



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:59 PM UTC

PDB ID : 7F77 / pdb_00007f77
Title : Crystal structure of glutamate dehydrogenase 3 from *Candida albicans*
Authors : Li, N.; Wang, W.; Zeng, X.; Liu, M.; Li, M.; Li, C.; Wang, M.
Deposited on : 2021-06-28
Resolution : 3.09 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

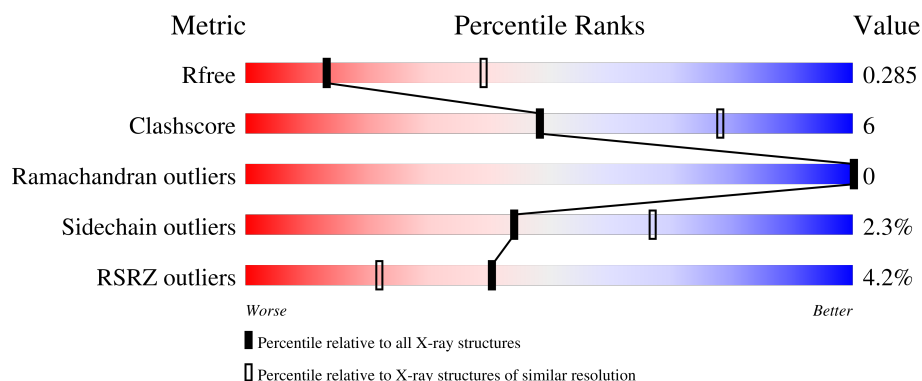
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	484	2% 74% 14% • 11%
1	B	484	5% 75% 12% 13%
1	C	484	4% 72% 14% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9733 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3295	2089	556	636	14			
1	B	420	Total	C	N	O	S	0	0	0
			3216	2039	543	620	14			
1	C	419	Total	C	N	O	S	0	0	0
			3205	2032	539	621	13			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A1D8PMH8
A	-18	GLY	-	expression tag	UNP A0A1D8PMH8
A	-17	SER	-	expression tag	UNP A0A1D8PMH8
A	-16	SER	-	expression tag	UNP A0A1D8PMH8
A	-15	HIS	-	expression tag	UNP A0A1D8PMH8
A	-14	HIS	-	expression tag	UNP A0A1D8PMH8
A	-13	HIS	-	expression tag	UNP A0A1D8PMH8
A	-12	HIS	-	expression tag	UNP A0A1D8PMH8
A	-11	HIS	-	expression tag	UNP A0A1D8PMH8
A	-10	HIS	-	expression tag	UNP A0A1D8PMH8
A	-9	SER	-	expression tag	UNP A0A1D8PMH8
A	-8	SER	-	expression tag	UNP A0A1D8PMH8
A	-7	GLY	-	expression tag	UNP A0A1D8PMH8
A	-6	LEU	-	expression tag	UNP A0A1D8PMH8
A	-5	VAL	-	expression tag	UNP A0A1D8PMH8
A	-4	PRO	-	expression tag	UNP A0A1D8PMH8
A	-3	ARG	-	expression tag	UNP A0A1D8PMH8
A	-2	GLY	-	expression tag	UNP A0A1D8PMH8
A	-1	SER	-	expression tag	UNP A0A1D8PMH8
A	0	HIS	-	expression tag	UNP A0A1D8PMH8
A	457	LEU	-	expression tag	UNP A0A1D8PMH8
A	458	GLU	-	expression tag	UNP A0A1D8PMH8
A	459	HIS	-	expression tag	UNP A0A1D8PMH8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	460	HIS	-	expression tag	UNP A0A1D8PMH8
A	461	HIS	-	expression tag	UNP A0A1D8PMH8
A	462	HIS	-	expression tag	UNP A0A1D8PMH8
A	463	HIS	-	expression tag	UNP A0A1D8PMH8
A	464	HIS	-	expression tag	UNP A0A1D8PMH8
B	-19	MET	-	initiating methionine	UNP A0A1D8PMH8
B	-18	GLY	-	expression tag	UNP A0A1D8PMH8
B	-17	SER	-	expression tag	UNP A0A1D8PMH8
B	-16	SER	-	expression tag	UNP A0A1D8PMH8
B	-15	HIS	-	expression tag	UNP A0A1D8PMH8
B	-14	HIS	-	expression tag	UNP A0A1D8PMH8
B	-13	HIS	-	expression tag	UNP A0A1D8PMH8
B	-12	HIS	-	expression tag	UNP A0A1D8PMH8
B	-11	HIS	-	expression tag	UNP A0A1D8PMH8
B	-10	HIS	-	expression tag	UNP A0A1D8PMH8
B	-9	SER	-	expression tag	UNP A0A1D8PMH8
B	-8	SER	-	expression tag	UNP A0A1D8PMH8
B	-7	GLY	-	expression tag	UNP A0A1D8PMH8
B	-6	LEU	-	expression tag	UNP A0A1D8PMH8
B	-5	VAL	-	expression tag	UNP A0A1D8PMH8
B	-4	PRO	-	expression tag	UNP A0A1D8PMH8
B	-3	ARG	-	expression tag	UNP A0A1D8PMH8
B	-2	GLY	-	expression tag	UNP A0A1D8PMH8
B	-1	SER	-	expression tag	UNP A0A1D8PMH8
B	0	HIS	-	expression tag	UNP A0A1D8PMH8
B	457	LEU	-	expression tag	UNP A0A1D8PMH8
B	458	GLU	-	expression tag	UNP A0A1D8PMH8
B	459	HIS	-	expression tag	UNP A0A1D8PMH8
B	460	HIS	-	expression tag	UNP A0A1D8PMH8
B	461	HIS	-	expression tag	UNP A0A1D8PMH8
B	462	HIS	-	expression tag	UNP A0A1D8PMH8
B	463	HIS	-	expression tag	UNP A0A1D8PMH8
B	464	HIS	-	expression tag	UNP A0A1D8PMH8
C	-19	MET	-	initiating methionine	UNP A0A1D8PMH8
C	-18	GLY	-	expression tag	UNP A0A1D8PMH8
C	-17	SER	-	expression tag	UNP A0A1D8PMH8
C	-16	SER	-	expression tag	UNP A0A1D8PMH8
C	-15	HIS	-	expression tag	UNP A0A1D8PMH8
C	-14	HIS	-	expression tag	UNP A0A1D8PMH8
C	-13	HIS	-	expression tag	UNP A0A1D8PMH8
C	-12	HIS	-	expression tag	UNP A0A1D8PMH8
C	-11	HIS	-	expression tag	UNP A0A1D8PMH8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	HIS	-	expression tag	UNP A0A1D8PMH8
C	-9	SER	-	expression tag	UNP A0A1D8PMH8
C	-8	SER	-	expression tag	UNP A0A1D8PMH8
C	-7	GLY	-	expression tag	UNP A0A1D8PMH8
C	-6	LEU	-	expression tag	UNP A0A1D8PMH8
C	-5	VAL	-	expression tag	UNP A0A1D8PMH8
C	-4	PRO	-	expression tag	UNP A0A1D8PMH8
C	-3	ARG	-	expression tag	UNP A0A1D8PMH8
C	-2	GLY	-	expression tag	UNP A0A1D8PMH8
C	-1	SER	-	expression tag	UNP A0A1D8PMH8
C	0	HIS	-	expression tag	UNP A0A1D8PMH8
C	457	LEU	-	expression tag	UNP A0A1D8PMH8
C	458	GLU	-	expression tag	UNP A0A1D8PMH8
C	459	HIS	-	expression tag	UNP A0A1D8PMH8
C	460	HIS	-	expression tag	UNP A0A1D8PMH8
C	461	HIS	-	expression tag	UNP A0A1D8PMH8
C	462	HIS	-	expression tag	UNP A0A1D8PMH8
C	463	HIS	-	expression tag	UNP A0A1D8PMH8
C	464	HIS	-	expression tag	UNP A0A1D8PMH8

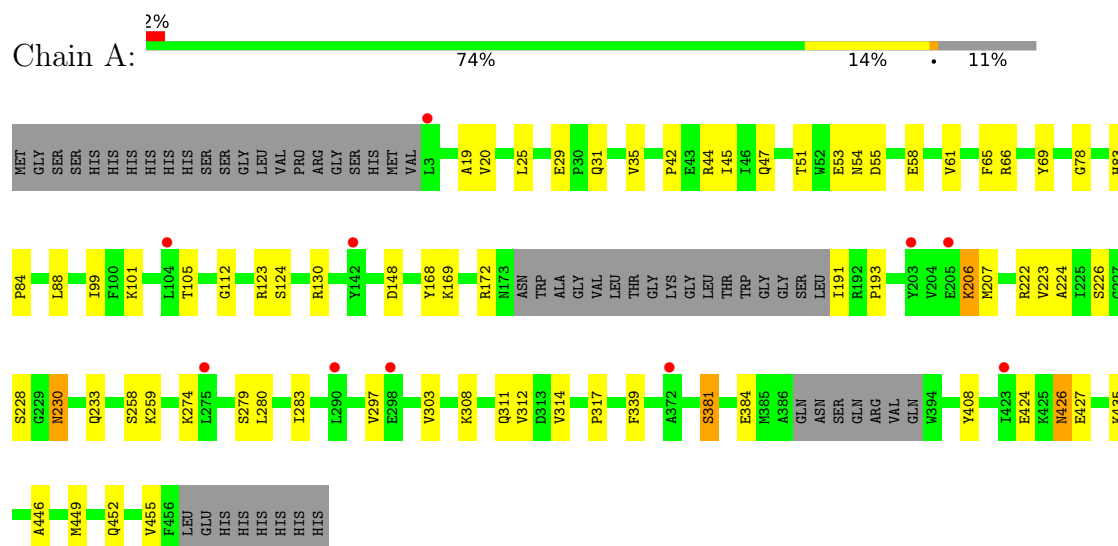
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	11	Total O 11 11	0	0
2	B	3	Total O 3 3	0	0
2	C	3	Total O 3 3	0	0

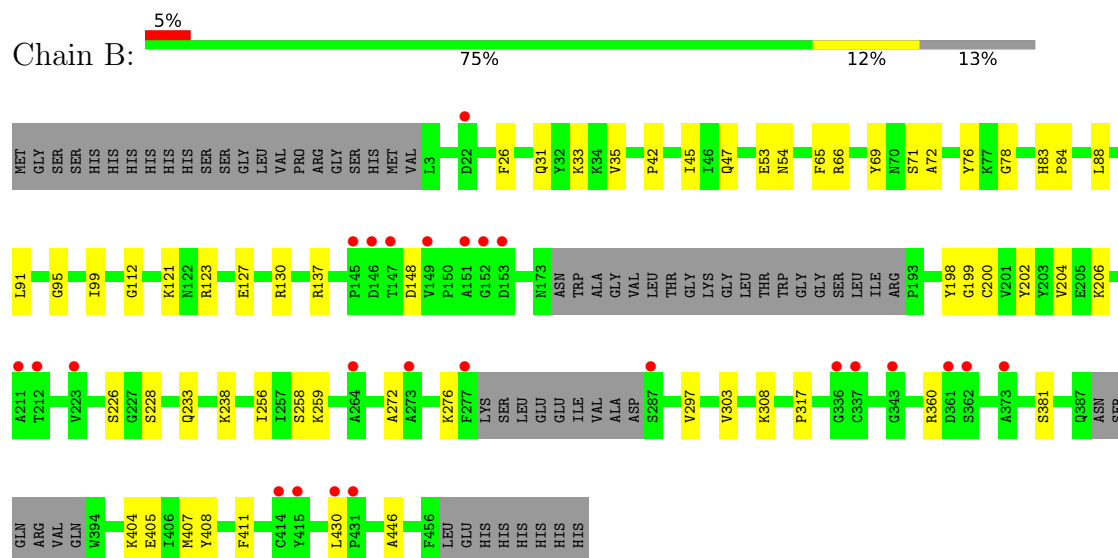
3 Residue-property plots [i](#)

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.

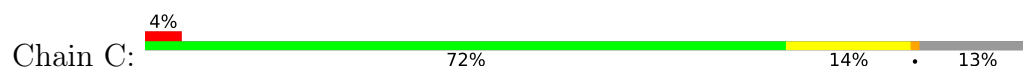
• Molecule 1: Glutamate dehydrogenase

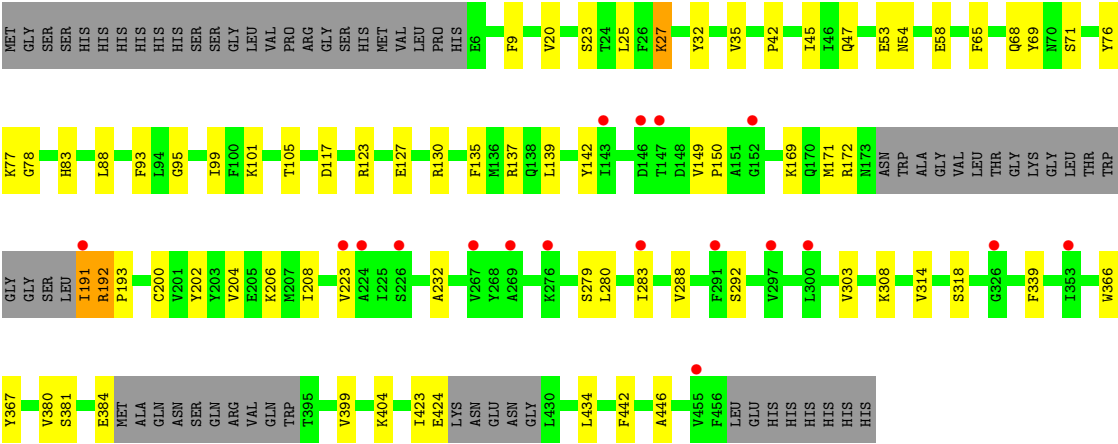


• Molecule 1: Glutamate dehydrogenase



• Molecule 1: Glutamate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.54Å 94.54Å 334.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.52 – 3.09 43.52 – 3.09	Depositor EDS
% Data completeness (in resolution range)	83.8 (43.52-3.09) 83.8 (43.52-3.09)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.241 , 0.290 0.238 , 0.285	Depositor DCC
R_{free} test set	1155 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9733	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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	0.17	0/3356	0.37	0/4524
1	B	0.16	0/3276	0.34	0/4414
1	C	0.16	0/3261	0.35	0/4393
All	All	0.16	0/9893	0.35	0/13331

There are no bond length outliers.

There are no bond angle outliers.

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	3295	0	3251	40	0
1	B	3216	0	3165	30	0
1	C	3205	0	3167	38	0
2	A	11	0	0	1	0
2	B	3	0	0	1	0
2	C	3	0	0	0	0
All	All	9733	0	9583	107	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 6.

All (107) 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:193:PRO:O	1:A:230:ASN:ND2	2.21	0.74
1:B:45:ILE:HD13	1:B:88:LEU:HD11	1.78	0.65
1:C:78:GLY:O	1:C:150:PRO:HA	1.99	0.63
1:A:45:ILE:HD13	1:A:88:LEU:HD11	1.83	0.61
1:C:45:ILE:HD13	1:C:88:LEU:HD11	1.84	0.59
1:C:42:PRO:HG2	1:C:45:ILE:HD11	1.84	0.59
1:A:51:THR:HG22	1:A:61:VAL:HG22	1.87	0.57
1:B:42:PRO:HG2	1:B:45:ILE:HD11	1.87	0.56
1:B:66:ARG:NH2	1:B:148:ASP:OD1	2.36	0.56
1:C:191:ILE:HD12	1:C:399:VAL:HG21	1.88	0.55
1:A:452:GLN:NE2	2:A:501:HOH:O	2.39	0.55
1:C:279:SER:O	1:C:283:ILE:HG23	2.08	0.54
1:A:381:SER:O	1:A:384:GLU:HB3	2.08	0.54
1:A:303:VAL:HG11	1:A:308:LYS:HE3	1.89	0.54
1:C:71:SER:HB3	1:C:76:TYR:CE1	2.43	0.53
1:B:35:VAL:HG21	1:B:446:ALA:HB1	1.91	0.53
1:B:303:VAL:HG11	1:B:308:LYS:HE3	1.89	0.53
1:B:272:ALA:O	1:B:276:LYS:HG2	2.10	0.52
1:A:69:TYR:CD1	1:A:99:ILE:HD11	2.44	0.52
1:A:168:TYR:CE1	1:A:172:ARG:HG3	2.45	0.52
1:B:53:GLU:O	1:B:130:ARG:HD2	2.09	0.52
1:C:303:VAL:HG11	1:C:308:LYS:HE3	1.92	0.52
1:A:78:GLY:HA3	1:A:112:GLY:O	2.10	0.52
1:C:223:VAL:HG22	1:C:314:VAL:HB	1.92	0.52
1:A:206:LYS:HG2	1:A:408:TYR:CD1	2.45	0.51
1:B:228:SER:O	1:B:233:GLN:NE2	2.40	0.51
1:A:426:ASN:N	1:A:426:ASN:OD1	2.43	0.51
1:B:95:GLY:O	1:B:99:ILE:HG13	2.11	0.51
1:C:77:LYS:HD2	1:C:149:VAL:HB	1.94	0.50
1:C:53:GLU:O	1:C:130:ARG:HD2	2.11	0.50
1:B:78:GLY:HA3	1:B:112:GLY:O	2.12	0.49
1:C:27:LYS:HD2	1:C:27:LYS:H	1.77	0.49
1:C:47:GLN:HG2	1:C:65:PHE:CD2	2.48	0.49
1:C:380:VAL:O	1:C:384:GLU:HG2	2.13	0.48
1:C:35:VAL:HG21	1:C:446:ALA:HB1	1.94	0.48
1:A:258:SER:HB3	1:A:297:VAL:HG12	1.96	0.48
1:A:42:PRO:HG2	1:A:45:ILE:HD11	1.95	0.48
1:C:32:TYR:HB3	1:C:442:PHE:HE2	1.79	0.47
1:B:200:CYS:O	1:B:204:VAL:HG23	2.15	0.47
1:B:404:LYS:HG2	1:B:408:TYR:CZ	2.49	0.47
1:A:279:SER:O	1:A:283:ILE:HG23	2.13	0.47
1:B:258:SER:HB3	1:B:297:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:OD2	1:A:124:SER:OG	2.30	0.46
1:C:83:HIS:O	1:C:117:ASP:HA	2.16	0.46
1:C:54:ASN:HA	1:C:127:GLU:HG2	1.96	0.46
1:B:199:GLY:HA2	1:B:407:MET:HG3	1.97	0.46
1:B:54:ASN:HA	1:B:127:GLU:HG2	1.97	0.46
1:C:69:TYR:CD1	1:C:99:ILE:HD11	2.51	0.46
1:A:47:GLN:HG2	1:A:65:PHE:CD2	2.51	0.46
1:A:83:HIS:CG	1:A:84:PRO:HD2	2.51	0.45
1:B:47:GLN:NE2	2:B:501:HOH:O	2.44	0.45
1:A:206:LYS:HA	1:A:206:LYS:HD2	1.56	0.45
1:C:101:LYS:O	1:C:105:THR:HG23	2.16	0.45
1:C:95:GLY:O	1:C:99:ILE:HG13	2.16	0.45
1:A:20:VAL:HG13	1:A:25:LEU:HD23	1.99	0.45
1:A:228:SER:OG	1:A:274:LYS:HE3	2.17	0.45
1:C:20:VAL:HG13	1:C:25:LEU:HD23	1.99	0.45
1:C:202:TYR:CD2	1:C:404:LYS:HG3	2.52	0.44
1:B:69:TYR:CD1	1:B:99:ILE:HD11	2.52	0.44
1:C:232:ALA:HB2	1:C:318:SER:HB2	2.00	0.44
1:A:44:ARG:HB2	1:A:44:ARG:CZ	2.47	0.44
1:A:228:SER:O	1:A:233:GLN:NE2	2.46	0.44
1:C:280:LEU:O	1:C:283:ILE:HG13	2.17	0.44
1:C:20:VAL:O	1:C:23:SER:OG	2.28	0.44
1:A:449:MET:HE2	1:A:455:VAL:HG23	2.00	0.44
1:B:83:HIS:CG	1:B:84:PRO:HD2	2.52	0.44
1:B:206:LYS:HB3	1:B:411:PHE:CD2	2.53	0.44
1:A:169:LYS:HZ2	1:B:72:ALA:HA	1.83	0.43
1:C:208:ILE:HG12	1:C:339:PHE:CE2	2.53	0.43
1:A:191:ILE:HG22	1:A:193:PRO:HD2	2.00	0.43
1:A:35:VAL:HG21	1:A:446:ALA:HB1	2.00	0.43
1:A:29:GLU:HG2	1:A:31:GLN:HE22	1.82	0.43
1:A:207:MET:HE2	1:A:339:PHE:HD1	1.82	0.43
1:C:200:CYS:O	1:C:204:VAL:HG23	2.18	0.43
1:A:280:LEU:O	1:A:283:ILE:HG13	2.18	0.43
1:C:192:ARG:N	1:C:193:PRO:CD	2.82	0.43
1:B:71:SER:HB3	1:B:76:TYR:CE1	2.55	0.42
1:A:19:ALA:HB1	1:A:435:LYS:HA	2.01	0.42
1:A:226:SER:OG	1:A:317:PRO:HA	2.19	0.42
1:B:47:GLN:HG2	1:B:65:PHE:CD2	2.55	0.42
1:A:223:VAL:HG22	1:A:314:VAL:HB	2.01	0.42
1:A:53:GLU:O	1:A:130:ARG:HD2	2.19	0.42
1:A:259:LYS:HE2	1:A:259:LYS:HB3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ARG:N	1:C:193:PRO:HD3	2.34	0.41
1:C:206:LYS:HD3	1:C:206:LYS:HA	1.70	0.41
1:A:222:ARG:NE	1:A:311:GLN:O	2.48	0.41
1:B:226:SER:OG	1:B:317:PRO:HA	2.20	0.41
1:C:9:PHE:N	1:C:93:PHE:HB2	2.35	0.41
1:B:256:ILE:HB	1:B:297:VAL:HG11	2.02	0.41
1:B:202:TYR:CZ	1:B:404:LYS:HE2	2.56	0.41
1:A:66:ARG:NH2	1:A:148:ASP:OD1	2.45	0.41
1:B:91:LEU:HD23	1:B:91:LEU:HA	1.93	0.41
1:B:360:ARG:HD2	1:B:430:LEU:O	2.21	0.41
1:C:367:TYR:HE2	1:C:434:LEU:HD13	1.86	0.41
1:A:424:GLU:HB2	1:A:427:GLU:HB2	2.01	0.41
1:C:42:PRO:HG3	1:C:69:TYR:CZ	2.56	0.41
1:C:68:GLN:HB3	1:C:76:TYR:CE1	2.55	0.41
1:B:26:PHE:CE2	1:B:33:LYS:HE3	2.57	0.40
1:B:202:TYR:CD2	1:B:404:LYS:HG3	2.56	0.40
1:B:198:TYR:CD1	1:B:238:LYS:HB2	2.57	0.40
1:C:135:PHE:CE2	1:C:139:LEU:HD22	2.55	0.40
1:C:288:VAL:O	1:C:292:SER:HB2	2.21	0.40
1:A:54:ASN:HD21	1:A:58:GLU:HB2	1.85	0.40
1:A:101:LYS:O	1:A:105:THR:HG23	2.22	0.40
1:A:224:ALA:HB2	1:A:312:VAL:HG21	2.03	0.40
1:C:54:ASN:HD21	1:C:58:GLU:HB2	1.86	0.40
1:C:137:ARG:O	1:C:171:MET:HE1	2.22	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	424/484 (88%)	412 (97%)	12 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	412/484 (85%)	402 (98%)	10 (2%)	0	100	100
1	C	411/484 (85%)	401 (98%)	10 (2%)	0	100	100
All	All	1247/1452 (86%)	1215 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	346/391 (88%)	341 (99%)	5 (1%)	59	73
1	B	337/391 (86%)	330 (98%)	7 (2%)	47	68
1	C	337/391 (86%)	326 (97%)	11 (3%)	33	60
All	All	1020/1173 (87%)	997 (98%)	23 (2%)	44	67

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ARG
1	A	206	LYS
1	A	230	ASN
1	A	381	SER
1	A	426	ASN
1	B	31	GLN
1	B	121	LYS
1	B	123	ARG
1	B	137	ARG
1	B	259	LYS
1	B	381	SER
1	B	405	GLU
1	C	27	LYS
1	C	123	ARG
1	C	142	TYR
1	C	169	LYS

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Mol	Chain	Res	Type
1	C	172	ARG
1	C	191	ILE
1	C	192	ARG
1	C	366	TRP
1	C	381	SER
1	C	423	ILE
1	C	424	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	98	GLN
1	A	138	GLN
1	A	295	HIS
1	A	359	ASN
1	A	363	ASN
1	B	10	GLN
1	B	138	GLN
1	B	363	ASN
1	B	419	GLN
1	B	426	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 [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	430/484 (88%)	0.11	10 (2%) 61 38	21, 38, 78, 93	0
1	B	420/484 (86%)	0.59	25 (5%) 27 14	25, 68, 123, 145	0
1	C	419/484 (86%)	0.43	18 (4%) 40 21	27, 64, 103, 122	0
All	All	1269/1452 (87%)	0.38	53 (4%) 40 22	21, 53, 108, 145	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	TYR	5.1
1	C	152	GLY	4.2
1	C	269	ALA	3.8
1	B	415	TYR	3.4
1	B	153	ASP	3.2
1	C	326	GLY	3.2
1	A	104	LEU	3.2
1	B	147	THR	3.1
1	B	336	GLY	3.1
1	C	226	SER	3.0
1	C	267	VAL	3.0
1	B	151	ALA	2.9
1	B	145	PRO	2.9
1	B	211	ALA	2.8
1	B	431	PRO	2.8
1	C	191	ILE	2.8
1	B	22	ASP	2.7
1	B	273	ALA	2.6
1	B	343	GLY	2.6
1	A	290	LEU	2.5
1	B	287	SER	2.4
1	C	283	ILE	2.4
1	C	146	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	276	LYS	2.4
1	B	362	SER	2.4
1	A	372	ALA	2.4
1	B	430	LEU	2.4
1	B	277	PHE	2.4
1	A	423	ILE	2.3
1	C	455	VAL	2.3
1	B	152	GLY	2.3
1	C	147	THR	2.3
1	B	146	ASP	2.3
1	A	275	LEU	2.3
1	B	361	ASP	2.3
1	B	212	THR	2.3
1	A	3	LEU	2.3
1	C	224	ALA	2.2
1	A	142	TYR	2.2
1	B	264	ALA	2.1
1	B	414	CYS	2.1
1	B	373	ALA	2.1
1	C	291	PHE	2.1
1	C	143	ILE	2.1
1	A	205	GLU	2.1
1	C	300	LEU	2.1
1	A	298	GLU	2.1
1	B	223	VAL	2.0
1	B	149	VAL	2.0
1	C	223	VAL	2.0
1	B	337	CYS	2.0
1	C	297	VAL	2.0
1	C	353	ILE	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.