4			
2	D	183	Total	C	N	O	S	0	0	0
			1363	862	228	268	5			

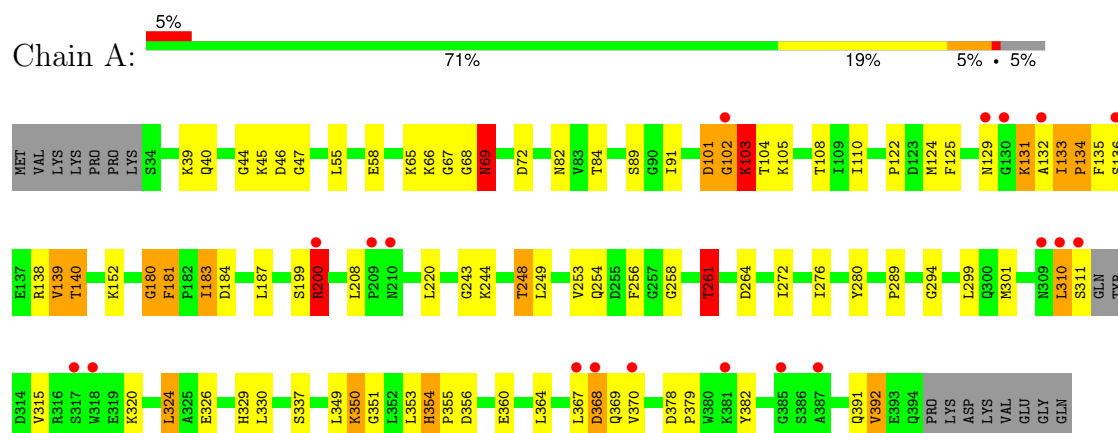
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total	O	0	0
			130	130		
3	B	55	Total	O	0	0
			55	55		
3	C	113	Total	O	0	0
			113	113		
3	D	51	Total	O	0	0
			51	51		

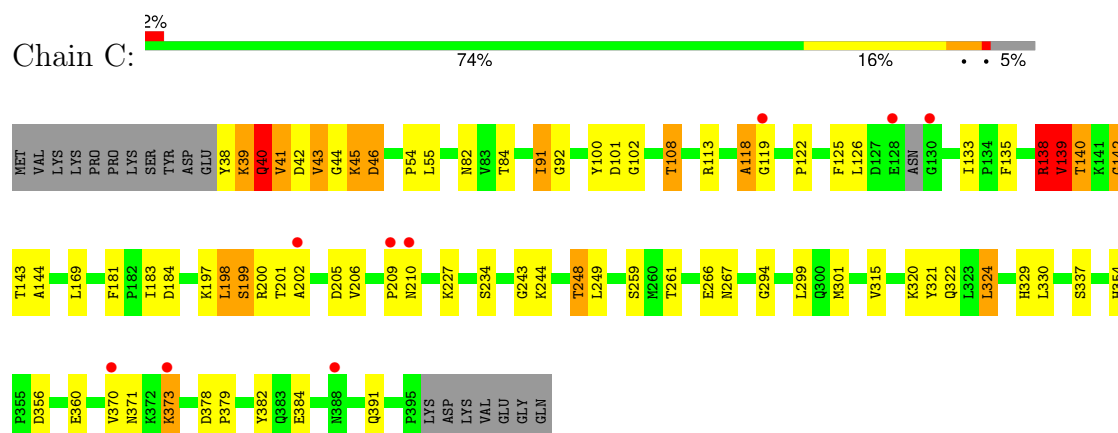
3 Residue-property plots [i](#)

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 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.

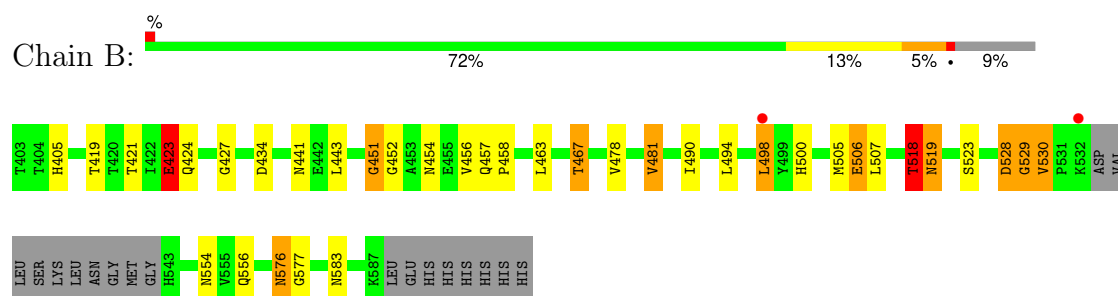
• Molecule 1: GAMMA-GLUTAMYLTRANSPEPTIDASE LARGE CHAIN



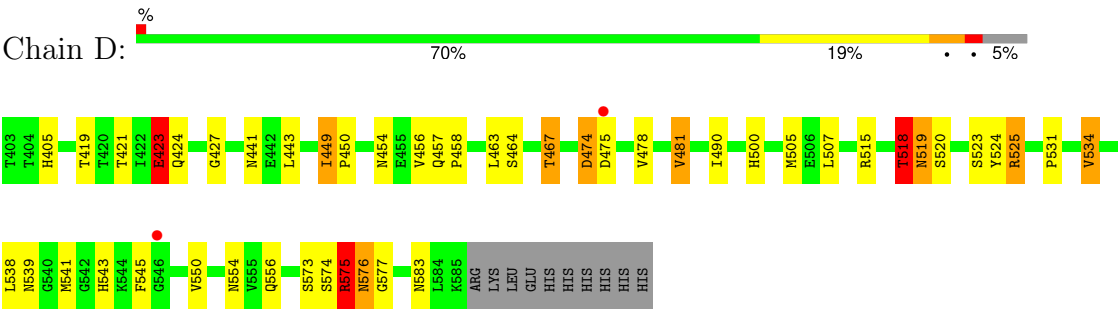
• Molecule 1: GAMMA-GLUTAMYLTRANSPEPTIDASE LARGE CHAIN



• Molecule 2: GAMMA-GLUTAMYLTRANSPEPTIDASE SMALL CHAIN



● Molecule 2: GAMMA-GLUTAMYLTRANSPEPTIDASE SMALL CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.26Å 108.77Å 161.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.17 – 1.85 90.17 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.6 (90.17-1.85) 97.9 (90.17-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.249 0.210 , 0.240	Depositor DCC
R_{free} test set	5358 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8372	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	1.17	12/2750 (0.4%)	1.47	35/3729 (0.9%)
1	C	1.16	11/2727 (0.4%)	1.45	36/3699 (1.0%)
2	B	1.05	1/1324 (0.1%)	1.17	16/1805 (0.9%)
2	D	1.10	2/1391 (0.1%)	1.19	16/1895 (0.8%)
All	All	1.14	26/8192 (0.3%)	1.37	103/11128 (0.9%)

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	20
1	C	0	18
2	B	0	4
2	D	0	3
All	All	0	45

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	197	LYS	C-N	16.65	1.56	1.33
1	C	373	LYS	C-O	-13.37	1.08	1.23
1	A	134	PRO	C-N	11.38	1.48	1.33
1	A	105	LYS	C-N	10.98	1.48	1.33
1	A	256	PHE	C-N	-10.29	1.18	1.33
1	C	143	THR	C-N	8.97	1.47	1.33
1	A	355	PRO	C-N	-8.80	1.21	1.34
1	C	384	GLU	C-N	7.67	1.48	1.33
1	A	261	THR	CB-CG2	-7.53	1.27	1.52
1	C	142	GLY	C-N	-7.48	1.23	1.33
1	A	253	VAL	C-N	7.12	1.42	1.33
1	A	103	LYS	CA-C	6.55	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	199	SER	C-N	6.13	1.43	1.33
1	C	144	ALA	C-N	-6.05	1.26	1.33
1	A	354	HIS	C-N	-5.73	1.26	1.34
1	C	261	THR	CB-CG2	-5.53	1.34	1.52
1	A	133	ILE	C-N	-5.36	1.21	1.33
2	D	467	THR	CA-CB	5.28	1.59	1.53
2	B	467	THR	CA-CB	5.24	1.59	1.53
1	A	248	THR	CA-CB	5.20	1.61	1.53
1	A	132	ALA	C-N	5.11	1.39	1.33
1	A	326	GLU	C-N	-5.11	1.27	1.33
1	C	248	THR	CA-CB	5.10	1.61	1.53
2	D	515	ARG	CZ-NH1	-5.09	1.25	1.32
1	C	41	VAL	CA-CB	5.08	1.63	1.55
1	C	138	ARG	CZ-NH2	-5.07	1.26	1.33

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	VAL	N-CA-C	-21.88	94.33	111.62
1	A	132	ALA	N-CA-C	-20.61	75.95	109.76
1	A	103	LYS	N-CA-C	-19.55	86.92	112.93
1	A	350	LYS	N-CA-C	-17.52	91.50	111.82
1	A	102	GLY	N-CA-C	-17.05	93.52	114.66
1	A	140	THR	N-CA-C	-16.75	93.65	114.75
1	C	373	LYS	CA-C-O	-14.38	106.62	121.29
1	C	267	ASN	N-CA-C	-14.26	95.96	113.50
1	C	200	ARG	N-CA-C	-14.16	93.11	114.64
1	C	40	GLN	N-CA-C	13.86	128.52	112.72
1	C	199	SER	N-CA-C	-13.49	96.83	113.28
1	A	104	THR	N-CA-C	-13.48	97.30	113.88
1	C	140	THR	N-CA-C	-13.06	94.78	114.64
1	C	244	LYS	N-CA-C	-12.75	96.20	112.90
1	A	244	LYS	N-CA-C	-12.68	96.29	112.90
2	D	577	GLY	N-CA-C	-12.64	92.92	112.89
1	A	40	GLN	N-CA-C	12.16	128.24	113.16
2	B	577	GLY	N-CA-C	-11.42	94.85	112.89
1	C	373	LYS	O-C-N	11.39	130.77	121.20
1	A	200	ARG	N-CA-C	-11.27	98.46	114.12
1	A	66	LYS	N-CA-C	-10.92	98.79	112.88
1	C	139	VAL	N-CA-C	-10.78	98.30	113.07
2	D	518	THR	CB-CA-C	-10.67	95.40	110.34
1	A	69	ASN	N-CA-C	10.66	125.06	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	371	ASN	O-C-N	10.13	135.98	122.82
1	C	198	LEU	O-C-N	-10.09	109.01	122.43
1	C	206	VAL	N-CA-CB	9.89	119.75	111.64
1	C	142	GLY	N-CA-C	9.52	125.14	114.67
1	C	101	ASP	N-CA-C	-9.34	91.46	107.99
1	C	197	LYS	N-CA-C	9.31	121.51	111.36
1	C	43	VAL	N-CA-C	9.04	123.21	109.20
1	A	379	PRO	N-CA-C	-8.93	102.22	114.27
1	C	102	GLY	N-CA-C	8.92	124.96	114.16
1	A	351	GLY	N-CA-C	-8.78	92.37	113.18
1	A	104	THR	N-CA-CB	8.65	122.09	110.59
1	A	369	GLN	N-CA-C	8.57	121.35	109.18
2	D	575	ARG	NE-CZ-NH2	-8.39	111.65	119.20
1	C	46	ASP	N-CA-C	-8.26	102.08	114.64
1	C	199	SER	CA-C-N	8.20	136.41	121.41
1	C	199	SER	C-N-CA	8.20	136.41	121.41
2	D	449	ILE	N-CA-C	8.07	116.93	107.73
1	A	129	ASN	N-CA-C	7.98	119.67	110.97
2	D	575	ARG	NE-CZ-NH1	7.93	129.43	121.50
1	A	136	SER	N-CA-C	-7.82	103.54	113.23
2	B	451	GLY	N-CA-C	7.80	131.68	113.18
1	C	92	GLY	N-CA-C	7.80	131.66	113.18
2	B	451	GLY	CA-C-N	7.77	136.65	121.41
2	B	451	GLY	C-N-CA	7.77	136.65	121.41
2	B	518	THR	CB-CA-C	-7.75	96.63	109.80
1	C	197	LYS	O-C-N	7.64	130.86	122.15
1	A	354	HIS	CA-C-N	7.50	127.38	119.05
1	A	354	HIS	C-N-CA	7.50	127.38	119.05
1	C	118	ALA	N-CA-C	7.48	119.51	111.36
2	B	481	VAL	CG1-CB-CG2	-7.13	95.12	110.80
1	A	104	THR	CA-C-N	7.02	134.07	123.05
1	A	104	THR	C-N-CA	7.02	134.07	123.05
2	D	575	ARG	CD-NE-CZ	6.85	133.99	124.40
1	A	261	THR	N-CA-CB	-6.81	100.17	111.20
1	C	144	ALA	CA-C-N	-6.76	112.33	121.80
1	C	144	ALA	C-N-CA	-6.76	112.33	121.80
2	D	507	LEU	CD1-CG-CD2	-6.70	96.05	110.80
2	B	576	ASN	N-CA-C	6.61	122.19	113.20
1	C	378	ASP	CA-C-N	6.61	127.13	119.47
1	C	378	ASP	C-N-CA	6.61	127.13	119.47
2	D	576	ASN	N-CA-C	6.56	122.12	113.20
2	D	481	VAL	CG1-CB-CG2	-6.53	96.43	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	421	THR	N-CA-C	6.52	118.76	108.79
1	A	139	VAL	CG1-CB-CG2	-6.39	96.75	110.80
1	A	67	GLY	CA-C-N	6.36	126.14	120.10
1	A	67	GLY	C-N-CA	6.36	126.14	120.10
1	A	378	ASP	N-CA-C	6.35	120.91	108.21
1	C	379	PRO	N-CA-C	6.29	122.94	113.81
2	D	478	VAL	CG1-CB-CG2	-6.21	97.14	110.80
2	B	530	VAL	CB-CA-C	6.20	117.81	110.68
2	D	450	PRO	N-CA-C	-6.18	101.92	111.13
1	A	200	ARG	N-CA-CB	6.11	119.31	110.88
1	C	118	ALA	O-C-N	-6.09	115.20	122.15
2	D	575	ARG	CB-CG-CD	6.04	125.19	111.30
2	B	507	LEU	CD1-CG-CD2	-5.94	97.74	110.80
1	C	39	LYS	N-CA-C	-5.88	100.08	109.96
2	B	528	ASP	CA-C-N	5.87	132.26	121.70
2	B	528	ASP	C-N-CA	5.87	132.26	121.70
1	A	140	THR	CB-CA-C	5.86	116.71	109.16
2	D	474	ASP	N-CA-C	5.79	123.12	110.80
1	A	108	THR	OG1-CB-CG2	-5.64	98.01	109.30
1	C	118	ALA	CA-C-N	5.61	132.41	121.41
1	C	118	ALA	C-N-CA	5.61	132.41	121.41
2	B	528	ASP	O-C-N	-5.52	116.15	122.89
2	B	451	GLY	O-C-N	-5.50	115.55	122.70
1	A	392	VAL	N-CA-C	5.50	116.04	108.12
1	A	58	GLU	CB-CA-C	-5.44	102.34	110.88
1	A	47	GLY	N-CA-C	5.36	125.88	113.18
1	C	43	VAL	N-CA-CB	-5.33	102.61	112.43
1	C	199	SER	O-C-N	-5.32	114.85	122.41
1	A	181	PHE	N-CA-CB	-5.32	100.91	110.37
2	D	449	ILE	CA-C-N	5.22	125.68	120.52
2	D	449	ILE	C-N-CA	5.22	125.68	120.52
2	B	421	THR	N-CA-C	5.21	116.76	108.79
1	A	310	LEU	N-CA-C	5.16	121.80	110.80
1	A	124	MET	N-CA-C	5.14	118.65	112.38
2	B	478	VAL	CG1-CB-CG2	-5.11	99.57	110.80
1	C	40	GLN	N-CA-CB	-5.05	103.17	110.70
2	B	506	GLU	CA-CB-CG	5.01	124.12	114.10

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ASP	Peptide
1	A	102	GLY	Peptide
1	A	103	LYS	Peptide
1	A	131	LYS	Peptide
1	A	135	PHE	Peptide
1	A	139	VAL	Peptide
1	A	180	GLY	Peptide
1	A	199	SER	Peptide
1	A	208	LEU	Peptide
1	A	243	GLY	Peptide
1	A	310	LEU	Peptide
1	A	349	LEU	Peptide
1	A	350	LYS	Peptide
1	A	353	LEU	Mainchain
1	A	368	ASP	Peptide
1	A	39	LYS	Peptide
1	A	46	ASP	Peptide
1	A	65	LYS	Peptide
1	A	68	GLY	Peptide
1	A	89	SER	Peptide
2	B	451	GLY	Peptide
2	B	528	ASP	Peptide
2	B	529	GLY	Peptide
2	B	576	ASN	Peptide
1	C	100	TYR	Peptide
1	C	118	ALA	Peptide
1	C	138	ARG	Peptide
1	C	139	VAL	Peptide
1	C	142	GLY	Mainchain
1	C	198	LEU	Mainchain,Peptide
1	C	199	SER	Peptide
1	C	201	THR	Peptide
1	C	205	ASP	Peptide
1	C	243	GLY	Peptide
1	C	266	GLU	Peptide
1	C	373	LYS	Mainchain
1	C	39	LYS	Peptide
1	C	40	GLN	Peptide
1	C	42	ASP	Peptide
1	C	45	LYS	Peptide
1	C	91	ILE	Peptide
2	D	449	ILE	Peptide
2	D	474	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	D	576	ASN	Peptide

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	2693	0	2615	39	0
1	C	2670	0	2577	39	0
2	B	1297	0	1243	29	0
2	D	1363	0	1327	47	0
3	A	130	0	0	2	0
3	B	55	0	0	4	0
3	C	113	0	0	5	0
3	D	51	0	0	1	0
All	All	8372	0	7762	128	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 (128) 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)
2:D:525:ARG:NH1	2:D:550:VAL:HG11	1.53	1.21
2:D:525:ARG:HH12	2:D:550:VAL:HG11	1.19	0.95
1:C:337:SER:OG	1:C:391:GLN:NE2	2.12	0.83
2:D:525:ARG:NH1	2:D:550:VAL:CG1	2.41	0.82
1:A:329:HIS:HE1	2:B:518:THR:CG2	1.93	0.81
2:B:452:GLY:HA3	3:B:2020:HOH:O	1.79	0.81
1:C:329:HIS:HE1	2:D:518:THR:CG2	1.98	0.77
1:C:45:LYS:HG2	2:D:583:ASN:HD22	1.50	0.76
2:D:424:GLN:H	2:D:441:ASN:HD21	1.33	0.76
1:C:329:HIS:HD2	3:C:2107:HOH:O	1.67	0.76
1:C:209:PRO:CA	1:C:210:ASN:N	2.50	0.75
1:A:360:GLU:OE2	1:A:382:TYR:OH	2.04	0.75
2:B:529:GLY:HA2	3:B:2041:HOH:O	1.87	0.74
2:D:525:ARG:HH12	2:D:550:VAL:CG1	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:HIS:HE1	2:B:518:THR:HG21	1.51	0.74
2:B:424:GLN:H	2:B:441:ASN:HD21	1.36	0.73
2:D:531:PRO:HB2	2:D:534:VAL:HG13	1.70	0.72
1:C:322:GLN:OE1	2:D:543:HIS:HE1	1.72	0.72
2:D:539:ASN:HD21	2:D:545:PHE:H	1.37	0.72
2:D:525:ARG:HH11	2:D:550:VAL:HG11	1.55	0.71
1:A:125:PHE:HB3	1:A:138:ARG:HD2	1.71	0.71
2:B:434:ASP:CB	3:B:2012:HOH:O	2.38	0.71
1:A:329:HIS:HD2	3:A:2110:HOH:O	1.73	0.70
1:C:329:HIS:HE1	2:D:518:THR:HG21	1.56	0.70
1:C:354:HIS:HD2	1:C:356:ASP:H	1.38	0.69
2:D:405:HIS:HD2	2:D:419:THR:OG1	1.76	0.68
1:A:152:LYS:NZ	3:A:2034:HOH:O	2.03	0.68
2:B:519:ASN:HD22	2:B:519:ASN:H	1.42	0.67
1:A:301:MET:HE2	2:B:490:ILE:HD12	1.78	0.65
1:C:301:MET:HE2	2:D:490:ILE:HD12	1.77	0.65
1:C:125:PHE:HB3	1:C:138:ARG:HD2	1.80	0.64
1:A:329:HIS:CE1	2:B:518:THR:HG21	2.32	0.64
1:A:44:GLY:HA2	2:B:583:ASN:HD21	1.61	0.64
2:D:538:LEU:HA	2:D:541:MET:HE3	1.80	0.64
1:C:354:HIS:CD2	1:C:356:ASP:H	2.17	0.62
2:D:519:ASN:H	2:D:519:ASN:HD22	1.47	0.62
1:A:69:ASN:C	1:A:69:ASN:HD22	2.07	0.61
1:C:108:THR:CG2	3:C:2016:HOH:O	2.48	0.61
2:B:405:HIS:HE1	3:B:2049:HOH:O	1.83	0.61
1:C:108:THR:HG22	3:C:2016:HOH:O	2.01	0.60
1:A:261:THR:HG22	1:A:264:ASP:H	1.65	0.60
1:C:84:THR:HA	1:C:181:PHE:CZ	2.37	0.60
1:C:315:VAL:O	1:C:320:LYS:HE3	2.01	0.59
1:A:82:ASN:ND2	1:A:91:ILE:H	2.01	0.59
2:B:405:HIS:HD2	2:B:419:THR:OG1	1.85	0.59
2:D:554:ASN:CG	2:D:575:ARG:HG3	2.28	0.58
2:B:427:GLY:HA2	2:B:441:ASN:HD22	1.70	0.57
1:C:40:GLN:HE22	2:D:573:SER:HA	1.68	0.57
2:D:518:THR:HG23	2:D:523:SER:O	2.05	0.57
2:D:519:ASN:ND2	2:D:523:SER:HB3	2.19	0.57
2:B:500:HIS:HD2	2:B:505:MET:O	1.88	0.56
1:C:329:HIS:CE1	2:D:518:THR:HG21	2.39	0.56
1:A:44:GLY:HA2	2:B:583:ASN:ND2	2.22	0.55
2:D:524:TYR:OH	2:D:543:HIS:HD2	1.89	0.55
1:A:84:THR:HA	1:A:181:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:500:HIS:HD2	2:D:505:MET:O	1.90	0.54
2:D:405:HIS:CD2	2:D:419:THR:OG1	2.61	0.54
1:A:329:HIS:CE1	2:B:518:THR:CG2	2.84	0.54
2:D:454:ASN:HD21	2:D:463:LEU:H	1.56	0.53
2:D:518:THR:CG2	2:D:523:SER:O	2.56	0.53
1:A:122:PRO:HA	2:B:456:VAL:HB	1.90	0.53
1:C:44:GLY:HA2	2:D:583:ASN:HD21	1.72	0.53
1:C:320:LYS:HD3	1:C:324:LEU:HD22	1.90	0.53
2:B:554:ASN:ND2	2:B:556:GLN:HE22	2.07	0.52
1:C:82:ASN:ND2	1:C:91:ILE:H	2.08	0.52
2:B:457:GLN:HE21	2:B:458:PRO:HD2	1.74	0.52
1:A:354:HIS:HD2	1:A:356:ASP:H	1.57	0.51
1:A:249:LEU:C	1:A:249:LEU:HD23	2.36	0.51
1:C:294:GLY:HA3	2:D:467:THR:OG1	2.11	0.51
1:A:294:GLY:HA3	2:B:467:THR:OG1	2.12	0.50
1:A:315:VAL:O	1:A:320:LYS:HE3	2.12	0.50
1:A:45:LYS:HG2	2:B:583:ASN:HD22	1.76	0.50
2:B:494:LEU:HG	2:B:498:LEU:HD22	1.93	0.50
2:D:554:ASN:ND2	2:D:556:GLN:HE22	2.11	0.49
1:A:337:SER:CB	1:A:391:GLN:HE22	2.26	0.49
1:C:133:ILE:O	1:C:138:ARG:HD3	2.13	0.49
1:C:360:GLU:OE2	1:C:382:TYR:OH	2.20	0.48
2:D:427:GLY:HA2	2:D:441:ASN:HD22	1.78	0.48
2:B:454:ASN:HD21	2:B:463:LEU:H	1.62	0.48
1:A:69:ASN:ND2	1:A:72:ASP:H	2.11	0.48
1:C:135:PHE:O	1:C:139:VAL:HG13	2.14	0.48
1:A:280:TYR:OH	2:B:498:LEU:HD12	2.14	0.47
2:B:423:GLU:HB3	2:B:441:ASN:ND2	2.30	0.47
1:A:200:ARG:CB	1:A:200:ARG:HH11	2.28	0.46
1:A:200:ARG:HH11	1:A:200:ARG:HB3	1.81	0.46
1:A:354:HIS:CD2	1:A:356:ASP:H	2.33	0.46
2:B:518:THR:CG2	2:B:523:SER:O	2.64	0.46
1:C:45:LYS:H	2:D:583:ASN:ND2	2.13	0.45
2:D:423:GLU:HB3	2:D:441:ASN:ND2	2.32	0.45
1:A:82:ASN:HD21	1:A:91:ILE:H	1.62	0.45
1:C:45:LYS:HG3	1:C:46:ASP:OD2	2.16	0.45
1:C:113:ARG:CZ	2:D:464:SER:HB2	2.47	0.45
2:D:539:ASN:HD21	2:D:545:PHE:N	2.09	0.45
2:D:405:HIS:HE1	3:D:2048:HOH:O	1.99	0.45
1:A:276:ILE:HG23	1:A:289:PRO:HB3	2.00	0.44
2:B:405:HIS:CD2	2:B:419:THR:OG1	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:LEU:C	1:C:249:LEU:HD23	2.42	0.44
1:C:321:TYR:CD2	2:D:534:VAL:HG21	2.53	0.44
2:D:519:ASN:HD21	2:D:523:SER:HB3	1.83	0.44
1:A:329:HIS:CE1	2:B:518:THR:HB	2.53	0.44
1:C:119:GLY:CA	1:C:259:SER:OG	2.66	0.44
2:B:518:THR:HG23	2:B:523:SER:O	2.18	0.44
2:D:457:GLN:HE21	2:D:458:PRO:HD2	1.82	0.44
1:A:133:ILE:O	1:A:134:PRO:C	2.61	0.43
2:D:454:ASN:ND2	2:D:463:LEU:H	2.16	0.43
1:C:82:ASN:HD21	1:C:91:ILE:HG12	1.82	0.43
1:A:320:LYS:HD3	1:A:324:LEU:HD22	2.01	0.43
1:C:82:ASN:HD21	1:C:91:ILE:H	1.66	0.43
1:A:133:ILE:O	1:A:138:ARG:HD3	2.19	0.43
1:C:43:VAL:HG12	1:C:44:GLY:N	2.33	0.42
1:C:329:HIS:CD2	3:C:2107:HOH:O	2.55	0.42
2:D:554:ASN:OD1	2:D:575:ARG:HG3	2.18	0.42
1:C:329:HIS:CE1	2:D:518:THR:CG2	2.89	0.42
2:D:518:THR:HG22	2:D:520:SER:O	2.19	0.42
2:D:519:ASN:HD22	2:D:519:ASN:N	2.12	0.42
2:D:574:SER:C	2:D:575:ARG:HG2	2.45	0.42
1:A:254:GLN:HA	1:A:258:GLY:O	2.20	0.41
1:C:122:PRO:HA	2:D:456:VAL:HB	2.02	0.41
1:C:227:LYS:HE2	1:C:227:LYS:HB3	1.83	0.41
1:A:183:ILE:HB	1:A:187:LEU:HD23	2.01	0.41
1:C:38:TYR:CD1	1:C:54:PRO:HB3	2.56	0.41
1:A:110:ILE:HD12	1:A:272:ILE:CD1	2.51	0.41
1:A:181:PHE:N	1:A:181:PHE:CD2	2.89	0.40
1:C:354:HIS:HD2	1:C:356:ASP:N	2.12	0.40
3:C:2080:HOH:O	2:D:475:ASP:HA	2.22	0.40
1:A:101:ASP:C	1:A:103:LYS:H	2.28	0.40
1:A:180:GLY:HA2	1:A:220:LEU:O	2.21	0.40
2:D:518:THR:HG21	2:D:524:TYR:CZ	2.56	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	355/376 (94%)	342 (96%)	13 (4%)	0	100	100
1	C	351/376 (93%)	338 (96%)	12 (3%)	1 (0%)	36	25
2	B	171/193 (89%)	162 (95%)	8 (5%)	1 (1%)	21	10
2	D	181/193 (94%)	175 (97%)	5 (3%)	1 (1%)	21	10
All	All	1058/1138 (93%)	1017 (96%)	38 (4%)	3 (0%)	36	25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	423	GLU
2	D	423	GLU
1	C	202	ALA

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	274/312 (88%)	256 (93%)	18 (7%)	15	4
1	C	272/312 (87%)	257 (94%)	15 (6%)	19	6
2	B	139/165 (84%)	131 (94%)	8 (6%)	18	6
2	D	149/165 (90%)	141 (95%)	8 (5%)	20	7
All	All	834/954 (87%)	785 (94%)	49 (6%)	18	5

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	69	ASN
1	A	131	LYS

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Mol	Chain	Res	Type
1	A	140	THR
1	A	183	ILE
1	A	184	ASP
1	A	200	ARG
1	A	248	THR
1	A	261	THR
1	A	299	LEU
1	A	311	SER
1	A	324	LEU
1	A	330	LEU
1	A	364	LEU
1	A	367	LEU
1	A	368	ASP
1	A	370	VAL
1	A	392	VAL
2	B	423	GLU
2	B	443	LEU
2	B	481	VAL
2	B	498	LEU
2	B	506	GLU
2	B	518	THR
2	B	519	ASN
2	B	530	VAL
1	C	41	VAL
1	C	55	LEU
1	C	108	THR
1	C	126	LEU
1	C	138	ARG
1	C	140	THR
1	C	169	LEU
1	C	183	ILE
1	C	184	ASP
1	C	234	SER
1	C	248	THR
1	C	299	LEU
1	C	324	LEU
1	C	330	LEU
1	C	370	VAL
2	D	423	GLU
2	D	443	LEU
2	D	481	VAL
2	D	518	THR

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Mol	Chain	Res	Type
2	D	519	ASN
2	D	525	ARG
2	D	534	VAL
2	D	575	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	82	ASN
1	A	267	ASN
1	A	281	GLN
1	A	329	HIS
1	A	354	HIS
1	A	391	GLN
2	B	405	HIS
2	B	424	GLN
2	B	441	ASN
2	B	454	ASN
2	B	457	GLN
2	B	500	HIS
2	B	519	ASN
2	B	554	ASN
2	B	576	ASN
2	B	583	ASN
1	C	40	GLN
1	C	82	ASN
1	C	281	GLN
1	C	329	HIS
1	C	354	HIS
1	C	362	GLN
1	C	388	ASN
1	C	391	GLN
2	D	405	HIS
2	D	441	ASN
2	D	454	ASN
2	D	457	GLN
2	D	500	HIS
2	D	519	ASN
2	D	539	ASN
2	D	543	HIS
2	D	554	ASN

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Mol	Chain	Res	Type
2	D	583	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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	256:PHE	C	257:GLY	N	1.18

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	359/376 (95%)	0.12	19 (5%) 32 35	7, 16, 31, 39	0
1	C	357/376 (94%)	0.09	9 (2%) 58 62	8, 17, 30, 38	0
2	B	175/193 (90%)	-0.06	2 (1%) 78 81	8, 15, 28, 37	0
2	D	183/193 (94%)	-0.04	2 (1%) 78 81	9, 15, 27, 34	0
All	All	1074/1138 (94%)	0.06	32 (2%) 52 56	7, 16, 30, 39	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	210	ASN	4.5
1	A	368	ASP	3.9
1	A	129	ASN	3.6
2	D	546	GLY	3.3
1	A	310	LEU	3.3
1	C	130	GLY	3.3
1	A	210	ASN	3.2
1	A	200	ARG	3.2
1	A	311	SER	3.1
1	A	370	VAL	3.0
1	C	128	GLU	2.9
1	A	385	GLY	2.9
1	C	370	VAL	2.8
1	A	130	GLY	2.8
1	A	318	TRP	2.7
1	C	388	ASN	2.7
2	B	532	LYS	2.7
2	D	475	ASP	2.6
1	C	373	LYS	2.6
1	A	367	LEU	2.6
2	B	498	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	102	GLY	2.4
1	A	136	SER	2.4
1	C	202	ALA	2.4
1	A	132	ALA	2.3
1	A	209	PRO	2.3
1	C	119	GLY	2.2
1	A	387	ALA	2.2
1	A	381	LYS	2.2
1	C	209	PRO	2.1
1	A	309	ASN	2.0
1	A	317	SER	2.0

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.