



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:33 am BST

PDB ID : 6K12
Title : Babesia microti lactate dehydrogenase apo form (BmLDH)
Authors : Long, Y.
Deposited on : 2019-05-09
Resolution : 2.79 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

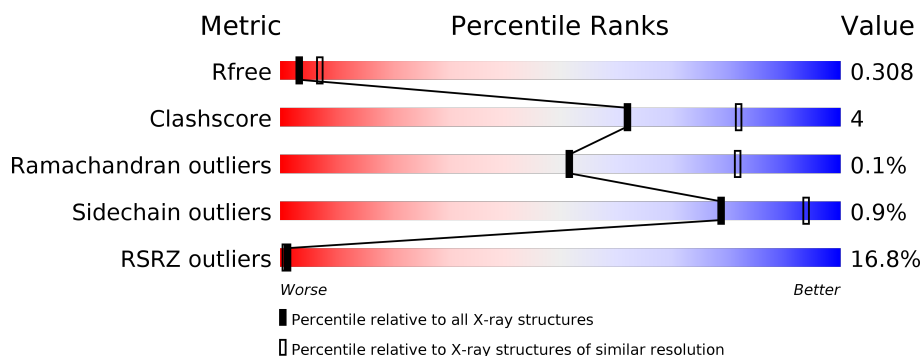
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	332	<div> <div>12%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>11%</div> </div> </div>
1	B	332	<div> <div>10%</div> <div> <div></div> <div>79%</div> <div>5%</div> <div>17%</div> </div> </div>
1	C	332	<div> <div>8%</div> <div> <div></div> <div>80%</div> <div>5%</div> <div>16%</div> </div> </div>
1	D	332	<div> <div>18%</div> <div> <div></div> <div>71%</div> <div>9%</div> <div>20%</div> </div> </div>
1	E	332	<div> <div>15%</div> <div> <div></div> <div>62%</div> <div>11%</div> <div>27%</div> </div> </div>
1	F	332	<div> <div>19%</div> <div> <div></div> <div>69%</div> <div>10%</div> <div>20%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25316 atoms, of which 12881 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.

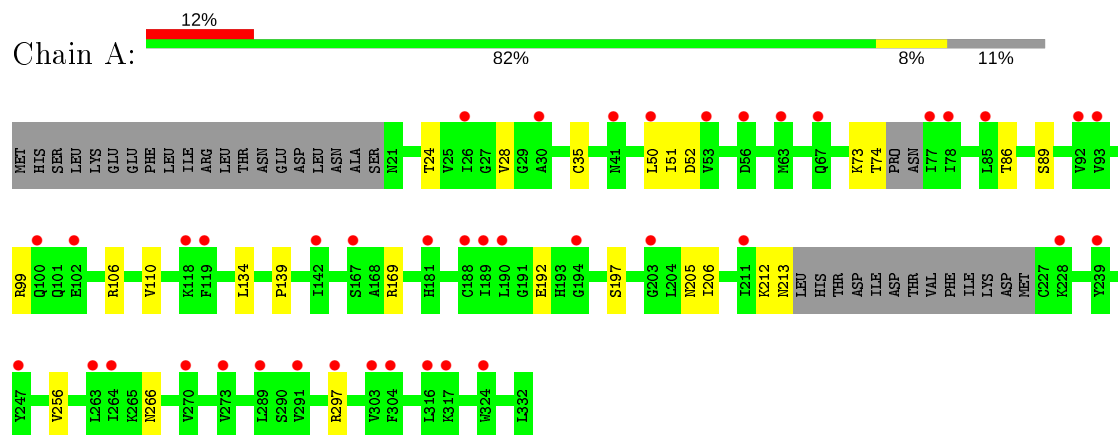
- Molecule 1 is a protein called L-lactate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	H	N	O	S	0	0	0
			4646	1459	2364	385	426	12			
1	B	277	Total	C	H	N	O	S	0	0	0
			4316	1364	2195	352	394	11			
1	C	280	Total	C	H	N	O	S	0	0	0
			4362	1377	2221	354	398	12			
1	D	265	Total	C	H	N	O	S	0	0	0
			4131	1310	2096	334	380	11			
1	E	244	Total	C	H	N	O	S	0	0	0
			3754	1181	1908	306	348	11			
1	F	265	Total	C	H	N	O	S	0	0	0
			4107	1289	2097	333	377	11			

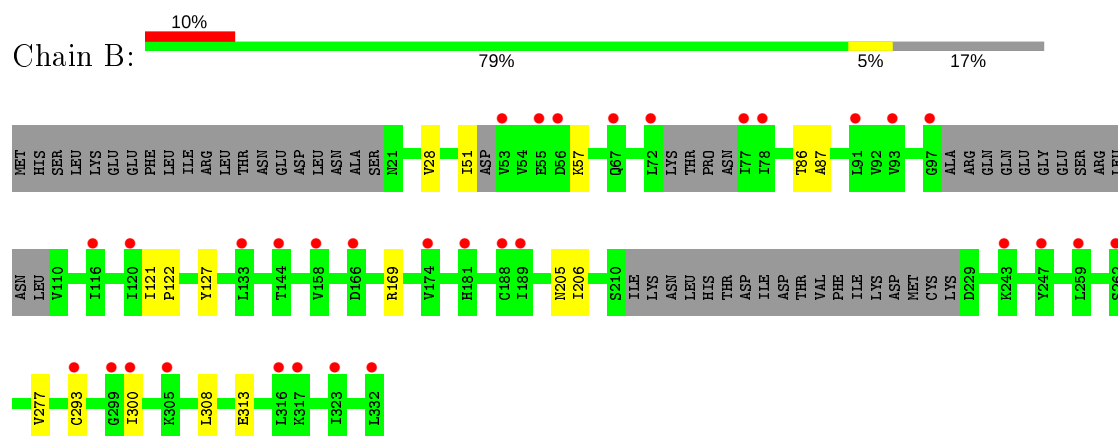
3 Residue-property plots [i](#)

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.

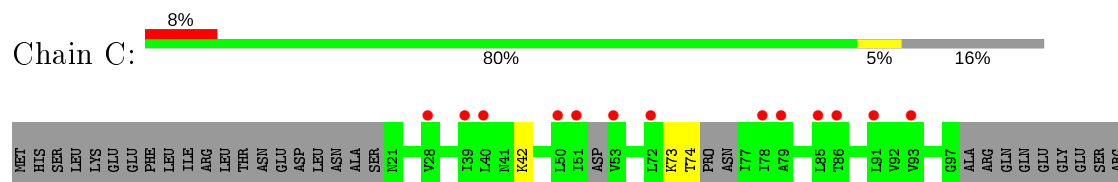
- Molecule 1: L-lactate dehydrogenase

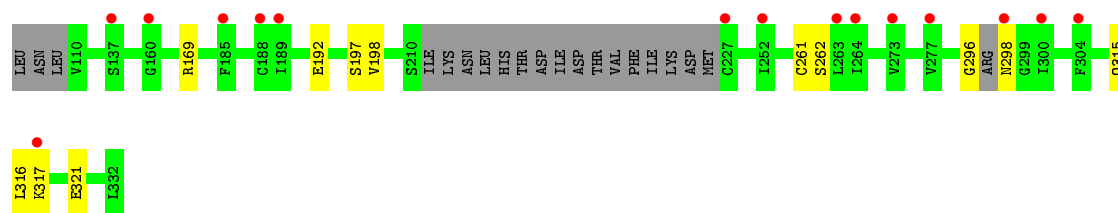


- Molecule 1: L-lactate dehydrogenase

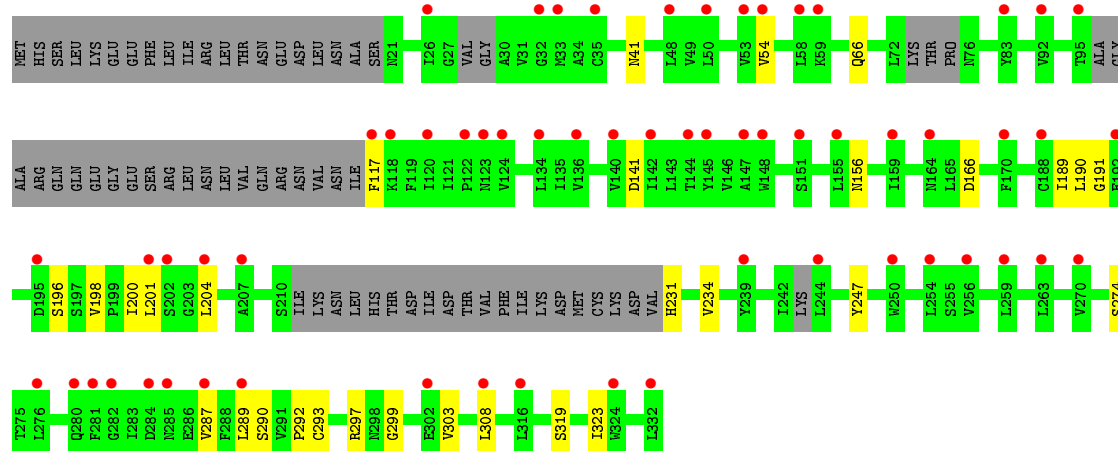


- Molecule 1: L-lactate dehydrogenase

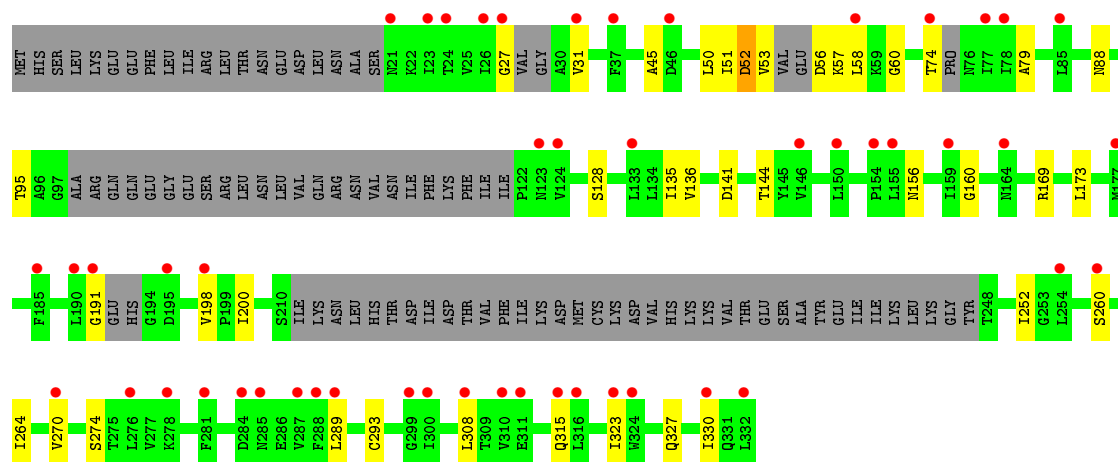




• Molecule 1: L-lactate dehydrogenase

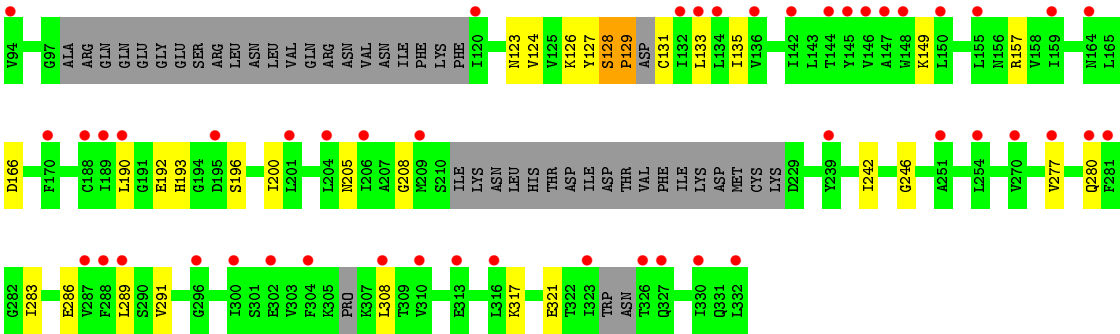


• Molecule 1: L-lactate dehydrogenase



• Molecule 1: L-lactate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	255.60Å 147.68Å 65.27Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	45.66 – 2.79 45.66 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.66-2.79) 99.1 (45.66-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, R_{free}	0.280 , 0.308 0.280 , 0.308	Depositor DCC
R_{free} test set	3009 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 20.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.019 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.477 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.477 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25316	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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	0.41	0/2315	0.47	0/3127
1	B	0.26	0/2152	0.44	0/2908
1	C	0.45	0/2171	0.46	0/2931
1	D	0.28	0/2065	0.44	0/2789
1	E	0.31	0/1869	0.48	1/2523 (0.0%)
1	F	0.42	0/2033	0.49	0/2741
All	All	0.36	0/12605	0.46	1/17019 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	53	VAL	N-CA-C	7.63	131.59	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2282	2364	2363	17	0
1	B	2121	2195	2194	8	0
1	C	2141	2221	2218	7	0
1	D	2035	2096	2095	19	0
1	E	1846	1908	1904	33	0
1	F	2010	2097	2091	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12435	12881	12865	111	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 4.

All (111) 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:E:289:LEU:HD21	1:E:323:ILE:CD1	1.42	1.48
1:E:289:LEU:CD2	1:E:323:ILE:HD11	1.67	1.25
1:F:128:SER:O	1:F:131:CYS:SG	1.93	1.25
1:E:289:LEU:CD2	1:E:323:ILE:CD1	2.16	1.23
1:F:124:VAL:O	1:F:128:SER:OG	1.64	1.14
1:E:289:LEU:HD21	1:E:323:ILE:HD12	1.33	1.08
1:E:289:LEU:HD21	1:E:323:ILE:HD11	1.05	1.04
1:D:66:GLN:O	1:E:169:ARG:NH2	2.06	0.87
1:F:131:CYS:O	1:F:157:ARG:NH1	2.12	0.83
1:C:317:LYS:O	1:C:321:GLU:HG3	1.88	0.74
1:E:198:VAL:HG21	1:E:315:GLN:HB3	1.70	0.73
1:E:31:VAL:HG13	1:E:252:ILE:HG21	1.71	0.72
1:E:198:VAL:CG2	1:E:315:GLN:HB3	2.19	0.72
1:A:73:LYS:O	1:A:74:THR:OG1	2.06	0.70
1:E:289:LEU:HD23	1:E:323:ILE:CD1	2.19	0.70
1:A:51:ILE:HD11	1:A:86:THR:HG22	1.75	0.68
1:A:51:ILE:HD11	1:A:86:THR:CG2	2.22	0.68
1:E:57:LYS:O	1:E:58:LEU:C	2.35	0.65
1:C:73:LYS:O	1:C:74:THR:OG1	2.14	0.64
1:C:42:LYS:HD2	1:C:261:CYS:SG	2.37	0.64
1:E:198:VAL:HG21	1:E:315:GLN:CB	2.29	0.62
1:A:51:ILE:CD1	1:A:86:THR:CG2	2.77	0.62
1:F:242:ILE:O	1:F:246:GLY:N	2.32	0.62
1:A:212:LYS:O	1:A:213:ASN:ND2	2.33	0.61
1:D:190:LEU:O	1:D:198:VAL:N	2.31	0.59
1:F:126:LYS:HB3	1:F:127:TYR:CD1	2.38	0.59
1:F:126:LYS:HB3	1:F:127:TYR:CE1	2.38	0.58
1:F:28:VAL:HG23	1:F:28:VAL:O	2.01	0.58
1:D:201:LEU:HD23	1:D:204:LEU:HD11	1.86	0.56
1:F:123:ASN:O	1:F:127:TYR:HD1	1.88	0.56
1:F:317:LYS:O	1:F:321:GLU:N	2.28	0.55
1:F:124:VAL:O	1:F:128:SER:N	2.38	0.55
1:C:296:GLY:O	1:C:298:ASN:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASN:HB2	1:A:297:ARG:HG3	1.88	0.54
1:F:200:ILE:HG23	1:F:308:LEU:HD13	1.88	0.54
1:D:231:HIS:O	1:D:234:VAL:N	2.34	0.54
1:A:205:ASN:OD1	1:A:206:ILE:N	2.41	0.53
1:F:192:GLU:OE1	1:F:196:SER:OG	2.18	0.53
1:D:287:VAL:HG13	1:D:323:ILE:HG21	1.91	0.52
1:E:50:LEU:O	1:E:51:ILE:HD13	2.09	0.52
1:B:308:LEU:HB2	1:B:313:GLU:HG2	1.91	0.51
1:E:198:VAL:HG13	1:E:315:GLN:OE1	2.09	0.51
1:E:169:ARG:HH11	1:E:173:LEU:HD21	1.77	0.49
1:C:262:SER:O	1:C:296:GLY:HA2	2.13	0.49
1:F:131:CYS:N	1:F:157:ARG:NH1	2.61	0.48
1:B:205:ASN:OD1	1:B:206:ILE:N	2.46	0.48
1:F:127:TYR:N	1:F:127:TYR:CD1	2.81	0.48
1:D:141:ASP:OD1	1:D:274:SER:OG	2.27	0.48
1:E:198:VAL:HG22	1:E:315:GLN:HB3	1.94	0.48
1:B:277:VAL:O	1:B:277:VAL:HG12	2.14	0.47
1:D:191:GLY:HA2	1:D:289:LEU:HD11	1.96	0.47
1:A:51:ILE:CD1	1:A:86:THR:HG22	2.41	0.47
1:D:289:LEU:HD12	1:D:290:SER:N	2.30	0.47
1:D:190:LEU:CD2	1:D:292:PRO:HD3	2.45	0.46
1:A:35:CYS:SG	1:A:256:VAL:HG11	2.55	0.46
1:F:28:VAL:HG11	1:F:58:LEU:HD23	1.98	0.46
1:A:106:ARG:O	1:A:110:VAL:HG23	2.16	0.46
1:C:192:GLU:O	1:C:197:SER:HB3	2.15	0.46
1:E:31:VAL:HG13	1:E:252:ILE:CG2	2.43	0.46
1:B:51:ILE:HD11	1:B:86:THR:CG2	2.46	0.45
1:E:95:THR:HG22	1:E:136:VAL:HB	1.99	0.45
1:D:190:LEU:HD12	1:D:200:ILE:HG12	1.97	0.45
1:E:289:LEU:CD2	1:E:323:ILE:HD12	2.15	0.45
1:E:57:LYS:O	1:E:60:GLY:N	2.50	0.45
1:F:205:ASN:OD1	1:F:208:GLY:N	2.50	0.45
1:D:166:ASP:HB2	1:D:189:ILE:HD11	1.98	0.44
1:E:200:ILE:HD12	1:E:308:LEU:HD13	1.99	0.44
1:B:28:VAL:O	1:B:57:LYS:HE2	2.17	0.44
1:A:110:VAL:HG22	1:A:139:PRO:HG3	1.98	0.44
1:D:190:LEU:CD1	1:D:200:ILE:HG12	2.48	0.44
1:F:47:GLU:HG3	1:F:76:ASN:HB3	1.99	0.44
1:B:293:CYS:HB3	1:B:300:ILE:HG23	2.00	0.43
1:F:31:VAL:O	1:F:33:MET:N	2.49	0.43
1:F:31:VAL:O	1:F:32:GLY:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:ALA:O	1:E:74:THR:HG22	2.18	0.43
1:D:200:ILE:HD12	1:D:308:LEU:HD13	2.01	0.43
1:F:280:GLN:O	1:F:283:ILE:HG12	2.18	0.43
1:E:27:GLY:HA2	1:E:52:ASP:OD2	2.18	0.43
1:F:190:LEU:HD22	1:F:291:VAL:HA	2.00	0.43
1:E:327:GLN:HA	1:E:330:ILE:CD1	2.49	0.43
1:D:231:HIS:CD2	1:D:231:HIS:C	2.92	0.43
1:E:289:LEU:HD23	1:E:323:ILE:HD11	1.78	0.43
1:B:121:ILE:N	1:B:122:PRO:CD	2.82	0.42
1:F:149:LYS:NZ	1:F:286:GLU:OE1	2.52	0.42
1:E:144:THR:HG21	1:E:160:GLY:HA3	2.01	0.42
1:F:133:LEU:HD13	1:F:135:ILE:HD11	2.00	0.42
1:E:50:LEU:O	1:E:79:ALA:HA	2.19	0.42
1:F:166:ASP:OD2	1:F:193:HIS:ND1	2.50	0.42
1:D:293:CYS:SG	1:D:303:VAL:HG22	2.60	0.42
1:E:135:ILE:HB	1:E:144:THR:HG22	2.01	0.42
1:A:28:VAL:CG1	1:A:50:LEU:HB3	2.50	0.41
1:D:54:VAL:CG2	1:D:54:VAL:O	2.68	0.41
1:E:270:VAL:HA	1:E:293:CYS:O	2.20	0.41
1:F:128:SER:HB2	1:F:131:CYS:SG	2.61	0.41
1:F:277:VAL:HG21	1:F:289:LEU:HG	2.02	0.41
1:A:99:ARG:O	1:A:99:ARG:HG3	2.20	0.41
1:A:134:LEU:HD12	1:A:134:LEU:HA	1.83	0.41
1:B:87:ALA:HA	1:B:127:TYR:HB3	2.02	0.41
1:D:196:SER:O	1:D:319:SER:OG	2.39	0.41
1:E:88:ASN:N	1:E:128:SER:OG	2.54	0.41
1:F:129:PRO:C	1:F:131:CYS:N	2.74	0.41
1:C:198:VAL:HG22	1:C:315:GLN:HB3	2.03	0.41
1:D:156:ASN:O	1:D:299:GLY:HA3	2.21	0.41
1:A:192:GLU:O	1:A:197:SER:HB3	2.21	0.40
1:A:266:ASN:CB	1:A:297:ARG:HG3	2.50	0.40
1:D:166:ASP:OD1	1:D:166:ASP:N	2.54	0.40
1:E:191:GLY:HA2	1:E:289:LEU:HD22	2.02	0.40
1:E:141:ASP:OD1	1:E:274:SER:OG	2.36	0.40
1:E:260:SER:O	1:E:264:ILE:HG12	2.22	0.40
1:A:24:THR:OG1	1:A:89:SER:OG	2.34	0.40
1:F:129:PRO:O	1:F:131:CYS:N	2.55	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	291/332 (88%)	274 (94%)	16 (6%)	1 (0%)	41	72
1	B	267/332 (80%)	258 (97%)	9 (3%)	0	100	100
1	C	268/332 (81%)	259 (97%)	9 (3%)	0	100	100
1	D	253/332 (76%)	237 (94%)	16 (6%)	0	100	100
1	E	230/332 (69%)	220 (96%)	10 (4%)	0	100	100
1	F	249/332 (75%)	223 (90%)	25 (10%)	1 (0%)	34	66
All	All	1558/1992 (78%)	1471 (94%)	85 (6%)	2 (0%)	51	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	28	VAL
1	A	52	ASP

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	259/293 (88%)	258 (100%)	1 (0%)	91	97
1	B	241/293 (82%)	240 (100%)	1 (0%)	91	97
1	C	244/293 (83%)	242 (99%)	2 (1%)	81	94
1	D	232/293 (79%)	228 (98%)	4 (2%)	60	87
1	E	211/293 (72%)	208 (99%)	3 (1%)	67	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	230/293 (78%)	228 (99%)	2 (1%)	78	94
All	All	1417/1758 (81%)	1404 (99%)	13 (1%)	78	94

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

Mol	Chain	Res	Type
1	A	169	ARG
1	B	169	ARG
1	C	169	ARG
1	C	316	LEU
1	D	41	ASN
1	D	117	PHE
1	D	247	TYR
1	D	297	ARG
1	E	52	ASP
1	E	56	ASP
1	E	156	ASN
1	F	128	SER
1	F	129	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [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	297/332 (89%)	1.07	41 (13%) 2 1	45, 56, 68, 95	0
1	B	277/332 (83%)	1.08	32 (11%) 4 2	43, 54, 63, 70	0
1	C	280/332 (84%)	1.05	28 (10%) 7 4	45, 56, 67, 73	0
1	D	265/332 (79%)	1.41	60 (22%) 0 0	54, 75, 103, 111	0
1	E	244/332 (73%)	1.38	50 (20%) 1 0	52, 71, 100, 108	0
1	F	265/332 (79%)	1.41	62 (23%) 0 0	53, 73, 96, 109	0
All	All	1628/1992 (81%)	1.23	273 (16%) 1 1	43, 62, 95, 111	0

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	308	LEU	8.3
1	F	59	LYS	7.3
1	E	285	ASN	7.2
1	D	332	LEU	6.0
1	D	144	THR	5.9
1	E	332	LEU	5.8
1	D	308	LEU	5.8
1	F	316	LEU	5.7
1	F	330	ILE	5.7
1	F	332	LEU	5.5
1	D	147	ALA	5.4
1	F	195	ASP	5.3
1	D	259	LEU	5.2
1	D	270	VAL	5.2
1	F	304	PHE	5.2
1	F	287	VAL	5.1
1	D	140	VAL	5.1
1	E	276	LEU	5.0
1	E	159	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	F	270	VAL	4.9
1	E	300	ILE	4.9
1	D	122	PRO	4.8
1	A	188	CYS	4.6
1	B	97	GLY	4.5
1	A	263	LEU	4.5
1	D	289	LEU	4.4
1	D	117	PHE	4.4
1	F	147	ALA	4.4
1	B	120	ILE	4.3
1	D	142	ILE	4.3
1	B	332	LEU	4.3
1	F	48	LEU	4.2
1	E	284	ASP	4.2
1	B	181	HIS	4.2
1	E	164	ASN	4.1
1	F	120	ILE	4.1
1	D	287	VAL	4.1
1	F	85	LEU	4.0
1	E	198	VAL	4.0
1	E	123	ASN	4.0
1	F	323	ILE	4.0
1	E	26	ILE	3.9
1	D	136	VAL	3.9
1	E	46	ASP	3.9
1	A	77	ILE	3.9
1	F	26	ILE	3.9
1	D	281	PHE	3.9
1	E	308	LEU	3.9
1	E	185	PHE	3.8
1	C	317	LYS	3.8
1	E	85	LEU	3.8
1	F	44	LEU	3.8
1	F	201	LEU	3.8
1	E	278	LYS	3.8
1	D	26	ILE	3.7
1	C	188	CYS	3.7
1	D	250	TRP	3.7
1	E	155	LEU	3.7
1	F	155	LEU	3.7
1	F	145	TYR	3.7
1	F	142	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	280	GLN	3.6
1	D	151	SER	3.6
1	A	181	HIS	3.6
1	D	285	ASN	3.6
1	C	53	VAL	3.5
1	B	299	GLY	3.5
1	D	282	GLY	3.5
1	E	190	LEU	3.5
1	D	95	THR	3.5
1	D	155	LEU	3.5
1	D	284	ASP	3.5
1	A	93	VAL	3.5
1	D	54	VAL	3.4
1	A	316	LEU	3.4
1	A	297	ARG	3.4
1	F	206	ILE	3.4
1	E	330	ILE	3.4
1	D	188	CYS	3.4
1	F	281	PHE	3.4
1	A	203	GLY	3.4
1	B	300	ILE	3.3
1	C	78	ILE	3.3
1	B	189	ILE	3.3
1	E	254	LEU	3.3
1	F	254	LEU	3.3
1	F	58	LEU	3.3
1	C	93	VAL	3.2
1	E	195	ASP	3.2
1	B	72	LEU	3.2
1	D	48	LEU	3.2
1	F	80	GLY	3.2
1	E	287	VAL	3.2
1	D	316	LEU	3.2
1	D	164	ASN	3.2
1	A	289	LEU	3.1
1	D	35	CYS	3.1
1	F	251	ALA	3.1
1	C	50	LEU	3.1
1	F	289	LEU	3.1
1	E	78	ILE	3.1
1	B	247	TYR	3.1
1	E	281	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	148	TRP	3.1
1	D	159	ILE	3.1
1	F	159	ILE	3.1
1	F	134	LEU	3.0
1	E	316	LEU	3.0
1	A	142	ILE	2.9
1	F	136	VAL	2.9
1	D	192	GLU	2.9
1	F	170	PHE	2.9
1	E	323	ILE	2.9
1	B	188	CYS	2.9
1	B	243	LYS	2.9
1	C	189	ILE	2.8
1	F	188	CYS	2.8
1	C	72	LEU	2.8
1	C	298	ASN	2.8
1	B	93	VAL	2.8
1	D	202	SER	2.8
1	E	288	PHE	2.8
1	F	61	GLU	2.8
1	D	148	TRP	2.8
1	B	259	LEU	2.8
1	A	63	MET	2.7
1	E	177	MET	2.7
1	A	53	VAL	2.7
1	F	209	MET	2.7
1	D	324	TRP	2.7
1	A	78	ILE	2.7
1	F	189	ILE	2.7
1	E	289	LEU	2.7
1	A	85	LEU	2.7
1	A	92	VAL	2.7
1	C	263	LEU	2.7
1	D	204	LEU	2.7
1	D	201	LEU	2.6
1	F	24	THR	2.6
1	A	270	VAL	2.6
1	E	146	VAL	2.6
1	C	137	SER	2.6
1	D	124	VAL	2.6
1	F	313	GLU	2.6
1	F	310	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	51	ILE	2.6
1	D	239	TYR	2.6
1	E	27	GLY	2.6
1	A	67	GLN	2.5
1	C	264	ILE	2.5
1	D	207	ALA	2.5
1	D	263	LEU	2.5
1	F	92	VAL	2.5
1	F	296	GLY	2.5
1	D	33	MET	2.5
1	D	280	GLN	2.5
1	C	39	ILE	2.5
1	C	300	ILE	2.5
1	D	120	ILE	2.5
1	D	254	LEU	2.5
1	D	134	LEU	2.5
1	B	77	ILE	2.5
1	C	185	PHE	2.5
1	D	145	TYR	2.5
1	F	288	PHE	2.5
1	D	195	ASP	2.5
1	B	67	GLN	2.4
1	C	86	THR	2.4
1	E	150	LEU	2.4
1	E	260	SER	2.4
1	F	277	VAL	2.4
1	B	78	ILE	2.4
1	D	83	TYR	2.4
1	C	85	LEU	2.4
1	F	190	LEU	2.4
1	E	324	TRP	2.4
1	B	116	ILE	2.4
1	B	158	VAL	2.4
1	E	31	VAL	2.4
1	A	102	GLU	2.4
1	B	317	LYS	2.4
1	E	311	GLU	2.4
1	F	302	GLU	2.4
1	A	291	VAL	2.4
1	F	53	VAL	2.4
1	B	316	LEU	2.4
1	C	273	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	247	TYR	2.4
1	B	262	SER	2.4
1	E	74	THR	2.4
1	F	132	ILE	2.4
1	F	239	TYR	2.3
1	A	50	LEU	2.3
1	A	119	PHE	2.3
1	D	92	VAL	2.3
1	F	40	LEU	2.3
1	C	277	VAL	2.3
1	E	154	PRO	2.3
1	F	150	LEU	2.3
1	B	133	LEU	2.3
1	F	144	THR	2.3
1	C	252	ILE	2.3
1	E	310	VAL	2.3
1	A	100	GLN	2.3
1	B	293	CYS	2.3
1	C	79	ALA	2.3
1	A	324	TRP	2.3
1	A	26	ILE	2.3
1	B	91	LEU	2.2
1	A	304	PHE	2.2
1	B	323	ILE	2.2
1	C	160	GLY	2.2
1	D	256	VAL	2.2
1	F	23	ILE	2.2
1	D	276	LEU	2.2
1	F	94	VAL	2.2
1	F	133	LEU	2.2
1	A	56	ASP	2.2
1	F	300	ILE	2.2
1	A	190	LEU	2.2
1	C	40	LEU	2.2
1	E	133	LEU	2.2
1	B	144	THR	2.2
1	C	304	PHE	2.2
1	A	211	ILE	2.2
1	A	303	VAL	2.2
1	C	91	LEU	2.2
1	E	58	LEU	2.2
1	F	73	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	194	GLY	2.2
1	C	227	CYS	2.2
1	A	239	TYR	2.1
1	E	270	VAL	2.1
1	E	23	ILE	2.1
1	D	59	LYS	2.1
1	A	167	SER	2.1
1	A	273	VAL	2.1
1	B	56	ASP	2.1
1	E	21	ASN	2.1
1	A	317	LYS	2.1
1	B	166	ASP	2.1
1	A	30	ALA	2.1
1	E	24	THR	2.1
1	A	189	ILE	2.1
1	B	174	VAL	2.1
1	D	58	LEU	2.1
1	E	124	VAL	2.1
1	F	326	THR	2.1
1	F	327	GLN	2.1
1	A	118	LYS	2.1
1	A	228	LYS	2.1
1	B	305	LYS	2.1
1	C	28	VAL	2.1
1	F	146	VAL	2.1
1	D	123	ASN	2.1
1	B	55	GLU	2.1
1	D	32	GLY	2.1
1	E	37	PHE	2.1
1	B	53	VAL	2.0
1	E	315	GLN	2.0
1	E	191	GLY	2.0
1	E	299	GLY	2.0
1	D	118	LYS	2.0
1	D	50	LEU	2.0
1	A	264	ILE	2.0
1	E	77	ILE	2.0
1	A	41	ASN	2.0
1	F	164	ASN	2.0
1	D	170	PHE	2.0
1	D	244	LEU	2.0
1	D	302	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	204	LEU	2.0
1	D	53	VAL	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 carbohydrates 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.