



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 08:20 PM GMT

PDB ID : 2DBU  
Title : Crystal Structure of Gamma-glutamyltranspeptidase from Escherichia coli  
Authors : Okada, T.; Wada, K.; Fukuyama, K.  
Deposited on : 2005-12-16  
Resolution : 1.95 Å (reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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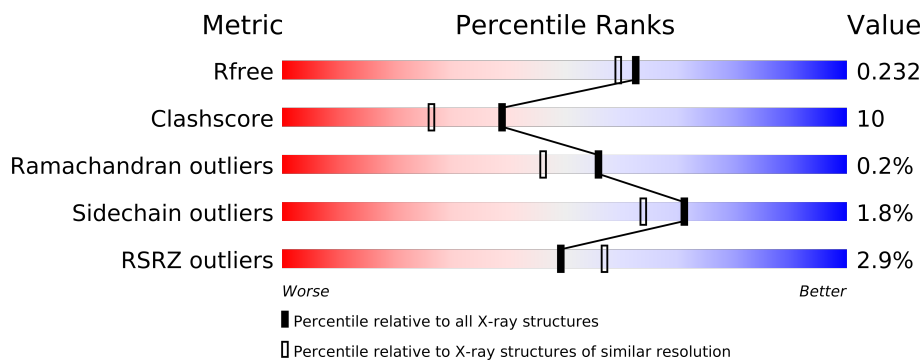
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	366	
1	C	366	
2	B	190	
2	D	190	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8846 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	359	Total	C	N	O	Se	0	0	0
			2716	1717	456	532	11			
1	C	358	Total	C	N	O	Se	0	0	0
			2711	1714	455	531	11			

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 1407	C 882	N 238	O 282	Se 5	0	0	0
2	D	190	Total 1407	C 882	N 238	O 282	Se 5	0	0	0

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 water.

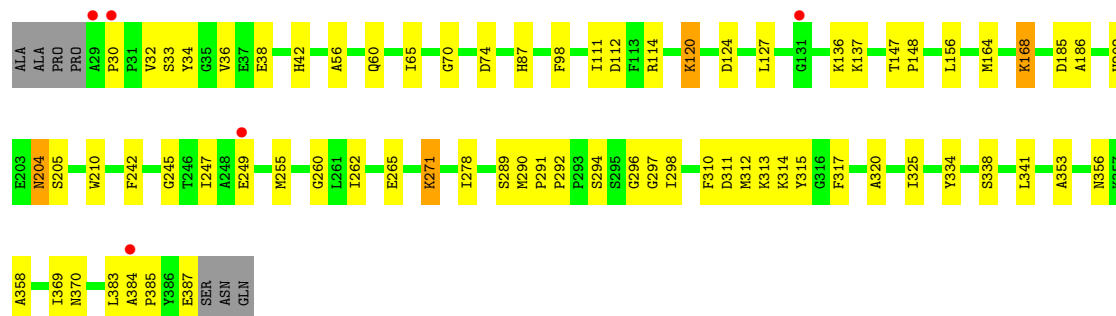
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	201	Total 201	O 201	0	0
3	B	105	Total 105	O 105	0	0
3	C	198	Total 198	O 198	0	0
3	D	101	Total 101	O 101	0	0

### 3 Residue-property plots

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.

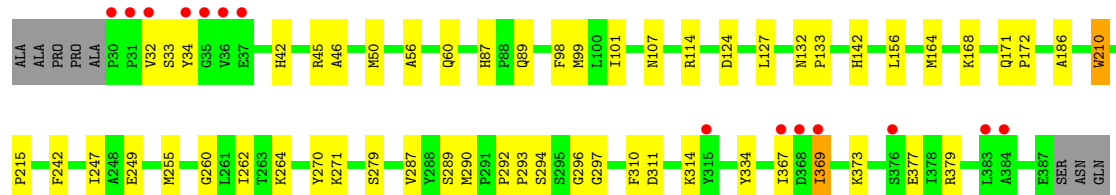
#### • Molecule 1: Gamma-glutamyltranspeptidase

Chain A: 



#### • Molecule 1: Gamma-glutamyltranspeptidase

Chain C: 



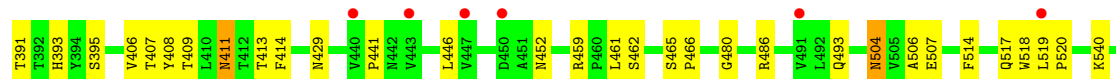
#### • Molecule 2: Gamma-glutamyltranspeptidase

Chain B: 



#### • Molecule 2: Gamma-glutamyltranspeptidase

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.70Å 126.90Å 128.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.39 – 1.95 46.39 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.7 (46.39-1.95) 96.6 (46.39-1.95)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.207 , 0.231 0.207 , 0.232	Depositor DCC
$R_{free}$ test set	4590 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.5	EDS
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 94641 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8846	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.30	0/2761	0.56	0/3721
1	C	0.31	0/2756	0.57	0/3713
2	B	0.31	0/1429	0.67	0/1937
2	D	0.31	0/1429	0.66	0/1937
All	All	0.30	0/8375	0.60	0/11308

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2716	0	2680	79	0
1	C	2711	0	2676	44	0
2	B	1407	0	1392	27	0
2	D	1407	0	1392	33	0
3	A	201	0	0	5	0
3	B	105	0	0	4	0
3	C	198	0	0	3	0
3	D	101	0	0	2	0
All	All	8846	0	8140	158	0



Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (158) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:ASP:HB3	1:A:164:MSE:HE3	1.20	1.13
1:A:70:GLY:HA3	1:A:164:MSE:HE2	1.16	1.13
1:A:34:TYR:HA	2:B:557:MSE:HE1	1.30	1.12
1:A:65:ILE:HG23	1:A:164:MSE:HE1	1.26	1.08
1:A:74:ASP:CB	1:A:164:MSE:HE3	1.92	0.98
1:A:70:GLY:CA	1:A:164:MSE:HE2	1.95	0.97
1:A:70:GLY:HA3	1:A:164:MSE:CE	1.98	0.94
1:A:65:ILE:CG2	1:A:164:MSE:HE1	2.01	0.90
1:A:34:TYR:CD2	2:B:557:MSE:HE3	2.09	0.87
2:B:557:MSE:HE2	3:B:1119:HOH:O	1.80	0.82
1:A:312:MSE:HA	1:A:312:MSE:HE2	1.61	0.82
1:A:34:TYR:HA	2:B:557:MSE:CE	2.10	0.81
2:B:532:ASP:O	2:B:535:LYS:HG2	1.81	0.80
2:D:504:ASN:ND2	2:D:507:GLU:H	1.82	0.78
1:A:30:PRO:HD3	1:A:313:LYS:HE2	1.67	0.77
2:D:493:GLN:HE22	2:D:514:PHE:H	1.30	0.76
1:C:290:MSE:HE3	2:D:466:PRO:HG2	1.66	0.75
1:A:98:PHE:CD1	1:A:290:MSE:HE2	2.22	0.74
1:C:249:GLU:OE1	1:C:264:LYS:HD2	1.88	0.73
1:A:310:PHE:HB3	1:A:312:MSE:HE3	1.69	0.72
1:A:290:MSE:HE3	1:A:291:PRO:HD2	1.71	0.72
1:A:310:PHE:CB	1:A:312:MSE:HE3	2.21	0.71
2:D:411:ASN:HB3	2:D:429:ASN:OD1	1.92	0.69
1:A:204:ASN:HD22	1:A:205:SER:H	1.42	0.68
1:A:30:PRO:CD	1:A:313:LYS:HE2	2.25	0.67
1:A:369:ILE:HG23	1:A:370:ASN:OD1	1.95	0.66
1:C:164:MSE:HE2	1:C:168:LYS:HB3	1.78	0.66
2:D:504:ASN:HD21	2:D:507:GLU:H	1.45	0.65
1:C:99:MSE:HG3	2:D:406:VAL:HG22	1.81	0.62
1:A:278:ILE:HG12	1:A:291:PRO:HB3	1.80	0.62
2:B:411:ASN:HB3	2:B:429:ASN:OD1	2.00	0.62
1:C:255:MSE:HG3	1:C:262:ILE:HB	1.83	0.61
1:A:136:LYS:HD3	1:A:137:LYS:N	2.16	0.61
1:A:36:VAL:HB	1:A:38:GLU:OE2	2.01	0.61
1:A:136:LYS:HD3	1:A:136:LYS:C	2.21	0.60
2:D:504:ASN:C	2:D:504:ASN:HD22	2.05	0.60
2:D:393:HIS:HD2	2:D:407:THR:OG1	1.85	0.58
2:B:452:ASN:HD21	2:B:461:LEU:H	1.51	0.58
1:C:89:GLN:HB2	2:D:413:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:164:MSE:CE	1:C:168:LYS:HB3	2.33	0.57
1:C:124:ASP:HB3	1:C:127:LEU:HD12	1.84	0.57
1:A:36:VAL:HG23	1:A:38:GLU:HG2	1.87	0.57
1:A:34:TYR:HD2	2:B:557:MSE:HE3	1.67	0.56
1:A:34:TYR:CE2	2:B:559:GLY:HA2	2.41	0.56
1:C:296:GLY:HA3	2:D:465:SER:OG	2.05	0.56
1:A:204:ASN:HD22	1:A:205:SER:N	2.04	0.55
1:A:255:MSE:HG3	1:A:262:ILE:HB	1.90	0.54
1:C:87:HIS:HE1	3:D:1502:HOH:O	1.91	0.54
1:A:334:TYR:CD2	2:B:517:GLN:HA	2.43	0.53
1:A:289:SER:HB3	1:A:297:GLY:HA2	1.90	0.53
1:C:210:TRP:CH2	1:C:215:PRO:HB3	2.44	0.53
1:C:290:MSE:HE3	2:D:466:PRO:CG	2.36	0.53
1:C:292:PRO:HA	1:C:294:SER:N	2.25	0.52
1:A:383:LEU:O	1:A:387:GLU:HG3	2.10	0.52
2:D:518:TRP:O	2:D:519:LEU:HD12	2.09	0.52
1:C:98:PHE:HB3	1:C:290:MSE:SE	2.59	0.52
1:A:202:HIS:HE1	3:A:1026:HOH:O	1.92	0.52
2:B:393:HIS:HD2	2:B:407:THR:OG1	1.91	0.52
1:C:373:LYS:HB2	1:C:373:LYS:NZ	2.24	0.52
1:A:265:GLU:HG3	3:A:1263:HOH:O	2.09	0.52
1:C:32:VAL:HG12	1:C:33:SER:N	2.25	0.51
1:C:156:LEU:C	1:C:156:LEU:HD23	2.30	0.51
1:A:310:PHE:HB2	1:A:312:MSE:HE3	1.93	0.51
1:C:142:HIS:HD2	1:C:255:MSE:HE2	1.76	0.51
2:B:557:MSE:CE	3:B:1119:HOH:O	2.47	0.51
2:D:518:TRP:CD2	2:D:519:LEU:HD13	2.46	0.50
1:C:311:ASP:CG	1:C:314:LYS:HG3	2.31	0.50
1:A:156:LEU:C	1:A:156:LEU:HD23	2.31	0.50
1:A:242:PHE:HA	1:A:247:ILE:HB	1.93	0.50
1:A:32:VAL:HG12	1:A:33:SER:N	2.27	0.50
2:B:489:THR:OG1	2:B:515:HIS:HD2	1.95	0.49
1:C:289:SER:HB3	1:C:297:GLY:HA2	1.94	0.49
1:A:38:GLU:H	1:A:38:GLU:CD	2.14	0.49
1:A:120:LYS:HD3	3:A:1149:HOH:O	2.11	0.49
1:A:353:ALA:HB2	1:A:387:GLU:HG2	1.94	0.49
1:C:255:MSE:SE	1:C:260:GLY:HA3	2.63	0.49
1:A:311:ASP:HB3	1:A:314:LYS:HE3	1.93	0.49
1:A:204:ASN:N	1:A:204:ASN:HD22	2.11	0.49
1:C:32:VAL:CG1	1:C:33:SER:N	2.75	0.49
1:A:56:ALA:O	1:A:60:GLN:HG3	2.12	0.49
1:A:185:ASP:HB3	1:C:45:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:533:THR:O	2:B:537:LEU:HD23	2.13	0.48
1:A:98:PHE:HB3	1:A:290:MSE:SE	2.64	0.48
2:D:504:ASN:HD22	2:D:506:ALA:N	2.12	0.48
1:C:99:MSE:SE	1:C:101:ILE:HD11	2.64	0.48
1:C:369:ILE:HD13	1:C:369:ILE:N	2.29	0.48
1:A:312:MSE:HE2	1:A:315:TYR:HD2	1.79	0.47
1:A:114:ARG:CZ	2:B:462:SER:HB2	2.44	0.47
1:A:87:HIS:HE1	3:B:1198:HOH:O	1.98	0.47
2:D:441:PRO:HA	2:D:446:LEU:O	2.14	0.47
1:A:356:ASN:OD1	1:A:358:ALA:N	2.48	0.47
1:C:56:ALA:O	1:C:60:GLN:HG3	2.16	0.46
1:A:290:MSE:HG2	2:B:466:PRO:HG2	1.97	0.46
1:A:320:ALA:HA	2:B:537:LEU:HD21	1.96	0.46
2:D:393:HIS:HE1	2:D:395:SER:OG	1.97	0.46
1:C:279:SER:HA	1:C:287:VAL:O	2.15	0.46
1:A:87:HIS:HD2	3:A:1046:HOH:O	1.99	0.45
1:A:312:MSE:HE1	1:A:325:ILE:HD12	1.97	0.45
2:B:413:THR:O	2:B:414:PHE:HB2	2.16	0.45
1:A:124:ASP:HB3	1:A:127:LEU:HD12	1.98	0.45
2:B:391:THR:HA	2:B:409:THR:HB	1.99	0.45
2:B:517:GLN:O	2:B:518:TRP:HB3	2.17	0.45
1:C:42:HIS:HD2	3:C:1511:HOH:O	2.00	0.45
1:A:296:GLY:HA3	2:B:465:SER:OG	2.16	0.45
1:C:171:GLN:HB3	1:C:172:PRO:HD3	1.98	0.45
2:D:504:ASN:HD22	2:D:506:ALA:H	1.63	0.45
1:C:377:GLU:HG2	1:C:377:GLU:O	2.16	0.45
2:D:504:ASN:ND2	2:D:504:ASN:C	2.70	0.45
1:A:245:GLY:O	1:A:249:GLU:HG3	2.16	0.45
1:A:255:MSE:SE	1:A:260:GLY:HA3	2.67	0.45
1:A:186:ALA:HB2	2:B:573:VAL:HG23	1.99	0.44
2:D:566:GLY:HA3	2:D:577:THR:HG21	2.00	0.44
2:B:566:GLY:HA3	2:B:577:THR:HG21	2.00	0.44
2:D:452:ASN:HD21	2:D:461:LEU:H	1.65	0.44
1:A:32:VAL:CG1	1:A:33:SER:N	2.80	0.44
2:D:517:GLN:O	2:D:518:TRP:HB3	2.17	0.44
1:C:310:PHE:CZ	1:C:367:ILE:HD11	2.53	0.44
1:C:334:TYR:CD2	2:D:517:GLN:HA	2.54	0.43
1:A:30:PRO:HB3	1:A:313:LYS:HE2	1.99	0.43
1:C:34:TYR:CE2	2:D:559:GLY:HA2	2.53	0.43
1:A:32:VAL:HG13	3:B:1183:HOH:O	2.19	0.43
1:A:290:MSE:CE	1:A:291:PRO:HD2	2.46	0.43
1:C:32:VAL:HG13	3:D:1431:HOH:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:292:PRO:HA	1:A:294:SER:N	2.33	0.43
1:C:114:ARG:CZ	2:D:462:SER:HB2	2.49	0.43
1:A:204:ASN:ND2	1:A:205:SER:N	2.68	0.42
1:A:111:ILE:HD12	1:A:156:LEU:HD22	2.01	0.42
1:A:278:ILE:HG12	1:A:291:PRO:CB	2.46	0.42
1:C:293:PRO:O	2:D:461:LEU:HD12	2.18	0.42
1:A:168:LYS:NZ	1:A:168:LYS:HB2	2.33	0.42
1:A:356:ASN:OD1	1:A:358:ALA:HB3	2.20	0.42
1:C:242:PHE:HA	1:C:247:ILE:HB	2.02	0.42
1:A:42:HIS:HD2	3:A:1490:HOH:O	2.03	0.42
1:A:312:MSE:HA	1:A:312:MSE:CE	2.40	0.42
2:D:413:THR:O	2:D:414:PHE:HB2	2.20	0.42
1:C:132:ASN:HA	1:C:133:PRO:HD3	1.96	0.42
1:C:87:HIS:HD2	3:C:1087:HOH:O	2.01	0.41
1:A:298:ILE:HD12	1:A:341:LEU:HD11	2.02	0.41
1:A:338:SER:HB2	2:B:447:VAL:HG23	2.02	0.41
2:D:519:LEU:HA	2:D:520:PRO:C	2.40	0.41
3:C:1037:HOH:O	2:D:459:ARG:HD2	2.19	0.41
2:D:393:HIS:CD2	2:D:480:GLY:HA3	2.55	0.41
1:C:369:ILE:O	2:D:540:LYS:HD3	2.19	0.41
2:D:573:VAL:O	2:D:574:ASP:HB2	2.21	0.41
1:A:112:ASP:OD1	1:A:112:ASP:C	2.59	0.41
1:A:312:MSE:CA	1:A:312:MSE:HE2	2.41	0.41
1:C:186:ALA:HB2	2:D:573:VAL:HG23	2.02	0.41
1:A:317:PHE:CZ	2:B:511:ALA:HB1	2.56	0.41
1:C:46:ALA:HB3	1:C:50:MSE:HE3	2.03	0.41
1:A:369:ILE:HG12	1:A:369:ILE:O	2.22	0.40
1:A:384:ALA:N	1:A:385:PRO:HD2	2.36	0.40
1:A:271:LYS:NZ	1:A:271:LYS:CB	2.83	0.40
2:B:452:ASN:ND2	2:B:461:LEU:H	2.17	0.40
2:B:393:HIS:HE1	2:B:395:SER:OG	2.05	0.40
1:A:147:THR:HA	1:A:148:PRO:HD3	1.92	0.40
2:D:391:THR:HA	2:D:409:THR:HB	2.02	0.40
1:C:310:PHE:CE2	1:C:367:ILE:HD11	2.57	0.40
1:C:270:TYR:CD2	1:C:271:LYS:N	2.90	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	357/366 (98%)	348 (98%)	9 (2%)	0	100	100
1	C	356/366 (97%)	348 (98%)	8 (2%)	0	100	100
2	B	188/190 (99%)	181 (96%)	6 (3%)	1 (0%)	38	23
2	D	188/190 (99%)	182 (97%)	5 (3%)	1 (0%)	38	23
All	All	1089/1112 (98%)	1059 (97%)	28 (3%)	2 (0%)	56	46

All (2) Ramachandran outliers are listed below:

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

### 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	282/276 (102%)	277 (98%)	5 (2%)	71	64
1	C	282/276 (102%)	278 (99%)	4 (1%)	78	73
2	B	154/149 (103%)	150 (97%)	4 (3%)	59	46
2	D	154/149 (103%)	151 (98%)	3 (2%)	69	62
All	All	872/850 (103%)	856 (98%)	16 (2%)	71	64

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

Mol	Chain	Res	Type
1	A	120	LYS

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Mol	Chain	Res	Type
1	A	168	LYS
1	A	204	ASN
1	A	210	TRP
1	A	271	LYS
2	B	408	TYR
2	B	430	GLN
2	B	486	ARG
2	B	519	LEU
1	C	107	ASN
1	C	210	TRP
1	C	369	ILE
1	C	379	ARG
2	D	408	TYR
2	D	486	ARG
2	D	504	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	87	HIS
1	A	107	ASN
1	A	201	ASN
1	A	202	HIS
1	A	204	ASN
1	A	250	GLN
1	A	253	GLN
2	B	393	HIS
2	B	452	ASN
2	B	515	HIS
1	C	42	HIS
1	C	87	HIS
1	C	107	ASN
1	C	132	ASN
1	C	171	GLN
1	C	201	ASN
1	C	237	ASN
1	C	366	GLN
2	D	393	HIS
2	D	452	ASN
2	D	493	GLN
2	D	497	ASN

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Mol	Chain	Res	Type
2	D	504	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

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	359/366 (98%)	0.12	5 (1%) 72 80	21, 32, 51, 60	0
1	C	358/366 (97%)	0.34	14 (3%) 37 43	19, 31, 57, 76	0
2	B	190/190 (100%)	0.36	4 (2%) 60 69	20, 28, 48, 60	0
2	D	190/190 (100%)	0.52	9 (4%) 30 36	19, 29, 51, 62	0
All	All	1097/1112 (98%)	0.30	32 (2%) 49 57	19, 31, 53, 76	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	32	VAL	5.3
1	C	31	PRO	4.7
2	D	440	VAL	4.5
1	C	35	GLY	4.3
1	C	36	VAL	4.0
2	D	560	PRO	3.8
2	D	561	ASP	3.7
1	C	30	PRO	3.5
2	D	443	VAL	3.4
2	D	450	ASP	3.1
1	C	383	LEU	3.0
2	B	543	LYS	3.0
2	B	537	LEU	2.9
2	D	447	VAL	2.8
1	C	315	TYR	2.7
2	B	450	ASP	2.6
1	C	37	GLU	2.6
2	B	448	GLY	2.6
1	C	369	ILE	2.6
1	C	34	TYR	2.5
1	A	131	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	249	GLU	2.4
1	C	367	ILE	2.3
1	C	368	ASP	2.3
2	D	519	LEU	2.3
1	C	384	ALA	2.3
1	A	30	PRO	2.3
2	D	491	VAL	2.2
1	A	384	ALA	2.2
1	A	29	ALA	2.1
2	D	543	LYS	2.1
1	C	376	SER	2.0

## 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.