



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:01 PM UTC

PDB ID : 2DBU / pdb_00002dbu
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 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

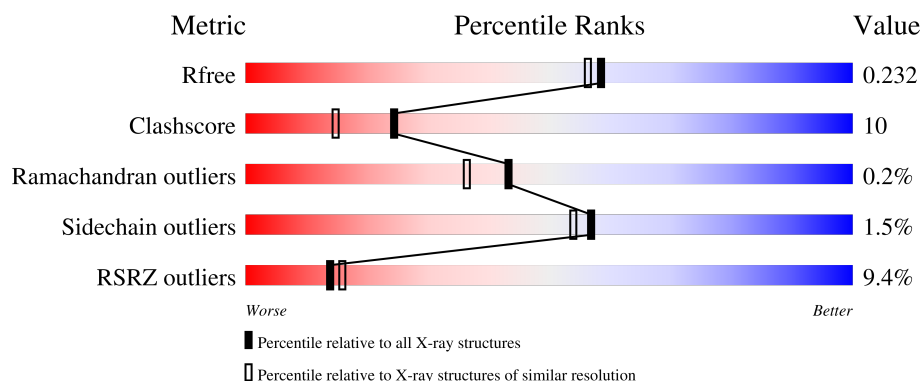
1 Overall quality at a glance

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	366	7% 77% 19% ..
1	C	366	9% 81% 16% ..
2	B	190	11% 78% 20% .
2	D	190	12% 77% 21% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8846 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
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

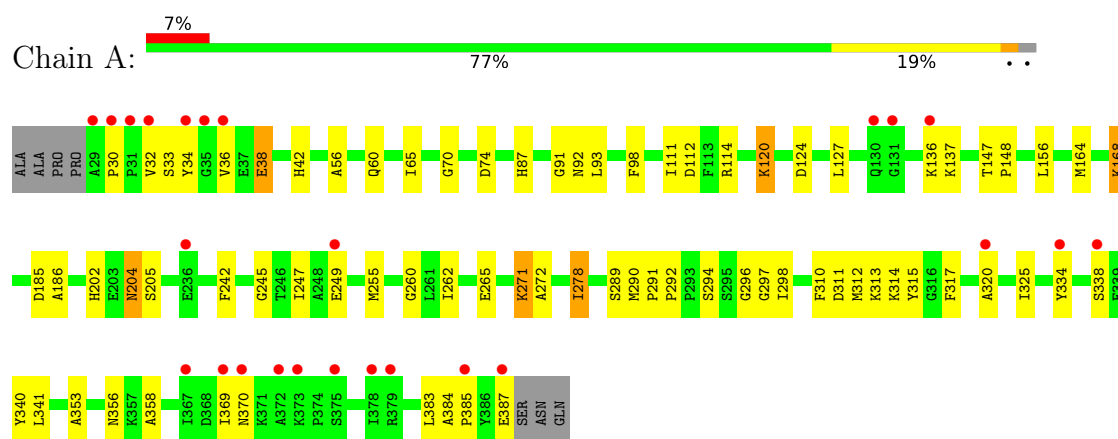
- Molecule 3 is water.

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

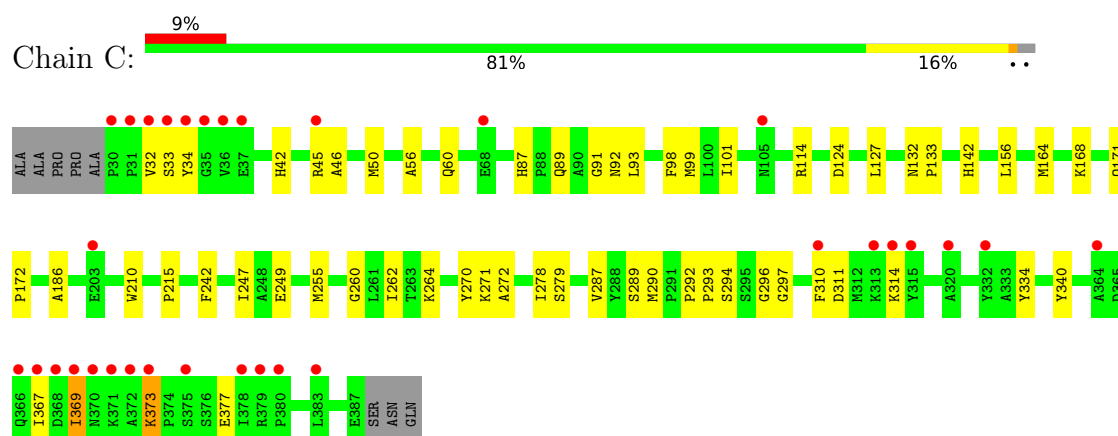
3 Residue-property plots [i](#)

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.

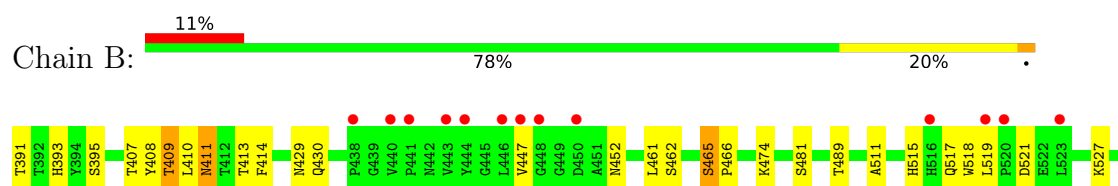
• Molecule 1: Gamma-glutamyltranspeptidase

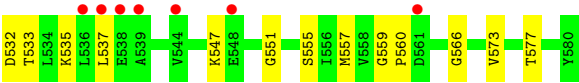


• Molecule 1: Gamma-glutamyltranspeptidase

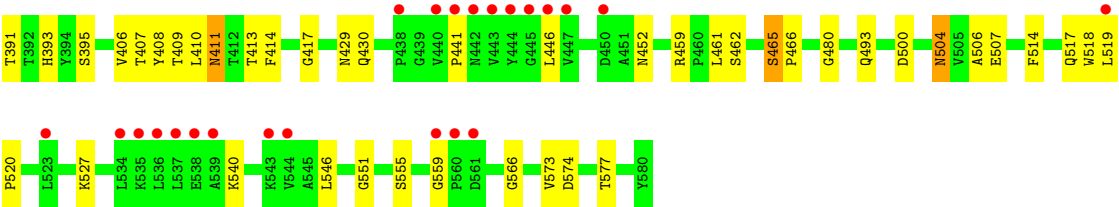
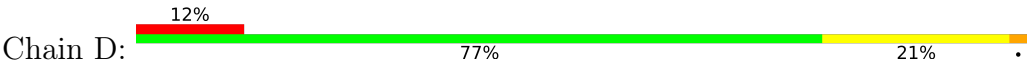


• Molecule 2: Gamma-glutamyltranspeptidase





● Molecule 2: Gamma-glutamyltranspeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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) 96.7 (46.39-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	4758 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8846	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.36	0/2761	0.89	6/3721 (0.2%)
1	C	0.36	0/2756	0.88	6/3713 (0.2%)
2	B	0.38	0/1429	1.01	8/1937 (0.4%)
2	D	0.38	0/1429	0.98	7/1937 (0.4%)
All	All	0.37	0/8375	0.92	27/11308 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	LEU	N-CA-C	-9.73	101.75	114.31
1	A	93	LEU	N-CA-C	-8.67	103.13	114.31
1	A	91	GLY	N-CA-C	-8.63	102.01	111.93
2	B	410	LEU	N-CA-C	-7.54	103.20	113.30
1	C	91	GLY	N-CA-C	-6.95	103.23	111.36
2	D	410	LEU	N-CA-C	-6.56	104.51	113.30
1	A	340	TYR	N-CA-C	6.29	121.09	113.17
1	A	272	ALA	N-CA-C	-6.27	101.20	110.48
1	A	92	ASN	N-CA-C	6.26	117.65	108.14
2	B	555	SER	N-CA-C	6.03	119.38	109.85
1	C	340	TYR	N-CA-C	6.01	120.61	113.28
1	C	278	ILE	N-CA-C	-5.94	101.13	109.21
2	B	547	LYS	N-CA-C	5.89	116.05	108.34
1	C	272	ALA	N-CA-C	-5.80	101.90	110.48
2	D	465	SER	N-CA-C	5.80	119.14	108.94
1	C	92	ASN	N-CA-C	5.79	116.94	108.14
2	B	465	SER	N-CA-C	5.77	119.02	109.79
2	D	555	SER	N-CA-C	5.70	118.85	109.85
2	D	527	LYS	N-CA-C	-5.61	102.60	110.50
2	B	551	GLY	N-CA-C	5.49	122.45	112.58
2	B	481	SER	N-CA-C	5.43	113.02	108.13
2	D	500	ASP	N-CA-C	5.39	116.97	111.14
2	B	527	LYS	N-CA-C	-5.36	102.94	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	417	GLY	N-CA-C	-5.30	107.96	115.43
2	B	409	THR	N-CA-C	5.26	116.14	108.14
1	A	278	ILE	N-CA-C	-5.23	100.92	108.87
2	D	551	GLY	N-CA-C	5.21	121.95	112.58

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	2716	0	2680	79	0
1	C	2711	0	2676	45	0
2	B	1407	0	1392	29	0
2	D	1407	0	1392	34	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	162	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 10.

All (162) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:136:LYS:HD3	1:A:136:LYS:C	2.21	0.65
2:D:504:ASN:HD22	2:D:504:ASN:C	2.05	0.65
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
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
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:156:LEU:C	1:C:156:LEU:HD23	2.30	0.56
1:C:296:GLY:HA3	2:D:465:SER:OG	2.05	0.56
1:C:311:ASP:CG	1:C:314:LYS:HG3	2.31	0.55
1:A:204:ASN:HD22	1:A:205:SER:N	2.04	0.55
1:A:156:LEU:C	1:A:156:LEU:HD23	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:H	1:A:38:GLU:CD	2.14	0.54
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:A:383:LEU:O	1:A:387:GLU:HG3	2.10	0.52
1:C:292:PRO:HA	1:C:294:SER:N	2.25	0.52
2:D:518:TRP:O	2:D:519:LEU:HD12	2.09	0.52
1:A:202:HIS:HE1	3:A:1026:HOH:O	1.92	0.52
1:C:98:PHE:HB3	1:C:290:MSE:SE	2.59	0.52
2:B:393:HIS:HD2	2:B:407:THR:OG1	1.91	0.52
1:C:373:LYS:NZ	1:C:373:LYS:HB2	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: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:A:32:VAL:HG12	1:A:33:SER:N	2.27	0.50
1:A:242:PHE:HA	1:A:247:ILE:HB	1.93	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: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
2:D:504:ASN:ND2	2:D:504:ASN:C	2.70	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:56:ALA:O	1:A:60:GLN:HG3	2.12	0.49
1:A:204:ASN:HD22	1:A:204:ASN:N	2.11	0.49
1:C:32:VAL:CG1	1:C:33:SER:N	2.75	0.49
1:A:185:ASP:HB3	1:C:45:ARG:NH1	2.28	0.48
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
1:C:99:MSE:SE	1:C:101:ILE:HD11	2.64	0.48
1:C:369:ILE:N	1:C:369:ILE:HD13	2.29	0.48
2:D:504:ASN:HD22	2:D:506:ALA:N	2.12	0.48
1:A:114:ARG:CZ	2:B:462:SER:HB2	2.44	0.47
1:A:312:MSE:HE2	1:A:315:TYR:HD2	1.79	0.47
1:A:87:HIS:HE1	3:B:1198:HOH:O	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:112:ASP:OD1	1:A:112:ASP:C	2.59	0.46
2:D:519:LEU:HA	2:D:520:PRO:C	2.40	0.46
1:A:87:HIS:HD2	3:A:1046:HOH:O	1.99	0.45
1:A:124:ASP:HB3	1:A:127:LEU:HD12	1.98	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
2:B:391:THR:HA	2:B:409:THR:HB	1.99	0.45
1:A:296:GLY:HA3	2:B:465:SER:OG	2.16	0.45
1:C:42:HIS:HD2	3:C:1511:HOH:O	2.00	0.45
1:C:171:GLN:HB3	1:C:172:PRO:HD3	1.98	0.45
2:B:474:LYS:HZ1	2:B:560:PRO:CB	2.29	0.45
1:C:377:GLU:O	1:C:377:GLU:HG2	2.16	0.45
2:D:504:ASN:HD22	2:D:506:ALA:H	1.63	0.45
1:A:245:GLY:O	1:A:249:GLU:HG3	2.16	0.45
2:B:517:GLN:O	2:B:518:TRP:HB3	2.17	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: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
2:D:566:GLY:HA3	2:D:577:THR:HG21	2.00	0.44
1:A:32:VAL:CG1	1:A:33:SER:N	2.80	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
2:D:517:GLN:O	2:D:518:TRP:HB3	2.17	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
2:D:546:LEU:C	2:D:546:LEU:HD13	2.43	0.43
1:A:290:MSE:CE	1:A:291:PRO:HD2	2.46	0.43
1:A:292:PRO:HA	1:A:294:SER:N	2.33	0.43
1:C:32:VAL:HG13	3:D:1431:HOH:O	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB2	1:A:168:LYS:NZ	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
1:C:132:ASN:HA	1:C:133:PRO:HD3	1.96	0.42
2:D:413:THR:O	2:D:414:PHE:HB2	2.20	0.42
1:A:298:ILE:HD12	1:A:341:LEU:HD11	2.02	0.41
1:C:87:HIS:HD2	3:C:1087:HOH:O	2.01	0.41
1:A:338:SER:HB2	2:B:447:VAL:HG23	2.02	0.41
3:C:1037:HOH:O	2:D:459:ARG:HD2	2.19	0.41
1:C:369:ILE:O	2:D:540:LYS:HD3	2.19	0.41
1:C:373:LYS:HB2	1:C:373:LYS:HZ2	1.86	0.41
2:D:393:HIS:CD2	2:D:480:GLY:HA3	2.55	0.41
2:D:573:VAL:O	2:D:574:ASP:HB2	2.21	0.41
1:A:312:MSE:HE2	1:A:312:MSE:CA	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:271:LYS:NZ	1:A:271:LYS:CB	2.83	0.40
1:A:369:ILE:O	1:A:369:ILE:HG12	2.22	0.40
1:A:384:ALA:N	1:A:385:PRO:HD2	2.36	0.40
2:B:521:ASP:C	2:B:521:ASP:OD2	2.64	0.40
2:B:452:ASN:ND2	2:B:461:LEU:H	2.17	0.40
1:A:147:THR:HA	1:A:148:PRO:HD3	1.92	0.40
2:B:393:HIS:HE1	2:B:395:SER:OG	2.05	0.40
2:D:391:THR:HA	2:D:409:THR:HB	2.02	0.40
1:C:270:TYR:CD2	1:C:271:LYS:N	2.90	0.40
1:C:310:PHE:CE2	1:C:367:ILE:HD11	2.57	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%)	24	16
2	D	188/190 (99%)	182 (97%)	5 (3%)	1 (0%)	24	16
All	All	1089/1112 (98%)	1059 (97%)	28 (3%)	2 (0%)	43	36

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	282/276 (102%)	277 (98%)	5 (2%)	51	47
1	C	282/276 (102%)	280 (99%)	2 (1%)	76	76
2	B	154/149 (103%)	151 (98%)	3 (2%)	50	45
2	D	154/149 (103%)	151 (98%)	3 (2%)	50	45
All	All	872/850 (103%)	859 (98%)	13 (2%)	57	54

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	120	LYS
1	A	168	LYS
1	A	204	ASN
1	A	271	LYS
2	B	408	TYR

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Mol	Chain	Res	Type
2	B	430	GLN
2	B	519	LEU
1	C	369	ILE
1	C	373	LYS
2	D	408	TYR
2	D	430	GLN
2	D	504	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	87	HIS
1	A	142	HIS
1	A	202	HIS
1	A	204	ASN
1	A	250	GLN
1	A	253	GLN
1	A	256	GLN
2	B	393	HIS
2	B	452	ASN
2	B	497	ASN
2	B	515	HIS
2	B	542	GLN
1	C	42	HIS
1	C	48	GLN
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	504	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	348/366 (95%)	0.52	25 (7%)	21 25	21, 32, 51, 60	0
1	C	347/366 (94%)	0.62	32 (9%)	14 16	19, 31, 57, 76	0
2	B	185/190 (97%)	0.50	20 (10%)	11 12	20, 28, 48, 60	0
2	D	185/190 (97%)	0.54	23 (12%)	8 9	19, 29, 51, 62	0
All	All	1065/1112 (95%)	0.55	100 (9%)	14 16	19, 31, 53, 76	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	30	PRO	5.5
1	C	35	GLY	5.2
1	C	32	VAL	5.1
1	C	36	VAL	5.1
2	D	440	VAL	5.0
1	C	369	ILE	4.6
2	D	443	VAL	4.4
1	C	367	ILE	4.4
1	A	372	ALA	4.2
2	D	560	PRO	4.1
2	D	561	ASP	4.1
1	C	368	ASP	4.1
2	B	447	VAL	4.0
2	B	537	LEU	4.0
2	B	448	GLY	3.9
2	B	536	LEU	3.8
2	B	440	VAL	3.8
2	B	444	TYR	3.8
1	A	36	VAL	3.7
2	D	447	VAL	3.7
2	B	539	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	369	ILE	3.5
1	A	35	GLY	3.3
1	C	34	TYR	3.3
1	C	315	TYR	3.3
1	C	372	ALA	3.3
2	D	544	VAL	3.2
1	C	37	GLU	3.2
2	B	438	PRO	3.1
2	D	444	TYR	3.1
2	D	445	GLY	3.1
1	A	378	ILE	3.0
2	B	519	LEU	3.0
2	B	561	ASP	3.0
2	D	537	LEU	3.0
2	D	442	ASN	3.0
1	C	31	PRO	2.9
1	A	30	PRO	2.9
2	D	539	ALA	2.9
1	C	379	ARG	2.9
1	A	34	TYR	2.9
1	A	370	ASN	2.9
2	B	450	ASP	2.9
1	A	385	PRO	2.8
2	B	548	GLU	2.8
2	D	536	LEU	2.8
1	A	31	PRO	2.8
1	C	33	SER	2.8
2	D	523	LEU	2.7
2	B	441	PRO	2.7
1	C	375	SER	2.7
1	A	236	GLU	2.7
1	A	379	ARG	2.6
1	A	136	LYS	2.6
1	A	32	VAL	2.6
2	D	450	ASP	2.6
1	A	131	GLY	2.6
2	B	520	PRO	2.5
1	A	320	ALA	2.5
1	C	371	LYS	2.5
2	D	519	LEU	2.4
2	B	443	VAL	2.4
1	A	334	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	523	LEU	2.4
2	D	543	LYS	2.4
2	D	441	PRO	2.4
1	A	387	GLU	2.4
1	C	310	PHE	2.4
1	A	249	GLU	2.4
1	C	370	ASN	2.4
1	C	105	ASN	2.3
1	A	338	SER	2.3
1	A	130	GLN	2.3
2	D	534	LEU	2.3
1	C	45	ARG	2.3
1	C	313	LYS	2.3
1	C	373	LYS	2.3
2	D	538	GLU	2.2
1	A	375	SER	2.2
1	C	366	GLN	2.2
1	C	383	LEU	2.2
1	C	378	ILE	2.2
2	B	544	VAL	2.2
2	D	438	PRO	2.2
2	D	446	LEU	2.1
2	D	535	LYS	2.1
1	C	320	ALA	2.1
1	C	203	GLU	2.1
2	B	516	HIS	2.1
2	B	446	LEU	2.1
1	A	29	ALA	2.1
2	B	538	GLU	2.1
1	A	367	ILE	2.0
1	A	373	LYS	2.0
1	C	314	LYS	2.0
1	C	364	ALA	2.0
1	C	68	GLU	2.0
2	D	559	GLY	2.0
1	C	332	TYR	2.0
1	C	380	PRO	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.