



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:53 AM GMT

PDB ID : 2V36  
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.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

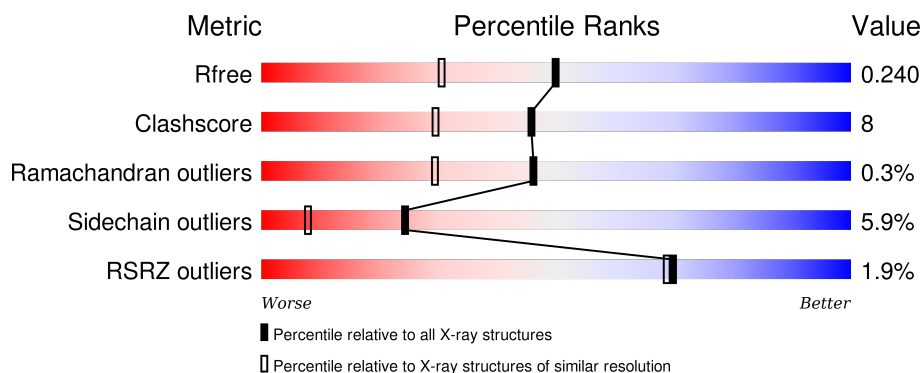
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>• • 5%</div> </div> </div>
1	C	376	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• • 5%</div> </div> </div>
2	B	193	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>• • 9%</div> </div> </div>
2	D	193	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>• • 5%</div> </div> </div>

## 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			

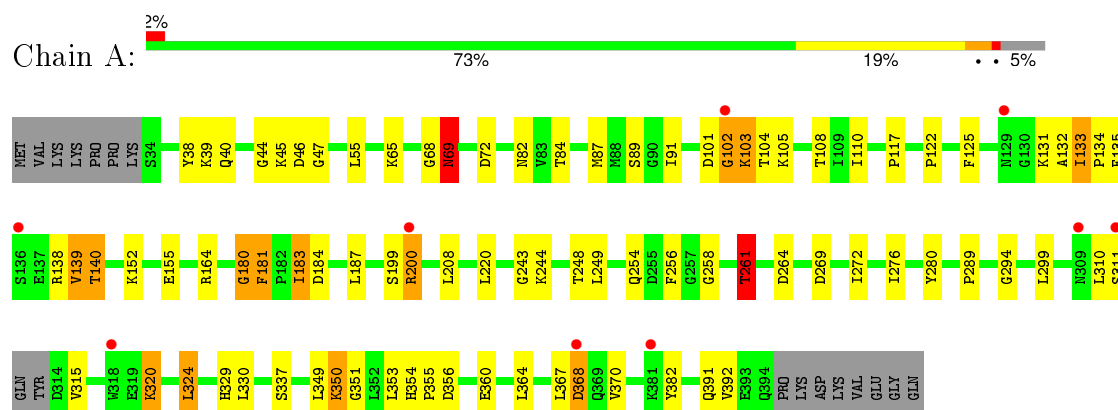
- Molecule 3 is water.

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		

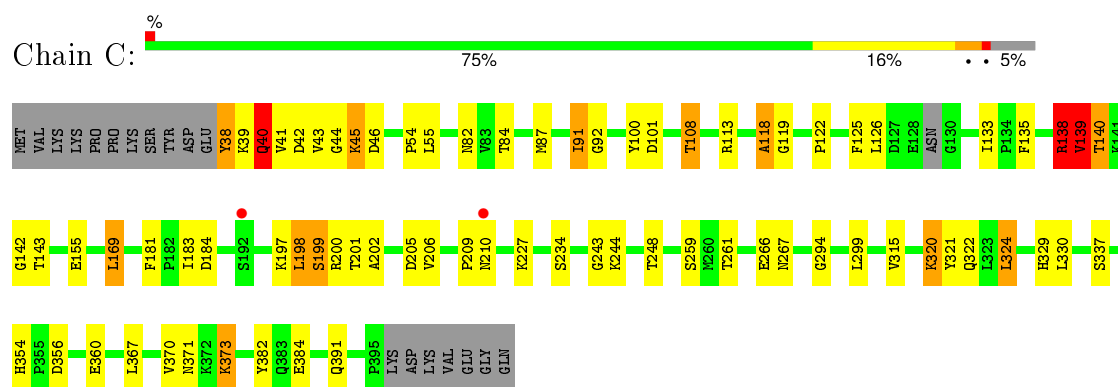
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

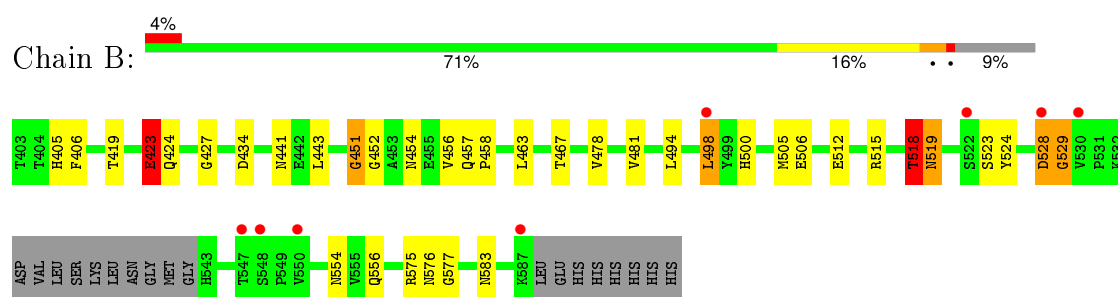
#### • Molecule 1: GAMMA-GLUTAMYLTRANSPEPTIDASE LARGE CHAIN



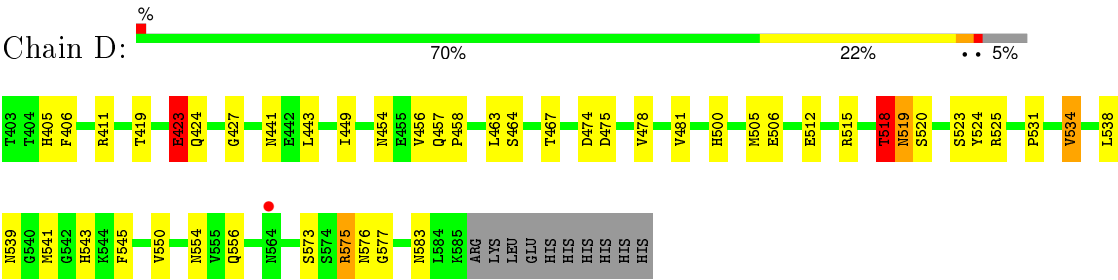
#### • Molecule 1: GAMMA-GLUTAMYLTRANSPEPTIDASE LARGE CHAIN



#### • 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, $\alpha$ , $\beta$ , $\gamma$	72.26Å 108.77Å 161.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.17 – 1.85 29.56 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.6 (90.17-1.85) 97.6 (29.56-1.85)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	5336 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.3	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 107238 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8372	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.94	12/2750 (0.4%)	0.99	18/3729 (0.5%)
1	C	0.93	9/2727 (0.3%)	1.01	20/3699 (0.5%)
2	B	0.99	10/1324 (0.8%)	1.01	10/1805 (0.6%)
2	D	0.97	7/1391 (0.5%)	1.13	12/1895 (0.6%)
All	All	0.95	38/8192 (0.5%)	1.03	60/11128 (0.5%)

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 (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	197	LYS	C-N	9.56	1.56	1.34
1	C	384	GLU	C-N	8.49	1.48	1.33
1	A	256	PHE	C-N	-8.33	1.18	1.33
1	A	139	VAL	CB-CG1	-7.91	1.36	1.52
1	C	139	VAL	CB-CG2	-7.87	1.36	1.52
2	D	481	VAL	CB-CG2	-7.74	1.36	1.52
1	C	373	LYS	C-O	-7.68	1.08	1.23
1	A	261	THR	CB-CG2	-7.47	1.27	1.52
2	B	524	TYR	CE1-CZ	-7.20	1.29	1.38
1	C	38	TYR	CE1-CZ	-7.10	1.29	1.38
1	A	133	ILE	C-N	-6.81	1.21	1.34
2	D	423	GLU	CD-OE2	6.73	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	406	PHE	CE1-CZ	-6.67	1.24	1.37
1	A	38	TYR	CE2-CZ	-6.66	1.29	1.38
1	A	105	LYS	C-N	6.33	1.48	1.34
2	D	478	VAL	CB-CG1	-6.30	1.39	1.52
1	A	134	PRO	C-N	6.22	1.48	1.34
1	A	139	VAL	CB-CG2	-6.22	1.39	1.52
2	D	478	VAL	CB-CG2	-6.04	1.40	1.52
2	B	524	TYR	CE2-CZ	-6.03	1.30	1.38
1	C	139	VAL	CB-CG1	-5.91	1.40	1.52
2	D	506	GLU	CD-OE1	-5.91	1.19	1.25
2	B	478	VAL	CB-CG2	-5.82	1.40	1.52
1	A	38	TYR	CG-CD1	-5.79	1.31	1.39
2	D	515	ARG	CZ-NH1	-5.71	1.25	1.33
1	C	143	THR	C-N	5.69	1.47	1.34
2	B	515	ARG	CZ-NH1	-5.52	1.25	1.33
2	B	524	TYR	CG-CD2	-5.52	1.31	1.39
2	B	524	TYR	CG-CD1	-5.51	1.31	1.39
1	A	38	TYR	CE1-CZ	-5.49	1.31	1.38
1	C	261	THR	CB-CG2	-5.47	1.34	1.52
1	A	38	TYR	CG-CD2	-5.42	1.32	1.39
2	B	406	PHE	CG-CD1	-5.40	1.30	1.38
2	B	481	VAL	CB-CG1	-5.35	1.41	1.52
1	A	355	PRO	C-N	-5.32	1.21	1.34
2	B	478	VAL	CB-CG1	-5.15	1.42	1.52
1	C	38	TYR	CE2-CZ	-5.02	1.32	1.38
2	D	406	PHE	CE2-CZ	-5.02	1.27	1.37

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	575	ARG	NE-CZ-NH1	18.26	129.43	120.30
2	D	575	ARG	NE-CZ-NH2	-17.30	111.65	120.30
1	A	132	ALA	N-CA-C	-12.98	75.95	111.00
2	B	481	VAL	CG1-CB-CG2	-9.86	95.12	110.90
1	C	138	ARG	NE-CZ-NH1	9.74	125.17	120.30
2	D	481	VAL	CG1-CB-CG2	-9.05	96.43	110.90
1	A	103	LYS	N-CA-C	-8.92	86.92	111.00
1	A	139	VAL	CG1-CB-CG2	-8.84	96.75	110.90
2	D	478	VAL	CG1-CB-CG2	-8.60	97.14	110.90
1	C	198	LEU	O-C-N	-8.56	109.01	122.70
1	C	371	ASN	O-C-N	8.30	135.98	122.70
1	A	351	GLY	N-CA-C	-8.29	92.37	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	577	GLY	N-CA-C	-8.07	92.92	113.10
1	A	102	GLY	N-CA-C	-7.83	93.52	113.10
2	D	515	ARG	NE-CZ-NH1	7.69	124.14	120.30
2	B	451	GLY	N-CA-C	7.43	131.68	113.10
1	C	92	GLY	N-CA-C	7.42	131.66	113.10
2	D	575	ARG	CD-NE-CZ	7.42	133.99	123.60
1	C	371	ASN	CA-C-N	-7.41	100.89	117.20
2	B	577	GLY	N-CA-C	-7.30	94.85	113.10
1	C	101	ASP	N-CA-C	-7.24	91.46	111.00
1	A	350	LYS	N-CA-C	-7.22	91.50	111.00
2	B	478	VAL	CG1-CB-CG2	-7.08	99.57	110.90
2	B	451	GLY	C-N-CA	6.83	136.65	122.30
1	C	200	ARG	N-CA-C	-6.62	93.11	111.00
1	C	40	GLN	N-CA-C	6.49	128.52	111.00
1	A	140	THR	N-CA-C	-6.43	93.65	111.00
1	C	373	LYS	CA-C-O	-6.42	106.62	120.10
1	A	40	GLN	N-CA-C	6.38	128.24	111.00
2	B	451	GLY	CA-C-N	6.22	128.65	116.20
1	A	104	THR	N-CA-CB	6.21	122.09	110.30
1	C	206	VAL	N-CA-C	-6.17	94.33	111.00
2	B	512	GLU	OE1-CD-OE2	-6.13	115.94	123.30
1	C	169	LEU	CB-CG-CD1	6.10	121.37	111.00
1	C	140	THR	N-CA-C	-6.01	94.78	111.00
2	D	518	THR	CB-CA-C	-6.00	95.40	111.60
1	C	199	SER	C-N-CA	5.88	136.41	121.70
1	A	155	GLU	OE1-CD-OE2	-5.83	116.30	123.30
2	D	506	GLU	OE1-CD-OE2	-5.83	116.30	123.30
2	B	575	ARG	NE-CZ-NH1	-5.75	117.42	120.30
2	D	411	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	267	ASN	N-CA-C	-5.57	95.96	111.00
2	B	518	THR	CB-CA-C	-5.55	96.63	111.60
1	C	244	LYS	N-CA-C	-5.48	96.20	111.00
1	A	244	LYS	N-CA-C	-5.45	96.29	111.00
2	D	512	GLU	OE1-CD-OE2	-5.44	116.77	123.30
1	A	181	PHE	N-CA-CB	-5.39	100.91	110.60
1	A	269	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	261	THR	N-CA-CB	-5.33	100.17	110.30
1	C	199	SER	N-CA-C	-5.25	96.83	111.00
2	D	575	ARG	CB-CG-CD	5.23	125.19	111.60
1	A	108	THR	OG1-CB-CG2	-5.21	98.01	110.00
1	A	69	ASN	N-CA-C	5.21	125.06	111.00
2	B	528	ASP	CA-C-N	5.16	126.53	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	155	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	C	118	ALA	CA-C-N	5.12	126.43	116.20
1	A	47	GLY	N-CA-C	5.11	125.88	113.10
1	C	197	LYS	O-C-N	5.10	130.86	122.70
1	C	373	LYS	O-C-N	5.09	130.77	121.10
1	A	104	THR	N-CA-C	-5.08	97.30	111.00

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

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Mol	Chain	Res	Type	Group
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
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	36	0
1	C	2670	0	2577	37	0
2	B	1297	0	1243	28	0
2	D	1363	0	1327	45	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	122	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 (122) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:525:ARG:HH12	2:D:550:VAL:CG1	2.00	0.74
2:B:529:GLY:HA2	3:B:2041:HOH:O	1.87	0.74
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
2:B:519:ASN:H	2:B:519:ASN:HD22	1.42	0.67
1:C:125:PHE:HB3	1:C:138:ARG:HD2	1.80	0.64
1:A:152:LYS:NZ	3:A:2034:HOH:O	2.03	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
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: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
1:A:69:ASN:C	1:A:69:ASN:HD22	2.07	0.58
2:B:427:GLY:HA2	2:B:441:ASN:HD22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:329:HIS:CE1	2:D:518:THR:HG21	2.39	0.56
2:B:500:HIS:HD2	2:B:505:MET:O	1.88	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
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
2:D:554:ASN:CG	2:D:575:ARG:HG3	2.28	0.54
1:A:329:HIS:CE1	2:B:518:THR:CG2	2.84	0.54
2:D:518:THR:CG2	2:D:523:SER:O	2.56	0.53
2:D:454:ASN:HD21	2:D:463:LEU:H	1.56	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: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:C:133:ILE:O	1:C:138:ARG:HD3	2.13	0.49
1:A:337:SER:CB	1:A:391:GLN:HE22	2.26	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:249:LEU:HD23	1:A:249:LEU:C	2.36	0.46
1:A:200:ARG:HH11	1:A:200:ARG:CB	2.28	0.46
1:A:200:ARG:HH11	1:A:200:ARG:HB3	1.81	0.46
2:B:518:THR:CG2	2:B:523:SER:O	2.64	0.46
1:A:354:HIS:CD2	1:A:356:ASP:H	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:519:ASN:HD21	2:D:523:SER:HB3	1.83	0.44
1:C:321:TYR:CD2	2:D:534:VAL:HG21	2.53	0.44
2:D:538:LEU:HA	2:D:541:MET:HE3	1.99	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
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:C:82:ASN:HD21	1:C:91:ILE:H	1.66	0.43
1:A:320:LYS:HD3	1:A:324:LEU:HD22	2.01	0.43
1:A:133:ILE:O	1:A:138:ARG:HD3	2.19	0.43
1:C:329:HIS:CD2	3:C:2107:HOH:O	2.55	0.42
1:C:43:VAL:HG12	1:C:44:GLY:N	2.33	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
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
2:D:518:THR:HG21	2:D:524:TYR:CZ	2.56	0.40
1:A:180:GLY:HA2	1:A:220:LEU:O	2.21	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%)	46	29
2	B	171/193 (89%)	162 (95%)	8 (5%)	1 (1%)	30	13
2	D	181/193 (94%)	175 (97%)	5 (3%)	1 (1%)	30	13
All	All	1058/1138 (93%)	1017 (96%)	38 (4%)	3 (0%)	46	29

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%)	253 (92%)	21 (8%)	16	3
1	C	272/312 (87%)	255 (94%)	17 (6%)	22	6
2	B	139/165 (84%)	133 (96%)	6 (4%)	35	16
2	D	149/165 (90%)	144 (97%)	5 (3%)	44	24
All	All	834/954 (87%)	785 (94%)	49 (6%)	24	8

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	87	MET
1	A	117	PRO
1	A	140	THR
1	A	164	ARG
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	320	LYS
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	498	LEU
2	B	506	GLU
2	B	518	THR
2	B	519	ASN
1	C	41	VAL
1	C	55	LEU
1	C	87	MET
1	C	108	THR
1	C	126	LEU
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	320	LYS
1	C	324	LEU
1	C	330	LEU
1	C	367	LEU

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Mol	Chain	Res	Type
1	C	370	VAL
2	D	423	GLU
2	D	443	LEU
2	D	518	THR
2	D	519	ASN
2	D	534	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) 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	441	ASN
2	B	454	ASN
2	B	457	GLN
2	B	500	HIS
2	B	519	ASN
2	B	554	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 carbohydrates 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](#)

There are no chain breaks in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	359/376 (95%)	0.05	9 (2%) 61 58	7, 16, 31, 39	0
1	C	357/376 (94%)	-0.04	2 (0%) 90 90	8, 17, 30, 38	0
2	B	175/193 (90%)	0.17	8 (4%) 36 34	8, 15, 28, 37	0
2	D	183/193 (94%)	-0.10	1 (0%) 91 91	9, 15, 27, 34	0
All	All	1074/1138 (94%)	0.02	20 (1%) 70 69	7, 16, 30, 39	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	ASN	5.1
1	A	318	TRP	3.5
1	A	368	ASP	3.1
1	A	311	SER	3.1
2	B	530	VAL	3.0
2	B	547	THR	2.9
1	C	210	ASN	2.8
2	B	550	VAL	2.5
2	D	564	ASN	2.4
2	B	498	LEU	2.4
2	B	522	SER	2.4
1	A	200	ARG	2.2
1	C	192	SER	2.2
1	A	102	GLY	2.2
2	B	587	LYS	2.1
1	A	309	ASN	2.1
1	A	381	LYS	2.1
2	B	528	ASP	2.1
1	A	136	SER	2.0
2	B	548	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 carbohydrates 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.