



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:06 PM UTC

PDB ID : 4AJ1 / pdb_00004aj1
Title : rat LDHA in complex with N-(2-(methylamino)-1,3-benzothiazol-6-yl) acetamide
Authors : Tucker, J.A.; Brassington, C.; Hassall, G.; Vogtherr, M.; Ward, R.; Tart, J.; Davies, G.
Deposited on : 2012-02-15
Resolution : 1.87 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

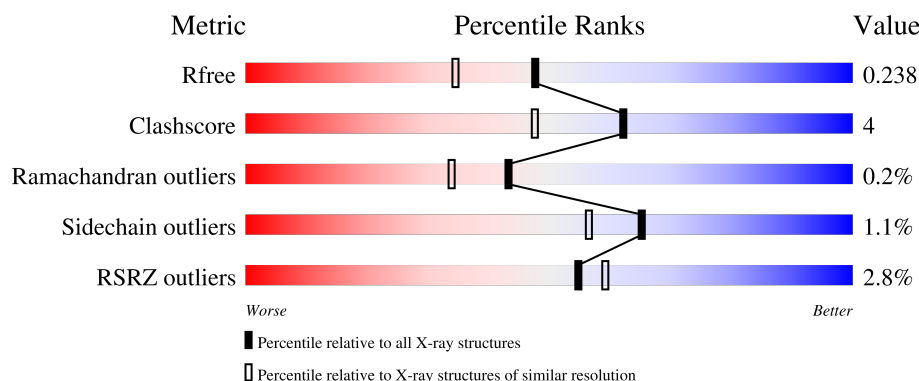
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	331	5% 89% 9% ..
1	B	331	2% 89% 10%
1	C	331	2% 91% 9%
1	D	331	2% 90% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MLI	A	1334	-	X	-	-

2 Entry composition [i](#)

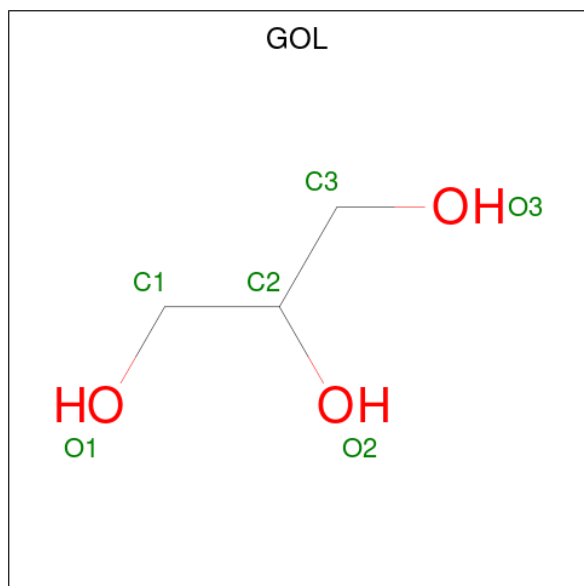
There are 6 unique types of molecules in this entry. The entry contains 11431 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 A CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	4	1
			2520	1609	428	470	13			
1	B	330	Total	C	N	O	S	0	6	0
			2559	1635	432	479	13			
1	C	330	Total	C	N	O	S	0	9	0
			2607	1665	438	491	13			
1	D	330	Total	C	N	O	S	0	8	0
			2574	1643	434	484	13			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



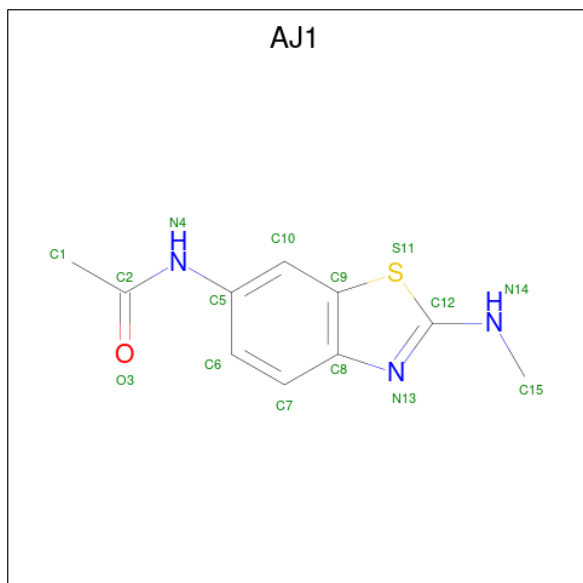
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

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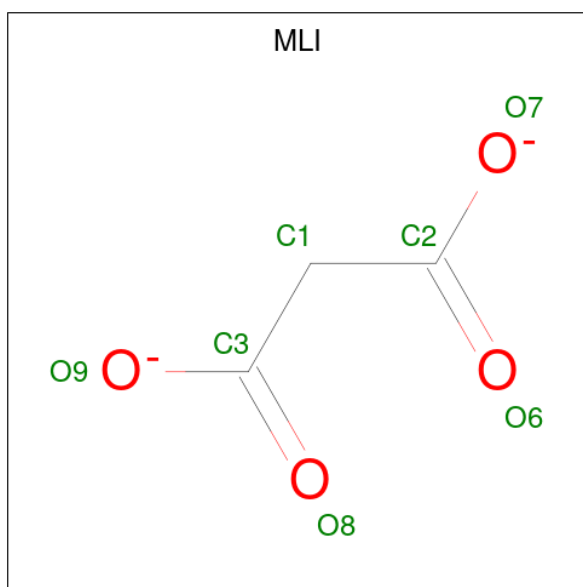
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is N-(2-METHYLAMINO)-1,3-BENZOTHIAZOL-6-YL)ACETAMIDE (CCD ID: AJ1) (formula: C₁₀H₁₁N₃OS).



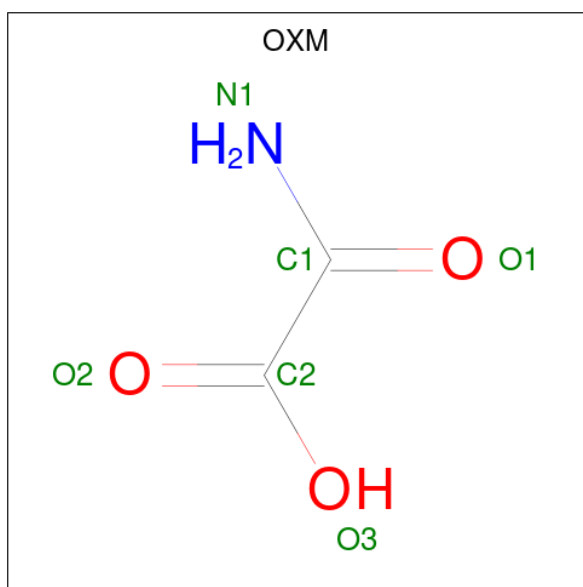
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	10	3	1	1		
3	B	1	Total	C	N	O	S	0	0
			15	10	3	1	1		
3	C	1	Total	C	N	O	S	0	0
			15	10	3	1	1		
3	D	1	Total	C	N	O	S	0	0
			15	10	3	1	1		

- Molecule 4 is MALONATE ION (CCD ID: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	3	4		
4	A	1	Total	C	O	0	0
			7	3	4		
4	B	1	Total	C	O	0	0
			7	3	4		
4	B	1	Total	C	O	0	0
			7	3	4		
4	C	1	Total	C	O	0	0
			7	3	4		
4	C	1	Total	C	O	0	0
			7	3	4		
4	D	1	Total	C	O	0	0
			7	3	4		
4	D	1	Total	C	O	0	0
			7	3	4		

- Molecule 5 is OXAMIC ACID (CCD ID: OXM) (formula: $C_2H_3NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			6	2	1	3		

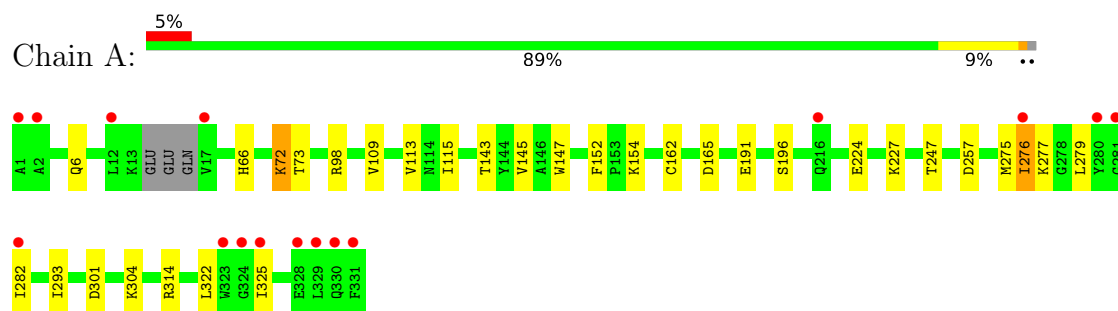
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	296	Total	O	0	0
			296	296		
6	B	277	Total	O	0	0
			277	277		
6	C	253	Total	O	0	0
			253	253		
6	D	199	Total	O	0	0
			199	199		

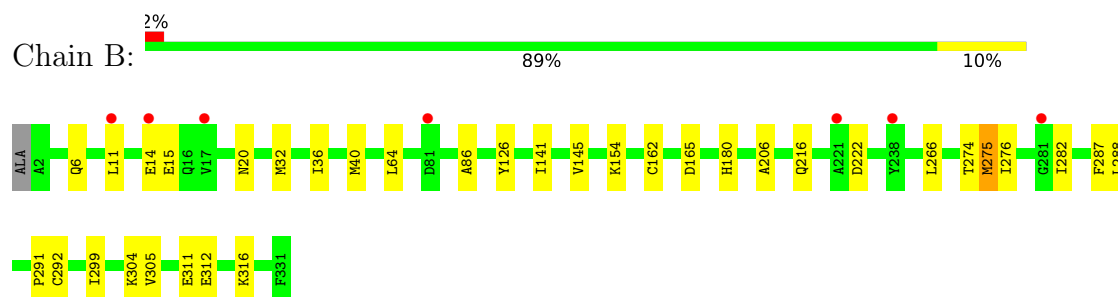
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

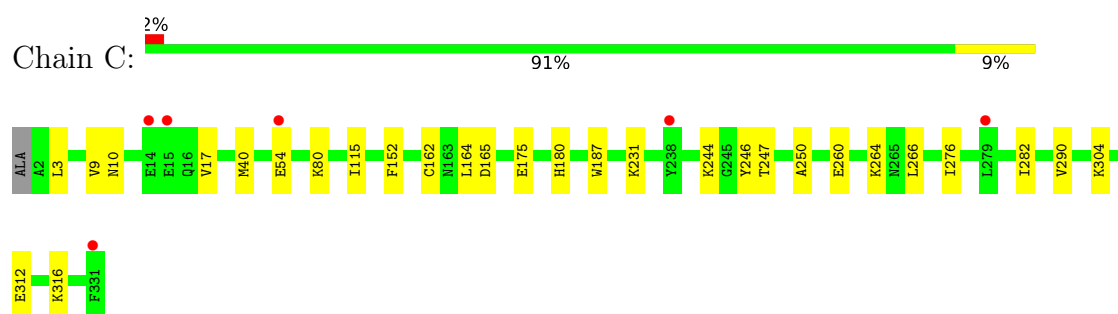
• Molecule 1: L-LACTATE DEHYDROGENASE A CHAIN



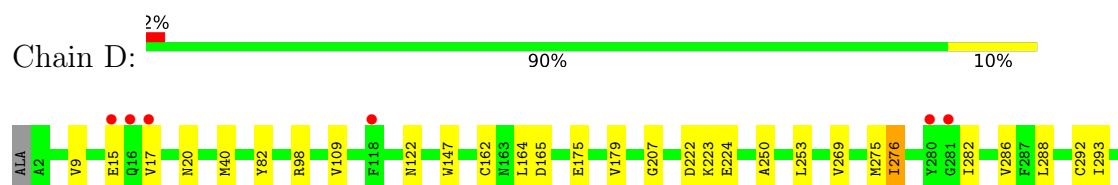
• Molecule 1: L-LACTATE DEHYDROGENASE A CHAIN



• Molecule 1: L-LACTATE DEHYDROGENASE A CHAIN



• Molecule 1: L-LACTATE DEHYDROGENASE A CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.24Å 81.91Å 128.87Å 90.00° 96.18° 90.00°	Depositor
Resolution (Å)	49.37 – 1.87 49.37 – 1.87	Depositor EDS
% Data completeness (in resolution range)	73.3 (49.37-1.87) 73.3 (49.37-1.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.173 , 0.231 0.181 , 0.238	Depositor DCC
R_{free} test set	3860 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11431	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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: AJ1, GOL, OXM, MLI

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	0.93	1/2562 (0.0%)	0.98	6/3474 (0.2%)
1	B	0.94	0/2602	0.95	0/3530
1	C	0.89	0/2652	0.93	3/3596 (0.1%)
1	D	0.88	0/2617	0.91	1/3551 (0.0%)
All	All	0.91	1/10433 (0.0%)	0.94	10/14151 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	HIS	CG-CD2	5.61	1.42	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	109	VAL	N-CA-C	7.43	117.56	110.42
1	C	290	VAL	N-CA-C	-6.28	101.92	109.01
1	A	152	PHE	CA-C-N	-5.71	113.90	119.78
1	A	152	PHE	C-N-CA	-5.71	113.90	119.78
1	A	109	VAL	N-CA-C	5.64	115.83	110.42
1	A	73	THR	CA-C-N	5.62	125.72	119.87
1	A	73	THR	C-N-CA	5.62	125.72	119.87
1	C	152	PHE	CA-C-N	-5.31	114.78	120.03
1	C	152	PHE	C-N-CA	-5.31	114.78	120.03
1	A	143	THR	N-CA-C	-5.09	105.65	111.14

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	2520	0	2552	24	0
1	B	2559	0	2601	23	0
1	C	2607	0	2640	22	0
1	D	2574	0	2611	29	0
2	A	6	0	8	3	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	1	0
3	A	15	0	11	1	0
3	B	15	0	11	0	0
3	C	15	0	11	1	0
3	D	15	0	11	0	0
4	A	14	0	4	0	0
4	B	14	0	4	0	0
4	C	14	0	4	0	0
4	D	14	0	4	0	0
5	D	6	0	2	1	0
6	A	296	0	0	7	0
6	B	277	0	0	3	1
6	C	253	0	0	2	1
6	D	199	0	0	1	0
All	All	11431	0	10498	85	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 4.

All (85) 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:C:276:ILE:HD13	1:C:282:ILE:HD13	1.58	0.83
1:D:276:ILE:HD13	1:D:282:ILE:HD12	1.69	0.74
1:B:11:LEU:HD11	1:D:302:VAL:HG23	1.71	0.72
1:A:276:ILE:HD13	1:A:282:ILE:HG21	1.72	0.70
1:D:98:ARG:NH1	6:D:2024:HOH:O	2.19	0.70
1:A:257:ASP:OD2	6:A:2191:HOH:O	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ILE:HD12	1:D:301:ASP:HB2	1.76	0.67
1:A:115:ILE:HG12	3:A:1333:AJ1:H153	1.78	0.65
1:B:276:ILE:HD13	1:B:282:ILE:HD13	1.78	0.65
1:A:154:LYS:NZ	6:A:2185:HOH:O	2.31	0.64
1:A:191:GLU:HG3	1:A:322:LEU:HD21	1.80	0.63
1:D:276:ILE:HD13	1:D:282:ILE:CD1	2.29	0.62
1:A:72:LYS:HG2	2:A:1332:GOL:H31	1.81	0.61
1:A:98:ARG:NH1	6:A:2027:HOH:O	2.33	0.60
1:A:196:SER:O	1:A:314[B]:ARG:NH2	2.33	0.60
1:D:17[B]:VAL:HG13	1:D:17[B]:VAL:O	2.01	0.59
1:A:147:TRP:CH2	1:A:275:MET:HE1	2.37	0.59
1:C:54[B]:GLU:H	1:C:54[B]:GLU:CD	2.10	0.58
1:B:288:LEU:HD12	1:B:288:LEU:C	2.28	0.57
1:A:276:ILE:CD1	1:A:282:ILE:HG21	2.35	0.57
1:B:6:GLN:O	1:D:304:LYS:HE3	2.06	0.55
1:D:276:ILE:CD1	1:D:282:ILE:HG21	2.36	0.55
1:A:279:LEU:CB	6:A:2280:HOH:O	2.54	0.53
1:C:162:CYS:HA	1:C:165:ASP:OD1	2.09	0.53
1:A:147:TRP:CH2	1:A:275:MET:CE	2.92	0.52
1:C:260:GLU:HG3	1:C:264[B]:LYS:HE3	1.90	0.52
1:B:20:ASN:ND2	6:B:2020:HOH:O	2.43	0.51
1:D:15:GLU:HG3	1:D:17[B]:VAL:HG12	1.92	0.51
1:C:276:ILE:CD1	1:C:282:ILE:HD13	2.35	0.51
1:A:72:LYS:HZ2	2:A:1332:GOL:H32	1.76	0.51
1:B:162:CYS:HA	1:B:165:ASP:OD1	2.11	0.50
1:B:11:LEU:HD11	1:D:302:VAL:CG2	2.40	0.50
1:B:291:PRO:HG2	1:B:305:VAL:CG2	2.41	0.50
1:B:292:CYS:HB3	1:B:299:ILE:HG23	1.94	0.50
1:B:312:GLU:HG2	1:B:316:LYS:HE3	1.94	0.49
1:A:314[B]:ARG:NH2	6:A:2220:HOH:O	2.44	0.49
1:D:17[B]:VAL:O	1:D:17[B]:VAL:CG1	2.59	0.49
1:D:162:CYS:HA	1:D:165:ASP:OD1	2.13	0.49
1:C:3:LEU:N	1:D:224:GLU:OE2	2.40	0.49
1:A:314[B]:ARG:NH1	6:A:2245:HOH:O	2.24	0.48
1:C:276:ILE:CD1	1:C:282:ILE:HG21	2.44	0.48
1:C:54[B]:GLU:HG3	1:C:80:LYS:HD2	1.95	0.48
1:B:154:LYS:HD3	1:B:275:MET:HE2	1.95	0.48
1:D:276:ILE:HD11	1:D:286:VAL:HB	1.94	0.48
1:A:6:GLN:O	1:C:304:LYS:HE3	2.15	0.47
1:C:115:ILE:HG12	3:C:1333:AJ1:H153	1.96	0.47
1:B:266:LEU:O	1:C:180:HIS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:HIS:HB2	1:C:266:LEU:O	2.15	0.46
1:A:72:LYS:HG2	2:A:1332:GOL:C3	2.45	0.46
1:D:40[A]:MET:HE2	1:D:40[A]:MET:HB3	1.88	0.45
6:B:2019:HOH:O	1:D:20:ASN:ND2	2.49	0.45
1:C:312:GLU:HG2	1:C:316:LYS:HE3	1.98	0.45
1:D:288:LEU:C	1:D:288:LEU:HD12	2.41	0.45
1:A:301:ASP:OD2	1:C:10:ASN:HA	2.16	0.44
1:C:276:ILE:HD13	1:C:282:ILE:CD1	2.39	0.44
1:D:164:LEU:HD11	1:D:250:ALA:HB1	1.98	0.44
1:A:162:CYS:HA	1:A:165:ASP:OD1	2.18	0.44
1:B:216:GLN:O	1:B:222:ASP:HB2	2.17	0.44
1:D:82:TYR:CG	1:D:122:ASN:HB3	2.53	0.44
1:D:269:VAL:HA	1:D:292:CYS:O	2.17	0.44
1:B:32:MET:HE1	1:B:64:LEU:HD11	2.00	0.43
1:B:276:ILE:CD1	1:B:282:ILE:HG21	2.46	0.43
1:A:314[B]:ARG:HE	1:A:314[B]:ARG:HB3	1.24	0.43
1:B:141:ILE:O	1:B:145:VAL:HG23	2.19	0.43
1:B:311:GLU:OE2	6:B:2260:HOH:O	2.21	0.43
1:D:276:ILE:HD13	1:D:282:ILE:HG21	2.00	0.43
1:A:227:LYS:HB2	6:A:2237:HOH:O	2.18	0.43
1:C:231:LYS:NZ	6:C:2204:HOH:O	2.51	0.43
1:B:36:ILE:O	1:B:40[B]:MET:HG2	2.19	0.42
1:D:293:ILE:HD12	1:D:301:ASP:CB	2.44	0.42
1:D:222:ASP:O	1:D:223:LYS:C	2.63	0.42
1:A:304:LYS:HG3	1:C:9:VAL:HG23	2.02	0.42
1:C:40[B]:MET:SD	1:D:253:LEU:HD21	2.60	0.42
1:B:304:LYS:HD3	1:D:9:VAL:CG2	2.50	0.42
1:A:113:VAL:HG22	1:A:145:VAL:HG21	2.01	0.41
1:B:86:ALA:HA	1:B:126:TYR:HB3	2.01	0.41
1:B:274:THR:O	1:B:287:PHE:HA	2.20	0.41
1:D:207:GLY:O	5:D:1332:OXM:N1	2.54	0.41
1:A:293:ILE:HD13	1:D:179:VAL:HG22	2.03	0.41
1:D:40[B]:MET:CE	2:D:1333:GOL:H12	2.51	0.41
1:D:147:TRP:CH2	1:D:275:MET:CE	3.04	0.41
1:C:164:LEU:HD11	1:C:250:ALA:HB1	2.04	0.40
1:C:175[B]:GLU:HG2	6:C:2163:HOH:O	2.21	0.40
1:B:206:ALA:HA	1:C:187:TRP:CZ2	2.56	0.40
1:C:244:LYS:HE2	1:C:246:TYR:O	2.21	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)
6:B:2145:HOH:O	6:C:2134:HOH:O[1_455]	2.15	0.05

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	328/331 (99%)	317 (97%)	11 (3%)	0	100	100
1	B	334/331 (101%)	325 (97%)	7 (2%)	2 (1%)	21	10
1	C	338/331 (102%)	328 (97%)	10 (3%)	0	100	100
1	D	336/331 (102%)	324 (96%)	12 (4%)	0	100	100
All	All	1336/1324 (101%)	1294 (97%)	40 (3%)	2 (0%)	43	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	GLU
1	B	14	GLU

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	275/286 (96%)	269 (98%)	6 (2%)	45	30
1	B	282/286 (99%)	281 (100%)	1 (0%)	84	79
1	C	288/286 (101%)	286 (99%)	2 (1%)	76	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	284/286 (99%)	279 (98%)	5 (2%)	51 38
All	All	1129/1144 (99%)	1115 (99%)	14 (1%)	65 53

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LYS
1	A	224	GLU
1	A	247	THR
1	A	276	ILE
1	A	277	LYS
1	A	325	ILE
1	B	275	MET
1	C	17	VAL
1	C	247	THR
1	D	175[A]	GLU
1	D	175[B]	GLU
1	D	276	ILE
1	D	316[A]	LYS
1	D	316[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	B	10	ASN
1	B	20	ASN
1	C	10	ASN
1	C	20	ASN
1	D	10	ASN
1	D	20	ASN
1	D	232	GLN

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](#)

17 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$
4	MLI	D	1335	-	6,6,6	1.35	0	7,7,7	2.00	3 (42%)
4	MLI	B	1335	-	6,6,6	1.06	0	7,7,7	2.28	4 (57%)
2	GOL	A	1332	-	5,5,5	0.52	0	5,5,5	0.92	0
4	MLI	C	1335	-	6,6,6	1.00	0	7,7,7	1.99	2 (28%)
4	MLI	B	1334	-	6,6,6	1.35	0	7,7,7	1.85	1 (14%)
4	MLI	A	1335	-	6,6,6	1.19	0	7,7,7	1.68	2 (28%)
4	MLI	A	1334	-	6,6,6	1.47	0	7,7,7	1.79	4 (57%)
4	MLI	C	1334	-	6,6,6	1.83	1 (16%)	7,7,7	1.43	1 (14%)
5	OXM	D	1332	-	5,5,5	3.15	1 (20%)	2,6,6	1.19	0
2	GOL	D	1333	-	5,5,5	0.39	0	5,5,5	0.76	0
2	GOL	B	1332	-	5,5,5	0.57	0	5,5,5	0.67	0
4	MLI	D	1336	-	6,6,6	1.21	0	7,7,7	1.71	3 (42%)
3	AJ1	D	1334	-	16,16,16	0.51	0	22,22,22	0.61	0
3	AJ1	B	1333	-	16,16,16	0.46	0	22,22,22	0.55	0
2	GOL	C	1332	-	5,5,5	0.47	0	5,5,5	0.61	0
3	AJ1	C	1333	-	16,16,16	0.59	0	22,22,22	0.66	0
3	AJ1	A	1333	-	16,16,16	0.69	0	22,22,22	0.59	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
4	MLI	D	1335	-	-	2/4/4/4	-
4	MLI	B	1335	-	-	2/4/4/4	-
2	GOL	A	1332	-	-	4/4/4/4	-
4	MLI	C	1335	-	-	2/4/4/4	-
4	MLI	B	1334	-	-	2/4/4/4	-
4	MLI	A	1335	-	-	2/4/4/4	-
4	MLI	A	1334	-	-	4/4/4/4	-
4	MLI	C	1334	-	-	2/4/4/4	-
5	OXM	D	1332	-	-	4/4/4/4	-
2	GOL	D	1333	-	-	2/4/4/4	-
2	GOL	B	1332	-	-	4/4/4/4	-
4	MLI	D	1336	-	-	3/4/4/4	-
3	AJ1	D	1334	-	-	2/6/6/6	0/2/2/2
3	AJ1	B	1333	-	-	0/6/6/6	0/2/2/2
2	GOL	C	1332	-	-	4/4/4/4	-
3	AJ1	C	1333	-	-	2/6/6/6	0/2/2/2
3	AJ1	A	1333	-	-	4/6/6/6	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1332	OXM	C1-C2	-6.83	1.47	1.55
4	C	1334	MLI	C1-C3	2.32	1.54	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1335	MLI	O8-C3-C1	-3.40	112.43	122.11
4	B	1335	MLI	O8-C3-C1	-3.33	112.64	122.11
4	B	1334	MLI	O8-C3-C1	-3.01	113.53	122.11
4	C	1335	MLI	O7-C2-O6	2.97	130.97	123.33
4	B	1335	MLI	O6-C2-C1	-2.85	113.99	122.11
4	C	1335	MLI	O8-C3-C1	-2.76	114.26	122.11
4	D	1336	MLI	O7-C2-O6	2.67	130.21	123.33
4	B	1335	MLI	O9-C3-O8	2.59	130.00	123.33
4	A	1335	MLI	O6-C2-C1	-2.56	114.81	122.11
4	A	1335	MLI	O7-C2-O6	2.49	129.74	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1335	MLI	O9-C3-O8	2.46	129.67	123.33
4	C	1334	MLI	C3-C1-C2	-2.45	104.30	112.95
4	A	1334	MLI	O9-C3-O8	2.45	129.63	123.33
4	D	1336	MLI	O8-C3-C1	-2.41	115.23	122.11
4	A	1334	MLI	O8-C3-C1	-2.34	115.44	122.11
4	B	1335	MLI	C3-C1-C2	-2.29	104.88	112.95
4	A	1334	MLI	O6-C2-C1	-2.14	116.03	122.11
4	D	1335	MLI	O7-C2-O6	2.12	128.79	123.33
4	A	1334	MLI	O7-C2-O6	2.11	128.76	123.33
4	D	1336	MLI	O9-C3-O8	2.04	128.58	123.33

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1332	GOL	O1-C1-C2-C3
2	B	1332	GOL	O1-C1-C2-O2
2	B	1332	GOL	O1-C1-C2-C3
2	B	1332	GOL	C1-C2-C3-O3
2	C	1332	GOL	O1-C1-C2-C3
2	D	1333	GOL	C1-C2-C3-O3
3	D	1334	AJ1	S11-C12-N14-C15
3	D	1334	AJ1	N13-C12-N14-C15
5	D	1332	OXM	N1-C1-C2-O2
5	D	1332	OXM	N1-C1-C2-O3
5	D	1332	OXM	O1-C1-C2-O2
5	D	1332	OXM	O1-C1-C2-O3
2	C	1332	GOL	O2-C2-C3-O3
2	A	1332	GOL	C1-C2-C3-O3
2	C	1332	GOL	C1-C2-C3-O3
2	A	1332	GOL	O1-C1-C2-O2
2	D	1333	GOL	O2-C2-C3-O3
2	A	1332	GOL	O2-C2-C3-O3
2	B	1332	GOL	O2-C2-C3-O3
2	C	1332	GOL	O1-C1-C2-O2
3	A	1333	AJ1	C1-C2-N4-C5
3	C	1333	AJ1	C6-C5-N4-C2
3	C	1333	AJ1	C10-C5-N4-C2
4	B	1335	MLI	C3-C1-C2-O7
3	A	1333	AJ1	O3-C2-N4-C5
4	A	1335	MLI	C3-C1-C2-O7
4	C	1335	MLI	C3-C1-C2-O7

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Mol	Chain	Res	Type	Atoms
4	A	1334	MLI	C2-C1-C3-O8
4	A	1334	MLI	C2-C1-C3-O9
4	A	1335	MLI	C3-C1-C2-O6
4	C	1335	MLI	C3-C1-C2-O6
4	D	1336	MLI	C3-C1-C2-O7
4	B	1335	MLI	C3-C1-C2-O6
4	C	1334	MLI	C3-C1-C2-O6
4	C	1334	MLI	C3-C1-C2-O7
4	D	1335	MLI	C2-C1-C3-O9
3	A	1333	AJ1	C6-C5-N4-C2
4	D	1335	MLI	C2-C1-C3-O8
4	D	1336	MLI	C3-C1-C2-O6
4	B	1334	MLI	C3-C1-C2-O7
4	A	1334	MLI	C3-C1-C2-O7
4	D	1336	MLI	C2-C1-C3-O9
3	A	1333	AJ1	C10-C5-N4-C2
4	A	1334	MLI	C3-C1-C2-O6
4	B	1334	MLI	C3-C1-C2-O6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1332	GOL	3	0
5	D	1332	OXM	1	0
2	D	1333	GOL	1	0
3	C	1333	AJ1	1	0
3	A	1333	AJ1	1	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	328/331 (99%)	0.08	16 (4%) 35 37	10, 24, 47, 76	4 (1%)
1	B	330/331 (99%)	-0.14	7 (2%) 63 70	10, 21, 39, 65	6 (1%)
1	C	330/331 (99%)	-0.05	6 (1%) 67 73	9, 23, 39, 64	9 (2%)
1	D	330/331 (99%)	0.18	8 (2%) 59 66	10, 27, 49, 63	8 (2%)
All	All	1318/1324 (99%)	0.02	37 (2%) 55 59	9, 24, 45, 76	27 (2%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	238[A]	TYR	6.0
1	D	331	PHE	4.9
1	A	329	LEU	4.7
1	A	331	PHE	4.4
1	A	1	ALA	3.7
1	B	281	GLY	3.5
1	C	54[A]	GLU	3.4
1	A	324	GLY	3.3
1	A	280	TYR	3.3
1	D	15	GLU	3.2
1	A	323	TRP	3.2
1	D	118	PHE	3.1
1	A	325	ILE	3.0
1	C	331	PHE	2.9
1	B	11	LEU	2.9
1	A	330	GLN	2.8
1	B	17	VAL	2.8
1	A	328	GLU	2.8
1	A	17	VAL	2.7
1	A	282	ILE	2.7
1	D	16	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	15	GLU	2.6
1	D	281	GLY	2.4
1	A	276	ILE	2.4
1	A	12	LEU	2.3
1	D	280	TYR	2.3
1	A	216	GLN	2.3
1	D	330	GLN	2.3
1	C	279	LEU	2.3
1	B	238	TYR	2.2
1	D	17[A]	VAL	2.2
1	C	14	GLU	2.2
1	A	2	ALA	2.2
1	B	81	ASP	2.2
1	B	14	GLU	2.1
1	B	221	ALA	2.1
1	A	281	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	GOL	B	1332	6/6	0.72	0.16	39,42,42,44	0
2	GOL	A	1332	6/6	0.77	0.14	33,37,41,47	0
3	AJ1	C	1333	15/15	0.78	0.15	34,47,54,55	0
3	AJ1	A	1333	15/15	0.81	0.14	29,40,43,43	0
2	GOL	C	1332	6/6	0.81	0.13	43,44,46,48	0
3	AJ1	D	1334	15/15	0.82	0.13	44,51,55,58	0
5	OXM	D	1332	6/6	0.83	0.12	46,47,52,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	D	1333	6/6	0.87	0.11	32,36,37,39	0
4	MLI	B	1335	7/7	0.94	0.06	23,24,25,25	0
4	MLI	B	1334	7/7	0.95	0.06	24,25,26,28	0
3	AJ1	B	1333	15/15	0.95	0.07	26,29,31,32	0
4	MLI	C	1334	7/7	0.95	0.06	23,25,27,29	0
4	MLI	D	1335	7/7	0.95	0.07	27,29,31,31	0
4	MLI	D	1336	7/7	0.95	0.06	25,25,27,28	0
4	MLI	A	1335	7/7	0.95	0.06	26,29,32,32	0
4	MLI	C	1335	7/7	0.96	0.07	21,23,27,27	0
4	MLI	A	1334	7/7	0.96	0.07	24,27,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.