



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:43 PM UTC

PDB ID : 2NQO / pdb_00002nqo
Title : Crystal Structure of Helicobacter pylori gamma-Glutamyltranspeptidase
Authors : Boanca, G.; Sand, A.; Okada, T.; Suzuki, H.; Kumagai, H.; Fukuyama, K.;
Barycki, J.J.
Deposited on : 2006-10-31
Resolution : 1.90 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
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

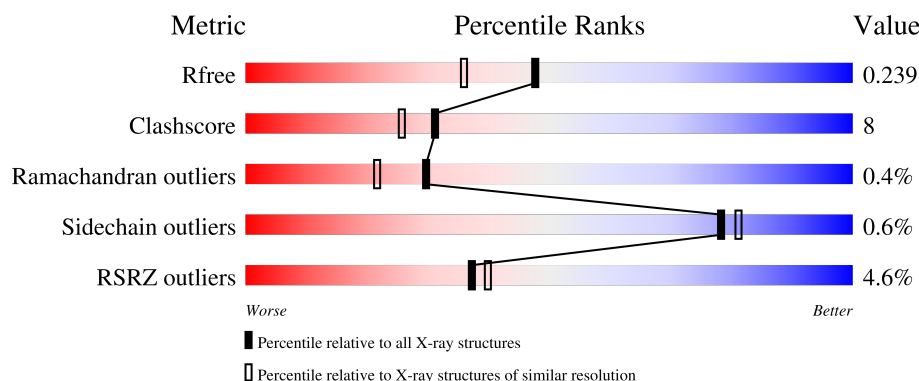
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	376	8% 71% 20% 8%
1	C	376	2% 78% 14% 7%
2	B	188	4% 74% 22% •
2	D	188	4% 77% 20% ••

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8679 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	347	Total	C	N	O	S	0	0	0
			2625	1674	450	492	9			
1	C	349	Total	C	N	O	S	0	0	0
			2646	1683	455	499	9			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	cloning artifact	UNP O25743
A	5	GLY	-	cloning artifact	UNP O25743
A	6	SER	-	cloning artifact	UNP O25743
A	7	SER	-	cloning artifact	UNP O25743
A	8	HIS	-	cloning artifact	UNP O25743
A	9	HIS	-	cloning artifact	UNP O25743
A	10	HIS	-	cloning artifact	UNP O25743
A	11	HIS	-	cloning artifact	UNP O25743
A	12	HIS	-	cloning artifact	UNP O25743
A	13	HIS	-	cloning artifact	UNP O25743
A	14	SER	-	cloning artifact	UNP O25743
A	15	SER	-	cloning artifact	UNP O25743
A	16	GLY	-	cloning artifact	UNP O25743
A	17	LEU	-	cloning artifact	UNP O25743
A	18	VAL	-	cloning artifact	UNP O25743
A	19	PRO	-	cloning artifact	UNP O25743
A	20	ARG	-	cloning artifact	UNP O25743
A	21	GLY	-	cloning artifact	UNP O25743
A	22	SER	-	cloning artifact	UNP O25743
A	23	HIS	-	cloning artifact	UNP O25743
A	24	MET	-	cloning artifact	UNP O25743
A	25	ALA	-	cloning artifact	UNP O25743
A	26	SER	-	cloning artifact	UNP O25743
C	4	MET	-	cloning artifact	UNP O25743
C	5	GLY	-	cloning artifact	UNP O25743

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	SER	-	cloning artifact	UNP O25743
C	7	SER	-	cloning artifact	UNP O25743
C	8	HIS	-	cloning artifact	UNP O25743
C	9	HIS	-	cloning artifact	UNP O25743
C	10	HIS	-	cloning artifact	UNP O25743
C	11	HIS	-	cloning artifact	UNP O25743
C	12	HIS	-	cloning artifact	UNP O25743
C	13	HIS	-	cloning artifact	UNP O25743
C	14	SER	-	cloning artifact	UNP O25743
C	15	SER	-	cloning artifact	UNP O25743
C	16	GLY	-	cloning artifact	UNP O25743
C	17	LEU	-	cloning artifact	UNP O25743
C	18	VAL	-	cloning artifact	UNP O25743
C	19	PRO	-	cloning artifact	UNP O25743
C	20	ARG	-	cloning artifact	UNP O25743
C	21	GLY	-	cloning artifact	UNP O25743
C	22	SER	-	cloning artifact	UNP O25743
C	23	HIS	-	cloning artifact	UNP O25743
C	24	MET	-	cloning artifact	UNP O25743
C	25	ALA	-	cloning artifact	UNP O25743
C	26	SER	-	cloning artifact	UNP O25743

- Molecule 2 is a protein called Gamma-glutamyltranspeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	186	Total	C	N	O	S	0	0	0
			1405	889	238	271	7			
2	D	186	Total	C	N	O	S	0	0	0
			1413	895	240	271	7			

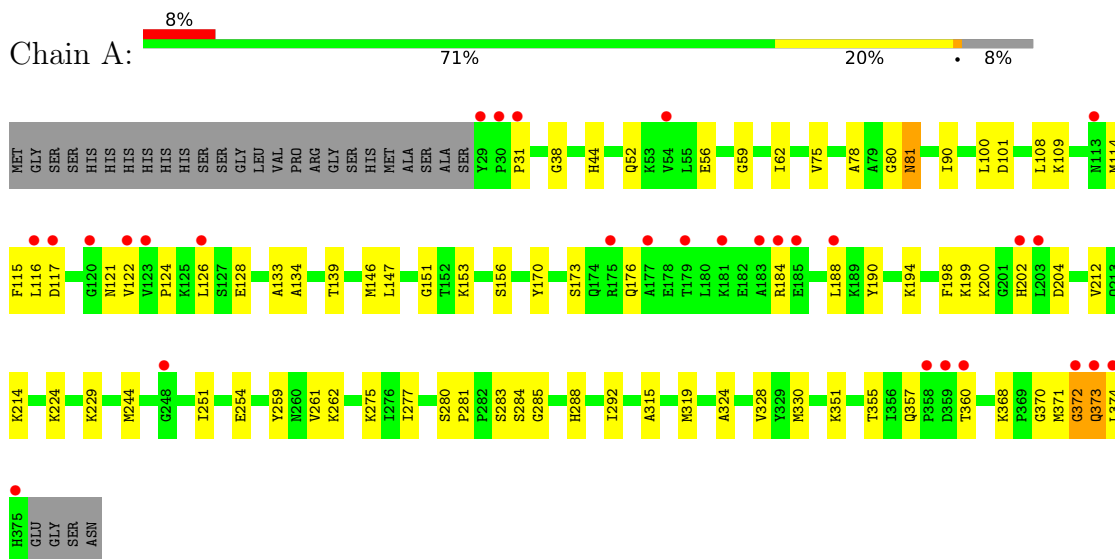
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total	O	0	0
			124	124		
3	B	97	Total	O	0	0
			97	97		
3	C	239	Total	O	0	0
			239	239		
3	D	130	Total	O	0	0
			130	130		

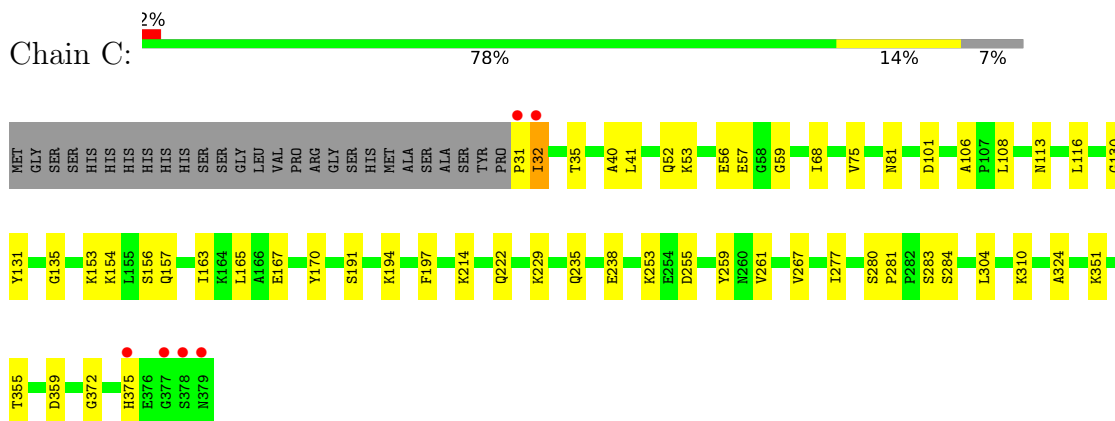
3 Residue-property plots [i](#)

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.

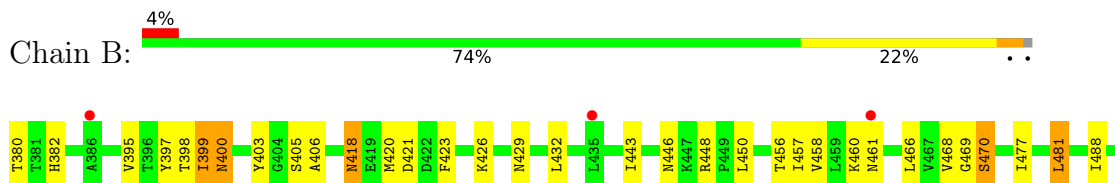
- Molecule 1: Gamma-glutamyltranspeptidase

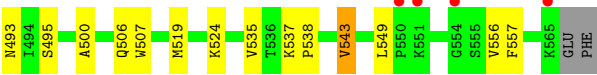


- Molecule 1: Gamma-glutamyltranspeptidase

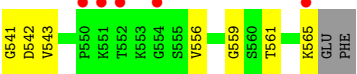
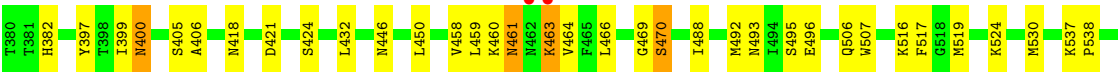
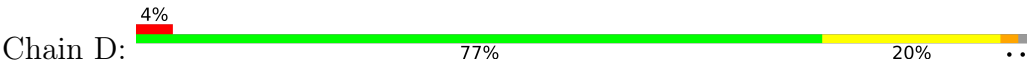


- Molecule 2: Gamma-glutamyltranspeptidase





● Molecule 2: Gamma-glutamyltranspeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.35Å 105.21Å 91.06Å 90.00° 91.99° 90.00°	Depositor
Resolution (Å)	28.19 – 1.90 28.19 – 1.91	Depositor EDS
% Data completeness (in resolution range)	91.5 (28.19-1.90) 91.6 (28.19-1.91)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 1.91Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.197 , 0.239 0.197 , 0.239	Depositor DCC
R_{free} test set	7720 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8679	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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	0.34	0/2672	0.91	10/3600 (0.3%)
1	C	0.37	0/2693	0.90	9/3624 (0.2%)
2	B	0.36	0/1434	0.98	9/1952 (0.5%)
2	D	0.40	0/1442	0.98	7/1960 (0.4%)
All	All	0.36	0/8241	0.93	35/11136 (0.3%)

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
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	399	ILE	N-CA-C	-8.48	102.89	111.88
2	D	399	ILE	N-CA-C	-8.18	103.21	111.88
2	B	395	VAL	N-CA-C	6.55	117.28	108.11
2	B	470	SER	N-CA-C	6.43	113.92	108.13
1	A	372	GLY	N-CA-C	-6.25	107.25	114.69
1	C	197	PHE	N-CA-C	6.19	120.53	112.92
2	D	424	SER	N-CA-C	-6.17	98.47	108.41
1	C	135	GLY	N-CA-C	-6.07	102.13	112.51
2	D	488	ILE	N-CA-C	6.03	116.21	110.42
1	A	80	GLY	N-CA-C	-5.92	105.12	111.93
1	A	324	ALA	N-CA-C	-5.92	104.75	111.14
1	A	44	HIS	CA-C-N	5.87	125.34	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	HIS	C-N-CA	5.87	125.34	119.24
2	D	493	ASN	N-CA-C	-5.86	102.97	110.53
2	B	418	ASN	N-CA-C	-5.85	103.42	110.44
1	A	330	MET	N-CA-C	5.81	119.11	109.46
2	D	470	SER	N-CA-C	5.81	113.36	108.13
1	C	130	GLY	N-CA-C	5.80	120.29	112.17
1	A	328	VAL	N-CA-C	5.66	116.87	112.12
2	B	493	ASN	N-CA-C	-5.65	103.24	110.53
1	A	81	ASN	N-CA-C	5.62	116.68	108.14
1	C	81	ASN	N-CA-C	5.52	116.62	107.73
1	C	131	TYR	N-CA-C	5.45	118.14	111.82
1	C	214	LYS	N-CA-C	5.41	116.86	111.07
2	B	488	ILE	N-CA-C	5.26	116.03	110.72
2	D	561	THR	N-CA-C	-5.23	103.00	110.59
1	C	324	ALA	N-CA-C	-5.22	105.59	111.28
1	C	32	ILE	N-CA-C	-5.19	104.34	110.21
2	D	541	GLY	N-CA-C	5.14	121.56	112.83
1	A	90	ILE	N-CA-C	5.11	116.07	108.46
1	A	134	ALA	N-CA-C	5.08	118.09	109.76
1	C	106	ALA	N-CA-C	-5.06	103.22	109.64
2	B	543	VAL	N-CA-C	5.03	115.53	108.89
2	B	500	ALA	N-CA-C	5.02	115.37	109.60
2	B	443	ILE	N-CA-C	5.01	115.51	108.89

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	TYR	Sidechain
1	C	259	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	2625	0	2685	58	0
1	C	2646	0	2702	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1405	0	1392	33	0
2	D	1413	0	1414	30	0
3	A	124	0	0	3	0
3	B	97	0	0	0	0
3	C	239	0	0	3	0
3	D	130	0	0	1	0
All	All	8679	0	8193	134	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 8.

All (134) 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:D:463:LYS:HE3	2:D:464:VAL:H	1.14	1.07
2:D:463:LYS:HE3	2:D:464:VAL:N	1.77	1.00
1:C:154:LYS:HD2	1:C:157:GLN:HE22	1.38	0.88
1:C:32:ILE:HD11	1:C:41:LEU:HD21	1.58	0.86
1:A:275:LYS:HE2	1:A:277:ILE:HD11	1.61	0.83
1:A:31:PRO:HG3	2:B:495:SER:HB2	1.62	0.80
1:A:292:ILE:HG21	2:B:481:LEU:HD11	1.65	0.77
1:A:373:GLN:HG2	1:A:374:LEU:H	1.52	0.72
1:C:52:GLN:O	1:C:56:GLU:HG3	1.93	0.69
2:D:460:LYS:O	2:D:460:LYS:HG3	1.94	0.68
1:A:108:LEU:HD23	2:B:446:ASN:HD21	1.60	0.67
2:B:519:MET:SD	2:B:524:LYS:HG2	2.34	0.66
1:A:292:ILE:CG2	2:B:481:LEU:HD11	2.25	0.66
1:A:244:MET:HE3	1:A:251:ILE:HD12	1.79	0.65
2:B:470:SER:HB2	2:B:543:VAL:HG22	1.78	0.65
1:A:355:THR:HG21	1:A:371:MET:HE1	1.81	0.62
1:A:108:LEU:CD2	2:B:446:ASN:HD21	2.12	0.62
1:C:31:PRO:HG3	2:D:495:SER:HB2	1.82	0.61
1:A:100:LEU:HD23	1:A:146:MET:HE2	1.81	0.61
2:B:382:HIS:CE1	2:B:469:GLY:HA3	2.36	0.61
2:D:400:ASN:HB3	2:D:418:ASN:OD1	2.02	0.60
2:D:460:LYS:O	2:D:461:ASN:HB2	2.01	0.59
1:A:31:PRO:HG3	2:B:495:SER:CB	2.32	0.59
1:A:373:GLN:HG2	1:A:374:LEU:N	2.18	0.59
1:A:75:VAL:HA	1:A:170:TYR:CZ	2.38	0.58
1:C:32:ILE:CD1	1:C:41:LEU:HD21	2.32	0.57
1:A:52:GLN:O	1:A:56:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:THR:HG22	2:D:556:VAL:HA	1.87	0.56
1:A:285:GLY:HA2	2:B:477:ILE:HG12	1.87	0.56
1:C:351:LYS:O	1:C:355:THR:HG23	2.06	0.56
2:B:458:VAL:HB	2:B:466:LEU:HB2	1.87	0.56
1:C:372:GLY:HA2	1:C:375:HIS:CD2	2.41	0.56
1:A:188:LEU:O	1:A:194:LYS:HD2	2.06	0.55
1:C:154:LYS:HD2	1:C:157:GLN:NE2	2.17	0.55
1:A:198:PHE:HB3	1:A:202:HIS:HA	1.87	0.54
1:A:357:GLN:HB2	1:A:360:THR:HG22	1.89	0.54
1:C:108:LEU:HD23	2:D:446:ASN:OD1	2.06	0.54
1:A:281:PRO:HA	1:A:283:SER:N	2.23	0.54
1:C:229:LYS:HG3	3:C:567:HOH:O	2.07	0.53
2:B:380:THR:HA	2:B:398:THR:HB	1.90	0.53
2:D:565:LYS:HD3	3:D:584:HOH:O	2.08	0.53
1:A:117:ASP:OD2	1:A:121:ASN:HB2	2.09	0.53
1:A:357:GLN:CB	1:A:360:THR:HG22	2.39	0.53
1:A:190:TYR:O	1:A:194:LYS:HG3	2.11	0.51
1:C:163:ILE:O	1:C:167:GLU:HG3	2.10	0.51
1:C:59:GLY:CA	1:C:153:LYS:HE3	2.40	0.51
1:C:156:SER:HB3	1:C:157:GLN:OE1	2.10	0.51
1:C:277:ILE:HD11	2:D:459:LEU:HD11	1.91	0.51
1:A:262:LYS:HG3	2:B:448:ARG:NH2	2.26	0.51
2:D:542:ASP:OD1	2:D:565:LYS:HB2	2.11	0.51
2:D:537:LYS:HB3	2:D:538:PRO:HD2	1.92	0.51
1:C:277:ILE:HD11	2:D:459:LEU:CD1	2.41	0.50
1:C:41:LEU:HD11	2:D:559:GLY:HA3	1.92	0.50
2:B:426:LYS:O	2:B:429:ASN:HB3	2.11	0.50
2:D:421:ASP:OD2	2:D:432:LEU:HG	2.11	0.50
1:A:128:GLU:OE1	2:B:432:LEU:HD21	2.12	0.49
1:A:116:LEU:HD23	1:A:122:VAL:HA	1.94	0.49
2:D:516:LYS:HE2	2:D:517:PHE:CZ	2.48	0.49
1:A:133:ALA:O	2:B:418:ASN:HA	2.12	0.49
1:C:53:LYS:O	1:C:57:GLU:HG3	2.11	0.49
1:A:184:ARG:O	1:A:188:LEU:HG	2.12	0.49
1:C:310:LYS:HD3	1:C:310:LYS:C	2.38	0.49
2:D:458:VAL:HB	2:D:466:LEU:HB2	1.95	0.49
1:C:284:SER:HB3	2:D:450:LEU:HD11	1.95	0.48
2:D:519:MET:SD	2:D:524:LYS:HG2	2.53	0.48
1:A:62:ILE:HD12	1:A:62:ILE:N	2.28	0.48
1:A:115:PHE:HA	1:A:126:LEU:HD23	1.96	0.48
2:D:537:LYS:HB3	2:D:538:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:ASN:HB3	2:B:418:ASN:OD1	2.14	0.47
2:B:481:LEU:C	2:B:481:LEU:HD23	2.39	0.47
1:C:53:LYS:HD3	3:C:494:HOH:O	2.14	0.47
2:D:460:LYS:O	2:D:461:ASN:CB	2.62	0.47
2:B:420:MET:O	2:B:423:PHE:HB2	2.15	0.47
2:B:537:LYS:HB3	2:B:538:PRO:HD2	1.96	0.47
2:D:506:GLN:O	2:D:507:TRP:HB3	2.14	0.47
1:C:222:GLN:NE2	1:C:235:GLN:OE1	2.48	0.46
2:D:470:SER:HB2	2:D:543:VAL:HG22	1.95	0.46
1:A:38:GLY:HA2	2:B:557:PHE:CD2	2.51	0.46
2:B:537:LYS:HB3	2:B:538:PRO:CD	2.46	0.46
2:D:382:HIS:CE1	2:D:469:GLY:HA3	2.49	0.46
1:A:108:LEU:HD13	1:A:254:GLU:OE2	2.16	0.46
2:D:492:MET:HB3	2:D:496:GLU:HB2	1.98	0.45
1:C:191:SER:HA	1:C:194:LYS:HE3	1.97	0.45
1:A:373:GLN:CG	1:A:374:LEU:H	2.21	0.45
1:A:108:LEU:HD23	2:B:446:ASN:ND2	2.30	0.45
1:C:75:VAL:HA	1:C:170:TYR:CZ	2.51	0.45
1:A:59:GLY:CA	1:A:153:LYS:HE3	2.47	0.45
1:C:304:LEU:HD12	1:C:310:LYS:HB3	1.99	0.45
1:A:156:SER:HA	1:A:224:LYS:HG3	1.99	0.44
1:A:184:ARG:HH11	1:A:184:ARG:HG3	1.82	0.44
1:C:101:ASP:OD1	1:C:101:ASP:C	2.60	0.44
2:D:463:LYS:CE	2:D:464:VAL:H	2.04	0.44
1:A:368:LYS:HE2	3:A:469:HOH:O	2.16	0.44
2:B:405:SER:O	2:B:406:ALA:HB3	2.18	0.44
1:C:238:GLU:OE2	1:C:253:LYS:HD2	2.17	0.44
1:A:198:PHE:HE1	1:A:204:ASP:OD1	2.01	0.44
1:A:109:LYS:HG3	1:A:109:LYS:O	2.16	0.44
1:A:101:ASP:OD1	1:A:101:ASP:C	2.61	0.44
1:C:267:VAL:HG13	1:C:280:SER:HB3	1.99	0.43
2:D:463:LYS:CE	2:D:464:VAL:N	2.65	0.43
1:A:351:LYS:O	1:A:355:THR:HG23	2.18	0.43
1:A:370:GLY:O	1:A:371:MET:HB2	2.18	0.43
1:C:113:ASN:HB3	1:C:116:LEU:HD12	2.00	0.43
1:A:370:GLY:C	1:A:372:GLY:H	2.27	0.43
1:A:261:VAL:HG22	3:A:503:HOH:O	2.19	0.43
1:C:108:LEU:HG	1:C:255:ASP:OD1	2.18	0.43
1:C:75:VAL:CG1	1:C:165:LEU:HD13	2.49	0.43
1:A:81:ASN:O	1:A:139:THR:HG21	2.19	0.42
1:A:147:LEU:HD12	1:A:151:GLY:HA3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:PRO:HA	1:C:283:SER:N	2.34	0.42
1:C:40:ALA:HB1	1:C:68:ILE:HD11	2.02	0.42
1:A:212:VAL:HG11	1:A:214:LYS:HE2	2.01	0.42
1:A:284:SER:HB3	2:B:450:LEU:HD11	2.01	0.42
1:A:114:MET:HE2	1:A:115:PHE:CZ	2.55	0.42
2:B:460:LYS:O	2:B:461:ASN:HB2	2.20	0.42
2:B:421:ASP:OD2	2:B:432:LEU:HG	2.20	0.41
2:B:468:VAL:HG22	2:B:469:GLY:N	2.35	0.41
2:B:456:THR:HG22	2:B:457:ILE:N	2.35	0.41
2:B:535:VAL:O	2:B:535:VAL:HG23	2.21	0.41
1:C:359:ASP:O	2:D:530:MET:HG2	2.21	0.41
2:D:405:SER:O	2:D:406:ALA:HB3	2.20	0.41
1:A:173:SER:OG	1:A:176:GLN:HG3	2.21	0.41
2:B:506:GLN:O	2:B:507:TRP:HB3	2.20	0.41
1:A:280:SER:HB2	1:A:281:PRO:CD	2.50	0.40
1:C:261:VAL:HG22	3:C:536:HOH:O	2.21	0.40
2:D:463:LYS:HE3	2:D:463:LYS:C	2.43	0.40
1:A:199:LYS:O	1:A:200:LYS:C	2.65	0.40
1:A:229:LYS:HG3	3:A:497:HOH:O	2.20	0.40
1:A:315:ALA:O	1:A:319:MET:HG3	2.22	0.40
1:A:78:ALA:HB2	2:B:403:TYR:CZ	2.56	0.40
1:A:262:LYS:HE2	1:A:262:LYS:HB3	1.99	0.40
1:A:122:VAL:O	1:A:124:PRO:HD3	2.21	0.40
1:A:288:HIS:O	1:A:292:ILE:HG13	2.21	0.40
2:B:549:LEU:HB2	2:B:556:VAL:CG1	2.52	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	345/376 (92%)	329 (95%)	15 (4%)	1 (0%)	36 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	347/376 (92%)	337 (97%)	10 (3%)	0	100	100
2	B	184/188 (98%)	177 (96%)	6 (3%)	1 (0%)	24	16
2	D	184/188 (98%)	174 (95%)	8 (4%)	2 (1%)	11	4
All	All	1060/1128 (94%)	1017 (96%)	39 (4%)	4 (0%)	30	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	GLN
2	B	400	ASN
2	D	461	ASN
2	D	400	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	272/297 (92%)	272 (100%)	0	100	100
1	C	275/297 (93%)	275 (100%)	0	100	100
2	B	155/159 (98%)	152 (98%)	3 (2%)	50	47
2	D	157/159 (99%)	155 (99%)	2 (1%)	61	61
All	All	859/912 (94%)	854 (99%)	5 (1%)	78	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	397	TYR
2	B	399	ILE
2	B	481	LEU
2	D	397	TYR
2	D	463	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	168	ASN
1	A	202	HIS
1	A	366	GLN
2	B	446	ASN
2	B	461	ASN
2	B	462	ASN
1	C	121	ASN
1	C	168	ASN
1	C	174	GLN
1	C	233	GLN
1	C	321	GLN
1	C	373	GLN
1	C	379	ASN
2	D	462	ASN
2	D	533	GLN
2	D	544	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 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 ⓘ

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	347/376 (92%)	0.77	29 (8%) 17 18	21, 35, 55, 73	0
1	C	349/376 (92%)	0.12	6 (1%) 69 72	15, 27, 42, 74	0
2	B	186/188 (98%)	0.39	7 (3%) 44 47	20, 30, 51, 68	0
2	D	186/188 (98%)	-0.08	7 (3%) 44 47	15, 23, 42, 60	0
All	All	1068/1128 (94%)	0.34	49 (4%) 37 40	15, 29, 51, 74	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	TYR	4.9
1	A	175	ARG	3.9
1	A	374	LEU	3.8
1	A	203	LEU	3.8
1	A	120	GLY	3.6
1	A	30	PRO	3.5
2	B	565	LYS	3.2
1	A	31	PRO	3.2
2	B	461	ASN	3.1
1	C	378	SER	3.1
1	A	177	ALA	3.1
1	A	123	VAL	3.0
1	A	202	HIS	3.0
1	C	377	GLY	3.0
1	A	373	GLN	3.0
2	B	550	PRO	2.9
1	A	375	HIS	2.8
1	C	31	PRO	2.8
1	A	179	THR	2.8
1	A	117	ASP	2.8
2	B	386	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	550	PRO	2.7
1	A	372	GLY	2.7
1	A	54	VAL	2.7
1	A	188	LEU	2.6
1	C	32	ILE	2.6
2	B	551	LYS	2.6
1	A	185	GLU	2.5
2	D	551	LYS	2.5
1	A	126	LEU	2.5
1	A	184	ARG	2.4
2	B	554	GLY	2.4
1	A	181	LYS	2.4
1	A	248	GLY	2.4
2	D	463	LYS	2.3
1	A	116	LEU	2.3
1	A	360	THR	2.3
2	D	565	LYS	2.3
1	C	379	ASN	2.3
2	B	435	LEU	2.2
1	C	375	HIS	2.2
2	D	552	THR	2.2
2	D	554	GLY	2.2
1	A	358	PRO	2.2
1	A	113	ASN	2.1
2	D	462	ASN	2.1
1	A	122	VAL	2.1
1	A	183	ALA	2.1
1	A	359	ASP	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.