



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:21 AM UTC

PDB ID : 4YE8 / pdb_00004ye8
Title : The crystal structure of the Y57H mutant of human GlnRS
Authors : Ognjenovic, J.; Wu, J.; Ling, J.; Simonovic, M.
Deposited on : 2015-02-23
Resolution : 3.30 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

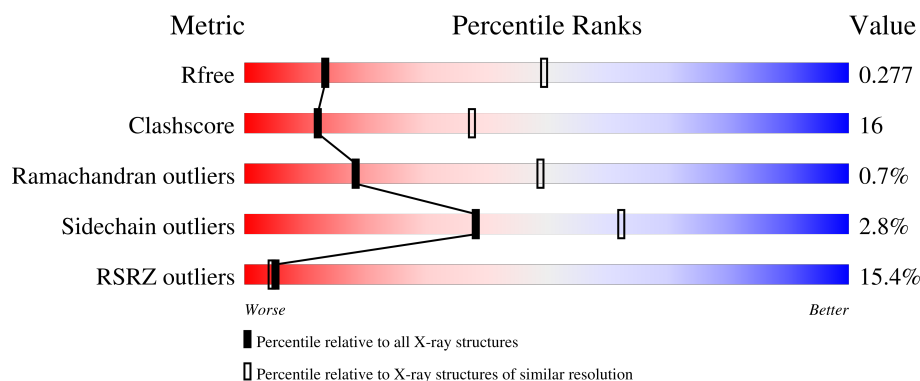
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	14% 59% 28% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5169 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	2	0
			5151	3265	907	950	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP P47897
A	57	HIS	TYR	engineered mutation	UNP P47897

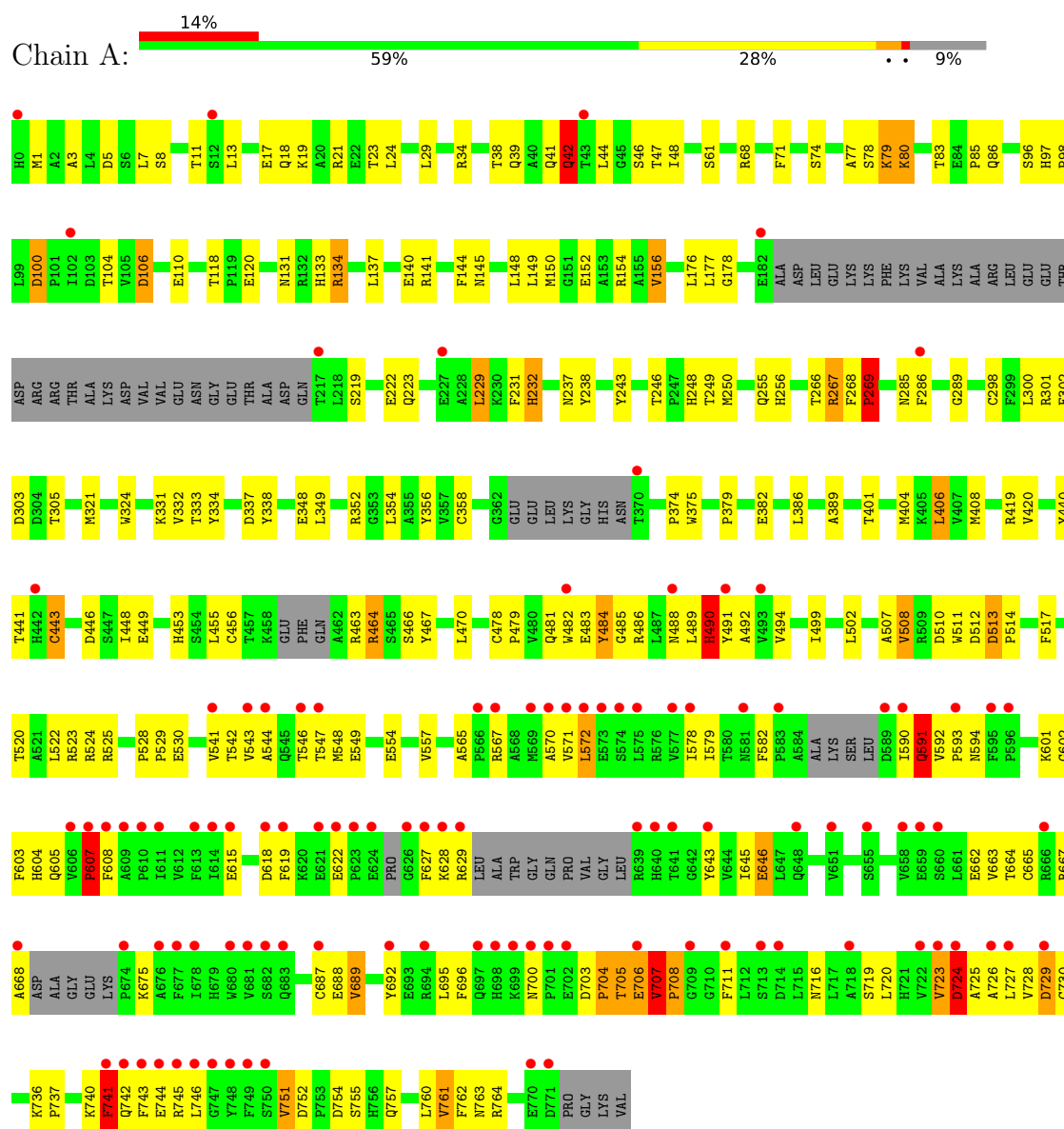
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	18	Total	O	0	0
			18	18		

3 Residue-property plots

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	333.09Å 58.26Å 85.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.87 – 3.30 33.87 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.87-3.30) 91.5 (33.87-3.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.221 , 0.274 0.228 , 0.277	Depositor DCC
R_{free} test set	2000 reflections (7.72%)	wwPDB-VP
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5169	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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	0.91	1/5275 (0.0%)	1.34	93/7199 (1.3%)

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	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	708	PRO	N-CD	6.50	1.56	1.47

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	743	PHE	N-CA-C	-18.81	79.30	109.59
1	A	707	VAL	N-CA-CB	-15.73	89.19	111.21
1	A	724	ASP	N-CA-C	15.61	131.73	111.75
1	A	607	PRO	CB-CA-C	-13.11	89.93	111.56
1	A	706	GLU	N-CA-C	-12.50	91.00	109.63
1	A	744	GLU	N-CA-CB	-12.46	88.49	110.42
1	A	627	PHE	N-CA-C	-11.87	89.61	109.80
1	A	628	LYS	N-CA-CB	-11.61	90.87	110.49
1	A	724	ASP	N-CA-CB	-11.36	92.19	110.14
1	A	723	VAL	CB-CA-C	11.29	129.81	111.29
1	A	707	VAL	N-CA-C	10.09	130.67	108.88
1	A	745	ARG	N-CA-C	9.94	124.06	111.24
1	A	608	PHE	N-CA-CB	-9.83	93.84	110.46
1	A	705	THR	N-CA-C	-9.45	90.68	110.80
1	A	646	GLU	N-CA-C	9.16	123.16	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	711	PHE	N-CA-C	-8.97	102.46	113.41
1	A	704	PRO	N-CA-C	-8.86	94.22	112.47
1	A	740	LYS	N-CA-C	8.64	122.42	110.24
1	A	592	VAL	CA-C-N	8.41	130.36	119.84
1	A	592	VAL	C-N-CA	8.41	130.36	119.84
1	A	507	ALA	N-CA-C	-7.89	103.45	113.23
1	A	178	GLY	CA-C-N	7.87	127.89	119.78
1	A	178	GLY	C-N-CA	7.87	127.89	119.78
1	A	740	LYS	CB-CA-C	-7.82	97.11	109.70
1	A	80	LYS	N-CA-C	-7.55	94.71	110.80
1	A	741	PHE	CB-CA-C	-7.54	95.41	110.42
1	A	156	VAL	N-CA-C	-7.25	106.82	113.71
1	A	645	ILE	N-CA-C	7.25	124.43	109.34
1	A	746	LEU	N-CA-C	-7.21	104.47	113.55
1	A	134	ARG	CA-C-N	-7.18	112.39	119.64
1	A	134	ARG	C-N-CA	-7.18	112.39	119.64
1	A	269	PRO	N-CA-C	7.01	119.25	110.70
1	A	222	GLU	N-CA-C	-6.95	105.42	114.04
1	A	484	TYR	N-CA-C	-6.90	101.63	110.53
1	A	549	GLU	CA-C-N	6.87	127.15	119.32
1	A	549	GLU	C-N-CA	6.87	127.15	119.32
1	A	705	THR	N-CA-CB	6.69	121.80	110.49
1	A	79	LYS	N-CA-C	-6.67	96.60	110.80
1	A	486	ARG	N-CA-C	6.59	120.49	111.39
1	A	716	ASN	N-CA-C	-6.58	99.18	109.25
1	A	466	SER	N-CA-C	-6.53	105.28	113.18
1	A	13	LEU	N-CA-C	-6.41	105.10	113.17
1	A	742	GLN	N-CA-CB	-6.36	99.76	110.83
1	A	231	PHE	CA-C-N	6.30	130.08	120.82
1	A	231	PHE	C-N-CA	6.30	130.08	120.82
1	A	743	PHE	CB-CA-C	6.23	120.59	109.38
1	A	601	LYS	N-CA-C	6.05	120.73	113.23
1	A	700	ASN	CA-C-N	-5.92	113.43	119.83
1	A	700	ASN	C-N-CA	-5.92	113.43	119.83
1	A	513	ASP	CA-C-N	5.89	127.20	119.84
1	A	513	ASP	C-N-CA	5.89	127.20	119.84
1	A	77	ALA	CB-CA-C	-5.86	101.68	110.88
1	A	604	HIS	CA-C-O	-5.85	115.27	121.88
1	A	420	VAL	N-CA-C	5.84	115.76	106.88
1	A	745	ARG	CB-CA-C	-5.80	101.28	110.86
1	A	80	LYS	N-CA-CB	5.77	120.25	110.49
1	A	106	ASP	N-CA-C	-5.76	105.00	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	TYR	N-CA-C	5.76	119.29	112.72
1	A	675	LYS	N-CA-C	5.75	118.27	108.67
1	A	622	GLU	CA-C-N	-5.73	114.05	119.90
1	A	622	GLU	C-N-CA	-5.73	114.05	119.90
1	A	443	CYS	N-CA-C	-5.72	105.40	112.72
1	A	18	GLN	CA-CB-CG	5.71	125.53	114.10
1	A	18	GLN	N-CA-C	-5.62	105.68	112.54
1	A	464	ARG	CB-CA-C	-5.60	100.89	110.24
1	A	100	ASP	CA-C-N	-5.58	112.86	119.05
1	A	100	ASP	C-N-CA	-5.58	112.86	119.05
1	A	592	VAL	N-CA-C	5.58	114.63	108.05
1	A	77	ALA	N-CA-C	5.57	117.03	111.07
1	A	544	ALA	N-CA-C	5.56	117.74	108.02
1	A	229	LEU	N-CA-CB	-5.54	102.25	111.06
1	A	543	VAL	N-CA-C	-5.54	97.81	109.34
1	A	736	LYS	CA-C-N	-5.49	114.94	120.21
1	A	736	LYS	C-N-CA	-5.49	114.94	120.21
1	A	42	GLN	N-CA-C	-5.45	106.63	113.28
1	A	729	ASP	CB-CA-C	-5.45	100.68	109.72
1	A	591	GLN	N-CA-C	5.45	117.22	107.80
1	A	726	ALA	N-CA-C	5.41	117.31	110.33
1	A	572	LEU	N-CA-C	5.40	117.99	111.40
1	A	546	THR	N-CA-C	-5.40	97.84	107.98
1	A	590	ILE	CA-C-N	-5.34	114.69	122.44
1	A	590	ILE	C-N-CA	-5.34	114.69	122.44
1	A	645	ILE	CB-CA-C	-5.34	102.52	111.29
1	A	490	HIS	N-CA-C	5.33	117.09	111.28
1	A	608	PHE	N-CA-C	5.30	118.06	107.62
1	A	507	ALA	CB-CA-C	5.23	120.17	109.55
1	A	232	HIS	N-CA-CB	-5.12	101.72	109.92
1	A	502	LEU	N-CA-C	-5.11	107.05	113.28
1	A	11	THR	N-CA-C	-5.07	106.94	113.23
1	A	543	VAL	CB-CA-C	-5.07	102.97	111.29
1	A	140	GLU	N-CA-C	-5.03	105.87	111.36
1	A	79	LYS	CB-CA-C	5.03	120.43	110.42
1	A	463	ARG	N-CA-C	-5.00	97.76	107.62

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	485	GLY	Peptide
1	A	724	ASP	Peptide

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	5151	0	4561	151	0
2	A	18	0	0	2	0
All	All	5169	0	4561	151	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 16.

All (151) 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:619:PHE:HA	1:A:629:ARG:CB	1.90	1.02
1:A:96:SER:C	1:A:98:PRO:HD3	1.90	0.95
1:A:618:ASP:O	1:A:629:ARG:CB	2.20	0.90
1:A:554:GLU:HA	1:A:557:VAL:HG12	1.57	0.85
1:A:514:PRO:HB3	1:A:525:ARG:HG3	1.59	0.83
1:A:267:ARG:HD2	1:A:269:PRO:HG3	1.60	0.82
1:A:528:PRO:HD2	1:A:557:VAL:HG23	1.60	0.81
1:A:488:ASN:O	1:A:547:THR:HA	1.81	0.81
1:A:582:PHE:CD1	1:A:665:CYS:SG	2.73	0.81
1:A:643:TYR:CB	1:A:667:ARG:HA	2.12	0.80
1:A:582:PHE:CE1	1:A:665:CYS:SG	2.78	0.76
1:A:692:TYR:O	1:A:764:ARG:NH2	2.20	0.73
1:A:78:SER:O	1:A:79:LYS:C	2.32	0.72
1:A:301:ARG:NH2	1:A:446:ASP:OD1	2.22	0.69
1:A:106:ASP:OD1	1:A:110:GLU:OE2	2.12	0.68
1:A:321:MET:HE1	1:A:523:ARG:HD2	1.74	0.68
1:A:141:ARG:NH2	1:A:177:LEU:O	2.28	0.67
1:A:68:ARG:NH2	1:A:98:PRO:O	2.28	0.67
1:A:133:HIS:NE2	1:A:152:GLU:OE2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ASN:O	1:A:547:THR:CA	2.43	0.66
1:A:97:HIS:N	1:A:98:PRO:CD	2.58	0.66
1:A:324:TRP:CE2	1:A:529:PRO:HG3	2.30	0.65
1:A:607:PRO:O	1:A:607:PRO:CD	2.43	0.65
1:A:286:PHE:HE2	1:A:455:LEU:HD22	1.62	0.65
1:A:301:ARG:NH1	1:A:449:GLU:OE1	2.30	0.65
1:A:530:GLU:H	1:A:530:GLU:CD	2.05	0.65
1:A:565:ALA:HB1	1:A:741:PHE:HA	1.79	0.63
1:A:689:VAL:HG22	1:A:762:PHE:HB2	1.79	0.63
1:A:5:ASP:N	1:A:5:ASP:OD1	2.31	0.62
1:A:7:LEU:HB2	1:A:24:LEU:HD11	1.81	0.61
1:A:488:ASN:O	1:A:548:MET:N	2.32	0.61
1:A:456:CYS:SG	1:A:481:GLN:NE2	2.73	0.61
1:A:582:PHE:HE1	1:A:665:CYS:HG	1.42	0.61
1:A:607:PRO:O	1:A:607:PRO:HD2	2.00	0.60
1:A:582:PHE:HD1	1:A:665:CYS:SG	2.19	0.60
1:A:754:ASP:HB2	1:A:761:VAL:HG11	1.84	0.60
1:A:594:ASN:ND2	1:A:603:PHE:HA	2.17	0.59
1:A:97:HIS:N	1:A:98:PRO:HD3	2.17	0.59
1:A:78:SER:O	1:A:80:LYS:N	2.36	0.59
1:A:514:PRO:HB3	1:A:525:ARG:CG	2.32	0.58
1:A:607:PRO:O	1:A:607:PRO:CG	2.52	0.57
1:A:646:GLU:O	1:A:664:THR:N	2.35	0.57
1:A:517:PHE:HA	1:A:522:LEU:HD21	1.86	0.57
1:A:703:ASP:O	1:A:705:THR:N	2.38	0.56
1:A:489:LEU:HA	1:A:548:MET:O	2.05	0.56
1:A:719:SER:OG	1:A:720:LEU:N	2.37	0.56
1:A:554:GLU:CA	1:A:557:VAL:HG12	2.33	0.55
1:A:582:PHE:HE1	1:A:665:CYS:SG	2.28	0.55
1:A:96:SER:C	1:A:98:PRO:CD	2.72	0.55
1:A:484:TYR:HA	1:A:542:THR:CB	2.36	0.55
1:A:667:ARG:O	1:A:668:ALA:HB3	2.07	0.55
1:A:46:SER:OG	1:A:47:THR:N	2.39	0.55
1:A:508:VAL:HG22	1:A:513:ASP:OD2	2.07	0.55
1:A:219:SER:O	1:A:223:GLN:HB2	2.09	0.53
1:A:570:ALA:HB2	1:A:728:VAL:HA	1.90	0.53
1:A:118:THR:HB	1:A:120:GLU:OE1	2.09	0.52
1:A:737:PRO:HA	1:A:751:VAL:HB	1.91	0.52
1:A:303:ASP:OD1	1:A:305:THR:HG23	2.10	0.52
1:A:338:TYR:OH	1:A:449:GLU:OE2	2.18	0.52
1:A:1:MET:C	1:A:3:ALA:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:LEU:C	1:A:696:PHE:HD2	2.18	0.52
1:A:176:LEU:HG	1:A:177:LEU:HD23	1.91	0.52
1:A:703:ASP:O	1:A:704:PRO:C	2.53	0.52
1:A:300:LEU:HD23	1:A:332:VAL:HG22	1.92	0.51
1:A:83:THR:OG1	1:A:85:PRO:HD2	2.10	0.51
1:A:482:TRP:C	1:A:483:GLU:HG3	2.36	0.51
1:A:137:LEU:HD13	1:A:144:PHE:CD2	2.45	0.51
1:A:567:ARG:HG2	1:A:594:ASN:O	2.10	0.51
1:A:324:TRP:CE2	1:A:523:ARG:HG3	2.45	0.50
1:A:757:GLN:N	1:A:757:GLN:OE1	2.44	0.50
1:A:17:GLU:O	1:A:21:ARG:N	2.40	0.50
1:A:386:LEU:HA	1:A:389:ALA:HB3	1.93	0.50
1:A:41:GLN:HB3	1:A:48:ILE:CD1	2.41	0.50
1:A:71:PHE:O	1:A:74:SER:OG	2.30	0.49
1:A:643:TYR:CA	1:A:667:ARG:HA	2.41	0.49
1:A:269:PRO:HA	1:A:301:ARG:O	2.12	0.49
1:A:494:VAL:HA	1:A:499:ILE:HD11	1.95	0.49
1:A:594:ASN:OD1	1:A:602:GLY:N	2.45	0.49
1:A:34:ARG:O	1:A:38:THR:HG23	2.13	0.49
1:A:492:ALA:HB2	1:A:517:PHE:CD1	2.48	0.49
1:A:232:HIS:CE1	1:A:453:HIS:CD2	3.00	0.48
1:A:29:LEU:HD13	1:A:61:SER:HA	1.95	0.48
1:A:68:ARG:O	1:A:71:PHE:HB3	2.12	0.48
1:A:591:GLN:HA	1:A:591:GLN:OE1	2.12	0.48
1:A:643:TYR:CB	1:A:667:ARG:CA	2.87	0.48
1:A:141:ARG:HA	1:A:177:LEU:HD13	1.95	0.48
1:A:441:THR:C	1:A:443:CYS:H	2.21	0.47
1:A:593:PRO:HA	1:A:603:PHE:CD1	2.48	0.47
1:A:268:PHE:HA	1:A:269:PRO:HD3	1.62	0.47
1:A:41:GLN:HA	1:A:44:LEU:HB3	1.96	0.47
1:A:374:PRO:HD2	1:A:375:TRP:CE3	2.50	0.47
1:A:511:TRP:CZ3	1:A:520:THR:HG21	2.50	0.47
1:A:356:TYR:CE2	1:A:358:CYS:HB2	2.50	0.47
1:A:406:LEU:HD11	1:A:408:MET:HG2	1.97	0.46
1:A:707:VAL:O	1:A:708:PRO:C	2.58	0.46
1:A:302:PHE:HB2	1:A:334:TYR:CD2	2.51	0.46
1:A:238:TYR:CD2	1:A:250:MET:HE1	2.51	0.46
1:A:83:THR:HG23	1:A:86:GLN:H	1.81	0.46
1:A:404:MET:HE2	1:A:440:TYR:HD1	1.80	0.46
1:A:349:LEU:HD23	1:A:349:LEU:HA	1.76	0.45
1:A:512:ASP:HB3	1:A:524:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ASP:OD1	1:A:8:SER:HB2	2.16	0.45
1:A:591:GLN:OE1	1:A:605:GLN:HA	2.17	0.45
1:A:593:PRO:HA	1:A:603:PHE:CG	2.52	0.45
1:A:618:ASP:C	1:A:629:ARG:CB	2.89	0.45
1:A:579:ILE:HA	1:A:663:VAL:H	1.82	0.44
1:A:131:ASN:OD1	1:A:134:ARG:NH1	2.50	0.44
1:A:490:HIS:N	1:A:548:MET:O	2.49	0.44
1:A:703:ASP:CB	1:A:704:PRO:HD2	2.48	0.44
1:A:255:GLN:O	1:A:256:HIS:C	2.61	0.44
1:A:578:ILE:O	1:A:662:GLU:HA	2.18	0.44
1:A:513:ASP:HA	1:A:514:PRO:HD3	1.87	0.44
1:A:19:LYS:O	1:A:23:THR:OG1	2.28	0.43
1:A:379:PRO:HD2	1:A:382:GLU:HB2	2.00	0.43
1:A:478:CYS:HA	1:A:479:PRO:HD3	1.82	0.43
1:A:470:LEU:HD23	1:A:470:LEU:HA	1.83	0.43
1:A:695:LEU:C	1:A:696:PHE:CD2	2.96	0.43
1:A:687:CYS:C	1:A:725:ALA:HA	2.43	0.43
1:A:688:GLU:HA	1:A:725:ALA:HA	2.00	0.43
1:A:145:ASN:HB3	1:A:148:LEU:HG	2.01	0.43
1:A:286:PHE:CE2	1:A:455:LEU:HD22	2.48	0.43
1:A:348:GLU:O	1:A:352:ARG:HG3	2.19	0.43
1:A:39:GLN:HA	1:A:42:GLN:HB3	2.01	0.43
1:A:255:GLN:NE2	2:A:803:HOH:O	2.51	0.42
1:A:729:ASP:OD1	1:A:730:CYS:N	2.52	0.42
1:A:723:VAL:CG1	1:A:724:ASP:N	2.83	0.42
1:A:154:ARG:C	1:A:156:VAL:H	2.26	0.42
1:A:510:ASP:C	1:A:512:ASP:H	2.27	0.42
1:A:570:ALA:HB1	1:A:727:LEU:O	2.19	0.42
1:A:571:VAL:HG11	1:A:615:GLU:CB	2.49	0.42
1:A:619:PHE:CA	1:A:629:ARG:CB	2.80	0.42
1:A:285:ASN:O	1:A:289:GLY:HA3	2.19	0.42
1:A:331:LYS:HE3	1:A:331:LYS:HB2	1.63	0.41
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.77	0.41
1:A:571:VAL:HG12	1:A:572:LEU:N	2.34	0.41
1:A:150:MET:HE2	1:A:150:MET:HB3	1.69	0.41
1:A:154:ARG:HA	1:A:154:ARG:HD3	1.78	0.41
1:A:334:TYR:O	1:A:337:ASP:HB2	2.20	0.41
1:A:237:ASN:HB3	1:A:243:TYR:CE1	2.55	0.41
1:A:246:THR:C	1:A:248:HIS:H	2.28	0.41
1:A:419[A]:ARG:HD3	2:A:807:HOH:O	2.20	0.41
1:A:448:ILE:HD13	1:A:448:ILE:HG21	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ARG:O	1:A:467:TYR:HB2	2.21	0.41
1:A:301:ARG:HA	1:A:333:THR:O	2.21	0.41
1:A:752:ASP:HB2	1:A:763:ASN:ND2	2.35	0.41
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.91	0.41
1:A:706:GLU:C	1:A:708:PRO:HD3	2.45	0.41
1:A:17:GLU:O	1:A:21:ARG:HG2	2.21	0.41
1:A:266:THR:O	1:A:298:CYS:HA	2.21	0.40
1:A:755:SER:HB2	1:A:760:LEU:HA	2.02	0.40
1:A:149:LEU:HD23	1:A:149:LEU:HA	1.82	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	695/776 (90%)	590 (85%)	100 (14%)	5 (1%)	18	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	PRO
1	A	541	VAL
1	A	707	VAL
1	A	100	ASP
1	A	607	PRO

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	461/666 (69%)	448 (97%)	13 (3%)	38	62

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

Mol	Chain	Res	Type
1	A	42	GLN
1	A	104	THR
1	A	229	LEU
1	A	249	THR
1	A	401	THR
1	A	406	LEU
1	A	490	HIS
1	A	508	VAL
1	A	591	GLN
1	A	689	VAL
1	A	741	PHE
1	A	751	VAL
1	A	761	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	232	HIS
1	A	306	ASN
1	A	426	HIS
1	A	481	GLN

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 [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	709/776 (91%)	0.55	109 (15%) 5 4	15, 63, 146, 165	2 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	687	CYS	6.3
1	A	698	HIS	5.6
1	A	624	GLU	5.3
1	A	621	GLU	5.0
1	A	571	VAL	4.9
1	A	608	PHE	4.9
1	A	488	ASN	4.7
1	A	593	PRO	4.4
1	A	623	PRO	4.4
1	A	668	ALA	4.4
1	A	677	PHE	4.2
1	A	676	ALA	4.2
1	A	714	ASP	4.0
1	A	741	PHE	3.9
1	A	711	PHE	3.9
1	A	699	LYS	3.8
1	A	570	ALA	3.7
1	A	611	ILE	3.6
1	A	697	GLN	3.6
1	A	607	PRO	3.5
1	A	745	ARG	3.5
1	A	491	TYR	3.4
1	A	682	SER	3.4
1	A	750	SER	3.4
1	A	724	ASP	3.4
1	A	546	THR	3.4
1	A	610	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	749	PHE	3.3
1	A	674	PRO	3.3
1	A	627	PHE	3.3
1	A	569	MET	3.3
1	A	702	GLU	3.3
1	A	729	ASP	3.3
1	A	583	PRO	3.2
1	A	771	ASP	3.2
1	A	629	ARG	3.2
1	A	744	GLU	3.2
1	A	643	TYR	3.1
1	A	590	ILE	3.1
1	A	589	ASP	3.1
1	A	613	PHE	3.1
1	A	640	HIS	3.0
1	A	628	LYS	3.0
1	A	614	ILE	3.0
1	A	727	LEU	3.0
1	A	747	GLY	3.0
1	A	619	PHE	3.0
1	A	575	LEU	2.9
1	A	701	PRO	2.9
1	A	618	ASP	2.9
1	A	641	THR	2.9
1	A	722	VAL	2.9
1	A	544	ALA	2.8
1	A	493	VAL	2.8
1	A	706	GLU	2.8
1	A	648	GLN	2.8
1	A	217	THR	2.8
1	A	748	TYR	2.7
1	A	543	VAL	2.7
1	A	680	TRP	2.7
1	A	547	THR	2.7
1	A	746	LEU	2.7
1	A	694	ARG	2.7
1	A	639	ARG	2.6
1	A	692	TYR	2.6
1	A	577	VAL	2.6
1	A	102	ILE	2.6
1	A	596	PRO	2.6
1	A	182	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	595	PHE	2.6
1	A	742	GLN	2.6
1	A	0	HIS	2.5
1	A	655	SER	2.5
1	A	581	ASN	2.5
1	A	659	GLU	2.5
1	A	718	ALA	2.5
1	A	43	THR	2.5
1	A	658	VAL	2.5
1	A	683	GLN	2.5
1	A	726	ALA	2.4
1	A	615	GLU	2.4
1	A	723	VAL	2.4
1	A	442	HIS	2.4
1	A	681	VAL	2.4
1	A	574	SER	2.4
1	A	626	GLY	2.4
1	A	743	PHE	2.4
1	A	622	GLU	2.4
1	A	578	ILE	2.3
1	A	609	ALA	2.3
1	A	678	ILE	2.3
1	A	770	GLU	2.3
1	A	606	VAL	2.3
1	A	666	ARG	2.3
1	A	713	SER	2.2
1	A	567	ARG	2.2
1	A	573	GLU	2.2
1	A	482	TRP	2.2
1	A	12	SER	2.2
1	A	709	GLY	2.2
1	A	541	VAL	2.1
1	A	700	ASN	2.1
1	A	286	PHE	2.1
1	A	227	GLU	2.1
1	A	660	SER	2.0
1	A	572	LEU	2.0
1	A	566	PRO	2.0
1	A	651	VAL	2.0
1	A	370	THR	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 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.