



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:55 AM UTC

PDB ID : 1U2L / pdb_00001u2l
Title : Crystal structure of the C-terminal domain from the catalase-peroxidase KatG of Escherichia coli (P1)
Authors : Carpena, X.; Melik-Adamyan, W.; Loewen, P.C.; Fita, I.
Deposited on : 2004-07-19
Resolution : 2.30 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

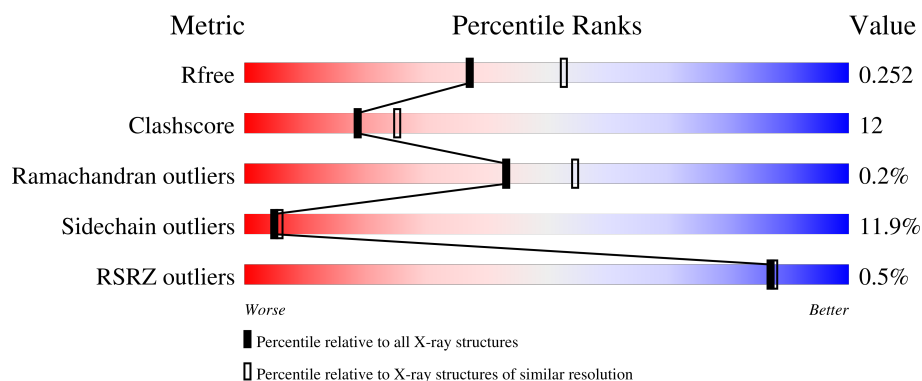
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	309	 72% 23% . .
1	B	309	 78% 20% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4931 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 Peroxidase/catalase HPI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2360	1495	404	454	7			
1	B	307	Total	C	N	O	S	0	0	0
			2360	1495	404	454	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	418	GLY	-	cloning artifact	UNP P13029
A	419	SER	-	cloning artifact	UNP P13029
A	420	HIS	-	cloning artifact	UNP P13029
A	421	MET	-	cloning artifact	UNP P13029
B	418	GLY	-	cloning artifact	UNP P13029
B	419	SER	-	cloning artifact	UNP P13029
B	420	HIS	-	cloning artifact	UNP P13029
B	421	MET	-	cloning artifact	UNP P13029

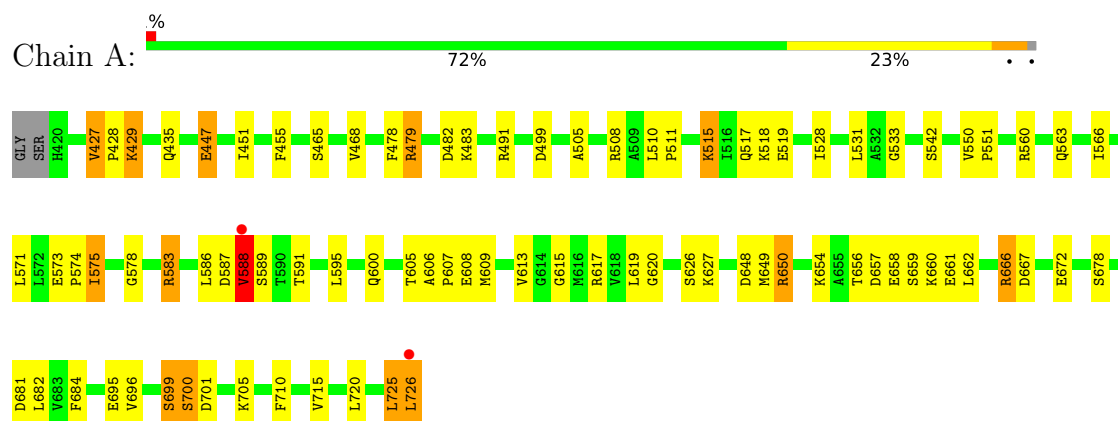
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	106	Total	O	0	0
			106	106		
2	B	105	Total	O	0	0
			105	105		

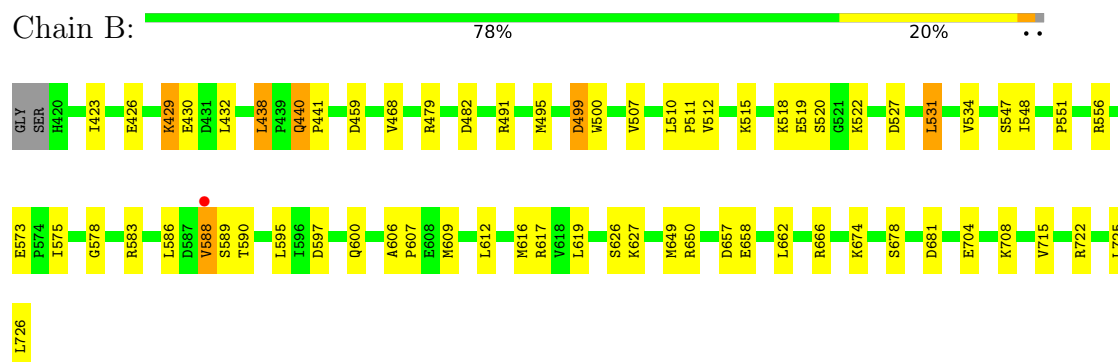
3 Residue-property plots

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: Peroxidase/catalase HPI



• Molecule 1: Peroxidase/catalase HPI



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.86Å 52.76Å 55.99Å 93.83° 90.71° 103.27°	Depositor
Resolution (Å)	25.00 – 2.30 25.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.30) 97.8 (25.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.175 , 0.251 0.176 , 0.252	Depositor DCC
R_{free} test set	1304 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4931	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.39% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.53	0/2403	0.83	0/3258
1	B	0.52	0/2403	0.80	0/3258
All	All	0.52	0/4806	0.82	0/6516

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	588	VAL	Peptide

5.2 Too-close contacts [i](#)

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	2360	0	2341	66	0
1	B	2360	0	2341	46	0
2	A	106	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	105	0	0	7	0
All	All	4931	0	4682	112	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 (112) 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:479:ARG:HH11	1:A:479:ARG:CG	1.76	0.98
1:A:479:ARG:HH11	1:A:479:ARG:CB	1.81	0.93
1:A:447:GLU:HG3	2:A:152:HOH:O	1.69	0.90
1:B:595:LEU:HD11	1:B:609:MET:SD	2.16	0.86
1:A:479:ARG:HH11	1:A:479:ARG:HG2	1.41	0.85
1:A:505:ALA:O	1:A:508:ARG:HG3	1.82	0.79
1:A:666:ARG:HG2	1:A:666:ARG:HH11	1.49	0.77
1:A:701:ASP:CA	2:A:131:HOH:O	2.32	0.77
1:A:605:THR:OG1	1:A:608:GLU:HG3	1.85	0.76
1:B:595:LEU:CD1	1:B:609:MET:SD	2.75	0.75
1:A:701:ASP:N	2:A:131:HOH:O	2.21	0.73
1:B:595:LEU:C	1:B:595:LEU:HD13	2.13	0.73
1:A:701:ASP:HA	2:A:131:HOH:O	1.88	0.72
1:A:479:ARG:HG2	1:A:479:ARG:NH1	2.03	0.70
1:B:479:ARG:NH2	1:B:482:ASP:OD1	2.24	0.68
1:A:587:ASP:O	1:A:588:VAL:HB	1.94	0.67
1:B:726:LEU:HD21	2:B:99:HOH:O	1.95	0.65
1:B:468:VAL:HG21	1:B:619:LEU:HD13	1.80	0.64
1:A:479:ARG:CB	1:A:479:ARG:NH1	2.59	0.63
1:A:578:GLY:HA3	1:A:595:LEU:HD23	1.82	0.60
1:A:479:ARG:HH11	1:A:479:ARG:HB3	1.65	0.60
1:A:666:ARG:HH11	1:A:666:ARG:CG	2.15	0.59
1:B:666:ARG:HG3	1:B:666:ARG:NH1	2.18	0.58
1:A:726:LEU:HG	2:A:194:HOH:O	2.01	0.58
1:A:588:VAL:CG1	1:A:588:VAL:O	2.51	0.57
1:B:666:ARG:HG3	1:B:666:ARG:HH11	1.68	0.57
1:A:595:LEU:CD1	1:A:609:MET:SD	2.93	0.57
1:A:662:LEU:HD23	2:A:109:HOH:O	2.04	0.57
1:A:551:PRO:HD2	1:A:715:VAL:HG21	1.85	0.57
1:B:491:ARG:HG3	2:B:51:HOH:O	2.04	0.56
1:B:573:GLU:OE2	2:B:186:HOH:O	2.18	0.56
1:A:491:ARG:NH1	2:A:115:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:VAL:HG12	1:B:507:VAL:O	2.04	0.56
1:B:657:ASP:C	1:B:657:ASP:OD2	2.49	0.55
1:B:578:GLY:HA3	1:B:595:LEU:HD23	1.89	0.55
1:A:726:LEU:HA	2:A:128:HOH:O	2.06	0.55
2:A:181:HOH:O	1:B:590:THR:HG23	2.06	0.55
1:B:438:LEU:CD2	2:B:93:HOH:O	2.55	0.55
1:B:678:SER:HB2	2:B:182:HOH:O	2.06	0.54
1:A:725:LEU:O	1:A:726:LEU:C	2.49	0.54
1:B:430:GLU:HG2	2:B:204:HOH:O	2.06	0.54
1:B:595:LEU:HD13	1:B:595:LEU:O	2.08	0.54
1:A:661:GLU:OE1	2:A:27:HOH:O	2.19	0.53
1:B:588:VAL:CG1	1:B:589:SER:N	2.70	0.53
1:B:612:LEU:O	1:B:616:MET:HG3	2.09	0.53
1:A:650:ARG:NE	1:A:667:ASP:OD2	2.43	0.52
1:B:520:SER:O	1:B:522:LYS:HG2	2.10	0.52
1:A:515:LYS:HE3	1:A:519:GLU:OE2	2.09	0.51
1:A:510:LEU:N	1:A:511:PRO:CD	2.73	0.51
1:A:560:ARG:HG2	1:A:563:GLN:HG3	1.91	0.51
1:A:666:ARG:CG	1:A:666:ARG:NH1	2.73	0.51
1:B:500:TRP:CD2	1:B:573:GLU:HG3	2.46	0.50
1:B:595:LEU:CD1	1:B:595:LEU:C	2.84	0.50
1:A:606:ALA:HB3	1:A:607:PRO:HD3	1.94	0.50
1:B:507:VAL:O	1:B:507:VAL:CG1	2.60	0.49
1:A:620:GLY:HA2	2:A:14:HOH:O	2.12	0.49
1:A:609:MET:O	1:A:613:VAL:HG23	2.13	0.49
1:A:617:ARG:NE	1:A:681:ASP:OD1	2.45	0.48
1:A:678:SER:HB2	2:A:27:HOH:O	2.13	0.48
1:B:510:LEU:HB2	1:B:511:PRO:HD3	1.94	0.48
1:B:429:LYS:HD2	1:B:432:LEU:CD1	2.43	0.48
1:B:510:LEU:N	1:B:511:PRO:CD	2.76	0.48
1:A:595:LEU:HD11	1:A:609:MET:SD	2.53	0.47
1:A:451:ILE:HG23	1:A:455:PHE:CE1	2.50	0.47
1:B:429:LYS:HA	1:B:429:LYS:HD3	1.56	0.47
1:A:468:VAL:HG21	1:A:619:LEU:HD13	1.96	0.47
1:B:500:TRP:CG	1:B:573:GLU:HG3	2.50	0.47
1:A:505:ALA:O	1:A:508:ARG:CG	2.59	0.47
1:B:510:LEU:N	1:B:511:PRO:HD2	2.29	0.47
1:A:613:VAL:HG21	1:A:684:PHE:CZ	2.51	0.46
1:A:510:LEU:HB2	1:A:511:PRO:HD3	1.98	0.46
1:B:440:GLN:NE2	1:B:441:PRO:O	2.46	0.46
1:A:666:ARG:CZ	1:A:666:ARG:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:LYS:N	1:B:627:LYS:HD2	2.30	0.45
1:B:429:LYS:HD2	1:B:432:LEU:HD11	1.99	0.45
1:B:527:ASP:OD1	1:B:556:ARG:HB2	2.17	0.45
1:A:429:LYS:HA	1:A:429:LYS:HD2	1.68	0.45
1:B:531:LEU:O	1:B:534:VAL:HB	2.17	0.45
1:B:551:PRO:HD2	1:B:715:VAL:HG21	1.99	0.44
1:A:575:ILE:HD13	2:A:83:HOH:O	2.17	0.44
1:A:595:LEU:HD13	1:A:609:MET:SD	2.57	0.44
1:A:619:LEU:HD23	1:A:619:LEU:HA	1.75	0.44
1:A:427:VAL:HG13	2:A:199:HOH:O	2.17	0.44
1:A:648:ASP:OD2	1:A:650:ARG:HB3	2.18	0.44
1:A:656:THR:O	1:A:657:ASP:HB3	2.18	0.44
1:A:615:GLY:HA3	1:A:710:PHE:CE1	2.53	0.43
1:B:606:ALA:HB3	1:B:607:PRO:HD3	2.00	0.43
1:A:583:ARG:HH21	1:A:591:THR:N	2.16	0.43
1:A:700:SER:O	1:A:701:ASP:HB2	2.17	0.43
1:A:427:VAL:HA	1:A:428:PRO:HD3	1.88	0.43
1:B:626:SER:HB3	2:B:150:HOH:O	2.18	0.43
1:A:451:ILE:CG2	1:A:455:PHE:HE1	2.32	0.43
1:B:606:ALA:N	1:B:607:PRO:CD	2.82	0.43
1:A:482:ASP:O	1:A:483:LYS:HB2	2.18	0.42
1:A:573:GLU:HA	1:A:574:PRO:HD3	1.85	0.42
1:A:479:ARG:HH12	1:A:482:ASP:CG	2.27	0.42
1:B:588:VAL:HG12	1:B:589:SER:N	2.35	0.42
1:A:479:ARG:NH1	1:A:482:ASP:OD2	2.53	0.42
1:A:533:GLY:HA3	2:A:140:HOH:O	2.19	0.42
1:A:696:VAL:O	1:A:699:SER:HB2	2.19	0.42
1:B:459:ASP:O	1:B:459:ASP:CG	2.62	0.42
1:A:478:PHE:CD2	1:A:720:LEU:HD13	2.54	0.42
1:B:495:MET:HE1	1:B:499:ASP:HB2	2.01	0.42
1:B:438:LEU:N	1:B:438:LEU:HD23	2.33	0.41
1:B:617:ARG:NE	1:B:681:ASP:OD1	2.47	0.41
1:A:666:ARG:HG2	1:A:666:ARG:NH1	2.25	0.41
1:A:606:ALA:N	1:A:607:PRO:CD	2.84	0.41
1:A:517:GLN:CG	1:A:528:ILE:HD12	2.51	0.41
1:B:722:ARG:HB3	1:B:725:LEU:HD12	2.02	0.41
1:A:550:VAL:HA	1:A:551:PRO:HD3	1.92	0.40
1:A:659:SER:O	1:A:660:LYS:HB2	2.19	0.40
1:B:657:ASP:OD2	1:B:658:GLU:N	2.54	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	305/309 (99%)	300 (98%)	4 (1%)	1 (0%)	36	46
1	B	305/309 (99%)	297 (97%)	8 (3%)	0	100	100
All	All	610/618 (99%)	597 (98%)	12 (2%)	1 (0%)	43	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	588	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	248/250 (99%)	214 (86%)	34 (14%)	3	4
1	B	248/250 (99%)	223 (90%)	25 (10%)	7	9
All	All	496/500 (99%)	437 (88%)	59 (12%)	5	6

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	427	VAL
1	A	429	LYS
1	A	435	GLN
1	A	447	GLU
1	A	465	SER

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Mol	Chain	Res	Type
1	A	479	ARG
1	A	499	ASP
1	A	515	LYS
1	A	518	LYS
1	A	531	LEU
1	A	542	SER
1	A	566	ILE
1	A	571	LEU
1	A	575	ILE
1	A	583	ARG
1	A	586	LEU
1	A	588	VAL
1	A	589	SER
1	A	600	GLN
1	A	626	SER
1	A	627	LYS
1	A	649	MET
1	A	650	ARG
1	A	654	LYS
1	A	658	GLU
1	A	666	ARG
1	A	672	GLU
1	A	682	LEU
1	A	695	GLU
1	A	699	SER
1	A	700	SER
1	A	705	LYS
1	A	725	LEU
1	A	726	LEU
1	B	423	ILE
1	B	426	GLU
1	B	429	LYS
1	B	438	LEU
1	B	440	GLN
1	B	499	ASP
1	B	512	VAL
1	B	515	LYS
1	B	518	LYS
1	B	519	GLU
1	B	531	LEU
1	B	547	SER
1	B	548	ILE

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Mol	Chain	Res	Type
1	B	575	ILE
1	B	583	ARG
1	B	586	LEU
1	B	588	VAL
1	B	597	ASP
1	B	600	GLN
1	B	649	MET
1	B	650	ARG
1	B	662	LEU
1	B	674	LYS
1	B	704	GLU
1	B	708	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	600	GLN
1	A	601	GLN
1	A	628	ASN
1	B	444	ASN
1	B	549	HIS
1	B	600	GLN
1	B	601	GLN
1	B	628	ASN

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	307/309 (99%)	-0.14	2 (0%) 84 85	11, 24, 46, 58	0
1	B	307/309 (99%)	-0.21	1 (0%) 90 90	10, 22, 47, 61	0
All	All	614/618 (99%)	-0.17	3 (0%) 87 87	10, 23, 46, 61	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	588	VAL	3.9
1	B	588	VAL	3.6
1	A	726	LEU	3.5

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.