



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:09 PM UTC

PDB ID : 3A75 / pdb_00003a75
Title : Crystal structure of glutamate complex of halotolerant γ -glutamyltranspeptidase from *Bacillus subtilis*
Authors : Wada, K.; Fukuyama, K.
Deposited on : 2009-09-14
Resolution : 1.95 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)	:	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

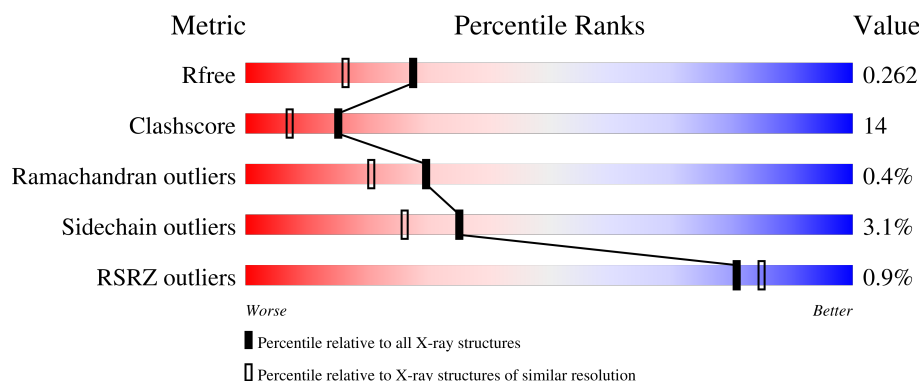
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	384	% 68% 22% • 7%
1	C	384	% 69% 21% • 7%
2	B	185	% 75% 21% • • •
2	D	185	% 71% 23% 5% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9133 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
			2778	1767	458	543	10			
1	C	358	Total	C	N	O	S	0	0	0
			2769	1762	457	540	10			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	expression tag	UNP P54422
A	20	ASN	-	expression tag	UNP P54422
A	21	HIS	-	expression tag	UNP P54422
A	22	LYS	-	expression tag	UNP P54422
A	23	VAL	-	expression tag	UNP P54422
A	24	HIS	-	expression tag	UNP P54422
A	25	HIS	-	expression tag	UNP P54422
A	26	HIS	-	expression tag	UNP P54422
A	27	HIS	-	expression tag	UNP P54422
A	28	HIS	-	expression tag	UNP P54422
A	29	HIS	-	expression tag	UNP P54422
A	30	ILE	-	expression tag	UNP P54422
A	31	GLU	-	expression tag	UNP P54422
A	32	GLY	-	expression tag	UNP P54422
A	33	ARG	-	expression tag	UNP P54422
A	34	HIS	-	expression tag	UNP P54422
A	35	MET	-	expression tag	UNP P54422
C	19	MET	-	expression tag	UNP P54422
C	20	ASN	-	expression tag	UNP P54422
C	21	HIS	-	expression tag	UNP P54422
C	22	LYS	-	expression tag	UNP P54422
C	23	VAL	-	expression tag	UNP P54422
C	24	HIS	-	expression tag	UNP P54422
C	25	HIS	-	expression tag	UNP P54422
C	26	HIS	-	expression tag	UNP P54422

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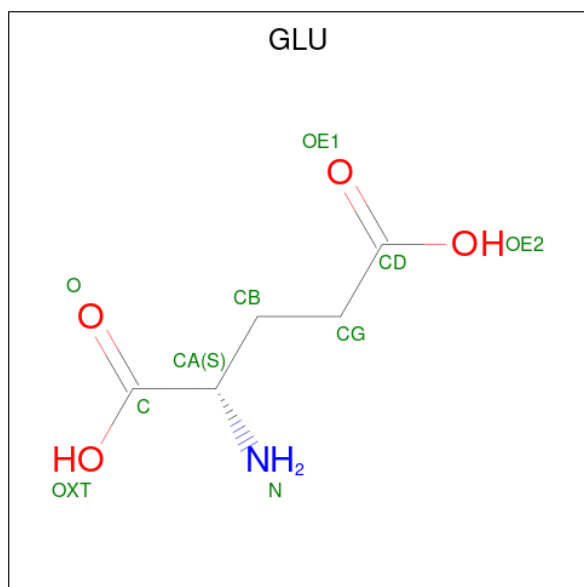
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Chain	Residue	Modelled	Actual	Comment	Reference
C	27	HIS	-	expression tag	UNP P54422
C	28	HIS	-	expression tag	UNP P54422
C	29	HIS	-	expression tag	UNP P54422
C	30	ILE	-	expression tag	UNP P54422
C	31	GLU	-	expression tag	UNP P54422
C	32	GLY	-	expression tag	UNP P54422
C	33	ARG	-	expression tag	UNP P54422
C	34	HIS	-	expression tag	UNP P54422
C	35	MET	-	expression tag	UNP P54422

- Molecule 2 is a protein called Gamma-glutamyltranspeptidase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	182	Total	C	N	O	S	0	0	0
			1378	869	229	275	5			
2	D	184	Total	C	N	O	S	0	0	0
			1398	881	235	277	5			

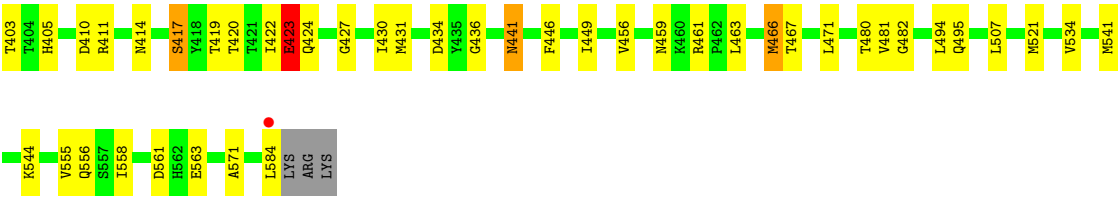
- Molecule 3 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



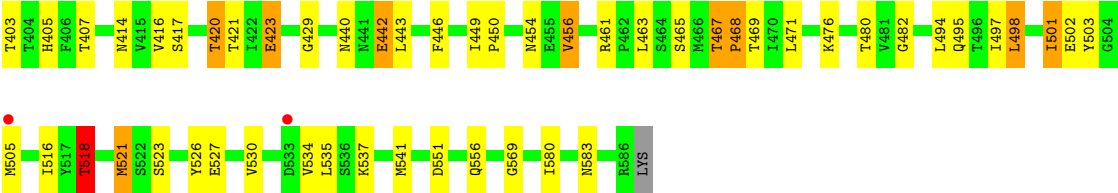
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	5	1	4		
3	D	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	269	Total 269	O 269	0	0
4	B	121	Total 121	O 121	0	0
4	C	261	Total 261	O 261	0	0
4	D	139	Total 139	O 139	0	0



● 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	49.40Å 98.89Å 227.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.86 – 1.95 24.86 – 1.95	Depositor EDS
% Data completeness (in resolution range)	93.1 (24.86-1.95) 93.2 (24.86-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.95Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.208 , 0.262 0.208 , 0.262	Depositor DCC
R_{free} test set	3895 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9133	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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	0.90	1/2836 (0.0%)	1.19	18/3834 (0.5%)
1	C	1.01	6/2827 (0.2%)	1.22	20/3822 (0.5%)
2	B	0.96	2/1406 (0.1%)	1.23	7/1913 (0.4%)
2	D	1.04	3/1426 (0.2%)	1.26	9/1938 (0.5%)
All	All	0.97	12/8495 (0.1%)	1.22	54/11507 (0.5%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	48	MET	SD-CE	-9.20	1.56	1.79
1	C	290	PRO	CA-C	8.93	1.56	1.51
1	C	88	MET	SD-CE	8.19	2.00	1.79
1	C	301	MET	SD-CE	-7.01	1.62	1.79
1	A	166	MET	SD-CE	6.31	1.95	1.79
2	B	541	MET	SD-CE	-6.27	1.63	1.79
2	B	466	MET	SD-CE	-6.20	1.64	1.79
2	D	456	VAL	CA-CB	6.13	1.61	1.54
1	C	285	ILE	CA-CB	-6.03	1.47	1.54
2	D	521	MET	SD-CE	-5.38	1.66	1.79
2	D	467	THR	CA-CB	5.09	1.59	1.53
1	C	328	MET	SD-CE	-5.08	1.66	1.79

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	518	THR	CB-CA-C	-10.25	95.28	110.24
1	C	312	GLN	N-CA-C	-10.14	100.32	112.89
1	C	290	PRO	N-CA-C	-7.31	103.45	110.47
1	A	288	THR	N-CA-C	7.28	120.20	109.42
2	D	501	ILE	N-CA-C	7.24	118.18	111.45
1	C	212	GLU	CA-C-N	7.19	126.95	119.76
1	C	212	GLU	C-N-CA	7.19	126.95	119.76
1	C	298	LEU	N-CA-C	-7.18	103.39	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	MET	N-CA-C	7.09	122.22	113.50
1	A	298	LEU	N-CA-C	-6.78	103.97	111.36
1	A	294	GLY	N-CA-C	6.65	120.22	112.50
1	A	310	LEU	N-CA-C	6.60	119.32	111.33
1	A	85	GLU	N-CA-C	-6.60	99.23	109.79
2	B	422	ILE	N-CA-C	-6.59	106.37	112.43
1	A	186	VAL	N-CA-C	6.53	116.69	110.42
2	D	450	PRO	N-CA-C	6.50	120.63	111.33
1	C	162	GLY	N-CA-C	6.44	118.90	111.36
1	C	288	THR	N-CA-C	6.41	117.73	109.65
1	C	368	ASP	N-CA-C	6.40	121.10	113.16
2	D	442	GLU	N-CA-C	6.37	119.04	111.33
1	A	312	GLN	N-CA-C	-6.20	105.56	113.01
1	C	85	GLU	N-CA-C	-6.18	99.91	109.79
2	B	441	ASN	N-CA-C	-6.02	103.38	111.87
1	A	100	TYR	N-CA-C	-5.95	99.53	109.24
1	A	357	TYR	N-CA-C	-5.82	104.30	111.40
1	C	133	ILE	CA-C-N	5.72	126.05	119.93
1	C	133	ILE	C-N-CA	5.72	126.05	119.93
1	C	357	TYR	N-CA-C	-5.66	105.19	111.36
2	D	465	SER	N-CA-C	-5.66	104.96	112.94
1	C	293	SER	N-CA-C	-5.64	106.40	113.28
1	A	276	ILE	N-CA-C	-5.63	100.47	108.58
2	B	417	SER	N-CA-C	-5.58	99.19	108.34
1	A	174	ILE	N-CA-C	-5.55	104.95	110.62
1	A	208	LEU	CA-C-N	5.53	126.75	119.84
1	A	208	LEU	C-N-CA	5.53	126.75	119.84
1	C	110	ILE	N-CA-C	-5.50	99.15	107.73
1	A	293	SER	N-CA-C	-5.48	106.64	113.38
2	B	555	VAL	N-CA-C	5.47	116.59	108.23
1	A	88	MET	N-CA-C	5.40	120.00	113.41
1	C	67	GLY	N-CA-C	5.40	122.77	115.32
2	B	507	LEU	N-CA-C	5.30	117.47	111.11
2	D	417	SER	N-CA-C	-5.29	99.48	108.26
2	D	429	GLY	N-CA-C	-5.26	108.37	115.21
1	A	268	TYR	N-CA-C	5.25	117.85	110.23
1	C	129	ASN	N-CA-C	5.23	118.68	112.72
1	C	338	TYR	N-CA-C	5.20	121.42	113.61
2	B	495	GLN	CA-CB-CG	-5.20	103.70	114.10
1	C	145	VAL	N-CA-C	5.18	116.20	108.54
2	D	551	ASP	N-CA-C	-5.17	103.21	110.50
1	A	110	ILE	N-CA-C	-5.15	99.69	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	468	PRO	N-CA-C	-5.11	103.17	111.03
1	A	83	VAL	N-CA-C	5.08	115.75	110.82
2	B	555	VAL	CB-CA-C	-5.01	104.89	110.96
1	C	214	LEU	N-CA-C	-5.00	103.54	110.35

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	2778	0	2762	83	0
1	C	2769	0	2756	83	0
2	B	1378	0	1355	40	0
2	D	1398	0	1381	65	0
3	B	10	0	5	0	0
3	D	10	0	5	1	0
4	A	269	0	0	8	0
4	B	121	0	0	5	0
4	C	261	0	0	6	0
4	D	139	0	0	7	0
All	All	9133	0	8264	226	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 14.

All (226) 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:B:480:THR:HB	4:B:715:HOH:O	1.31	1.22
1:C:78:GLN:HE22	2:D:420:THR:HG21	1.07	1.11
1:C:372:LYS:HA	2:D:521:MET:HE3	1.09	1.07
1:C:78:GLN:NE2	2:D:420:THR:HG21	1.75	1.01
2:B:419:THR:HG22	2:B:466:MET:HE2	1.06	1.01
2:B:419:THR:CG2	2:B:466:MET:HE2	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:GLY:H	2:D:440:ASN:HD21	1.14	0.94
1:C:351:GLY:H	1:C:383:GLN:HE21	1.16	0.92
1:A:111:ASP:HB3	1:A:271:THR:HG22	1.49	0.91
2:D:440:ASN:HD22	2:D:442:GLU:H	1.18	0.88
2:D:407:THR:HG23	2:D:416:VAL:O	1.72	0.88
1:C:114:GLU:OE2	2:D:442:GLU:HG3	1.74	0.87
1:C:372:LYS:HA	2:D:521:MET:CE	2.01	0.87
2:D:442:GLU:CG	4:D:716:HOH:O	2.22	0.86
2:B:424:GLN:H	2:B:441:ASN:HD21	1.17	0.85
1:C:276:ILE:HG12	1:C:289:PRO:HB3	1.60	0.84
2:D:503:TYR:HB3	2:D:505:MET:HE2	1.59	0.84
1:C:183:ILE:HD11	1:C:220:LEU:HB2	1.65	0.77
1:A:271:THR:HG23	1:A:273:ASP:OD1	1.85	0.77
1:A:102:GLY:H	2:B:414:ASN:ND2	1.84	0.76
1:A:53:HIS:HD2	1:A:55:LEU:H	1.32	0.75
1:C:394:GLN:HE22	2:D:449:ILE:H	1.33	0.75
1:A:394:GLN:HE22	2:B:449:ILE:H	1.31	0.75
1:A:197:LYS:HA	1:A:200:ARG:HD2	1.69	0.73
1:C:287:THR:HG23	2:D:469:THR:OG1	1.87	0.73
1:C:311:SER:HB3	2:D:502:GLU:HG3	1.71	0.72
1:C:233:ARG:HD2	4:C:584:HOH:O	1.88	0.72
1:C:325:ALA:HA	1:C:328:MET:CE	2.20	0.72
2:B:556:GLN:HE21	2:B:571:ALA:HA	1.56	0.71
1:C:48:MET:HE3	1:C:49:VAL:O	1.92	0.70
2:D:407:THR:HG21	2:D:480:THR:OG1	1.92	0.70
1:A:351:GLY:H	1:A:383:GLN:HE21	1.40	0.69
1:A:271:THR:HG21	2:B:461:ARG:HH12	1.57	0.69
1:A:337:SER:CB	1:A:391:GLN:HE22	2.06	0.69
1:C:48:MET:HE1	2:D:580:ILE:N	2.08	0.68
1:A:276:ILE:HD11	1:A:289:PRO:HA	1.74	0.67
1:A:103:LYS:HD2	4:A:837:HOH:O	1.94	0.67
1:C:183:ILE:HG12	1:C:187:LEU:HD23	1.77	0.67
2:D:442:GLU:HG3	4:D:716:HOH:O	1.91	0.66
1:A:249:LEU:C	1:A:249:LEU:HD23	2.19	0.66
2:B:403:THR:HG23	2:B:466:MET:CE	2.25	0.66
1:C:235:LYS:HB2	1:C:239:ALA:HB2	1.77	0.66
1:C:288:THR:HG21	2:D:468:PRO:HG2	1.79	0.65
1:C:367:LEU:HD23	1:C:367:LEU:C	2.23	0.64
2:D:454:ASN:HD21	2:D:463:LEU:H	1.45	0.64
2:B:403:THR:HG23	2:B:466:MET:HE3	1.78	0.64
1:C:287:THR:HG22	1:C:288:THR:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:GLU:CD	2:D:442:GLU:HG3	2.23	0.63
1:C:325:ALA:HA	1:C:328:MET:HE3	1.80	0.63
2:D:495:GLN:HE22	2:D:516:ILE:H	1.47	0.63
1:A:82:ASN:HD21	1:A:91:ILE:H	1.45	0.62
1:C:160:LYS:HG2	1:C:161:TRP:CE2	2.34	0.62
1:A:207:PHE:C	1:A:209:PRO:HD3	2.24	0.62
1:C:354:HIS:HD2	1:C:356:ASP:H	1.48	0.62
1:A:260:MET:SD	1:A:265:LEU:HD21	2.40	0.61
1:A:53:HIS:CD2	1:A:55:LEU:H	2.15	0.61
1:A:276:ILE:HG13	1:A:289:PRO:HB3	1.82	0.61
1:A:263:LYS:NZ	1:A:267:ASN:HD21	1.98	0.61
1:C:82:ASN:ND2	1:C:91:ILE:H	1.98	0.61
1:A:194:TYR:HD1	1:A:197:LYS:HD3	1.66	0.60
2:B:423:GLU:HB3	2:B:441:ASN:ND2	2.16	0.60
1:A:301:MET:HE2	2:B:494:LEU:HD22	1.83	0.60
1:A:82:ASN:ND2	1:A:91:ILE:H	2.01	0.59
4:C:637:HOH:O	2:D:476:LYS:HG2	2.02	0.59
1:A:307:HIS:HD2	4:A:477:HOH:O	1.86	0.59
2:B:427:GLY:HA2	2:B:441:ASN:HD22	1.66	0.58
1:C:200:ARG:HH11	1:C:200:ARG:HG2	1.67	0.58
1:C:207:PHE:C	1:C:209:PRO:HD3	2.28	0.58
1:C:354:HIS:CD2	1:C:356:ASP:H	2.21	0.58
1:C:329:HIS:NE2	2:D:518:THR:HG21	2.18	0.58
1:A:263:LYS:HZ3	1:A:267:ASN:HD21	1.51	0.58
2:D:518:THR:HG23	2:D:523:SER:O	2.03	0.58
2:D:442:GLU:CD	4:D:716:HOH:O	2.45	0.58
1:C:233:ARG:CD	4:C:584:HOH:O	2.46	0.58
1:A:247:LYS:NZ	1:A:251:ASP:OD2	2.38	0.57
1:A:271:THR:CG2	1:A:273:ASP:OD1	2.52	0.57
2:D:407:THR:CG2	2:D:416:VAL:O	2.50	0.57
1:C:146:GLY:H	2:D:440:ASN:ND2	1.94	0.57
1:C:82:ASN:HD21	1:C:91:ILE:H	1.52	0.57
1:A:293:SER:HB3	2:B:463:LEU:HD11	1.88	0.56
2:B:521:MET:O	2:B:544:LYS:HD2	2.06	0.56
1:A:46:ASP:OD2	2:B:584:LEU:N	2.35	0.56
1:C:45:LYS:HE2	4:C:484:HOH:O	2.06	0.55
1:C:78:GLN:HE22	2:D:420:THR:CG2	1.98	0.55
1:A:209:PRO:HD2	1:A:212:GLU:O	2.07	0.55
1:A:185:SER:O	1:A:189:GLU:HG3	2.07	0.55
1:C:155:GLU:HB2	1:C:237:THR:HG21	1.88	0.55
1:C:113:ARG:CZ	2:D:442:GLU:OE1	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:MET:CE	1:C:49:VAL:O	2.55	0.54
1:A:196:GLU:O	1:A:200:ARG:HG3	2.07	0.54
2:D:421:THR:HG23	4:D:716:HOH:O	2.07	0.54
1:A:238:ASP:HB2	4:A:577:HOH:O	2.06	0.54
2:B:544:LYS:NZ	4:B:746:HOH:O	2.41	0.54
2:B:420:THR:C	2:B:466:MET:HE1	2.32	0.54
1:C:276:ILE:HD11	1:C:349:LEU:HD11	1.89	0.53
1:A:276:ILE:CG1	1:A:289:PRO:HB3	2.38	0.53
2:B:417:SER:HB2	2:B:480:THR:HG23	1.90	0.53
1:A:390:LYS:HE2	4:A:690:HOH:O	2.08	0.53
1:C:48:MET:HE3	1:C:49:VAL:H	1.73	0.53
1:C:183:ILE:CD1	1:C:220:LEU:HB2	2.37	0.52
1:A:372:LYS:HE2	4:A:831:HOH:O	2.08	0.52
2:D:420:THR:HG23	4:D:599:HOH:O	2.09	0.52
1:C:113:ARG:NH1	2:D:442:GLU:OE1	2.43	0.52
1:A:102:GLY:H	2:B:414:ASN:HD22	1.55	0.51
1:A:110:ILE:CD1	1:A:272:ILE:HD12	2.40	0.51
1:A:110:ILE:HD13	1:A:272:ILE:HD12	1.92	0.51
1:C:288:THR:CG2	2:D:468:PRO:HG2	2.40	0.51
2:D:527:GLU:O	2:D:530:VAL:HG23	2.11	0.51
1:A:212:GLU:HG3	1:A:215:LYS:NZ	2.26	0.51
2:B:417:SER:HB2	2:B:480:THR:CG2	2.41	0.51
2:B:556:GLN:HE21	2:B:571:ALA:CA	2.22	0.51
1:C:263:LYS:HD2	1:C:263:LYS:C	2.36	0.51
2:D:440:ASN:HD22	2:D:442:GLU:N	1.98	0.50
1:C:48:MET:HE2	2:D:569:GLY:HA3	1.93	0.50
2:D:403:THR:OG1	3:D:601:GLU:OE1	2.29	0.50
1:C:371:ASN:O	2:D:521:MET:CE	2.60	0.50
1:A:53:HIS:HD2	1:A:55:LEU:N	2.07	0.50
2:D:518:THR:CG2	2:D:523:SER:O	2.60	0.50
1:C:115:ARG:HG2	2:D:461:ARG:HG2	1.93	0.49
1:C:299:LEU:O	1:C:303:LYS:HG3	2.11	0.49
1:A:186:VAL:HG21	4:B:136:HOH:O	2.11	0.49
1:C:209:PRO:HG2	1:C:214:LEU:HD21	1.93	0.49
2:B:446:PHE:CD2	2:B:456:VAL:HG22	2.48	0.49
1:C:270:ILE:HD12	1:C:270:ILE:C	2.37	0.49
2:D:537:LYS:O	2:D:541:MET:HG3	2.13	0.49
1:A:290:PRO:HA	1:A:292:SER:N	2.27	0.49
1:A:82:ASN:ND2	1:A:91:ILE:HG23	2.28	0.48
1:C:329:HIS:NE2	2:D:518:THR:CG2	2.76	0.48
1:A:111:ASP:CB	1:A:271:THR:HG22	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:GLY:H	2:D:414:ASN:ND2	2.11	0.48
4:C:718:HOH:O	2:D:502:GLU:HB2	2.14	0.48
2:B:424:GLN:H	2:B:441:ASN:ND2	1.99	0.48
2:D:497:ILE:HG23	2:D:501:ILE:HD12	1.95	0.48
1:A:301:MET:HE2	2:B:494:LEU:CD2	2.43	0.48
1:A:337:SER:HB3	1:A:391:GLN:HE22	1.77	0.48
2:B:405:HIS:CE1	2:B:482:GLY:HA3	2.49	0.48
2:B:467:THR:HG22	2:B:467:THR:O	2.14	0.47
1:C:393:GLU:HA	4:C:554:HOH:O	2.14	0.47
1:C:318:TRP:CH2	1:C:367:LEU:HD21	2.49	0.47
2:D:526:TYR:CE1	2:D:535:LEU:HD21	2.48	0.47
1:A:152:LYS:HG2	1:A:241:TYR:CE1	2.49	0.47
2:D:440:ASN:ND2	2:D:442:GLU:HB2	2.30	0.47
1:A:208:LEU:O	1:A:209:PRO:C	2.57	0.47
1:C:200:ARG:HG2	1:C:200:ARG:NH1	2.28	0.47
2:D:454:ASN:ND2	2:D:463:LEU:H	2.12	0.47
1:A:276:ILE:CD1	1:A:289:PRO:HA	2.44	0.47
1:A:281:GLN:HE21	1:A:281:GLN:HA	1.80	0.47
1:C:325:ALA:HA	1:C:328:MET:HE2	1.97	0.47
1:C:351:GLY:H	1:C:383:GLN:NE2	1.98	0.47
1:A:185:SER:HB3	1:A:216:GLU:OE2	2.15	0.46
1:A:337:SER:CB	1:A:391:GLN:NE2	2.77	0.46
1:A:358:ILE:O	1:A:362:GLN:HG3	2.15	0.46
2:D:494:LEU:HG	2:D:498:LEU:HD22	1.97	0.46
2:B:558:ILE:N	4:B:715:HOH:O	2.47	0.46
1:C:183:ILE:HG12	1:C:187:LEU:CD2	2.42	0.46
1:C:194:TYR:CD1	1:C:197:LYS:HE3	2.50	0.46
1:C:276:ILE:HD13	1:C:276:ILE:HA	1.81	0.46
1:A:270:ILE:C	1:A:270:ILE:HD12	2.40	0.46
1:A:183:ILE:HB	1:A:187:LEU:HD23	1.98	0.46
1:C:288:THR:HG21	2:D:468:PRO:CG	2.45	0.46
1:C:371:ASN:O	2:D:521:MET:HE2	2.15	0.46
1:A:235:LYS:HB2	1:A:239:ALA:HB2	1.97	0.45
2:B:424:GLN:N	2:B:441:ASN:HD21	1.97	0.45
1:C:89:SER:HB2	2:D:420:THR:HB	1.99	0.45
2:D:405:HIS:CE1	2:D:482:GLY:HA3	2.52	0.45
1:C:321:TYR:CD2	2:D:534:VAL:HG11	2.52	0.45
1:C:357:TYR:O	1:C:361:ARG:HG2	2.17	0.45
2:D:498:LEU:HA	2:D:498:LEU:HD12	1.71	0.45
1:A:301:MET:CE	2:B:494:LEU:HD22	2.47	0.45
1:C:358:ILE:O	1:C:362:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:SER:HB3	1:A:391:GLN:NE2	2.32	0.44
1:C:115:ARG:HG2	2:D:461:ARG:CG	2.47	0.44
1:A:277:TRP:HA	1:A:285:ILE:O	2.17	0.44
2:B:431:MET:SD	2:B:436:GLY:HA2	2.58	0.44
1:C:308:PHE:O	1:C:309:ASN:C	2.59	0.44
1:C:297:PHE:O	1:C:301:MET:HG3	2.17	0.44
1:A:133:ILE:O	1:A:134:PRO:C	2.61	0.44
1:A:209:PRO:HG2	1:A:214:LEU:CD2	2.48	0.44
1:C:276:ILE:HG22	1:C:299:LEU:CD1	2.48	0.43
2:D:476:LYS:NZ	4:D:653:HOH:O	2.51	0.43
1:A:281:GLN:HA	1:A:281:GLN:NE2	2.34	0.43
1:A:249:LEU:C	1:A:249:LEU:CD2	2.88	0.43
1:C:288:THR:HG21	2:D:468:PRO:HD2	2.00	0.43
1:A:123:ASP:HB2	1:A:126:LEU:HD12	2.00	0.43
1:A:209:PRO:HB2	4:A:656:HOH:O	2.17	0.43
1:A:281:GLN:HE21	1:A:281:GLN:CA	2.31	0.43
1:A:155:GLU:HB2	1:A:237:THR:HG21	2.00	0.43
1:C:192:SER:O	1:C:195:GLN:HG3	2.18	0.43
2:D:503:TYR:O	2:D:505:MET:HE2	2.19	0.43
2:D:471:LEU:CD2	2:D:501:ILE:HD11	2.49	0.43
1:A:112:SER:HB2	4:A:447:HOH:O	2.18	0.43
1:C:65:LYS:HB2	1:C:65:LYS:HE3	1.69	0.43
1:A:129:ASN:HB3	4:A:623:HOH:O	2.19	0.42
1:A:201:THR:O	1:A:204:LYS:HG2	2.19	0.42
1:C:351:GLY:N	1:C:383:GLN:HE21	1.99	0.42
2:B:427:GLY:HA2	2:B:441:ASN:ND2	2.33	0.42
1:C:71:ILE:HD12	1:C:71:ILE:N	2.34	0.42
1:A:69:ASN:HB2	2:B:410:ASP:OD2	2.19	0.42
1:A:321:TYR:CD2	2:B:534:VAL:HG11	2.54	0.42
1:A:53:HIS:CD2	1:A:54:PRO:HD2	2.54	0.42
1:A:201:THR:HG21	2:B:430:ILE:HA	2.01	0.42
1:A:338:TYR:HB3	1:A:348:PRO:HD2	2.02	0.42
1:A:351:GLY:H	1:A:383:GLN:NE2	2.15	0.42
1:A:212:GLU:HA	1:A:213:PRO:HD2	1.87	0.41
1:C:43:VAL:HG12	1:C:44:GLY:N	2.35	0.41
1:C:84:THR:HA	1:C:181:PHE:CZ	2.55	0.41
1:A:124:MET:HE3	1:A:125:PHE:CZ	2.55	0.41
1:C:44:GLY:HA2	2:D:583:ASN:HD21	1.84	0.41
1:C:160:LYS:HG2	1:C:161:TRP:CD2	2.55	0.41
1:C:212:GLU:HA	1:C:213:PRO:HD3	1.78	0.41
1:A:53:HIS:HA	1:A:54:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:SER:CB	2:B:420:THR:HG23	2.51	0.41
1:A:151:LEU:HG	1:A:237:THR:HG22	2.03	0.41
1:A:115:ARG:HD2	2:B:459:ASN:ND2	2.35	0.41
2:B:561:ASP:OD1	2:B:563:GLU:HB2	2.21	0.41
2:D:467:THR:HG22	2:D:467:THR:O	2.21	0.41
2:D:535:LEU:HD23	4:D:613:HOH:O	2.21	0.41
1:C:45:LYS:H	2:D:583:ASN:ND2	2.19	0.41
2:D:405:HIS:O	2:D:556:GLN:HG3	2.21	0.41
2:D:446:PHE:CD2	2:D:456:VAL:HG22	2.56	0.41
1:A:301:MET:HE2	1:A:301:MET:HB3	1.84	0.40
1:C:111:ASP:OD1	1:C:111:ASP:C	2.64	0.40
1:C:48:MET:HE3	1:C:49:VAL:N	2.36	0.40
1:A:241:TYR:C	1:A:242:LYS:HG3	2.46	0.40
2:B:411:ARG:HG3	4:B:213:HOH:O	2.22	0.40
2:B:417:SER:CB	2:B:480:THR:CG2	2.99	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	357/384 (93%)	349 (98%)	7 (2%)	1 (0%)	36	28
1	C	356/384 (93%)	345 (97%)	10 (3%)	1 (0%)	36	28
2	B	180/185 (97%)	174 (97%)	5 (3%)	1 (1%)	21	12
2	D	182/185 (98%)	175 (96%)	6 (3%)	1 (0%)	24	16
All	All	1075/1138 (94%)	1043 (97%)	28 (3%)	4 (0%)	30	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	PRO
2	B	423	GLU
2	D	423	GLU
1	C	209	PRO

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	296/319 (93%)	288 (97%)	8 (3%)	39	32
1	C	295/319 (92%)	284 (96%)	11 (4%)	30	20
2	B	154/157 (98%)	150 (97%)	4 (3%)	40	33
2	D	156/157 (99%)	151 (97%)	5 (3%)	34	25
All	All	901/952 (95%)	873 (97%)	28 (3%)	35	26

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	SER
1	A	139	VAL
1	A	196	GLU
1	A	209	PRO
1	A	238	ASP
1	A	249	LEU
1	A	271	THR
1	A	367	LEU
2	B	423	GLU
2	B	434	ASP
2	B	471	LEU
2	B	481	VAL
1	C	58	GLU
1	C	138	ARG
1	C	160	LYS
1	C	175	LYS
1	C	184	ASP
1	C	231	LEU

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Mol	Chain	Res	Type
1	C	263	LYS
1	C	289	PRO
1	C	290	PRO
1	C	306	ASP
1	C	315	VAL
2	D	420	THR
2	D	423	GLU
2	D	443	LEU
2	D	498	LEU
2	D	518	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	82	ASN
1	A	267	ASN
1	A	281	GLN
1	A	307	HIS
1	A	309	ASN
1	A	346	ASN
1	A	383	GLN
1	A	391	GLN
1	A	394	GLN
2	B	414	ASN
2	B	424	GLN
2	B	441	ASN
2	B	459	ASN
2	B	556	GLN
1	C	78	GLN
1	C	82	ASN
1	C	222	GLN
1	C	354	HIS
1	C	362	GLN
1	C	383	GLN
1	C	391	GLN
1	C	394	GLN
2	D	414	ASN
2	D	440	ASN
2	D	454	ASN
2	D	495	GLN
2	D	583	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	$\# Z > 2$
3	GLU	D	601	-	8,9,9	1.18	0	8,11,11	0.95	0
3	GLU	B	600	-	8,9,9	1.10	0	8,11,11	0.83	0

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
3	GLU	D	601	-	-	3/9/9/9	-
3	GLU	B	600	-	-	0/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	601	GLU	CA-CB-CG-CD
3	D	601	GLU	OE2-CD-CG-CB
3	D	601	GLU	OE1-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	601	GLU	1	0

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 [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	359/384 (93%)	0.05	4 (1%) 78 83	10, 23, 43, 55	0
1	C	358/384 (93%)	-0.09	3 (0%) 82 86	9, 20, 38, 51	0
2	B	182/185 (98%)	-0.21	1 (0%) 87 90	11, 19, 32, 51	0
2	D	184/185 (99%)	-0.19	2 (1%) 78 83	8, 17, 35, 50	0
All	All	1083/1138 (95%)	-0.08	10 (0%) 81 85	8, 20, 40, 55	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	505	MET	2.8
2	B	584	LEU	2.7
1	A	185	SER	2.5
1	C	209	PRO	2.5
2	D	533	ASP	2.5
1	C	38	TYR	2.4
1	A	184	ASP	2.3
1	A	209	PRO	2.2
1	A	239	ALA	2.1
1	C	395	PRO	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLU	B	600	10/10	0.90	0.09	22,31,42,49	0
3	GLU	D	601	10/10	0.91	0.10	14,22,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.