Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 10:06 AM EDT

PDB ID	:	4OTU
Title	:	Crystal structure of the gamma-glutamyltranspeptidase from Bacillus licheniformis in complex with L-Glutamate
Authors	:	Merlino, A.
Deposited on	:	2014-02-14
Resolution	:	3.02 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:

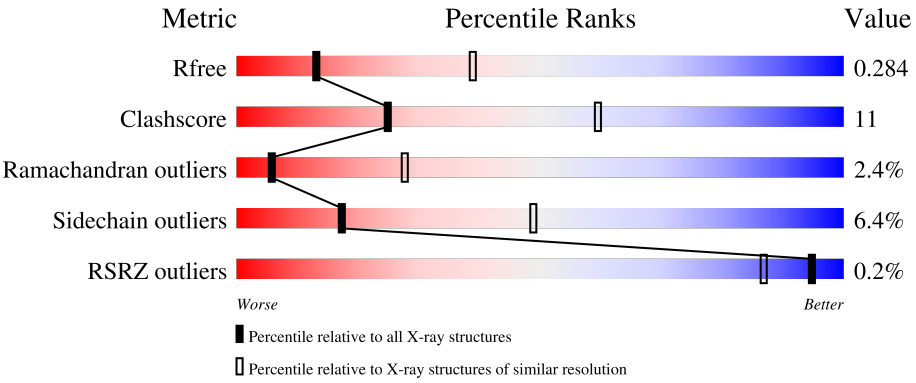
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 <=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	398	66% 22% · 9%
2	B	187	73% 23% ·· ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GLU	B	602	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4222 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 glutamyl transpeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2800	1774	462	550	14	0	0	0

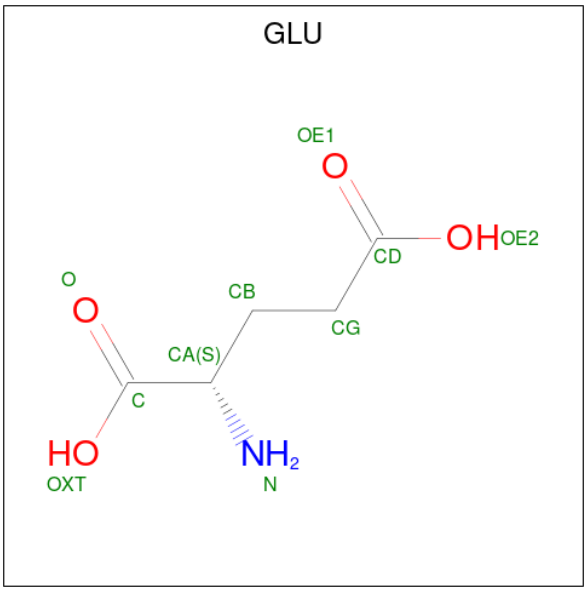
- Molecule 2 is a protein called Gamma-glutamyltranspeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	182	1410	893	233	280	4	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	B	1	1	1	0	0

- Molecule 4 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



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

- Molecule 5 is water.

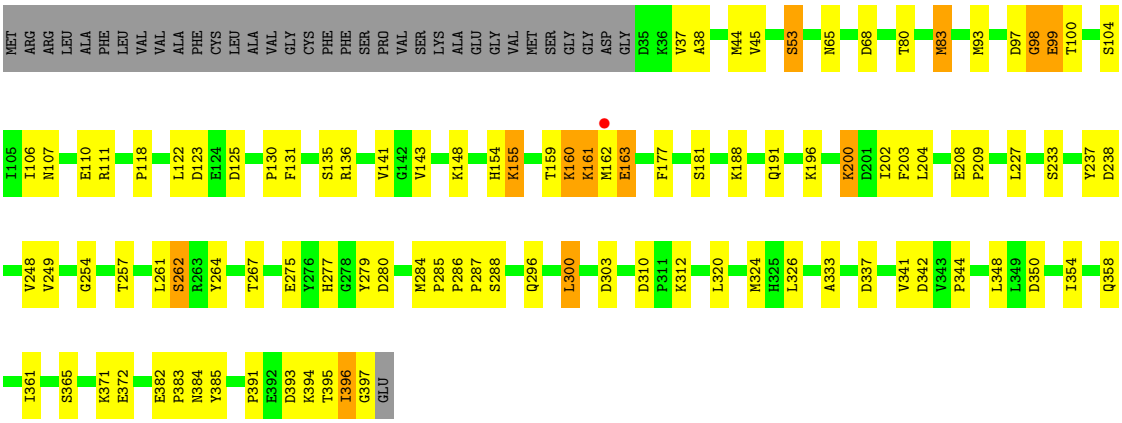
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			1	1		

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 glutamyl transpeptidase

Chain A:



• Molecule 2: Gamma-glutamyltranspeptidase

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.63Å 60.47Å 145.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.99 – 3.02 27.99 – 3.03	Depositor EDS
% Data completeness (in resolution range)	91.6 (27.99-3.02) 91.8 (27.99-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 3.05Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.202 , 0.288 0.204 , 0.284	Depositor DCC
R_{free} test set	485 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	50.2	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 2.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.089 for k,h,-l	Xtriage
Reported twinning fraction	0.101 for H, K, L 0.899 for K, H, -L	Depositor
Outliers	0 of 10094 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4222	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.54	0/2861	0.79	0/3861
2	B	0.56	0/1441	0.73	0/1961
All	All	0.55	0/4302	0.77	0/5822

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	53	SER	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	2800	0	2754	67	0
2	B	1410	0	1367	38	0
3	B	1	0	0	0	0
4	B	10	0	5	8	0
5	B	1	0	0	0	0
All	All	4222	0	4126	90	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 11.

All (90) 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:98:GLY:HA3	1:A:99:GLU:CB	2.11	0.80
1:A:161:LYS:CB	1:A:162:MET:HA	2.16	0.75
2:B:476:THR:O	2:B:553:SER:OG	2.03	0.75
2:B:399:THR:HG1	4:B:602:GLU:CD	1.90	0.74
1:A:161:LYS:HB3	1:A:162:MET:HA	1.70	0.74
1:A:111:ARG:NH1	2:B:455:ASN:O	2.22	0.71
2:B:399:THR:OG1	4:B:602:GLU:OE1	2.08	0.71
1:A:159:THR:O	1:A:160:LYS:HG3	1.95	0.67
1:A:320:LEU:O	1:A:324:MET:HG3	1.97	0.65
1:A:161:LYS:CG	1:A:162:MET:HA	2.27	0.65
1:A:300:LEU:HD12	1:A:354:ILE:HG23	1.78	0.64
1:A:45:VAL:HG22	2:B:404:VAL:HG22	1.80	0.64
1:A:248:VAL:HG21	2:B:429:PRO:HD3	1.80	0.63
1:A:98:GLY:HA3	1:A:99:GLU:HB2	1.81	0.63
1:A:238:ASP:OD1	1:A:262:SER:HB3	1.98	0.63
2:B:403:THR:OG1	2:B:476:THR:HG21	1.99	0.62
1:A:333:ALA:HB2	1:A:372:GLU:HG2	1.79	0.62
2:B:517:LEU:O	2:B:540:LYS:NZ	2.30	0.62
1:A:131:PHE:O	1:A:135:SER:HB2	2.00	0.62
2:B:399:THR:OG1	4:B:602:GLU:CD	2.38	0.62
1:A:107:ASN:HB3	1:A:267:THR:HG23	1.83	0.61
1:A:275:GLU:HA	1:A:279:TYR:O	2.01	0.60
1:A:249:VAL:HG12	1:A:254:GLY:HA3	1.82	0.60
1:A:393:ASP:O	1:A:395:THR:N	2.31	0.59
1:A:80:THR:HA	1:A:177:PHE:CZ	2.39	0.58
1:A:287:PRO:HB3	1:A:337:ASP:HA	1.85	0.58
2:B:467:VAL:HG11	2:B:497:PHE:CZ	2.39	0.58
2:B:399:THR:HG23	2:B:417:THR:HB	1.85	0.57
1:A:98:GLY:HA3	1:A:99:GLU:HB3	1.83	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:461:SER:N	4:B:602:GLU:OXT	2.31	0.57
1:A:188:LYS:O	1:A:191:GLN:HG3	2.05	0.56
2:B:443:ASP:OD2	2:B:450:ASN:HB3	2.05	0.56
1:A:141:VAL:HG22	2:B:424:THR:HG21	1.89	0.55
1:A:65:ASN:ND2	1:A:68:ASP:OD2	2.40	0.54
1:A:143:VAL:HG13	1:A:261:LEU:HD13	1.91	0.53
1:A:296:GLN:NE2	1:A:348:LEU:O	2.42	0.52
1:A:161:LYS:HA	1:A:163:GLU:H	1.74	0.52
2:B:484:THR:HG22	2:B:513:TYR:CG	2.45	0.51
1:A:382:GLU:HB2	1:A:383:PRO:HD2	1.93	0.50
1:A:310:ASP:OD1	1:A:312:LYS:N	2.38	0.49
1:A:161:LYS:HG2	1:A:163:GLU:N	2.27	0.49
1:A:37:VAL:HG12	1:A:38:ALA:N	2.28	0.49
1:A:123:ASP:OD1	1:A:125:ASP:N	2.40	0.49
1:A:118:PRO:HG3	2:B:453:GLN:NE2	2.28	0.48
1:A:154:HIS:NE2	1:A:160:LYS:O	2.30	0.48
1:A:200:LYS:HB2	1:A:204:LEU:HD12	1.96	0.47
1:A:350:ASP:O	1:A:354:ILE:HG12	2.14	0.47
1:A:154:HIS:O	1:A:155:LYS:CB	2.62	0.47
1:A:396:ILE:HG13	1:A:397:GLY:N	2.29	0.47
1:A:208:GLU:HB3	1:A:209:PRO:CD	2.45	0.47
2:B:484:THR:HG22	2:B:513:TYR:CD1	2.50	0.47
1:A:333:ALA:CB	1:A:372:GLU:HG2	2.45	0.46
1:A:248:VAL:HG21	2:B:429:PRO:CD	2.44	0.45
2:B:423:GLY:C	2:B:437:ASN:HD22	2.20	0.45
1:A:208:GLU:HB3	1:A:209:PRO:HD2	1.98	0.45
1:A:344:PRO:O	1:A:348:LEU:HG	2.17	0.45
1:A:280:ASP:HB2	2:B:468:PHE:HB2	1.99	0.44
1:A:341:VAL:HA	1:A:384:ASN:HD21	1.82	0.44
2:B:529:ASP:OD1	2:B:530:VAL:HG23	2.17	0.44
2:B:403:THR:CB	2:B:476:THR:HG21	2.48	0.44
2:B:417:THR:HG21	4:B:602:GLU:HB2	1.98	0.44
1:A:83:MET:HB3	2:B:422:PHE:CE1	2.51	0.44
1:A:303:ASP:OD2	1:A:358:GLN:NE2	2.31	0.44
1:A:148:LYS:HG3	1:A:237:TYR:CE2	2.52	0.44
2:B:520:TYR:HB2	2:B:540:LYS:O	2.18	0.43
2:B:399:THR:HA	2:B:417:THR:CB	2.48	0.43
1:A:280:ASP:O	2:B:468:PHE:N	2.48	0.43
1:A:385:TYR:CD2	2:B:449:ALA:HB2	2.54	0.43
1:A:161:LYS:HG2	1:A:162:MET:HA	1.97	0.43
1:A:44:MET:HB3	2:B:405:THR:HG22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:MET:HB3	1:A:106:ILE:HB	2.01	0.42
2:B:441:ASP:OD2	4:B:602:GLU:N	2.52	0.42
1:A:118:PRO:HA	2:B:452:VAL:HB	2.00	0.42
1:A:97:ASP:HB3	1:A:100:THR:HB	2.01	0.42
2:B:399:THR:OG1	4:B:602:GLU:CG	2.67	0.42
1:A:286:PRO:HA	1:A:288:SER:N	2.35	0.42
1:A:110:GLU:OE1	2:B:438:GLU:HG2	2.19	0.42
1:A:161:LYS:HG2	1:A:162:MET:C	2.40	0.42
1:A:107:ASN:HB3	1:A:267:THR:CG2	2.48	0.41
1:A:136:ARG:HD3	1:A:196:LYS:HE2	2.02	0.41
2:B:476:THR:O	2:B:553:SER:CB	2.68	0.41
1:A:202:ILE:HG23	1:A:203:PHE:CD1	2.56	0.41
2:B:484:THR:HG22	2:B:513:TYR:CD2	2.56	0.41
1:A:284:MET:HA	1:A:285:PRO:HD2	1.90	0.41
1:A:248:VAL:CG2	2:B:429:PRO:HD3	2.50	0.41
1:A:326:LEU:HD12	1:A:361:ILE:HD11	2.02	0.41
1:A:159:THR:O	1:A:160:LYS:CG	2.68	0.40
1:A:203:PHE:CZ	2:B:434:PHE:HE2	2.39	0.40
2:B:419:GLU:HA	4:B:602:GLU:HG3	2.03	0.40
1:A:143:VAL:HG11	1:A:264:TYR:HB2	2.04	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	361/398 (91%)	326 (90%)	24 (7%)	11 (3%)	4 22
2	B	180/187 (96%)	167 (93%)	11 (6%)	2 (1%)	14 48
All	All	541/585 (92%)	493 (91%)	35 (6%)	13 (2%)	6 28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	GLU
1	A	155	LYS
1	A	391	PRO
1	A	394	LYS
1	A	53	SER
1	A	98	GLY
2	B	419	GLU
1	A	163	GLU
1	A	396	ILE
1	A	160	LYS
1	A	365	SER
2	B	480	PRO
1	A	161	LYS

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	297/325 (91%)	283 (95%)	14 (5%)	26 61
2	B	158/162 (98%)	143 (90%)	15 (10%)	8 31
All	All	455/487 (93%)	426 (94%)	29 (6%)	17 49

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	MET
1	A	104	SER
1	A	122	LEU
1	A	130	PRO
1	A	181	SER
1	A	200	LYS
1	A	227	LEU
1	A	233	SER
1	A	257	THR
1	A	262	SER
1	A	277	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	300	LEU
1	A	342	ASP
1	A	371	LYS
2	B	399	THR
2	B	403	THR
2	B	414	TYR
2	B	416	THR
2	B	419	GLU
2	B	470	ASP
2	B	483	THR
2	B	514	THR
2	B	532	ARG
2	B	537	PHE
2	B	543	SER
2	B	561	LYS
2	B	562	THR
2	B	574	THR
2	B	576	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	78	ASN
1	A	137	HIS
1	A	139	ASN
1	A	191	GLN
1	A	390	GLN
2	B	437	ASN
2	B	453	GLN
2	B	550	ASN
2	B	552	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
4	GLU	B	602	-	8,9,9	1.21	1 (12%)	10,11,11	1.32	2 (20%)

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
4	GLU	B	602	-	-	3/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	GLU	OXT-C	-2.68	1.21	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	602	GLU	OXT-C-O	-2.37	118.70	124.09
4	B	602	GLU	OXT-C-CA	2.01	120.21	113.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	602	GLU	OXT-C-CA-N
4	B	602	GLU	O-C-CA-N
4	B	602	GLU	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	GLU	8	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

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^{th} 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	363/398 (91%)	-0.40	1 (0%) 94 83	27, 50, 69, 101	0
2	B	182/187 (97%)	-0.57	0 100 100	19, 38, 60, 67	0
All	All	545/585 (93%)	-0.46	1 (0%) 95 87	19, 45, 68, 101	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	MET	2.6

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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(Å^2)	Q<0.9
4	GLU	B	602	10/10	0.95	0.23	16,16,16,17	10
3	MG	B	601	1/1	0.98	0.24	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.