



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:17 AM UTC

PDB ID : 4YE9 / pdb_00004ye9
Title : The crystal structure of the G45V mutant of human GlnRS
Authors : Ognjenovic, J.; Wu, J.; Ling, J.; Simonovic, M.
Deposited on : 2015-02-23
Resolution : 2.70 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

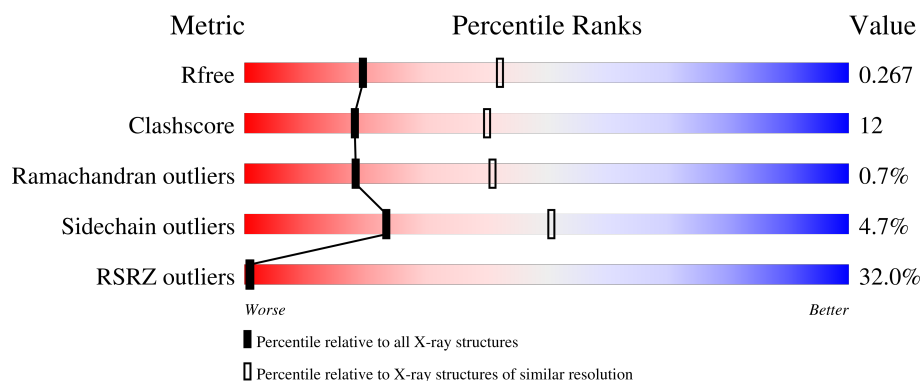
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	776	29% 68% 21% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5288 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 Glutamine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	709	Total	C	N	O	S	0	5	0
			5201	3307	919	947	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP P47897
A	45	VAL	GLY	engineered mutation	UNP P47897

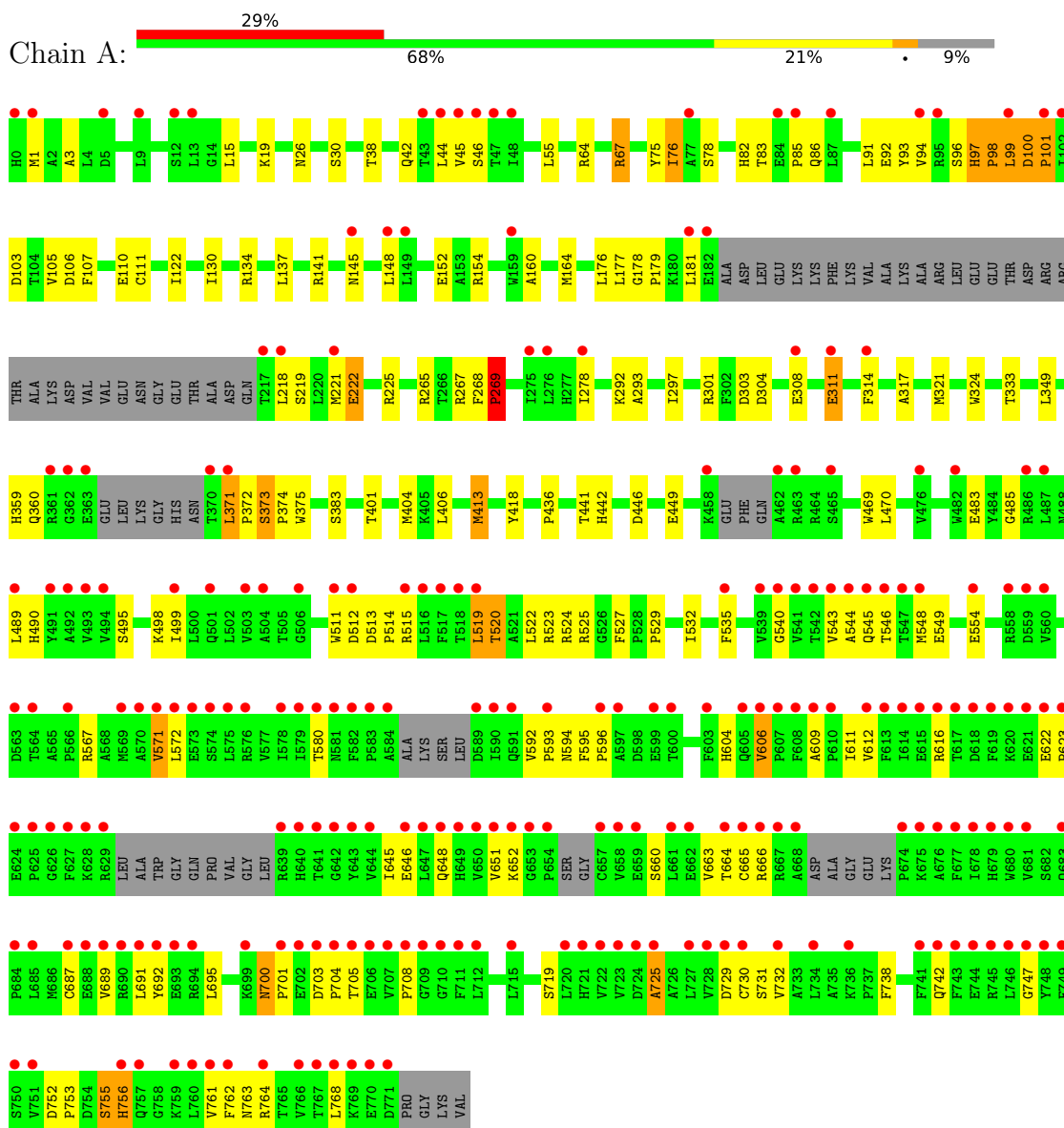
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	87	Total	O	0	0
			87	87		

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: Glutamine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	336.94Å 58.52Å 86.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.50 – 2.70 48.50 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.50-2.70) 89.5 (48.50-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.46 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.228 , 0.262 0.232 , 0.267	Depositor DCC
R_{free} test set	2000 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 83.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5288	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% 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	0.66	1/5336 (0.0%)	1.18	40/7283 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	HIS	C-N	5.80	1.38	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	622	GLU	CB-CA-C	-18.85	93.48	110.44
1	A	623	PRO	N-CA-CB	-13.82	88.74	103.25
1	A	99	LEU	CB-CA-C	-13.70	83.69	110.27
1	A	98	PRO	CB-CA-C	-12.39	93.67	110.52
1	A	99	LEU	N-CA-C	11.01	126.30	113.19
1	A	622	GLU	N-CA-C	-10.57	87.88	108.59
1	A	78	SER	N-CA-C	-9.37	94.86	109.76
1	A	46	SER	N-CA-C	-8.77	96.04	110.17
1	A	595	PHE	CA-C-N	8.10	127.67	119.24
1	A	595	PHE	C-N-CA	8.10	127.67	119.24
1	A	719	SER	CB-CA-C	-7.99	107.36	116.63
1	A	222	GLU	N-CA-C	-7.72	104.47	114.04
1	A	612	VAL	N-CA-C	7.62	118.82	110.21
1	A	373	SER	CA-C-N	7.39	127.10	119.56
1	A	373	SER	C-N-CA	7.39	127.10	119.56
1	A	611	ILE	N-CA-C	7.08	124.07	109.34
1	A	269	PRO	N-CA-C	6.96	119.19	110.70
1	A	616	ARG	N-CA-C	-6.88	99.19	109.86
1	A	178	GLY	CA-C-N	6.77	128.31	119.84
1	A	178	GLY	C-N-CA	6.77	128.31	119.84
1	A	45	VAL	N-CA-C	6.68	123.22	109.34
1	A	606	VAL	CA-C-N	6.45	127.90	119.84
1	A	606	VAL	C-N-CA	6.45	127.90	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	HIS	CA-C-N	-6.39	114.31	120.83
1	A	97	HIS	C-N-CA	-6.39	114.31	120.83
1	A	609	ALA	CA-C-N	6.29	126.26	120.03
1	A	609	ALA	C-N-CA	6.29	126.26	120.03
1	A	76	ILE	CB-CA-C	-5.96	104.18	110.62
1	A	67	ARG	N-CA-C	-5.96	105.50	112.89
1	A	622	GLU	CA-C-N	5.93	127.26	119.84
1	A	622	GLU	C-N-CA	5.93	127.26	119.84
1	A	44	LEU	N-CA-C	5.73	117.53	111.28
1	A	700	ASN	CA-C-N	-5.72	113.65	119.83
1	A	700	ASN	C-N-CA	-5.72	113.65	119.83
1	A	540	GLY	N-CA-C	5.63	126.52	113.18
1	A	725	ALA	CB-CA-C	5.60	117.84	110.06
1	A	549	GLU	CA-C-N	5.32	124.77	119.24
1	A	549	GLU	C-N-CA	5.32	124.77	119.24
1	A	513	ASP	CA-C-N	5.24	125.93	120.12
1	A	513	ASP	C-N-CA	5.24	125.93	120.12

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	5201	0	4668	119	0
2	A	87	0	0	3	0
All	All	5288	0	4668	119	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 12.

All (119) 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:524:ARG:NH1	1:A:753:PRO:HG2	1.38	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:O	1:A:101:PRO:HD3	1.49	1.11
1:A:311:GLU:OE1	1:A:314:PHE:HE2	1.33	1.08
1:A:311:GLU:OE1	1:A:314:PHE:CE2	2.05	1.07
1:A:99:LEU:O	1:A:101:PRO:CD	2.05	1.05
1:A:752:ASP:OD1	1:A:753:PRO:HD3	1.59	1.03
1:A:752:ASP:CG	1:A:753:PRO:CD	2.38	0.97
1:A:524:ARG:NH1	1:A:753:PRO:CG	2.31	0.93
1:A:524:ARG:HH12	1:A:753:PRO:HG2	1.37	0.88
1:A:524:ARG:HH11	1:A:753:PRO:HG2	1.39	0.87
1:A:752:ASP:CG	1:A:753:PRO:HD2	2.00	0.87
1:A:752:ASP:OD1	1:A:753:PRO:CD	2.25	0.84
1:A:752:ASP:CG	1:A:753:PRO:HD3	2.05	0.77
1:A:567:ARG:HG3	1:A:596:PRO:HD2	1.71	0.72
1:A:651:VAL:HG12	1:A:652:LYS:H	1.53	0.72
1:A:525:ARG:NH2	1:A:554:GLU:OE1	2.26	0.68
1:A:99:LEU:O	1:A:101:PRO:HD2	1.93	0.68
1:A:221:MET:HE1	1:A:292:LYS:HD3	1.78	0.66
1:A:301:ARG:NH1	1:A:449:GLU:OE1	2.29	0.66
1:A:103:ASP:OD1	1:A:105:VAL:HG12	1.97	0.65
1:A:371:LEU:HG	1:A:372:PRO:HD2	1.79	0.65
1:A:651:VAL:HB	1:A:660:SER:O	1.97	0.64
1:A:691:LEU:HG	1:A:764:ARG:HD2	1.82	0.61
1:A:512:ASP:HB3	1:A:520:THR:HG23	1.85	0.59
1:A:692:TYR:H	1:A:764:ARG:HD3	1.68	0.59
1:A:404:MET:HE3	1:A:470:LEU:HD13	1.85	0.59
1:A:752:ASP:OD2	1:A:753:PRO:HD2	2.04	0.58
1:A:92:GLU:OE2	1:A:96:SER:HB3	2.05	0.57
1:A:665:CYS:SG	1:A:666:ARG:N	2.78	0.57
1:A:83:THR:HG23	1:A:86:GLN:H	1.70	0.57
1:A:225:ARG:NH1	1:A:293:ALA:O	2.38	0.56
1:A:567:ARG:HD3	1:A:742:GLN:HB3	1.87	0.56
1:A:333:THR:HG21	1:A:449:GLU:OE2	2.05	0.56
1:A:38:THR:O	1:A:42:GLN:HG2	2.07	0.55
1:A:218:LEU:HG	1:A:219:SER:H	1.71	0.55
1:A:604:HIS:CD2	1:A:731:SER:HB3	2.41	0.55
1:A:76:ILE:HG22	1:A:76:ILE:O	2.06	0.55
1:A:700:ASN:HB3	1:A:701:PRO:HD2	1.88	0.55
1:A:729:ASP:OD1	1:A:730:CYS:N	2.36	0.54
1:A:704:PRO:HA	1:A:708:PRO:HD2	1.91	0.53
1:A:75:TYR:CD2	1:A:107:PHE:HE2	2.27	0.53
1:A:571:VAL:HG22	1:A:572:LEU:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:O	1:A:152:GLU:HG3	2.10	0.52
1:A:324:TRP:CZ2	1:A:523:ARG:HG3	2.44	0.52
1:A:648:GLN:H	1:A:663:VAL:HA	1.76	0.51
1:A:99:LEU:C	1:A:101:PRO:CD	2.82	0.51
1:A:691:LEU:HA	1:A:764:ARG:HG2	1.92	0.51
1:A:689:VAL:HG22	1:A:762:PHE:HB2	1.92	0.51
1:A:756:HIS:N	1:A:756:HIS:ND1	2.59	0.50
1:A:219:SER:HB3	1:A:222:GLU:CD	2.36	0.50
1:A:278:ILE:HA	1:A:519:LEU:HD21	1.94	0.50
1:A:651:VAL:HG12	1:A:652:LYS:N	2.26	0.49
1:A:515:ARG:HE	1:A:692:TYR:HD1	1.60	0.49
1:A:179:PRO:HB2	1:A:181:LEU:HD21	1.93	0.49
1:A:360:GLN:HE21	1:A:371:LEU:HD23	1.77	0.48
1:A:265:ARG:HG2	1:A:297:ILE:HD11	1.94	0.48
1:A:523:ARG:HG2	1:A:738:PHE:CE1	2.48	0.48
1:A:269:PRO:HA	1:A:301:ARG:O	2.14	0.48
1:A:26:ASN:O	1:A:30:SER:HB3	2.14	0.47
1:A:755:SER:C	1:A:756:HIS:ND1	2.73	0.47
1:A:406:LEU:HD22	1:A:469:TRP:CD2	2.50	0.47
1:A:511:TRP:CZ3	1:A:520:THR:HG21	2.50	0.47
1:A:93:TYR:CD1	1:A:107:PHE:HD1	2.32	0.46
1:A:703:ASP:O	1:A:705:THR:N	2.42	0.46
1:A:764:ARG:O	1:A:764:ARG:HG3	2.14	0.46
1:A:514:PRO:HB3	1:A:525:ARG:HB2	1.98	0.46
1:A:55:LEU:HD23	1:A:55:LEU:HA	1.81	0.45
1:A:141:ARG:NH1	2:A:802:HOH:O	2.50	0.45
1:A:512:ASP:O	1:A:524:ARG:HD3	2.17	0.45
1:A:324:TRP:CE2	1:A:529:PRO:HG3	2.52	0.45
1:A:96:SER:OG	1:A:97:HIS:CD2	2.70	0.45
1:A:83:THR:OG1	1:A:85:PRO:HD2	2.16	0.45
1:A:145:ASN:OD1	1:A:148:LEU:HD12	2.17	0.44
1:A:755:SER:HB2	1:A:761:VAL:H	1.81	0.44
1:A:747:GLY:HA2	1:A:768:LEU:HD11	1.99	0.44
1:A:164:MET:HE3	1:A:164:MET:HB3	1.88	0.44
1:A:729:ASP:CG	1:A:730:CYS:H	2.24	0.44
1:A:304:ASP:OD1	1:A:304:ASP:N	2.50	0.44
1:A:359:HIS:HB2	1:A:375:TRP:CH2	2.53	0.44
1:A:485:GLY:HA3	1:A:545:GLN:H	1.82	0.44
1:A:1:MET:C	1:A:3:ALA:H	2.25	0.43
1:A:268:PHE:HA	1:A:269:PRO:HD3	1.77	0.43
1:A:360:GLN:NE2	1:A:371:LEU:HD23	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:GLU:O	1:A:664:THR:N	2.50	0.43
1:A:695:LEU:HD23	1:A:695:LEU:O	2.18	0.43
1:A:154:ARG:NH1	1:A:160:ALA:O	2.48	0.43
1:A:176:LEU:HG	1:A:177:LEU:HD23	2.00	0.43
1:A:490:HIS:HB3	1:A:700:ASN:HA	2.00	0.43
1:A:96:SER:O	1:A:98:PRO:HD3	2.19	0.43
1:A:303:ASP:OD1	1:A:442:HIS:NE2	2.44	0.42
1:A:567:ARG:NH1	1:A:596:PRO:HG2	2.34	0.42
1:A:544:ALA:C	1:A:546:THR:N	2.77	0.42
1:A:495:SER:HB3	1:A:498:LYS:HB2	2.01	0.42
1:A:154:ARG:HA	1:A:154:ARG:HD3	1.73	0.42
1:A:317:ALA:O	1:A:321:MET:HG2	2.18	0.42
1:A:489:LEU:HD22	1:A:548:MET:HB3	2.00	0.42
1:A:592:VAL:HA	1:A:593:PRO:HD3	1.90	0.42
1:A:55:LEU:HD11	1:A:82:HIS:HA	2.01	0.42
1:A:67:ARG:HH22	1:A:100:ASP:HA	1.85	0.42
1:A:64:ARG:HB2	2:A:865:HOH:O	2.20	0.42
1:A:418:TYR:CZ	1:A:436:PRO:HB3	2.55	0.42
1:A:532:ILE:O	1:A:535:PHE:HB3	2.20	0.42
1:A:267:ARG:HD2	1:A:446:ASP:OD1	2.20	0.42
1:A:687:CYS:C	1:A:725:ALA:HA	2.45	0.42
1:A:489:LEU:CD2	1:A:548:MET:HB3	2.50	0.42
1:A:106:ASP:O	1:A:110:GLU:HG3	2.20	0.41
1:A:645:ILE:O	1:A:646:GLU:C	2.63	0.41
1:A:729:ASP:CG	1:A:730:CYS:N	2.79	0.41
1:A:373:SER:HA	1:A:374:PRO:HD3	1.82	0.41
1:A:324:TRP:NE1	1:A:529:PRO:HG3	2.35	0.41
1:A:86:GLN:HG2	1:A:111:CYS:O	2.21	0.41
1:A:413:MET:HE3	1:A:413:MET:HB3	1.76	0.41
1:A:522:LEU:HB3	1:A:527:PHE:CD2	2.56	0.41
1:A:594:ASN:OD1	1:A:594:ASN:N	2.53	0.41
1:A:134:ARG:HD3	2:A:811:HOH:O	2.20	0.41
1:A:580:THR:H	1:A:664:THR:HA	1.86	0.41
1:A:91:LEU:HD23	1:A:91:LEU:HA	1.81	0.40
1:A:75:TYR:HD1	1:A:75:TYR:HA	1.69	0.40
1:A:692:TYR:HE2	1:A:763:ASN:OD1	2.03	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	698/776 (90%)	610 (87%)	83 (12%)	5 (1%)	18	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	269	PRO
1	A	543	VAL
1	A	101	PRO
1	A	732	VAL

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	472/667 (71%)	450 (95%)	22 (5%)	23	51

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	19	LYS
1	A	94	VAL
1	A	122	ILE
1	A	130	ILE
1	A	137	LEU

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Mol	Chain	Res	Type
1	A	308	GLU
1	A	311	GLU
1	A	349	LEU
1	A	371	LEU
1	A	383	SER
1	A	401	THR
1	A	413	MET
1	A	441	THR
1	A	483	GLU
1	A	499	ILE
1	A	519	LEU
1	A	520	THR
1	A	571	VAL
1	A	606	VAL
1	A	755	SER
1	A	756	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	175	HIS
1	A	698	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	709/776 (91%)	1.56	227 (32%) 1 1	37, 92, 164, 186	5 (0%)

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	462	ALA	8.0
1	A	458	LYS	7.5
1	A	674	PRO	6.0
1	A	657	CYS	5.9
1	A	771	ASP	5.7
1	A	680	TRP	5.2
1	A	629	ARG	5.2
1	A	570	ALA	5.1
1	A	654	PRO	5.1
1	A	218	LEU	4.9
1	A	597	ALA	4.8
1	A	619	PHE	4.8
1	A	584	ALA	4.8
1	A	517	PHE	4.8
1	A	668	ALA	4.7
1	A	182	GLU	4.7
1	A	676	ALA	4.6
1	A	617	THR	4.6
1	A	543	VAL	4.6
1	A	665	CYS	4.5
1	A	616	ARG	4.4
1	A	582	PHE	4.4
1	A	541	VAL	4.4
1	A	627	PHE	4.4
1	A	569	MET	4.4
1	A	618	ASP	4.3
1	A	275	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	363	GLU	4.3
1	A	651	VAL	4.3
1	A	463	ARG	4.3
1	A	5	ASP	4.2
1	A	684	PRO	4.2
1	A	581	ASN	4.2
1	A	748	TYR	4.1
1	A	516	LEU	4.1
1	A	712	LEU	4.1
1	A	644	VAL	4.1
1	A	761	VAL	4.1
1	A	573	GLU	4.1
1	A	540	GLY	4.0
1	A	679	HIS	4.0
1	A	648	GLN	4.0
1	A	625	PRO	4.0
1	A	687	CYS	3.9
1	A	749	PHE	3.9
1	A	159	TRP	3.9
1	A	482[A]	TRP	3.9
1	A	580	THR	3.8
1	A	691	LEU	3.8
1	A	707	VAL	3.8
1	A	518	THR	3.8
1	A	767	THR	3.8
1	A	647	LEU	3.8
1	A	486	ARG	3.8
1	A	576	ARG	3.8
1	A	741	PHE	3.8
1	A	745	ARG	3.8
1	A	589	ASP	3.7
1	A	658	VAL	3.7
1	A	1	MET	3.7
1	A	744	GLU	3.7
1	A	743	PHE	3.7
1	A	606	VAL	3.7
1	A	650	VAL	3.7
1	A	705	THR	3.7
1	A	725	ALA	3.7
1	A	711	PHE	3.7
1	A	607	PRO	3.7
1	A	702	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	596	PRO	3.6
1	A	511	TRP	3.6
1	A	681	VAL	3.6
1	A	626	GLY	3.6
1	A	46	SER	3.6
1	A	0	HIS	3.5
1	A	708	PRO	3.5
1	A	675	LYS	3.5
1	A	575	LEU	3.5
1	A	701	PRO	3.5
1	A	688	GLU	3.5
1	A	623	PRO	3.5
1	A	768	LEU	3.5
1	A	613	PHE	3.4
1	A	762	PHE	3.4
1	A	615	GLU	3.4
1	A	579	ILE	3.4
1	A	678	ILE	3.4
1	A	574	SER	3.4
1	A	506	GLY	3.4
1	A	603	PHE	3.4
1	A	217	THR	3.3
1	A	659	GLU	3.3
1	A	563	ASP	3.3
1	A	747	GLY	3.3
1	A	571	VAL	3.3
1	A	689	VAL	3.3
1	A	643	TYR	3.3
1	A	149	LEU	3.3
1	A	706	GLU	3.3
1	A	664	THR	3.2
1	A	609	ALA	3.2
1	A	641	THR	3.2
1	A	608	PHE	3.2
1	A	13	LEU	3.2
1	A	546	THR	3.2
1	A	362	GLY	3.2
1	A	276	LEU	3.1
1	A	487	LEU	3.1
1	A	101	PRO	3.1
1	A	87	LEU	3.1
1	A	544	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	692	TYR	3.1
1	A	622	GLU	3.1
1	A	43	THR	3.1
1	A	690	ARG	3.1
1	A	770	GLU	3.1
1	A	499	ILE	3.1
1	A	667	ARG	3.1
1	A	732	VAL	3.0
1	A	44	LEU	3.0
1	A	703	ASP	3.0
1	A	757	GLN	3.0
1	A	102	ILE	3.0
1	A	685	LEU	3.0
1	A	370	THR	3.0
1	A	649	HIS	3.0
1	A	677	PHE	3.0
1	A	612	VAL	2.9
1	A	465	SER	2.9
1	A	605	GLN	2.9
1	A	599	GLU	2.9
1	A	710	GLY	2.9
1	A	628	LYS	2.8
1	A	759	LYS	2.8
1	A	760	LEU	2.8
1	A	766	VAL	2.8
1	A	45	VAL	2.8
1	A	624	GLU	2.8
1	A	583	PRO	2.8
1	A	593	PRO	2.8
1	A	493	VAL	2.8
1	A	494	VAL	2.8
1	A	566	PRO	2.7
1	A	750	SER	2.7
1	A	503	VAL	2.7
1	A	547	THR	2.7
1	A	47	THR	2.7
1	A	560	VAL	2.7
1	A	600	THR	2.7
1	A	48	ILE	2.7
1	A	746	LEU	2.7
1	A	764	ARG	2.7
1	A	693	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	314	PHE	2.7
1	A	559	ASP	2.7
1	A	683	GLN	2.6
1	A	742	GLN	2.6
1	A	578	ILE	2.6
1	A	694	ARG	2.6
1	A	590	ILE	2.6
1	A	84	GLU	2.6
1	A	12	SER	2.6
1	A	642	GLY	2.6
1	A	709	GLY	2.6
1	A	564	THR	2.6
1	A	720	LEU	2.6
1	A	727	LEU	2.6
1	A	734	LEU	2.6
1	A	515	ARG	2.6
1	A	621	GLU	2.6
1	A	729	ASP	2.5
1	A	9	LEU	2.5
1	A	620	LYS	2.5
1	A	311	GLU	2.5
1	A	554	GLU	2.5
1	A	489	LEU	2.5
1	A	640	HIS	2.5
1	A	501	GLN	2.5
1	A	542	THR	2.5
1	A	639	ARG	2.5
1	A	94	VAL	2.4
1	A	751	VAL	2.4
1	A	769	LYS	2.4
1	A	181	LEU	2.4
1	A	736	LYS	2.4
1	A	519	LEU	2.4
1	A	614	ILE	2.4
1	A	646	GLU	2.4
1	A	653	GLY	2.4
1	A	558	ARG	2.3
1	A	666	ARG	2.3
1	A	85	PRO	2.3
1	A	539	VAL	2.3
1	A	492	ALA	2.3
1	A	504	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	756	HIS	2.3
1	A	591	GLN	2.3
1	A	715	LEU	2.3
1	A	652	LYS	2.3
1	A	278	ILE	2.2
1	A	491	TYR	2.2
1	A	145	ASN	2.2
1	A	148	LEU	2.2
1	A	721	HIS	2.2
1	A	77	ALA	2.2
1	A	610	PRO	2.2
1	A	723	VAL	2.2
1	A	95	ARG	2.2
1	A	545	GLN	2.2
1	A	661	LEU	2.2
1	A	722	VAL	2.2
1	A	361	ARG	2.1
1	A	730	CYS	2.1
1	A	699	LYS	2.1
1	A	221	MET	2.1
1	A	548	MET	2.1
1	A	512	ASP	2.1
1	A	728	VAL	2.1
1	A	535	PHE	2.1
1	A	308	GLU	2.1
1	A	99	LEU	2.1
1	A	724	ASP	2.1
1	A	662	GLU	2.1
1	A	704	PRO	2.1
1	A	371	LEU	2.1
1	A	572	LEU	2.0
1	A	476	VAL	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 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.