



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 05:57 PM EDT

PDB ID : 2DG5  
Title : Crystal Structure of Gamma-glutamyl transpeptidase from Escherichia coli in complex with hydrolyzed Glutathione  
Authors : Okada, T.; Wada, K.; Fukuyama, K.  
Deposited on : 2006-03-08  
Resolution : 1.60 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

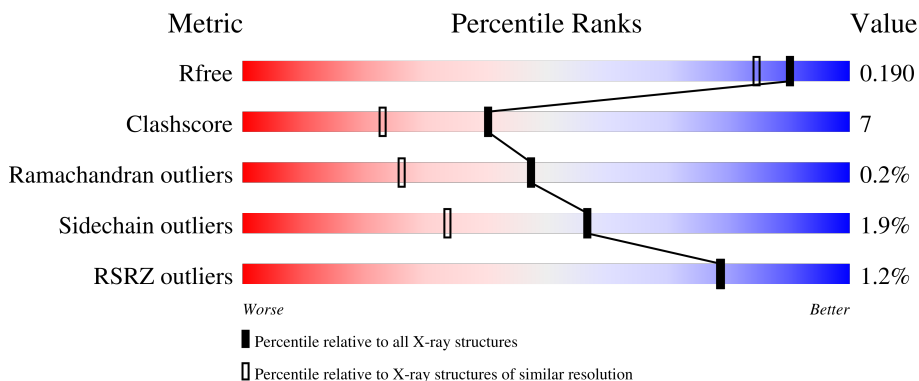
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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  $\geq 3$ , 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	366	 81% 13% . .
1	C	366	 2% 84% 11% . .
2	B	190	 89% 11% .
2	D	190	 86% 13% .

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9031 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	351	2661	1680	448	522	11	0	0	0
1	C	351	2661	1680	448	522	11	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MSE	MET	modified residue	UNP P18956
A	99	MSE	MET	modified residue	UNP P18956
A	116	MSE	MET	modified residue	UNP P18956
A	125	MSE	MET	modified residue	UNP P18956
A	164	MSE	MET	modified residue	UNP P18956
A	233	MSE	MET	modified residue	UNP P18956
A	255	MSE	MET	modified residue	UNP P18956
A	290	MSE	MET	modified residue	UNP P18956
A	312	MSE	MET	modified residue	UNP P18956
A	323	MSE	MET	modified residue	UNP P18956
A	326	MSE	MET	modified residue	UNP P18956
C	50	MSE	MET	modified residue	UNP P18956
C	99	MSE	MET	modified residue	UNP P18956
C	116	MSE	MET	modified residue	UNP P18956
C	125	MSE	MET	modified residue	UNP P18956
C	164	MSE	MET	modified residue	UNP P18956
C	233	MSE	MET	modified residue	UNP P18956
C	255	MSE	MET	modified residue	UNP P18956
C	290	MSE	MET	modified residue	UNP P18956
C	312	MSE	MET	modified residue	UNP P18956
C	323	MSE	MET	modified residue	UNP P18956
C	326	MSE	MET	modified residue	UNP P18956

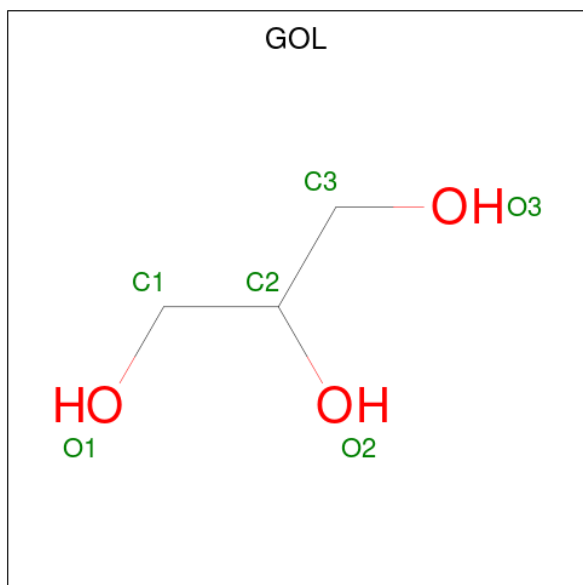
- Molecule 2 is a protein called Gamma-glutamyltranspeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	190	Total	C	N	O	Se	0	0	0
			1407	882	238	282	5			
2	D	190	Total	C	N	O	Se	0	0	0
			1407	882	238	282	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	431	MSE	MET	modified residue	UNP P18956
B	464	MSE	MET	modified residue	UNP P18956
B	494	MSE	MET	modified residue	UNP P18956
B	550	MSE	MET	modified residue	UNP P18956
B	557	MSE	MET	modified residue	UNP P18956
D	431	MSE	MET	modified residue	UNP P18956
D	464	MSE	MET	modified residue	UNP P18956
D	494	MSE	MET	modified residue	UNP P18956
D	550	MSE	MET	modified residue	UNP P18956
D	557	MSE	MET	modified residue	UNP P18956

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

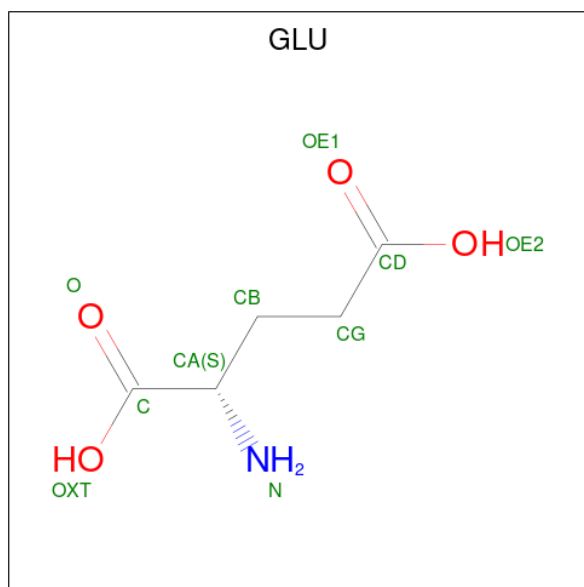


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

- Molecule 5 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



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

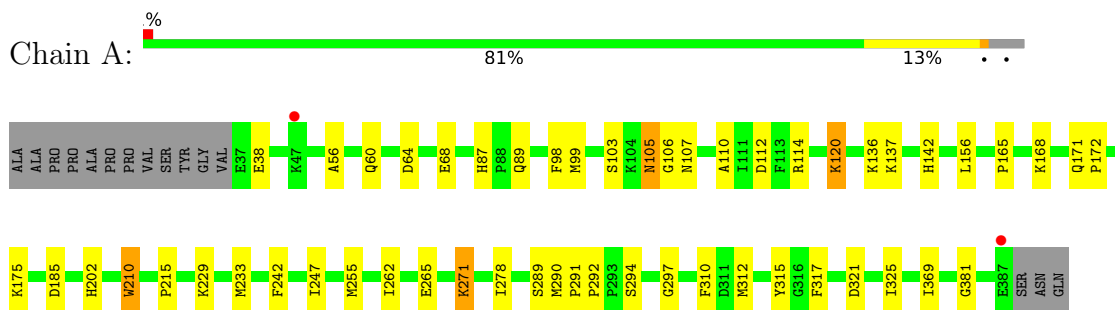
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	292	Total O 292 292	0	0
6	B	156	Total O 156 156	0	0
6	C	278	Total O 278 278	0	0
6	D	141	Total O 141 141	0	0

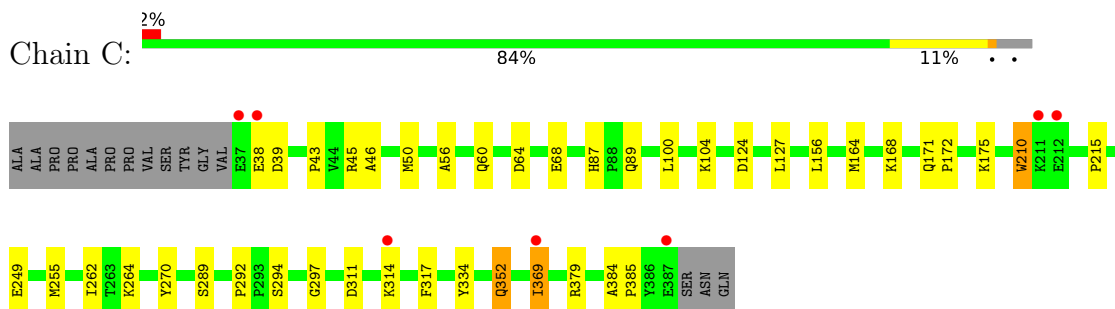
### 3 Residue-property plots [i](#)

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.

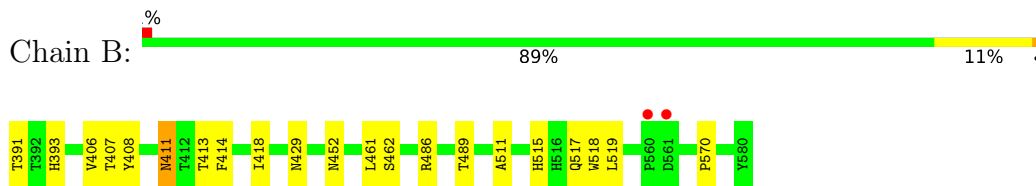
- Molecule 1: Gamma-glutamyltranspeptidase



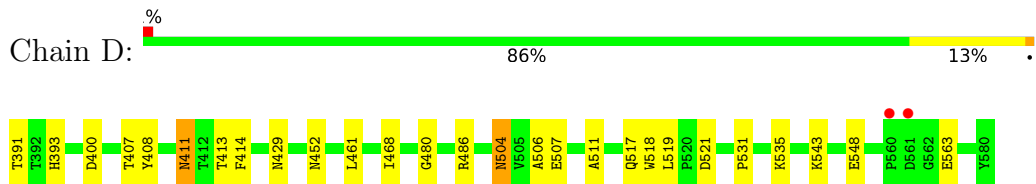
- Molecule 1: Gamma-glutamyltranspeptidase



- Molecule 2: Gamma-glutamyltranspeptidase



- Molecule 2: Gamma-glutamyltranspeptidase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.14Å 126.60Å 129.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.34 – 1.60 46.33 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.8 (46.34-1.60) 97.9 (46.33-1.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.64 (at 1.60Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.179 , 0.195 0.175 , 0.190	Depositor DCC
$R_{free}$ test set	8457 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.2	Xtrriage
Anisotropy	0.534	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.009 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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, 0.333 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: CA, GOL

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	0.28	0/2703	0.58	0/3639
1	C	0.27	0/2703	0.57	0/3639
2	B	0.28	0/1429	0.69	0/1937
2	D	0.28	0/1429	0.68	0/1937
All	All	0.28	0/8264	0.61	0/11152

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	C	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	C	270	TYR	Sidechain

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2661	0	2626	56	0
1	C	2661	0	2626	32	0
2	B	1407	0	1392	16	0
2	D	1407	0	1392	24	0
3	A	6	0	8	1	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	10	0	5	3	0
5	D	10	0	5	2	0
6	A	292	0	0	3	0
6	B	156	0	0	2	0
6	C	278	0	0	1	0
6	D	141	0	0	0	0
All	All	9031	0	8054	116	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 7.

All (116) 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:PHE:CD1	1:A:290:MSE:HE2	2.04	0.93
2:B:391:THR:OG1	5:B:601:GLU:CD	2.10	0.91
1:A:290:MSE:HE3	1:A:291:PRO:HD2	1.56	0.87
1:A:310:PHE:CB	1:A:312:MSE:HE3	2.06	0.86
2:D:391:THR:OG1	5:D:602:GLU:CD	2.17	0.82
1:A:98:PHE:HD1	1:A:290:MSE:HE2	1.46	0.78
1:C:38:GLU:OE2	1:C:43:PRO:HD2	1.83	0.78
2:D:504:ASN:ND2	2:D:507:GLU:H	1.82	0.78
1:A:310:PHE:HB2	1:A:312:MSE:HE3	1.66	0.76
1:A:310:PHE:HB3	1:A:312:MSE:HE3	1.71	0.71
1:A:312:MSE:HA	1:A:312:MSE:HE2	1.72	0.71
1:A:136:LYS:HD3	1:A:137:LYS:N	2.07	0.69
1:A:171:GLN:HG3	1:A:175:LYS:HZ2	1.59	0.67
1:A:38:GLU:HA	2:D:548:GLU:HA	1.75	0.67
2:D:518:TRP:CD2	2:D:519:LEU:HD13	2.31	0.66
1:C:311:ASP:OD1	1:C:314:LYS:HG3	1.96	0.66
2:D:393:HIS:HD2	2:D:407:THR:OG1	1.80	0.65
1:A:168:LYS:NZ	1:A:168:LYS:HB3	2.12	0.65
1:C:369:ILE:H	1:C:369:ILE:HD13	1.62	0.64
2:B:411:ASN:HB3	2:B:429:ASN:OD1	1.99	0.63
1:C:171:GLN:HG3	1:C:175:LYS:NZ	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:GLN:HE21	1:C:352:GLN:H	1.48	0.62
2:D:411:ASN:HB3	2:D:429:ASN:OD1	1.99	0.62
2:D:504:ASN:HD22	2:D:504:ASN:C	2.02	0.62
2:D:521:ASP:O	2:D:543:LYS:HE3	2.00	0.61
2:B:393:HIS:HD2	2:B:407:THR:OG1	1.82	0.61
1:A:136:LYS:HD3	1:A:136:LYS:C	2.21	0.60
2:D:452:ASN:HD21	2:D:461:LEU:H	1.50	0.60
1:C:369:ILE:HD13	1:C:369:ILE:N	2.16	0.59
1:C:352:GLN:H	1:C:352:GLN:NE2	2.00	0.58
1:C:104:LYS:HD3	2:D:400:ASP:HB3	1.85	0.58
1:C:171:GLN:HG3	1:C:175:LYS:HZ2	1.69	0.58
1:A:105:ASN:ND2	1:A:107:ASN:H	2.02	0.57
2:B:452:ASN:HD21	2:B:461:LEU:H	1.53	0.57
2:B:391:THR:OG1	5:B:601:GLU:CG	2.51	0.57
1:C:210:TRP:CH2	1:C:215:PRO:HB3	2.40	0.57
2:B:489:THR:OG1	2:B:515:HIS:HD2	1.89	0.55
1:C:89:GLN:HB2	2:D:413:THR:HG23	1.86	0.55
1:A:271:LYS:NZ	1:A:271:LYS:HB3	2.21	0.55
1:C:289:SER:HB3	1:C:297:GLY:HA2	1.88	0.55
1:A:120:LYS:HD2	6:A:1175:HOH:O	2.09	0.53
1:C:255:MSE:HG3	1:C:262:ILE:HB	1.91	0.53
1:A:255:MSE:HG3	1:A:262:ILE:HB	1.90	0.53
2:D:531:PRO:O	2:D:535:LYS:HG3	2.09	0.52
1:C:369:ILE:H	1:C:369:ILE:CD1	2.21	0.52
1:A:105:ASN:C	1:A:105:ASN:HD22	2.11	0.51
1:A:171:GLN:HG3	1:A:175:LYS:NZ	2.24	0.51
1:A:156:LEU:C	1:A:156:LEU:HD23	2.31	0.50
1:C:164:MSE:HE2	1:C:168:LYS:HB3	1.92	0.50
2:D:391:THR:OG1	5:D:602:GLU:CG	2.59	0.50
1:A:210:TRP:CH2	1:A:215:PRO:HB3	2.46	0.50
2:D:517:GLN:O	2:D:518:TRP:HB3	2.11	0.50
1:C:56:ALA:O	1:C:60:GLN:HG3	2.13	0.48
1:C:156:LEU:C	1:C:156:LEU:HD23	2.33	0.48
1:A:105:ASN:ND2	1:A:105:ASN:C	2.67	0.48
2:B:570:PRO:HA	6:B:1862:HOH:O	2.12	0.48
1:C:64:ASP:O	1:C:68:GLU:HG3	2.13	0.48
1:A:171:GLN:HB3	1:A:172:PRO:HD3	1.96	0.47
1:A:142:HIS:HD2	1:A:255:MSE:HE2	1.79	0.47
1:A:289:SER:HB3	1:A:297:GLY:HA2	1.96	0.47
1:A:321:ASP:HB3	1:A:369:ILE:HD11	1.96	0.47
1:C:124:ASP:HB3	1:C:127:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:PRO:HG2	1:A:168:LYS:HG3	1.96	0.47
2:D:504:ASN:HD21	2:D:507:GLU:H	1.57	0.47
1:A:98:PHE:HB3	1:A:290:MSE:SE	2.65	0.47
2:B:517:GLN:O	2:B:518:TRP:HB3	2.14	0.46
2:D:413:THR:O	2:D:414:PHE:HB2	2.15	0.46
1:A:87:HIS:HE1	6:B:1737:HOH:O	1.99	0.46
1:C:249:GLU:HA	1:C:264:LYS:HD3	1.98	0.46
2:D:452:ASN:ND2	2:D:461:LEU:H	2.14	0.45
2:D:504:ASN:HD22	2:D:506:ALA:N	2.15	0.45
1:A:56:ALA:O	1:A:60:GLN:HG3	2.17	0.45
1:C:100:LEU:HD23	2:D:468:ILE:HG13	1.99	0.45
1:C:171:GLN:HB3	1:C:172:PRO:HD3	1.99	0.45
1:C:292:PRO:HA	1:C:294:SER:N	2.32	0.45
1:A:312:MSE:HE2	1:A:312:MSE:CA	2.44	0.45
1:C:87:HIS:HD2	6:C:1102:HOH:O	1.99	0.44
1:C:314:LYS:HB3	1:C:314:LYS:NZ	2.32	0.44
2:B:413:THR:O	2:B:414:PHE:HB2	2.17	0.44
2:D:518:TRP:O	2:D:519:LEU:HD12	2.17	0.44
1:A:103:SER:HB2	1:A:105:ASN:ND2	2.33	0.44
1:A:292:PRO:HA	1:A:294:SER:N	2.32	0.44
1:A:317:PHE:CZ	2:B:511:ALA:HB1	2.53	0.43
1:A:105:ASN:HD22	1:A:106:GLY:N	2.16	0.43
1:A:278:ILE:HG12	1:A:291:PRO:HB3	2.00	0.43
1:C:369:ILE:N	1:C:369:ILE:CD1	2.82	0.43
2:D:393:HIS:CD2	2:D:480:GLY:HA3	2.54	0.43
1:A:168:LYS:HB3	1:A:168:LYS:HZ2	1.82	0.43
1:A:87:HIS:HD2	6:A:1078:HOH:O	2.02	0.43
1:A:381:GLY:HA2	3:A:703:GOL:H11	2.00	0.43
1:A:99:MSE:HG3	2:B:406:VAL:HG22	2.00	0.42
1:A:242:PHE:HA	1:A:247:ILE:HB	2.00	0.42
1:A:89:GLN:HB3	2:B:413:THR:HG23	2.02	0.42
1:A:185:ASP:HB3	1:C:45:ARG:NH1	2.34	0.42
1:A:312:MSE:HE1	1:A:325:ILE:CD1	2.50	0.42
1:C:384:ALA:N	1:C:385:PRO:HD2	2.35	0.42
1:A:156:LEU:HD23	1:A:156:LEU:O	2.20	0.41
2:B:452:ASN:ND2	2:B:461:LEU:H	2.16	0.41
2:B:391:THR:CB	5:B:601:GLU:CD	2.89	0.41
2:D:504:ASN:HD22	2:D:506:ALA:H	1.67	0.41
1:A:112:ASP:OD1	1:A:112:ASP:C	2.59	0.41
1:A:312:MSE:HE1	1:A:325:ILE:HD12	2.02	0.41
1:A:114:ARG:CZ	2:B:462:SER:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:ALA:HB3	1:C:50:MSE:HE3	2.02	0.41
1:A:312:MSE:HE2	1:A:315:TYR:CD1	2.56	0.41
1:A:64:ASP:O	1:A:68:GLU:HG3	2.21	0.41
1:A:171:GLN:HE21	1:A:175:LYS:NZ	2.17	0.41
1:A:110:ALA:HB1	1:A:290:MSE:HE1	2.03	0.41
1:A:165:PRO:HD2	1:A:168:LYS:HD3	2.03	0.41
1:C:317:PHE:CZ	2:D:511:ALA:HB1	2.56	0.41
1:A:229:LYS:HE3	1:A:233:MSE:SE	2.71	0.41
1:C:334:TYR:CD2	2:D:517:GLN:HA	2.57	0.40
1:C:171:GLN:HE21	1:C:171:GLN:HA	1.86	0.40
1:A:265:GLU:HG3	6:A:1294:HOH:O	2.21	0.40
1:A:202:HIS:CE1	2:B:418:ILE:HG12	2.57	0.40
1:A:310:PHE:HB3	1:A:312:MSE:CE	2.44	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	349/366 (95%)	342 (98%)	7 (2%)	0	100	100
1	C	349/366 (95%)	342 (98%)	7 (2%)	0	100	100
2	B	188/190 (99%)	182 (97%)	5 (3%)	1 (0%)	29	11
2	D	188/190 (99%)	181 (96%)	6 (3%)	1 (0%)	29	11
All	All	1074/1112 (97%)	1047 (98%)	25 (2%)	2 (0%)	47	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	411	ASN
2	D	411	ASN

### 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	276/276 (100%)	272 (99%)	4 (1%)	67	47
1	C	276/276 (100%)	271 (98%)	5 (2%)	59	36
2	B	154/149 (103%)	151 (98%)	3 (2%)	57	34
2	D	154/149 (103%)	150 (97%)	4 (3%)	46	21
All	All	860/850 (101%)	844 (98%)	16 (2%)	57	34

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	120	LYS
1	A	210	TRP
1	A	271	LYS
2	B	408	TYR
2	B	486	ARG
2	B	519	LEU
1	C	39	ASP
1	C	210	TRP
1	C	352	GLN
1	C	369	ILE
1	C	379	ARG
2	D	408	TYR
2	D	486	ARG
2	D	504	ASN
2	D	563	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	87	HIS
1	A	105	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	107	ASN
1	A	171	GLN
1	A	250	GLN
1	A	253	GLN
1	A	370	ASN
2	B	393	HIS
2	B	452	ASN
2	B	515	HIS
1	C	42	HIS
1	C	87	HIS
1	C	132	ASN
1	C	171	GLN
1	C	201	ASN
1	C	352	GLN
1	C	370	ASN
2	D	393	HIS
2	D	452	ASN
2	D	497	ASN
2	D	504	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
5	GLU	B	601	-	8,9,9	0.90	0	10,11,11	2.91	3 (30%)
5	GLU	D	602	-	8,9,9	1.67	1 (12%)	10,11,11	4.54	3 (30%)
3	GOL	A	703	-	5,5,5	0.32	0	5,5,5	0.26	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
5	GLU	B	601	-	-	0/9/9/9	-
5	GLU	D	602	-	-	1/9/9/9	-
3	GOL	A	703	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	602	GLU	CG-CD	4.09	1.60	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	602	GLU	OE2-CD-OE1	-13.12	90.59	123.30
5	B	601	GLU	OE2-CD-OE1	6.11	138.53	123.30
5	B	601	GLU	CB-CG-CD	5.46	126.99	112.51
5	D	602	GLU	CB-CG-CD	4.36	124.08	112.51
5	D	602	GLU	OE1-CD-CG	-3.29	112.53	123.08
5	B	601	GLU	OE1-CD-CG	-3.25	112.62	123.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	602	GLU	OE2-CD-CG-CB

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601	GLU	3	0
5	D	602	GLU	2	0
3	A	703	GOL	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, 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	340/366 (92%)	-0.29	2 (0%) 89 89	9, 14, 24, 40	0
1	C	340/366 (92%)	-0.12	7 (2%) 63 62	8, 15, 26, 45	0
2	B	185/190 (97%)	-0.23	2 (1%) 80 80	9, 12, 20, 38	0
2	D	185/190 (97%)	-0.21	2 (1%) 80 80	9, 12, 24, 37	0
All	All	1050/1112 (94%)	-0.21	13 (1%) 79 78	8, 13, 25, 45	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	38	GLU	5.9
2	D	560	PRO	4.1
2	D	561	ASP	4.1
1	C	37	GLU	3.7
1	C	387	GLU	3.1
2	B	561	ASP	3.1
1	C	369	ILE	2.7
1	C	211	LYS	2.5
1	A	387	GLU	2.5
1	C	212	GLU	2.4
1	A	47	LYS	2.3
1	C	314	LYS	2.3
2	B	560	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	GOL	A	703	6/6	0.87	0.17	24,27,28,28	0
5	GLU	B	601	10/10	0.90	0.11	10,11,19,20	0
5	GLU	D	602	10/10	0.92	0.11	8,9,19,22	0
4	CA	B	701	1/1	0.99	0.06	13,13,13,13	0
4	CA	D	702	1/1	0.99	0.06	12,12,12,12	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.