



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:00 am BST

PDB ID : 2V6M
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

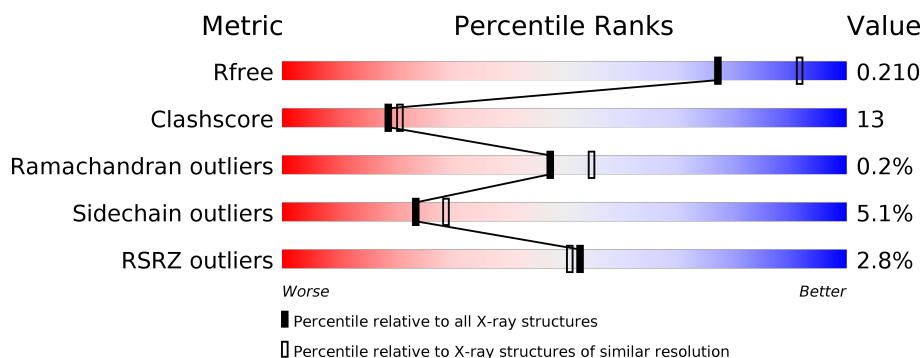
1 Overall quality at a glance

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	310	<div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	B	310	<div> <div>3%</div> <div>71%</div> <div>23%</div> <div>.</div> <div>.</div> </div>
1	C	310	<div> <div>4%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
1	D	310	<div> <div>5%</div> <div>70%</div> <div>27%</div> <div>..</div> </div>

2 Entry composition [i](#)

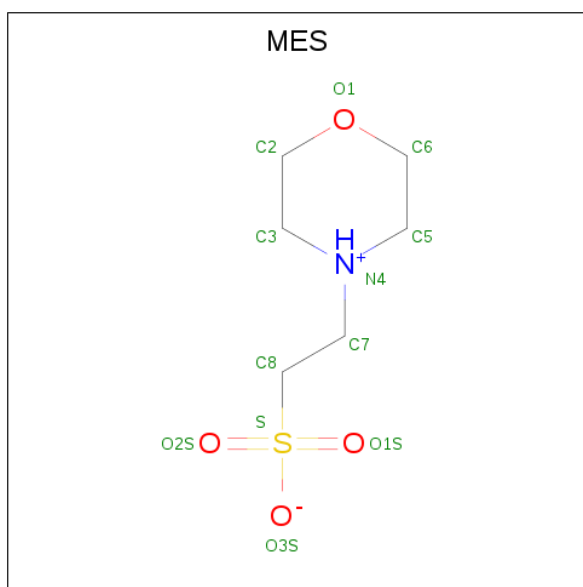
There are 3 unique types of molecules in this entry. The entry contains 9633 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

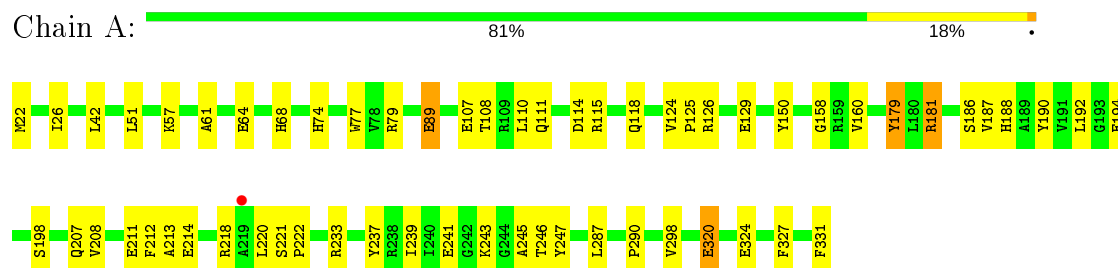
- Molecule 3 is water.

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		

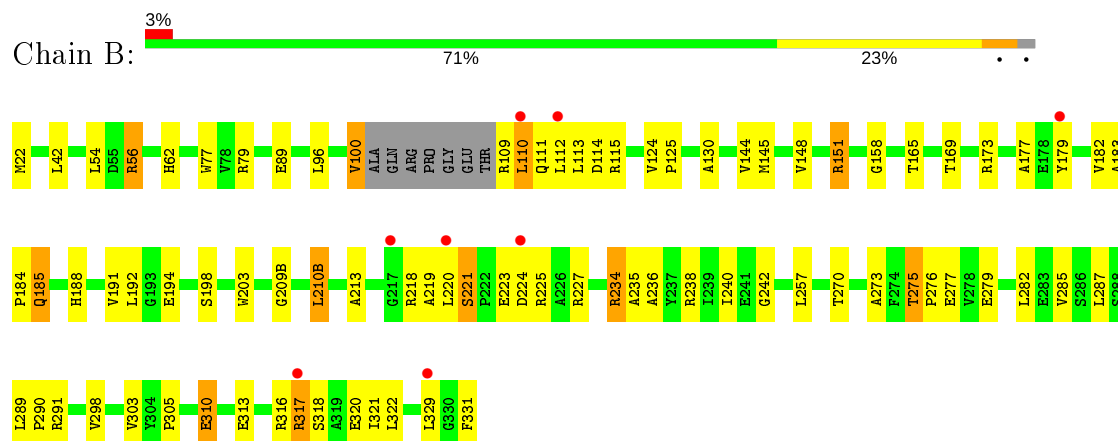
3 Residue-property plots [i](#)

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.

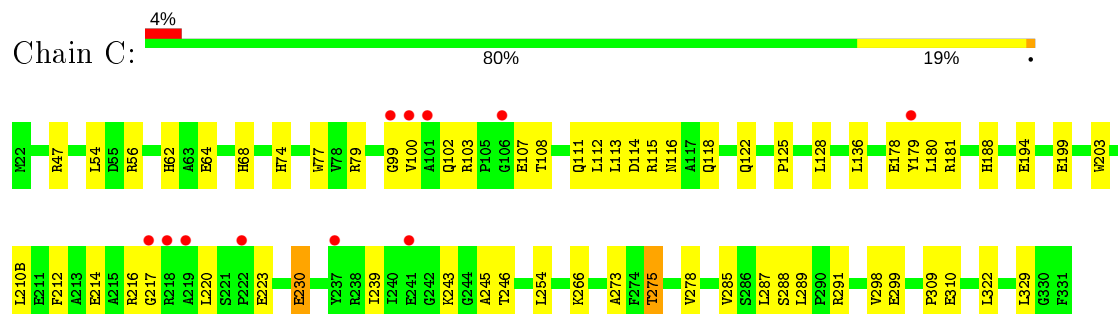
• Molecule 1: L-LACTATE DEHYDROGENASE



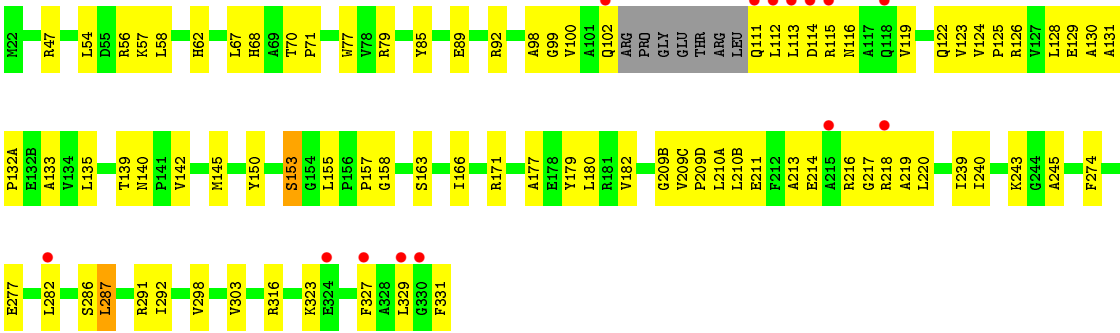
• Molecule 1: L-LACTATE DEHYDROGENASE



• Molecule 1: L-LACTATE DEHYDROGENASE



• Molecule 1: L-LACTATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.09 Å 135.30 Å 85.64 Å 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 2.20 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.196 , 0.218 0.186 , 0.210	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)	0.34 , 55.5	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 [i](#)

5.1 Standard geometry [i](#)

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	0.54	5/2334 (0.2%)	0.61	1/3176 (0.0%)
1	B	0.35	0/2267	0.52	0/3083
1	C	0.43	0/2345	0.63	0/3191
1	D	0.35	0/2293	0.54	0/3118
All	All	0.43	5/9239 (0.1%)	0.58	1/12568 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	TYR	CD1-CE1	-5.94	1.30	1.39
1	A	320	GLU	CG-CD	5.43	1.60	1.51
1	A	179	TYR	CB-CG	-5.37	1.43	1.51
1	A	179	TYR	CD2-CE2	-5.27	1.31	1.39
1	A	320	GLU	CB-CG	5.02	1.61	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ARG	NE-CZ-NH1	5.98	123.29	120.30

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	2294	0	2327	50	0
1	B	2230	0	2270	70	0
1	C	2305	0	2343	61	1
1	D	2255	0	2301	62	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	6	0
3	C	95	0	0	9	0
3	D	108	0	0	9	0
All	All	9633	0	9279	241	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 13.

All (241) 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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:108:THR:HG22	1:C:111:GLN:CD	2.13	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:HG2	1:D:92:ARG:O	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:C:266:LYS:NZ	1:C:299:GLU:OE2	2.31	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	1:D:92:ARG:O	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
2:D:1332:MES:H72	3:D:1088:HOH:O	2.04	0.56
1:D:142:VAL:HG12	3:D:1037:HOH:O	2.05	0.56
1:D:327:PHE:CD1	1:D:327:PHE:C	2.79	0.55
1:D:329:LEU:HD12	3:D:1031:HOH:O	2.04	0.55
1:A:188:HIS:CD2	1:A:188:HIS:O	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:C:99:GLY:HA2	1:C:116:ASN:ND2	2.22	0.55
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:181:ARG:NE	1:A:218:ARG:HH12	2.06	0.54
1:A:74:HIS:HE1	3:A:1007:HOH:O	1.90	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:179:TYR:CZ	1:C:220:LEU:HD23	2.47	0.50
1:A:179:TYR:C	1:A:179:TYR:CD1	2.84	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:HG3	1:D:316:ARG:HH11	1.77	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:C:107:GLU:CD	1:C:115:ARG:HH11	2.15	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: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: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:279:GLU:O	1:B:316:ARG:HG3	2.14	0.48
1:B:79:ARG:NH2	3:B:1039:HOH:O	2.46	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:A:22:MET:HE3	3:A:1009:HOH:O	2.12	0.48
1:B:303:VAL:HG22	1:C:212:PHE:CE1	2.48	0.48
1:C:246:THR:HG21	3:C:1074:HOH:O	2.13	0.48
1:C:62:HIS:HE1	3:C:1014:HOH:O	1.95	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: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: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:D:113:LEU:O	1:D:114:ASP:C	2.53	0.47
1:A:243:LYS:HD2	1:B:62:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:218:ARG:O	1:B:219:ALA:C	2.51	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:B:287:LEU:C	1:B:287:LEU:HD12	2.36	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:A:211:GLU:O	1:A:212:PHE:C	2.55	0.45
1:D:153:SER:OG	1:D:155:LEU:CB	2.65	0.45
1:B:290:PRO:HG2	1:B:305:PRO:HD3	1.99	0.44
1:B:194:GLU:HB2	1:B:322:LEU:HD11	1.99	0.44
1:C:203:TRP:HZ3	1:C:220:LEU:HD13	1.82	0.44
1:D:287:LEU:HD12	1:D:287:LEU:C	2.36	0.44
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: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:D:98:ALA:O	1:D:99:GLY:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:TYR:CZ	1:D:126:ARG:HD3	2.53	0.43
1:D:316:ARG:HD2	1:D:316:ARG:C	2.39	0.43
1:D:171:ARG:HD2	1:D:171:ARG:HA	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: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:158:GLY:HA2	1:A:298:VAL:CG2	2.49	0.43
1:B:56:ARG:CG	1:B:56:ARG:HH11	2.32	0.43
1:C:214:GLU:C	1:C:216:ARG:H	2.22	0.43
1:B:185:GLN:CG	3:C:1079:HOH:O	2.52	0.43
1:B:213:ALA:HB2	1:B:220:LEU:HD23	2.00	0.42
1:B:203:TRP:CE2	1:B:225:ARG:HG3	2.54	0.42
1:B:192:LEU:CD2	1:B:290:PRO:HD3	2.49	0.42
1:D:291:ARG:NH1	3:D:1094:HOH:O	2.48	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
2:B:1332:MES:C2	3:B:1092:HOH:O	2.67	0.42
1:B:275:THR:HA	1:B:276:PRO:HD3	1.83	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:D:100:VAL:HG12	1:D:116:ASN:OD1	2.18	0.42
1:D:209(C):VAL:CG1	1:D:209(D):PRO:HD2	2.49	0.42
1:B:210(B):LEU:HA	1:B:210(B):LEU:HD12	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: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:D:58:LEU:HD11	1:D:62:HIS:CE1	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	308/310 (99%)	295 (96%)	12 (4%)	1 (0%)	41	46
1	B	299/310 (96%)	287 (96%)	12 (4%)	0	100	100
1	C	308/310 (99%)	296 (96%)	11 (4%)	1 (0%)	41	46
1	D	299/310 (96%)	285 (95%)	13 (4%)	1 (0%)	41	46
All	All	1214/1240 (98%)	1163 (96%)	48 (4%)	3 (0%)	47	55

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%)	220 (97%)	6 (3%)	44	57
1	B	221/232 (95%)	202 (91%)	19 (9%)	10	10
1	C	230/232 (99%)	220 (96%)	10 (4%)	29	36
1	D	225/232 (97%)	214 (95%)	11 (5%)	25	31
All	All	902/928 (97%)	856 (95%)	46 (5%)	24	29

All (46) 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	186	SER
1	A	287	LEU
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	151	ARG
1	B	185	GLN
1	B	198	SER
1	B	210(B)	LEU
1	B	221	SER
1	B	234	ARG

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Mol	Chain	Res	Type
1	B	257	LEU
1	B	275	THR
1	B	310	GLU
1	B	317	ARG
1	B	318	SER
1	B	329	LEU
1	C	47	ARG
1	C	54	LEU
1	C	56	ARG
1	C	128	LEU
1	C	178	GLU
1	C	223	GLU
1	C	230	GLU
1	C	275	THR
1	C	278	VAL
1	C	287	LEU
1	D	47	ARG
1	D	54	LEU
1	D	56	ARG
1	D	57	LYS
1	D	67	LEU
1	D	111	GLN
1	D	122	GLN
1	D	153	SER
1	D	210(B)	LEU
1	D	216	ARG
1	D	287	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) 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	A	207	GLN
1	B	185	GLN
1	B	207	GLN
1	C	60	GLN
1	C	62	HIS
1	C	68	HIS

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Mol	Chain	Res	Type
1	C	74	HIS
1	C	116	ASN
1	C	195	HIS
1	C	207	GLN
1	D	60	GLN
1	D	62	HIS
1	D	68	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	C	1332	-	12,12,12	1.97	1 (8%)	14,16,16	3.74	9 (64%)
2	MES	D	1332	-	12,12,12	1.62	1 (8%)	14,16,16	1.43	3 (21%)
2	MES	B	1332	-	12,12,12	1.48	1 (8%)	14,16,16	0.83	0

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	C	1332	-	-	4/6/14/14	0/1/1/1
2	MES	D	1332	-	-	5/6/14/14	0/1/1/1
2	MES	B	1332	-	-	0/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1332	MES	C8-S	-6.39	1.68	1.77
2	D	1332	MES	C8-S	4.74	1.84	1.77
2	B	1332	MES	C8-S	4.08	1.83	1.77

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1332	MES	O1S-S-C8	7.79	116.30	106.92
2	C	1332	MES	O3S-S-O1S	-5.62	97.54	111.27
2	C	1332	MES	O3S-S-C8	4.67	113.32	105.77
2	C	1332	MES	C5-N4-C3	4.40	118.74	108.83
2	C	1332	MES	C7-N4-C5	4.10	121.72	111.23
2	C	1332	MES	C2-C3-N4	3.57	115.52	110.10
2	C	1332	MES	C7-N4-C3	3.21	119.43	111.23
2	C	1332	MES	C6-C5-N4	-3.17	105.29	110.10
2	D	1332	MES	O1S-S-C8	2.82	110.31	106.92
2	D	1332	MES	O2S-S-C8	2.81	110.30	106.92
2	C	1332	MES	O1-C2-C3	2.69	117.71	111.80
2	D	1332	MES	O3S-S-C8	2.03	109.05	105.77

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	D	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

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Mol	Chain	Res	Type	Atoms
2	D	1332	MES	C7-C8-S-O2S

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 [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	310/310 (100%)	-0.32	1 (0%) 94 93	13, 24, 49, 71	6 (1%)
1	B	303/310 (97%)	-0.15	8 (2%) 56 53	13, 27, 53, 69	1 (0%)
1	C	310/310 (100%)	-0.08	11 (3%) 44 42	18, 33, 55, 76	4 (1%)
1	D	303/310 (97%)	-0.07	14 (4%) 32 31	19, 32, 62, 72	4 (1%)
All	All	1226/1240 (98%)	-0.16	34 (2%) 53 51	13, 30, 54, 76	15 (1%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	329	LEU	5.1
1	C	217	GLY	5.0
1	C	218	ARG	4.5
1	D	114	ASP	4.0
1	C	99	GLY	3.9
1	A	219	ALA	3.9
1	C	237	TYR	3.8
1	D	327	PHE	3.8
1	D	113	LEU	3.4
1	B	110	LEU	3.3
1	C	222	PRO	3.3
1	C	219	ALA	3.1
1	D	115	ARG	3.0
1	D	112	LEU	2.9
1	B	112	LEU	2.7
1	B	220	LEU	2.7
1	C	101	ALA	2.6
1	B	179	TYR	2.6
1	D	111	GLN	2.5
1	D	330	GLY	2.4
1	B	329	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	324	GLU	2.3
1	C	100	VAL	2.3
1	C	241	GLU	2.2
1	D	282	LEU	2.2
1	D	118	GLN	2.2
1	B	224	ASP	2.2
1	C	106	GLY	2.2
1	D	218	ARG	2.1
1	C	179	TYR	2.1
1	D	215	ALA	2.1
1	D	102	GLN	2.1
1	B	217	GLY	2.1
1	B	317	ARG	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](#)

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(\AA^2)	Q<0.9
2	MES	C	1332	12/12	0.86	0.21	66,67,69,69	0
2	MES	B	1332	12/12	0.86	0.17	69,70,73,74	0
2	MES	D	1332	12/12	0.90	0.16	61,62,65,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.