



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:23 am BST

PDB ID : 3PQE
Title : Crystal structure of L-lactate dehydrogenase from *Bacillus subtilis* with H171C mutation
Authors : Zhang, Y.; Garavito, R.M.
Deposited on : 2010-11-26
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

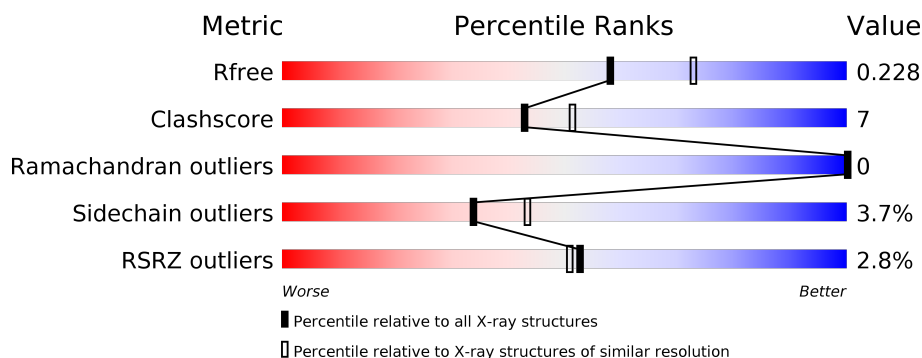
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	326	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 84%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> % 84% 12% • </div> </div>
1	B	326	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 83%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> % 83% 12% • • </div> </div>
1	C	326	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 16%, green 76%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> 4% 76% 16% • 6% </div> </div>
1	D	326	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 18%, green 75%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> 5% 75% 18% 6% </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9845 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 L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2397	1527	401	460	9			
1	B	314	Total	C	N	O	S	0	0	0
			2397	1527	401	460	9			
1	C	305	Total	C	N	O	S	0	0	0
			2331	1488	387	447	9			
1	D	306	Total	C	N	O	S	0	0	0
			2342	1494	391	448	9			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	CYS	HIS	ENGINEERED MUTATION	UNP P13714
A	321	HIS	-	EXPRESSION TAG	UNP P13714
A	322	HIS	-	EXPRESSION TAG	UNP P13714
A	323	HIS	-	EXPRESSION TAG	UNP P13714
A	324	HIS	-	EXPRESSION TAG	UNP P13714
A	325	HIS	-	EXPRESSION TAG	UNP P13714
A	326	HIS	-	EXPRESSION TAG	UNP P13714
B	171	CYS	HIS	ENGINEERED MUTATION	UNP P13714
B	321	HIS	-	EXPRESSION TAG	UNP P13714
B	322	HIS	-	EXPRESSION TAG	UNP P13714
B	323	HIS	-	EXPRESSION TAG	UNP P13714
B	324	HIS	-	EXPRESSION TAG	UNP P13714
B	325	HIS	-	EXPRESSION TAG	UNP P13714
B	326	HIS	-	EXPRESSION TAG	UNP P13714
C	171	CYS	HIS	ENGINEERED MUTATION	UNP P13714
C	321	HIS	-	EXPRESSION TAG	UNP P13714
C	322	HIS	-	EXPRESSION TAG	UNP P13714
C	323	HIS	-	EXPRESSION TAG	UNP P13714
C	324	HIS	-	EXPRESSION TAG	UNP P13714
C	325	HIS	-	EXPRESSION TAG	UNP P13714
C	326	HIS	-	EXPRESSION TAG	UNP P13714

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Chain	Residue	Modelled	Actual	Comment	Reference
D	171	CYS	HIS	ENGINEERED MUTATION	UNP P13714
D	321	HIS	-	EXPRESSION TAG	UNP P13714
D	322	HIS	-	EXPRESSION TAG	UNP P13714
D	323	HIS	-	EXPRESSION TAG	UNP P13714
D	324	HIS	-	EXPRESSION TAG	UNP P13714
D	325	HIS	-	EXPRESSION TAG	UNP P13714
D	326	HIS	-	EXPRESSION TAG	UNP P13714

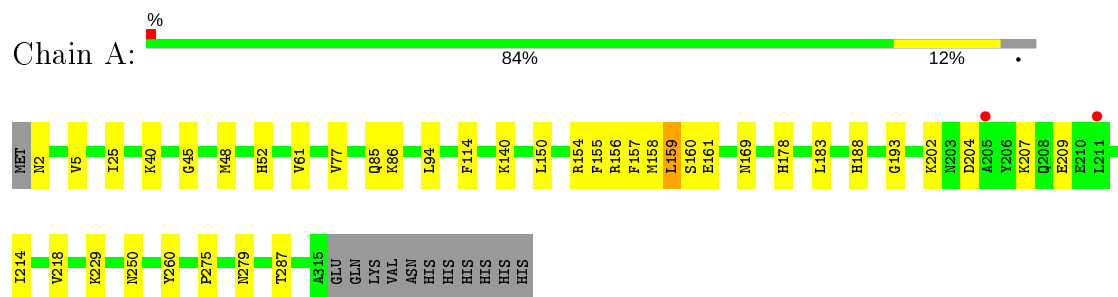
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	157	Total 157	O 157	0	0
2	B	154	Total 154	O 154	0	0
2	C	29	Total 29	O 29	0	0
2	D	38	Total 38	O 38	0	0

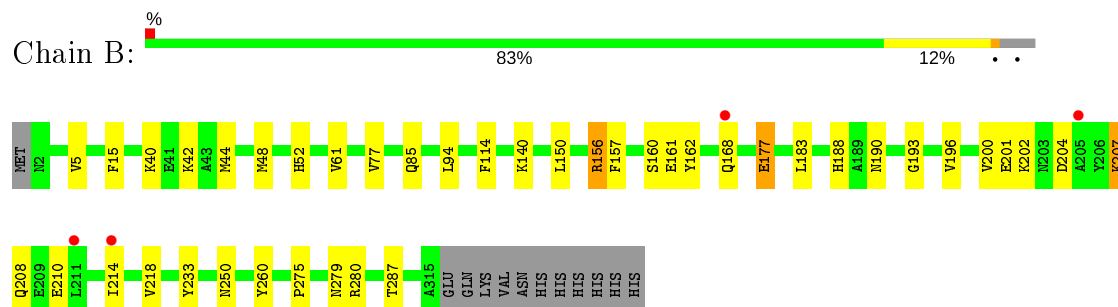
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

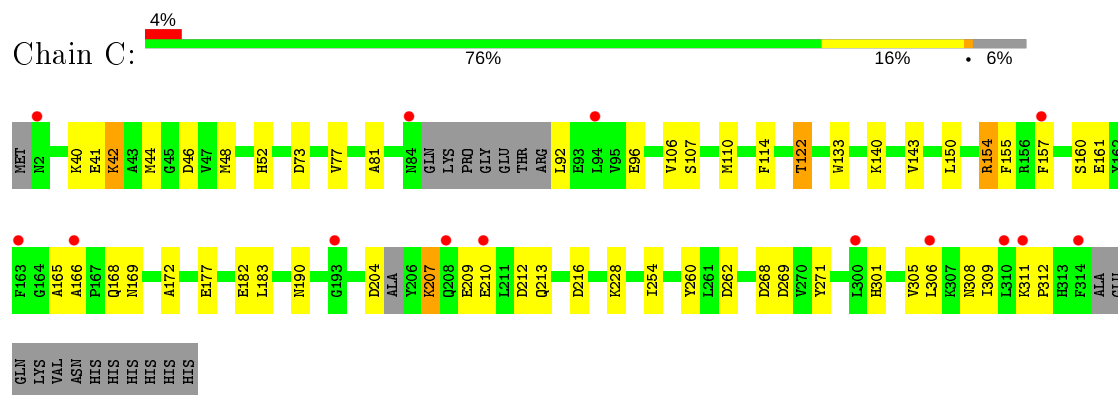
• Molecule 1: L-lactate dehydrogenase



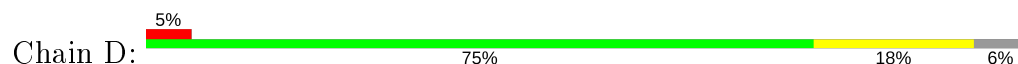
• Molecule 1: L-lactate dehydrogenase

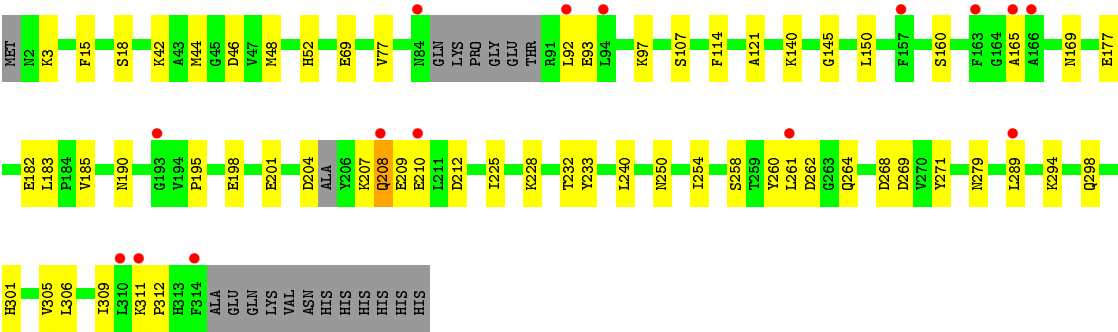


• Molecule 1: L-lactate dehydrogenase



• Molecule 1: L-lactate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	133.41 Å 133.41 Å 99.33 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.93 – 2.20 26.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (26.93-2.20) 99.5 (26.93-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 2.20 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6 _289)	Depositor
R, R_{free}	0.201 , 0.235 0.196 , 0.228	Depositor DCC
R_{free} test set	2993 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.487 for -h,-k,l 0.027 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9845	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.49	0/2443	0.54	0/3311
1	B	0.49	0/2443	0.54	0/3311
1	C	0.34	0/2374	0.46	0/3215
1	D	0.33	0/2385	0.47	0/3229
All	All	0.42	0/9645	0.50	0/13066

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	2397	0	2384	31	0
1	B	2397	0	2384	35	0
1	C	2331	0	2315	40	0
1	D	2342	0	2328	40	0
2	A	157	0	0	6	0
2	B	154	0	0	4	0
2	C	29	0	0	1	0
2	D	38	0	0	0	0
All	All	9845	0	9411	129	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 7.

All (129) 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:B:156:ARG:HG2	1:B:156:ARG:HH11	1.12	1.13
1:B:85:GLN:HB3	1:B:94:LEU:HD22	1.43	1.00
1:B:156:ARG:NH1	1:B:156:ARG:HG2	1.82	0.90
1:A:48:MET:CE	1:D:228:LYS:HD2	2.08	0.84
1:A:159:LEU:N	2:A:462:HOH:O	2.07	0.81
1:C:311:LYS:HG3	1:C:312:PRO:HD3	1.63	0.80
1:C:209:GLU:HA	1:C:212:ASP:HB2	1.67	0.76
1:C:254:ILE:HD12	1:D:169:ASN:HB3	1.70	0.74
1:C:81:ALA:O	1:C:122:THR:HG21	1.89	0.72
1:A:156:ARG:C	2:A:462:HOH:O	2.28	0.71
1:A:48:MET:HE2	1:D:228:LYS:HD2	1.70	0.71
1:A:158:MET:N	2:A:462:HOH:O	2.25	0.70
1:A:48:MET:HE1	1:D:228:LYS:HD2	1.72	0.70
1:B:48:MET:CE	1:C:228:LYS:HD2	2.23	0.68
1:B:156:ARG:CG	1:B:156:ARG:HH11	1.97	0.68
1:A:52:HIS:CE1	1:D:150:LEU:HD21	2.30	0.66
1:A:155:PHE:O	2:A:462:HOH:O	2.12	0.66
1:B:162:TYR:HE1	1:B:210:GLU:HG2	1.62	0.65
1:B:48:MET:HE1	1:C:228:LYS:HD2	1.77	0.65
1:D:160:SER:HB2	1:D:165:ALA:O	1.97	0.64
1:D:294:LYS:HE3	1:D:298:GLN:HE22	1.62	0.64
1:C:160:SER:HB2	1:C:165:ALA:O	1.99	0.62
1:C:301:HIS:O	1:C:305:VAL:HG23	2.00	0.61
1:B:190:ASN:C	2:B:478:HOH:O	2.39	0.61
1:C:140:LYS:HD2	1:C:260:TYR:CD2	2.36	0.60
1:A:188:HIS:HD2	1:B:193:GLY:O	1.83	0.60
1:A:85:GLN:HB2	1:A:94:LEU:HD22	1.83	0.60
1:D:140:LYS:HD2	1:D:260:TYR:CD2	2.37	0.59
1:D:177:GLU:HB2	1:D:306:LEU:HD11	1.85	0.59
1:A:161:GLU:O	1:A:161:GLU:HG2	2.04	0.58
1:D:301:HIS:O	1:D:305:VAL:HG23	2.03	0.58
1:B:52:HIS:CE1	1:C:150:LEU:HD21	2.39	0.58
1:D:93:GLU:O	1:D:97:LYS:HG3	2.03	0.58
1:B:44:MET:O	1:B:48:MET:HE3	2.03	0.58
1:A:178:HIS:HD2	2:A:372:HOH:O	1.87	0.57
1:A:193:GLY:O	1:B:188:HIS:HD2	1.88	0.57
1:B:204:ASP:O	1:B:207:LYS:HE2	2.06	0.55
1:D:262:ASP:HA	1:D:268:ASP:HA	1.89	0.55
1:A:214:ILE:O	1:A:218:VAL:HG23	2.07	0.54
1:C:169:ASN:ND2	1:D:254:ILE:H	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:O	1:A:158:MET:HG3	2.08	0.54
1:D:305:VAL:O	1:D:309:ILE:HG13	2.07	0.54
1:B:162:TYR:CE1	1:B:210:GLU:HG2	2.41	0.53
1:D:225:ILE:HG21	1:D:232:THR:HG22	1.90	0.52
1:D:311:LYS:HB2	1:D:312:PRO:HD3	1.90	0.52
1:C:177:GLU:O	1:C:182:GLU:HB3	2.10	0.52
1:B:156:ARG:HD3	2:B:390:HOH:O	2.10	0.52
1:D:77:VAL:HG23	1:D:114:PHE:CE1	2.45	0.52
1:D:225:ILE:CG2	1:D:232:THR:HG22	2.40	0.52
1:D:185:VAL:HG11	1:D:289:LEU:HD13	1.92	0.52
1:D:44:MET:O	1:D:48:MET:HG3	2.11	0.51
1:A:2:ASN:HB3	1:A:5:VAL:O	2.11	0.50
1:D:294:LYS:HE3	1:D:298:GLN:NE2	2.24	0.50
1:A:45:GLY:HA2	1:A:48:MET:HE3	1.93	0.50
1:A:140:LYS:HD2	1:A:260:TYR:CD2	2.46	0.50
1:D:260:TYR:OH	1:D:269:ASP:HA	2.12	0.50
1:A:204:ASP:O	1:A:207:LYS:HE2	2.11	0.49
1:C:305:VAL:O	1:C:309:ILE:HG13	2.12	0.49
1:D:260:TYR:CZ	1:D:269:ASP:HA	2.47	0.49
1:C:92:LEU:O	1:C:96:GLU:HG3	2.13	0.49
1:C:169:ASN:HB2	1:D:254:ILE:HD12	1.95	0.49
1:D:250:ASN:OD1	1:D:279:ASN:HB2	2.13	0.49
1:B:157:PHE:CE2	1:B:161:GLU:OE2	2.66	0.49
1:C:157:PHE:CE2	1:C:161:GLU:OE1	2.66	0.49
1:B:275:PRO:HB2	1:B:287:THR:HB	1.94	0.48
1:D:177:GLU:O	1:D:182:GLU:HB3	2.13	0.48
1:C:155:PHE:CE2	1:C:172:ALA:HB1	2.48	0.48
1:C:311:LYS:CG	1:C:312:PRO:HD3	2.39	0.48
1:B:140:LYS:HD2	1:B:260:TYR:CD2	2.48	0.48
1:B:214:ILE:O	1:B:218:VAL:HG23	2.14	0.48
1:A:250:ASN:OD1	1:A:279:ASN:HB2	2.13	0.48
1:B:150:LEU:HD21	1:C:52:HIS:CE1	2.49	0.47
1:A:158:MET:SD	2:A:457:HOH:O	2.60	0.47
1:A:150:LEU:HD21	1:D:52:HIS:CE1	2.49	0.47
1:A:40:LYS:HE3	1:A:40:LYS:HB3	1.80	0.47
1:C:77:VAL:HG23	1:C:114:PHE:CE1	2.50	0.47
1:D:195:PRO:HG2	1:D:198:GLU:HG3	1.97	0.47
1:B:177:GLU:O	1:B:177:GLU:HG2	2.12	0.47
1:A:25:ILE:HG12	1:A:61:VAL:HG11	1.95	0.47
1:B:202:LYS:HB2	1:B:202:LYS:NZ	2.30	0.47
1:A:158:MET:O	1:A:161:GLU:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ARG:NH2	1:D:3:LYS:HD3	2.30	0.46
1:A:77:VAL:HG23	1:A:114:PHE:CE1	2.51	0.46
1:B:196:VAL:O	1:B:200:VAL:HG23	2.16	0.46
1:C:154:ARG:NH1	2:C:348:HOH:O	2.46	0.46
1:D:177:GLU:HG3	1:D:306:LEU:HD21	1.96	0.45
1:B:77:VAL:HG23	1:B:114:PHE:CE1	2.51	0.45
1:D:42:LYS:HA	1:D:42:LYS:HD2	1.82	0.45
1:D:145:GLY:HA3	1:D:258:SER:HB2	1.99	0.44
1:B:250:ASN:OD1	1:B:279:ASN:HB2	2.17	0.44
1:C:207:LYS:N	1:C:207:LYS:HD2	2.32	0.44
1:C:40:LYS:HE3	1:C:41:GLU:OE1	2.18	0.44
1:C:262:ASP:HA	1:C:268:ASP:HA	2.00	0.44
1:C:177:GLU:HG3	1:C:306:LEU:HD21	1.99	0.44
1:C:260:TYR:OH	1:C:269:ASP:HA	2.18	0.43
1:C:157:PHE:HE2	1:C:161:GLU:OE1	2.00	0.43
1:D:208:GLN:HE21	1:D:208:GLN:HA	1.83	0.43
1:B:42:LYS:NZ	2:B:435:HOH:O	2.51	0.43
1:C:133:TRP:HA	1:C:143:VAL:HG21	2.00	0.43
1:B:48:MET:HE2	1:C:228:LYS:HD2	1.99	0.43
1:C:260:TYR:CZ	1:C:269:ASP:HA	2.53	0.43
1:A:209:GLU:HA	1:A:209:GLU:OE2	2.18	0.43
1:C:106:VAL:O	1:C:110:MET:HG2	2.18	0.43
1:A:159:LEU:HA	1:A:159:LEU:HD12	1.73	0.42
1:B:204:ASP:HA	2:B:342:HOH:O	2.19	0.42
1:D:260:TYR:HB2	1:D:271:TYR:CZ	2.54	0.42
1:C:213:GLN:HA	1:C:216:ASP:OD2	2.20	0.42
1:D:15:PHE:HB3	1:D:233:TYR:CD2	2.54	0.42
1:C:44:MET:O	1:C:48:MET:HG3	2.19	0.42
1:D:261:LEU:HD22	1:D:264:GLN:HB2	2.00	0.42
1:C:260:TYR:HB2	1:C:271:TYR:CZ	2.55	0.42
1:D:145:GLY:CA	1:D:258:SER:HB2	2.49	0.42
1:A:157:PHE:CD2	1:A:157:PHE:C	2.93	0.42
1:A:275:PRO:HB2	1:A:287:THR:HB	2.01	0.42
1:C:169:ASN:HD21	1:D:254:ILE:H	1.67	0.41
1:B:40:LYS:HE3	1:B:40:LYS:HB3	1.90	0.41
1:B:61:VAL:O	1:B:61:VAL:HG13	2.19	0.41
1:B:15:PHE:HB3	1:B:233:TYR:CD2	2.55	0.41
1:C:309:ILE:H	1:C:309:ILE:HG13	1.65	0.41
1:B:207:LYS:HD3	1:B:207:LYS:N	2.36	0.41
1:B:168:GLN:HG2	1:B:168:GLN:H	1.65	0.41
1:B:202:LYS:CB	1:B:202:LYS:NZ	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ALA:HB1	1:C:168:GLN:OE1	2.21	0.41
1:C:204:ASP:O	1:C:207:LYS:HE3	2.20	0.41
1:C:73:ASP:OD1	1:C:73:ASP:N	2.53	0.41
1:D:209:GLU:HA	1:D:212:ASP:HB3	2.03	0.40
1:D:121:ALA:HB2	1:D:240:LEU:HD21	2.03	0.40
1:A:61:VAL:HG13	1:A:61:VAL:O	2.21	0.40
1:C:42:LYS:HB3	1:C:42:LYS:HE2	1.90	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	312/326 (96%)	301 (96%)	11 (4%)	0	100	100
1	B	312/326 (96%)	301 (96%)	11 (4%)	0	100	100
1	C	299/326 (92%)	284 (95%)	15 (5%)	0	100	100
1	D	300/326 (92%)	291 (97%)	9 (3%)	0	100	100
All	All	1223/1304 (94%)	1177 (96%)	46 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	255/267 (96%)	248 (97%)	7 (3%)	44	57
1	B	255/267 (96%)	247 (97%)	8 (3%)	40	51
1	C	249/267 (93%)	239 (96%)	10 (4%)	31	40
1	D	250/267 (94%)	238 (95%)	12 (5%)	25	32
All	All	1009/1068 (94%)	972 (96%)	37 (4%)	34	43

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LYS
1	A	159	LEU
1	A	160	SER
1	A	169	ASN
1	A	183	LEU
1	A	202	LYS
1	A	229	LYS
1	B	5	VAL
1	B	156	ARG
1	B	160	SER
1	B	177	GLU
1	B	183	LEU
1	B	201	GLU
1	B	207	LYS
1	B	208	GLN
1	C	42	LYS
1	C	46	ASP
1	C	107	SER
1	C	122	THR
1	C	154	ARG
1	C	183	LEU
1	C	190	ASN
1	C	207	LYS
1	C	210	GLU
1	C	308	ASN
1	D	18	SER
1	D	46	ASP
1	D	69	GLU
1	D	92	LEU
1	D	107	SER
1	D	183	LEU
1	D	190	ASN
1	D	201	GLU

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Mol	Chain	Res	Type
1	D	204	ASP
1	D	207	LYS
1	D	208	GLN
1	D	210	GLU

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

Mol	Chain	Res	Type
1	A	52	HIS
1	A	213	GLN
1	B	6	ASN
1	B	52	HIS
1	C	169	ASN
1	C	203	ASN
1	D	52	HIS
1	D	188	HIS
1	D	203	ASN
1	D	208	GLN
1	D	249	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

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	314/326 (96%)	-0.03	2 (0%) 89 88	27, 40, 65, 81	0
1	B	314/326 (96%)	-0.02	4 (1%) 77 75	27, 40, 66, 81	0
1	C	305/326 (93%)	0.22	14 (4%) 32 31	39, 63, 92, 103	0
1	D	306/326 (93%)	0.21	15 (4%) 29 28	39, 64, 93, 110	0
All	All	1239/1304 (95%)	0.09	35 (2%) 53 51	27, 51, 86, 110	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	94	LEU	4.3
1	C	193	GLY	4.3
1	C	94	LEU	4.2
1	A	205	ALA	4.0
1	C	314	PHE	3.8
1	D	193	GLY	3.7
1	D	314	PHE	3.6
1	D	163	PHE	3.4
1	C	163	PHE	3.3
1	D	210	GLU	3.1
1	D	208	GLN	2.9
1	A	211	LEU	2.9
1	B	205	ALA	2.9
1	D	157	PHE	2.8
1	D	310	LEU	2.8
1	D	311	LYS	2.7
1	C	310	LEU	2.7
1	C	208	GLN	2.7
1	D	92	LEU	2.7
1	C	157	PHE	2.6
1	B	168	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	166	ALA	2.6
1	C	306	LEU	2.5
1	C	311	LYS	2.4
1	D	261	LEU	2.4
1	D	84	ASN	2.4
1	D	289	LEU	2.4
1	C	210	GLU	2.3
1	C	166	ALA	2.3
1	C	300	LEU	2.3
1	C	2	ASN	2.2
1	B	214	ILE	2.2
1	C	84	ASN	2.2
1	B	211	LEU	2.2
1	D	165	ALA	2.1

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 carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.