



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:44 AM UTC

PDB ID : 2V6M / pdb_00002v6m
Title : Crystal structure of lactate dehydrogenase from *Thermus Thermophilus* HB8 (Apo form)
Authors : Coquelle, N.; Fioravanti, E.; Weik, M.; Vellieux, F.
Deposited on : 2007-07-19
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 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

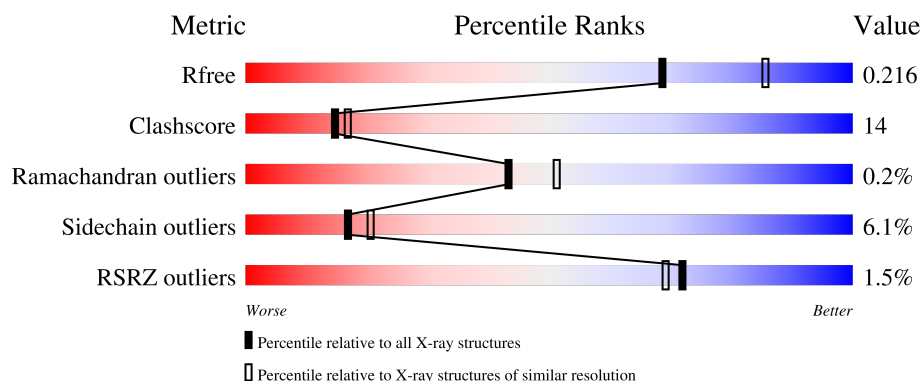
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

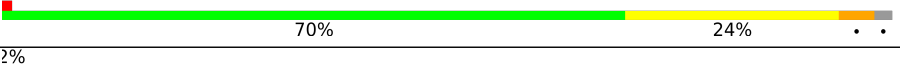
The reported resolution of this entry is 2.20 Å.

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	310	 77% 22% .
1	B	310	 70% 24% . .
1	C	310	 78% 20% .
1	D	310	 70% 27% . .

2 Entry composition [i](#)

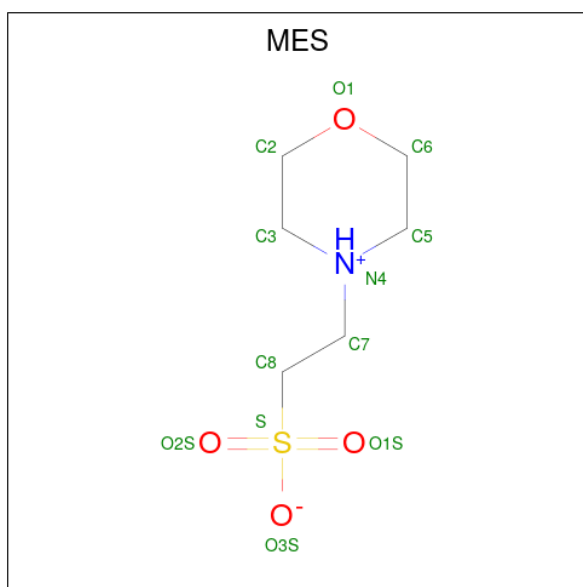
There are 3 unique types of molecules in this entry. The entry contains 9633 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	310	Total	C	N	O	S	0	0	0
			2294	1455	412	424	3			
1	B	303	Total	C	N	O	S	0	0	0
			2230	1418	397	412	3			
1	C	310	Total	C	N	O	S	0	0	0
			2305	1462	411	429	3			
1	D	303	Total	C	N	O	S	0	0	0
			2255	1433	402	417	3			

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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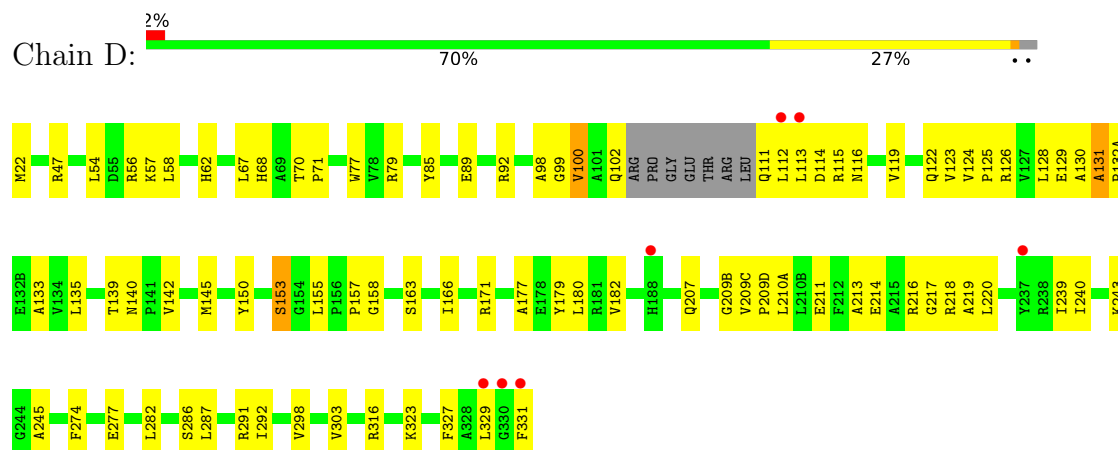
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total	O	0	0
			163	163		
3	B	147	Total	O	0	0
			147	147		
3	C	95	Total	O	0	0
			95	95		
3	D	108	Total	O	0	0
			108	108		

● Molecule 1: L-LACTATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.09Å 135.30Å 85.64Å 90.00° 94.04° 90.00°	Depositor
Resolution (Å)	29.22 – 2.20 29.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.22-2.20) 99.7 (29.22-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.196 , 0.218 0.194 , 0.216	Depositor DCC
R_{free} test set	3087 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9633	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MES

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	0.66	4/2334 (0.2%)	0.89	2/3176 (0.1%)
1	B	0.46	0/2267	0.78	2/3083 (0.1%)
1	C	0.56	0/2345	0.92	4/3191 (0.1%)
1	D	0.43	0/2293	0.84	2/3118 (0.1%)
All	All	0.54	4/9239 (0.0%)	0.86	10/12568 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	GLN	C-O	-7.09	1.15	1.24
1	A	177	ALA	C-O	-5.78	1.17	1.24
1	A	219	ALA	CA-CB	-5.35	1.44	1.53
1	A	178	GLU	C-O	-5.03	1.17	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	131	ALA	CA-C-N	6.66	126.36	119.56
1	D	131	ALA	C-N-CA	6.66	126.36	119.56
1	C	316	ARG	N-CA-C	-6.62	104.06	111.28
1	A	219	ALA	N-CA-C	5.94	120.26	112.89
1	A	178	GLU	N-CA-C	-5.94	104.75	112.23
1	C	97	ALA	N-CA-C	-5.53	103.40	111.30
1	C	166	ILE	N-CA-C	5.35	116.08	110.62
1	B	275	THR	CA-C-N	5.33	124.79	119.24
1	B	275	THR	C-N-CA	5.33	124.79	119.24
1	C	112	LEU	N-CA-C	-5.02	105.89	111.36

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	2294	0	2327	55	0
1	B	2230	0	2270	73	0
1	C	2305	0	2343	64	1
1	D	2255	0	2301	65	1
2	B	12	0	13	3	0
2	C	12	0	12	0	0
2	D	12	0	13	2	0
3	A	163	0	0	5	0
3	B	147	0	0	7	0
3	C	95	0	0	9	0
3	D	108	0	0	9	0
All	All	9633	0	9279	255	1

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 14.

All (255) 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:188:HIS:HB3	3:C:1064:HOH:O	1.52	1.06
1:B:313:GLU:HG3	1:B:317:ARG:HH11	1.16	1.04
1:C:108:THR:HG22	1:C:111:GLN:OE1	1.58	1.04
1:B:234:ARG:HG2	3:B:1115:HOH:O	1.66	0.95
2:B:1332:MES:H61	3:B:1146:HOH:O	1.70	0.90
1:B:313:GLU:HG3	1:B:317:ARG:NH1	1.87	0.89
1:A:188:HIS:CE1	1:A:190:TYR:CE2	2.62	0.88
1:A:221:SER:HB2	1:A:222:PRO:HD2	1.56	0.85
1:B:223:GLU:HG3	3:B:1113:HOH:O	1.77	0.83
1:C:179:TYR:CE2	1:C:220:LEU:HD23	2.13	0.82
1:A:181:ARG:HE	1:A:218:ARG:NH1	1.78	0.81
1:B:110:LEU:HA	1:B:113:LEU:HB3	1.63	0.80
1:D:102:GLN:HB3	1:D:112:LEU:HD11	1.62	0.80
1:B:185:GLN:HG3	3:C:1079:HOH:O	1.80	0.79
1:A:239:ILE:HG21	1:A:246:THR:HG22	1.62	0.79
1:D:85:TYR:CE2	1:D:126:ARG:HD3	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:O	1:A:68:HIS:HD2	1.67	0.77
1:C:179:TYR:HD2	1:C:180:LEU:HD12	1.51	0.75
1:D:329:LEU:CD1	3:D:1031:HOH:O	2.34	0.74
1:C:108:THR:HG22	1:C:111:GLN:CD	2.13	0.73
1:C:107:GLU:OE2	1:C:115:ARG:HD3	1.89	0.73
1:C:275:THR:HG23	1:C:285:VAL:O	1.89	0.72
1:A:22:MET:HE3	3:A:1009:HOH:O	1.89	0.72
1:C:107:GLU:OE2	1:C:115:ARG:CD	2.38	0.71
1:B:194:GLU:OE1	1:B:321:ILE:HD11	1.89	0.71
1:A:188:HIS:HE1	1:A:190:TYR:CE2	2.10	0.69
1:D:303:VAL:HG12	3:D:1095:HOH:O	1.92	0.69
1:A:211:GLU:O	1:A:214:GLU:HB2	1.93	0.68
1:C:114:ASP:O	1:C:118:GLN:HG2	1.94	0.68
1:C:179:TYR:CD2	1:C:180:LEU:HD12	2.29	0.68
1:A:118:GLN:NE2	3:A:1067:HOH:O	2.27	0.68
1:C:239:ILE:HG21	1:C:246:THR:HG22	1.77	0.67
1:B:183:ALA:HB1	1:B:185:GLN:HE21	1.60	0.67
1:A:64:GLU:O	1:A:68:HIS:CD2	2.48	0.66
1:A:181:ARG:NE	1:A:218:ARG:NH1	2.43	0.66
1:A:207:GLN:NE2	1:D:209(B):GLY:HA2	2.10	0.66
1:A:213:ALA:HB1	1:A:218:ARG:O	1.95	0.66
1:C:179:TYR:HD2	1:C:180:LEU:CD1	2.08	0.66
1:D:92:ARG:O	1:D:92:ARG:HG2	1.94	0.65
1:C:179:TYR:CE2	1:C:220:LEU:CD2	2.80	0.65
1:B:165:THR:HG21	1:B:191:VAL:O	1.96	0.64
3:C:1051:HOH:O	1:D:68:HIS:HE1	1.78	0.64
1:C:108:THR:HG22	1:C:111:GLN:CG	2.27	0.64
1:C:64:GLU:O	1:C:68:HIS:HD2	1.81	0.64
1:C:103:ARG:HB2	1:C:107:GLU:HB2	1.78	0.64
1:B:213:ALA:CB	1:B:220:LEU:HD23	2.27	0.64
1:C:179:TYR:CD2	1:C:220:LEU:HD21	2.33	0.64
1:C:266:LYS:NZ	1:C:299:GLU:OE2	2.31	0.63
1:B:192:LEU:HD22	1:B:289:LEU:HA	1.82	0.61
1:A:77:TRP:CZ2	1:A:79:ARG:HD3	2.36	0.60
1:B:144:VAL:O	1:B:148:VAL:HG13	2.00	0.60
1:D:327:PHE:CD1	1:D:327:PHE:C	2.79	0.60
1:A:108:THR:N	1:A:111:GLN:OE1	2.27	0.60
1:C:100:VAL:H	1:C:116:ASN:HD21	1.49	0.60
1:A:194:GLU:OE1	1:A:198:SER:HB3	2.02	0.60
1:A:158:GLY:HA2	1:A:298:VAL:HG23	1.83	0.59
1:D:128:LEU:HD11	1:D:135:LEU:HD21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ARG:O	1:B:112:LEU:HB3	2.02	0.59
1:C:245:ALA:HB1	3:C:1073:HOH:O	2.02	0.59
1:C:273:ALA:O	1:C:275:THR:HG22	2.01	0.59
1:D:112:LEU:O	1:D:115:ARG:HB2	2.01	0.59
1:D:150:TYR:CE1	1:D:157:PRO:HA	2.38	0.59
1:A:221:SER:HB2	1:A:222:PRO:CD	2.30	0.59
1:B:111:GLN:O	1:B:114:ASP:HB2	2.02	0.59
1:A:239:ILE:CG2	1:A:246:THR:HG22	2.34	0.58
1:B:221:SER:O	1:B:224:ASP:N	2.36	0.58
1:A:187:VAL:HG22	1:A:208:VAL:HG22	1.85	0.57
1:D:180:LEU:HD21	1:D:220:LEU:HD21	1.86	0.57
1:C:136:LEU:HD12	1:C:254:LEU:HD22	1.86	0.57
1:D:92:ARG:O	1:D:92:ARG:CG	2.52	0.57
1:A:188:HIS:CE1	1:A:190:TYR:CZ	2.92	0.57
1:B:273:ALA:O	1:B:275:THR:HG22	2.05	0.57
1:C:179:TYR:CD2	1:C:220:LEU:CD2	2.88	0.57
1:B:100:VAL:HG13	1:B:115:ARG:HH11	1.70	0.57
1:B:151:ARG:HD2	1:B:331:PHE:OXT	2.05	0.57
1:B:209(B):GLY:HA3	1:C:188:HIS:CE1	2.39	0.56
1:B:203:TRP:CZ2	1:B:225:ARG:HG3	2.39	0.56
1:D:142:VAL:HG12	3:D:1037:HOH:O	2.05	0.56
2:D:1332:MES:H72	3:D:1088:HOH:O	2.04	0.56
1:D:329:LEU:HD12	3:D:1031:HOH:O	2.04	0.55
1:A:188:HIS:O	1:A:188:HIS:CD2	2.60	0.55
1:B:321:ILE:HG13	1:B:322:LEU:N	2.21	0.55
1:D:139:THR:HG22	1:D:145:MET:HG3	1.89	0.55
1:A:179:TYR:CD1	1:A:179:TYR:C	2.84	0.55
1:C:99:GLY:HA2	1:C:116:ASN:ND2	2.22	0.55
1:B:22:MET:HE2	3:B:1001:HOH:O	2.06	0.54
1:C:107:GLU:CD	1:C:115:ARG:HH11	2.15	0.54
1:B:113:LEU:HD21	1:B:144:VAL:HG11	1.90	0.54
1:C:107:GLU:OE2	1:C:115:ARG:HD2	2.07	0.54
1:C:210(B):LEU:CD2	1:C:220:LEU:HD12	2.38	0.54
1:D:77:TRP:CE2	1:D:79:ARG:HD3	2.42	0.54
1:A:77:TRP:CE2	1:A:79:ARG:HD3	2.43	0.54
1:A:74:HIS:HE1	3:A:1007:HOH:O	1.90	0.54
1:A:181:ARG:NE	1:A:218:ARG:HH12	2.06	0.54
1:A:192:LEU:HD22	1:A:290:PRO:HD3	1.90	0.53
1:D:209(C):VAL:HG13	1:D:209(D):PRO:HD2	1.91	0.53
1:B:110:LEU:HA	1:B:113:LEU:CB	2.37	0.53
2:D:1332:MES:H61	3:D:1025:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:THR:N	1:D:71:PRO:CD	2.72	0.52
1:B:179:TYR:HE2	1:B:220:LEU:HD22	1.74	0.52
1:D:124:VAL:N	1:D:125:PRO:HD2	2.24	0.52
1:D:239:ILE:O	1:D:243:LYS:HG2	2.09	0.52
1:D:327:PHE:HA	1:D:331:PHE:O	2.09	0.52
1:D:113:LEU:O	1:D:114:ASP:C	2.53	0.51
1:D:163:SER:O	1:D:166:ILE:HG12	2.10	0.51
1:D:112:LEU:HD23	1:D:115:ARG:HD3	1.93	0.51
1:C:74:HIS:HE1	3:C:1008:HOH:O	1.92	0.51
1:C:99:GLY:CA	1:C:116:ASN:ND2	2.74	0.51
1:C:230:GLU:O	1:C:230:GLU:HG3	2.11	0.51
1:C:309:PRO:HD2	1:C:310:GLU:OE2	2.10	0.51
1:A:188:HIS:HE1	1:A:190:TYR:CZ	2.29	0.51
1:C:108:THR:HG23	1:C:111:GLN:H	1.76	0.51
1:B:218:ARG:O	1:B:219:ALA:C	2.51	0.50
1:C:179:TYR:CZ	1:C:220:LEU:HD23	2.47	0.50
1:A:61:ALA:HB2	1:B:242:GLY:HA3	1.94	0.50
1:C:113:LEU:HG	1:C:329:LEU:HD11	1.93	0.50
1:C:194:GLU:HG3	1:C:322:LEU:HD21	1.93	0.50
1:D:316:ARG:HH11	1:D:316:ARG:HG3	1.77	0.50
1:B:287:LEU:C	1:B:287:LEU:HD12	2.36	0.50
2:B:1332:MES:H21	3:B:1092:HOH:O	2.12	0.50
1:A:192:LEU:CD2	1:A:290:PRO:HD3	2.43	0.49
1:C:194:GLU:O	1:C:199:GLU:HB3	2.12	0.49
1:A:188:HIS:CE1	1:D:209(B):GLY:HA3	2.48	0.49
1:A:211:GLU:O	1:A:212:PHE:C	2.55	0.49
1:D:213:ALA:HB2	1:D:220:LEU:HD23	1.93	0.49
1:B:89:GLU:HA	1:B:130:ALA:O	2.12	0.49
1:C:77:TRP:CE2	1:C:79:ARG:HD3	2.48	0.49
1:D:180:LEU:HD11	1:D:210(A):LEU:HD11	1.94	0.49
1:D:287:LEU:C	1:D:287:LEU:HD12	2.36	0.49
1:B:177:ALA:HB1	1:B:182:VAL:O	2.13	0.49
1:B:316:ARG:NH1	1:B:320:GLU:OE2	2.46	0.49
1:D:98:ALA:O	1:D:99:GLY:C	2.56	0.48
1:B:275:THR:HG23	1:B:285:VAL:O	2.13	0.48
1:B:310:GLU:OE1	1:B:310:GLU:O	2.32	0.48
1:B:79:ARG:NH2	3:B:1039:HOH:O	2.46	0.48
1:B:279:GLU:O	1:B:316:ARG:HG3	2.14	0.48
1:B:179:TYR:CE2	1:B:220:LEU:HD13	2.49	0.48
1:D:119:VAL:O	1:D:123:VAL:HG23	2.14	0.48
1:D:316:ARG:HD2	1:D:316:ARG:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:VAL:HG22	1:C:212:PHE:CE1	2.48	0.48
1:C:62:HIS:HE1	3:C:1014:HOH:O	1.95	0.48
1:C:246:THR:HG21	3:C:1074:HOH:O	2.13	0.48
1:B:303:VAL:HG22	1:C:212:PHE:CZ	2.49	0.48
1:D:129:GLU:OE2	3:D:1034:HOH:O	2.20	0.48
1:D:140:ASN:ND2	3:D:1037:HOH:O	2.46	0.48
1:A:320:GLU:O	1:A:324:GLU:HG3	2.14	0.48
1:C:214:GLU:C	1:C:216:ARG:H	2.22	0.48
1:A:26:ILE:HB	1:A:51:LEU:HD23	1.95	0.47
1:D:274:PHE:HA	1:D:286:SER:OG	2.14	0.47
1:A:211:GLU:O	1:A:214:GLU:N	2.48	0.47
1:B:289:LEU:O	1:B:291:ARG:HG3	2.14	0.47
1:A:89:GLU:C	1:A:89:GLU:CD	2.82	0.47
1:C:136:LEU:CD1	1:C:254:LEU:CD2	2.92	0.47
1:C:239:ILE:CG2	1:C:246:THR:HG22	2.43	0.47
1:A:243:LYS:HD2	1:B:62:HIS:CE1	2.50	0.46
1:B:192:LEU:HD21	1:B:290:PRO:HD3	1.97	0.46
1:C:136:LEU:CD1	1:C:254:LEU:HD22	2.45	0.46
1:D:85:TYR:CD2	1:D:126:ARG:HD3	2.49	0.46
1:D:77:TRP:CZ2	1:D:79:ARG:HD3	2.50	0.46
1:B:223:GLU:O	1:B:227:ARG:HB2	2.15	0.46
1:B:77:TRP:CZ2	1:B:79:ARG:HD3	2.51	0.46
1:D:153:SER:OG	1:D:155:LEU:HB2	2.15	0.46
1:B:169:THR:O	1:B:173:ARG:HG3	2.16	0.46
1:C:210(B):LEU:HD23	1:C:220:LEU:HD12	1.98	0.46
1:A:243:LYS:HE3	1:A:245:ALA:O	2.15	0.46
1:C:100:VAL:HG21	1:C:115:ARG:CZ	2.46	0.46
1:C:243:LYS:HE2	1:C:245:ALA:O	2.15	0.46
1:B:213:ALA:HB1	1:B:220:LEU:CD2	2.47	0.45
1:C:99:GLY:HA2	1:C:116:ASN:HD22	1.80	0.45
1:C:118:GLN:O	1:C:122:GLN:HG2	2.16	0.45
1:D:22:MET:HE1	1:D:92:ARG:NH1	2.32	0.45
1:D:240:ILE:HD13	1:D:245:ALA:HA	1.98	0.45
1:B:236:ALA:O	1:B:240:ILE:HG13	2.17	0.45
1:D:131:ALA:N	1:D:132(A):PRO:HD3	2.31	0.45
1:D:153:SER:OG	1:D:155:LEU:N	2.45	0.45
1:D:153:SER:OG	1:D:155:LEU:CB	2.65	0.45
1:B:194:GLU:HB2	1:B:322:LEU:HD11	1.99	0.44
1:B:290:PRO:HG2	1:B:305:PRO:HD3	1.99	0.44
1:C:216:ARG:O	1:C:217:GLY:C	2.60	0.44
1:C:203:TRP:HZ3	1:C:220:LEU:HD13	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ARG:NH1	1:A:129:GLU:OE2	2.46	0.44
1:B:184:PRO:HD2	1:B:185:GLN:NE2	2.32	0.44
1:B:213:ALA:CB	1:B:220:LEU:CD2	2.94	0.44
1:D:158:GLY:HA2	1:D:298:VAL:CG2	2.47	0.44
1:B:100:VAL:HG13	1:B:115:ARG:NH1	2.33	0.44
1:D:316:ARG:HG3	1:D:316:ARG:NH1	2.32	0.44
1:A:150:TYR:HA	1:A:160:VAL:HG21	2.00	0.44
1:A:287:LEU:C	1:A:287:LEU:HD12	2.43	0.44
1:C:102:GLN:HB2	1:C:112:LEU:HD22	1.98	0.44
1:D:179:TYR:O	1:D:218:ARG:HD3	2.16	0.44
1:B:277:GLU:HB3	1:B:282:LEU:HD23	1.98	0.44
1:D:282:LEU:O	1:D:323:LYS:HD2	2.18	0.44
1:A:107:GLU:OE2	1:A:115:ARG:HD3	2.18	0.43
1:A:233:ARG:NH2	3:A:1127:HOH:O	2.50	0.43
1:D:85:TYR:CZ	1:D:126:ARG:HD3	2.53	0.43
1:D:171:ARG:HA	1:D:171:ARG:HD2	1.88	0.43
1:A:221:SER:CB	1:A:222:PRO:CD	2.94	0.43
1:D:214:GLU:O	1:D:217:GLY:N	2.37	0.43
1:B:124:VAL:HB	1:B:125:PRO:HD3	2.01	0.43
1:C:140:ASN:HA	1:C:141:PRO:C	2.43	0.43
1:B:158:GLY:HA2	1:B:298:VAL:CG2	2.48	0.43
1:A:124:VAL:N	1:A:125:PRO:HD2	2.34	0.43
1:A:214:GLU:C	1:A:216:ARG:H	2.25	0.43
1:A:308:SER:O	1:A:309:PRO:C	2.61	0.43
1:A:158:GLY:HA2	1:A:298:VAL:CG2	2.49	0.43
1:B:56:ARG:HH11	1:B:56:ARG:CG	2.32	0.43
1:D:114:ASP:O	1:D:115:ARG:C	2.62	0.43
1:B:185:GLN:CG	3:C:1079:HOH:O	2.52	0.43
1:B:192:LEU:CD2	1:B:290:PRO:HD3	2.49	0.42
1:B:203:TRP:CE2	1:B:225:ARG:HG3	2.54	0.42
1:B:213:ALA:HB2	1:B:220:LEU:HD23	2.00	0.42
1:D:291:ARG:NH1	3:D:1094:HOH:O	2.48	0.42
1:B:185:GLN:CD	1:B:185:GLN:H	2.25	0.42
1:C:103:ARG:CZ	1:C:103:ARG:HB3	2.49	0.42
1:A:208:VAL:HG11	1:A:212:PHE:CE2	2.54	0.42
1:B:275:THR:HA	1:B:276:PRO:HD3	1.83	0.42
2:B:1332:MES:C2	3:B:1092:HOH:O	2.67	0.42
1:B:235:ALA:HA	1:B:238:ARG:NH1	2.34	0.42
1:D:92:ARG:O	1:D:133:ALA:HA	2.19	0.42
1:A:263:THR:O	1:A:264:ASP:C	2.63	0.42
1:D:100:VAL:HG12	1:D:116:ASN:OD1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ALA:C	1:D:132(A):PRO:HD3	2.44	0.42
1:D:209(C):VAL:CG1	1:D:209(D):PRO:HD2	2.49	0.42
1:B:210(B):LEU:HD12	1:B:210(B):LEU:HA	1.88	0.42
1:D:131:ALA:HB1	1:D:133:ALA:HB2	2.02	0.42
1:C:122:GLN:O	1:C:125:PRO:HD2	2.20	0.42
1:C:180:LEU:O	1:C:181:ARG:HB2	2.19	0.42
1:A:220:LEU:HD23	1:A:220:LEU:HA	1.81	0.42
1:C:108:THR:CG2	1:C:111:GLN:OE1	2.48	0.42
1:A:89:GLU:HG3	1:A:89:GLU:O	2.19	0.41
1:B:100:VAL:CG1	1:B:115:ARG:NH1	2.83	0.41
1:B:221:SER:HB3	1:B:224:ASP:OD2	2.21	0.41
1:B:109:ARG:C	1:B:111:GLN:N	2.78	0.41
1:A:237:TYR:CE1	1:A:241:GLU:OE2	2.73	0.41
1:A:327:PHE:HA	1:A:331:PHE:O	2.21	0.41
1:C:108:THR:CG2	1:C:111:GLN:HB2	2.51	0.41
1:B:100:VAL:CG1	1:B:115:ARG:HH11	2.33	0.41
1:B:313:GLU:CG	1:B:317:ARG:NH1	2.72	0.41
1:C:214:GLU:C	1:C:216:ARG:N	2.78	0.41
1:A:57:LYS:HE2	3:A:1011:HOH:O	2.21	0.41
1:B:277:GLU:CB	1:B:282:LEU:HD23	2.50	0.41
1:D:58:LEU:HD11	1:D:62:HIS:CE1	2.55	0.41
1:D:89:GLU:HA	1:D:130:ALA:O	2.21	0.41
1:B:145:MET:O	1:B:148:VAL:HG22	2.21	0.41
1:D:277:GLU:HB3	1:D:282:LEU:HD23	2.02	0.41
1:D:292:ILE:O	1:D:298:VAL:HA	2.20	0.41
1:B:192:LEU:HD11	1:B:305:PRO:HG3	2.03	0.40
1:C:107:GLU:OE1	1:C:115:ARG:NH1	2.53	0.40
1:D:177:ALA:HB1	1:D:182:VAL:O	2.21	0.40
1:C:291:ARG:HD2	1:C:298:VAL:HG11	2.03	0.40
1:B:165:THR:HG23	1:B:270:THR:OG1	2.22	0.40
1:C:288:SER:O	1:C:289:LEU:HD23	2.21	0.40
1:D:128:LEU:N	1:D:128:LEU:CD1	2.85	0.40
1:C:245:ALA:CB	3:C:1073:HOH:O	2.65	0.40
1:D:150:TYR:HE1	1:D:157:PRO:HA	1.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ASP:OD2	1:D:211:GLU:OE2[2_545]	2.08	0.12

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	308/310 (99%)	295 (96%)	12 (4%)	1 (0%)	36	42
1	B	299/310 (96%)	287 (96%)	12 (4%)	0	100	100
1	C	308/310 (99%)	296 (96%)	11 (4%)	1 (0%)	36	42
1	D	299/310 (96%)	285 (95%)	13 (4%)	1 (0%)	36	42
All	All	1214/1240 (98%)	1163 (96%)	48 (4%)	3 (0%)	43	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	219	ALA
1	A	247	TYR
1	C	217	GLY

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	226/232 (97%)	217 (96%)	9 (4%)	28	38
1	B	221/232 (95%)	199 (90%)	22 (10%)	7	7
1	C	230/232 (99%)	217 (94%)	13 (6%)	18	23
1	D	225/232 (97%)	214 (95%)	11 (5%)	22	29
All	All	902/928 (97%)	847 (94%)	55 (6%)	17	20

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	89	GLU
1	A	110	LEU
1	A	114	ASP
1	A	178	GLU
1	A	186	SER
1	A	209(C)	VAL
1	A	209(D)	PRO
1	A	278	VAL
1	B	22	MET
1	B	42	LEU
1	B	54	LEU
1	B	56	ARG
1	B	96	LEU
1	B	100	VAL
1	B	110	LEU
1	B	148	VAL
1	B	151	ARG
1	B	185	GLN
1	B	198	SER
1	B	209(C)	VAL
1	B	209(D)	PRO
1	B	221	SER
1	B	234	ARG
1	B	257	LEU
1	B	275	THR
1	B	310	GLU
1	B	317	ARG
1	B	318	SER
1	B	324	GLU
1	B	329	LEU
1	C	54	LEU
1	C	56	ARG
1	C	128	LEU
1	C	136	LEU
1	C	178	GLU
1	C	209(C)	VAL
1	C	209(D)	PRO
1	C	223	GLU
1	C	230	GLU
1	C	275	THR
1	C	278	VAL
1	C	287	LEU

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Mol	Chain	Res	Type
1	C	310	GLU
1	D	47	ARG
1	D	54	LEU
1	D	56	ARG
1	D	57	LYS
1	D	67	LEU
1	D	100	VAL
1	D	111	GLN
1	D	122	GLN
1	D	153	SER
1	D	207	GLN
1	D	216	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	62	HIS
1	A	68	HIS
1	A	74	HIS
1	A	188	HIS
1	B	185	GLN
1	B	188	HIS
1	B	207	GLN
1	C	60	GLN
1	C	62	HIS
1	C	68	HIS
1	C	74	HIS
1	C	116	ASN
1	C	140	ASN
1	C	195	HIS
1	C	207	GLN
1	D	60	GLN
1	D	62	HIS
1	D	68	HIS
1	D	188	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	MES	D	1332	-	12,12,12	1.64	1 (8%)	15,16,16	1.23	2 (13%)
2	MES	B	1332	-	12,12,12	1.51	2 (16%)	15,16,16	0.81	0
2	MES	C	1332	-	12,12,12	2.00	1 (8%)	15,16,16	3.36	9 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	D	1332	-	-	5/6/14/14	0/1/1/1
2	MES	B	1332	-	-	0/6/14/14	0/1/1/1
2	MES	C	1332	-	-	4/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1332	MES	C8-S	-6.54	1.68	1.77
2	D	1332	MES	C8-S	4.75	1.84	1.77
2	B	1332	MES	C8-S	4.08	1.83	1.77
2	B	1332	MES	O1S-S	2.00	1.50	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1332	MES	O1S-S-C8	6.33	116.30	106.73
2	C	1332	MES	O3S-S-O1S	-5.54	97.54	111.40
2	C	1332	MES	C5-N4-C3	4.60	118.74	108.84
2	C	1332	MES	C7-N4-C5	3.93	121.72	111.24
2	C	1332	MES	O3S-S-C8	3.74	113.32	106.00
2	C	1332	MES	C2-C3-N4	3.55	115.52	110.12
2	C	1332	MES	C6-C5-N4	-3.18	105.29	110.12
2	C	1332	MES	C7-N4-C3	3.07	119.43	111.24
2	C	1332	MES	O1-C2-C3	2.76	117.71	111.77
2	D	1332	MES	O1S-S-C8	2.37	110.31	106.73
2	D	1332	MES	O2S-S-C8	2.37	110.30	106.73

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1332	MES	C8-C7-N4-C3
2	C	1332	MES	C7-C8-S-O1S
2	C	1332	MES	C7-C8-S-O3S
2	C	1332	MES	C7-C8-S-O2S
2	D	1332	MES	C8-C7-N4-C3
2	D	1332	MES	C8-C7-N4-C5
2	D	1332	MES	C7-C8-S-O1S
2	D	1332	MES	C7-C8-S-O2S
2	D	1332	MES	C7-C8-S-O3S

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1332	MES	2	0
2	B	1332	MES	3	0

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	310/310 (100%)	-0.35	4 (1%) 75 73	13, 24, 49, 71	6 (1%)
1	B	303/310 (97%)	-0.20	3 (0%) 79 77	13, 27, 53, 69	1 (0%)
1	C	310/310 (100%)	-0.13	5 (1%) 70 67	18, 32, 55, 76	4 (1%)
1	D	303/310 (97%)	-0.01	7 (2%) 61 58	19, 32, 62, 72	4 (1%)
All	All	1226/1240 (98%)	-0.17	19 (1%) 72 69	13, 30, 54, 76	15 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	ARG	3.7
1	C	99	GLY	3.4
1	D	113	LEU	3.2
1	A	219	ALA	2.8
1	D	329	LEU	2.8
1	B	220	LEU	2.8
1	B	110	LEU	2.7
1	D	330	GLY	2.5
1	A	209(A)	GLY	2.5
1	A	304	TYR	2.4
1	C	100	VAL	2.4
1	D	237	TYR	2.3
1	C	101	ALA	2.3
1	C	54	LEU	2.3
1	C	215	ALA	2.3
1	D	331	PHE	2.3
1	D	112	LEU	2.1
1	D	188	HIS	2.1
1	A	217	GLY	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MES	C	1332	12/12	0.83	0.16	66,67,69,69	0
2	MES	D	1332	12/12	0.86	0.14	61,62,65,66	0
2	MES	B	1332	12/12	0.87	0.14	69,70,73,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.