Full wwPDB X-ray Structure Validation Report (i)

Apr 21, 2024 – 04:28 am BST

PDB ID	:	4AJ1
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 (i) 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 (i)) were used in the production of this report:

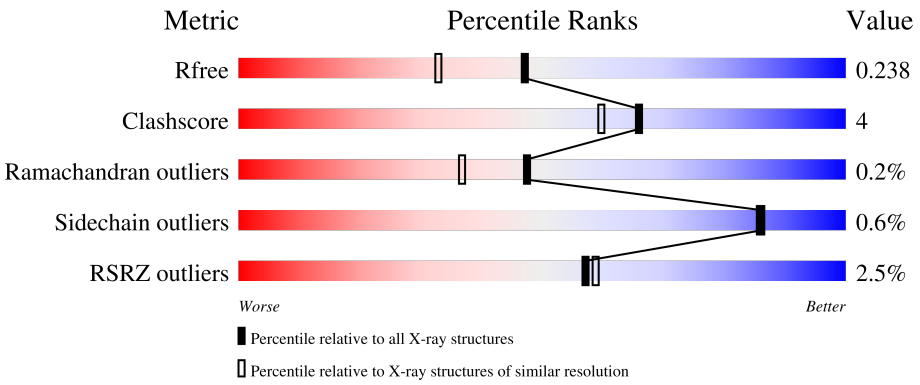
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 <=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	3% 91% 8%
1	B	331	2% 89% 11%
1	C	331	2% 91% 9%
1	D	331	3% 91% 9%

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)

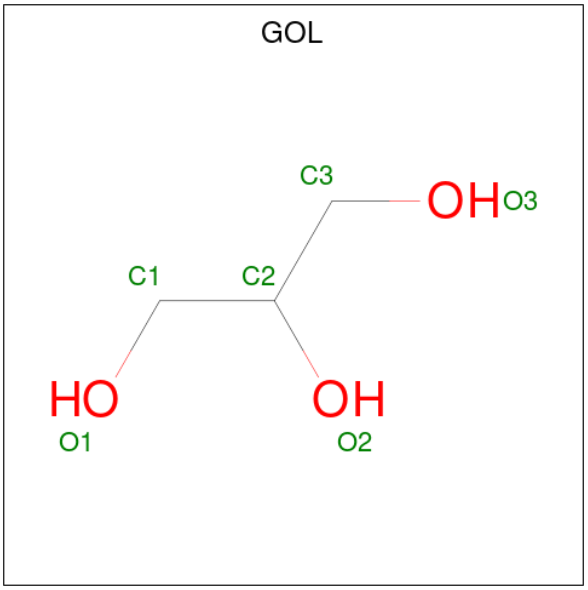
There are 6 unique types of molecules in this entry. The entry contains 11431 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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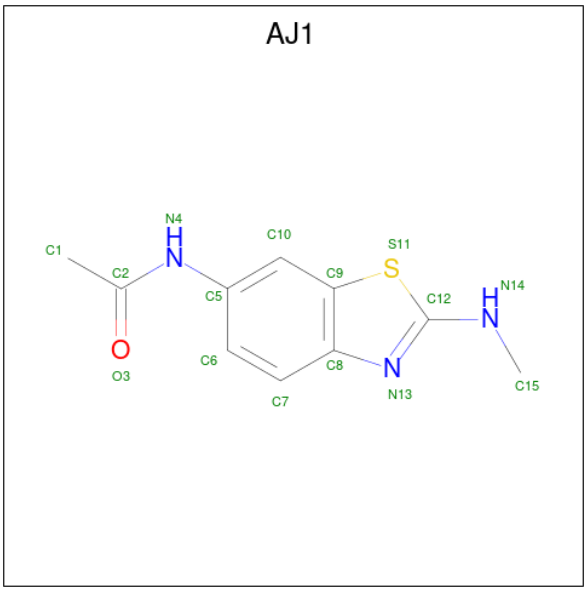
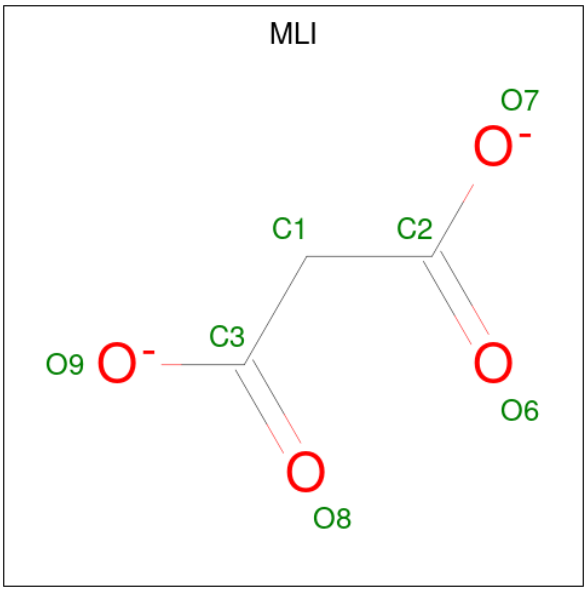
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	C	1	6	3	3		0	0
			Total	C	O			
2	D	1	6	3	3		0	0

- Molecule 3 is N-(2-METHYLAMINO)-1,3-BENZOTHIAZOL-6-YL)ACETAMIDE (three-letter code: AJ1) (formula: $C_{10}H_{11}N_3OS$).



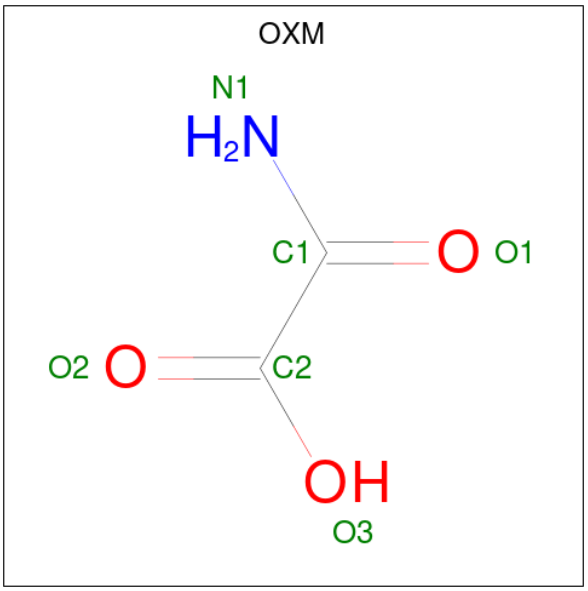
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	15	10	3	1	1	0	0
			Total	C	N	O	S		
3	B	1	15	10	3	1	1	0	0
			Total	C	N	O	S		
3	C	1	15	10	3	1	1	0	0
			Total	C	N	O	S		
3	D	1	15	10	3	1	1	0	0

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



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

- Molecule 5 is OXAMIC ACID (three-letter code: OXM) (formula: $C_2H_3NO_3$).



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

- Molecule 6 is water.

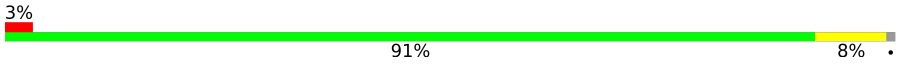
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	296	296	296	0	0
			Total	O		
6	B	277	277	277	0	0
			Total	O		
6	C	253	253	253	0	0
			Total	O		
6	D	199	199	199	0	0

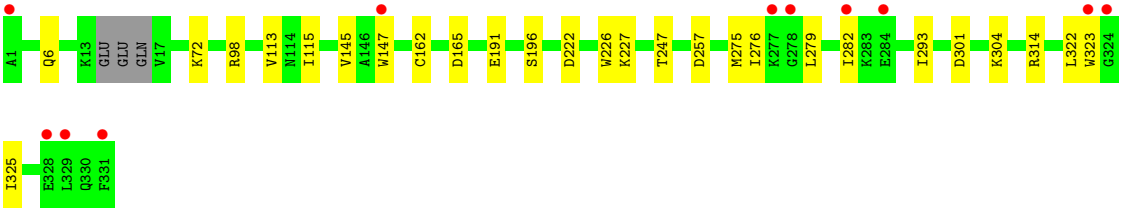
3 Residue-property plots (i)

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

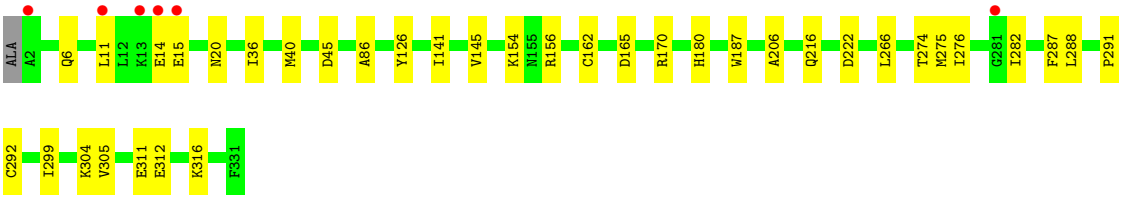
Chain A:





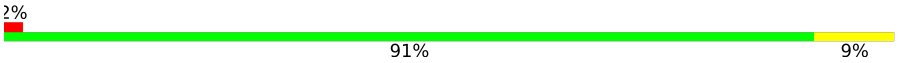
• Molecule 1: L-LACTATE DEHYDROGENASE A CHAIN

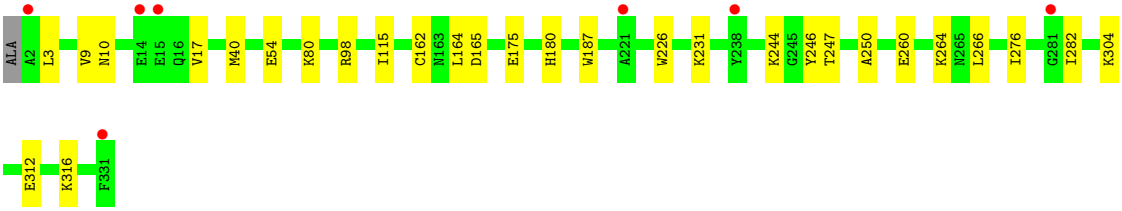
Chain B:



• Molecule 1: L-LACTATE DEHYDROGENASE A CHAIN

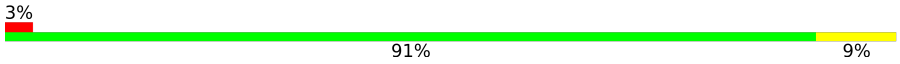
Chain C:

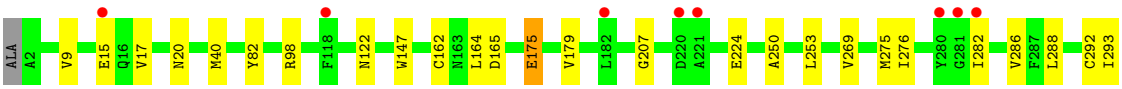


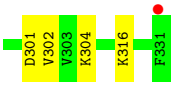


• Molecule 1: L-LACTATE DEHYDROGENASE A CHAIN

Chain D:






D301
V302
V303
K304
K316
F331

4 Data and refinement statistics (i)

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 40.96 – 1.87	Depositor EDS
% Data completeness (in resolution range)	73.3 (49.37-1.87) 73.3 (40.96-1.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (4.95%)	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 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, OXM, MLI, GOL

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	0.69	2/2562 (0.1%)	0.75	1/3474 (0.0%)
1	B	0.70	1/2602 (0.0%)	0.78	5/3530 (0.1%)
1	C	0.67	1/2652 (0.0%)	0.73	0/3596
1	D	0.67	0/2617	0.71	0/3551
All	All	0.68	4/10433 (0.0%)	0.74	6/14151 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	226	TRP	CD2-CE2	5.51	1.48	1.41
1	A	323	TRP	CD2-CE2	5.41	1.47	1.41
1	B	187	TRP	CD2-CE2	5.40	1.47	1.41
1	A	226	TRP	CD2-CE2	5.16	1.47	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	170	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	45	ASP	CB-CG-OD1	6.71	124.34	118.30
1	B	170	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	156	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	156	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	222	ASP	CB-CG-OD1	5.09	122.89	118.30

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	2520	0	2552	23	0
1	B	2559	0	2601	22	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	6	0
6	B	277	0	0	3	1
6	C	253	0	0	2	1
6	D	199	0	0	2	0
All	All	11431	0	10498	83	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 (83) 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:D:175[B]:GLU:OE1	6:D:2133:HOH:O	1.71	1.08
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ASP:OD2	6:A:2191:HOH:O	2.11	0.67
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: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: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:C:54[B]:GLU:H	1:C:54[B]:GLU:CD	2.10	0.55
1:D:276:ILE:CD1	1:D:282:ILE:HG21	2.36	0.55
1:A:147:TRP:CH2	1:A:275:MET:HE1	2.43	0.54
1:A:279:LEU:CB	6:A:2280:HOH:O	2.54	0.53
1:B:288:LEU:HD12	1:B:288:LEU:C	2.28	0.53
1:C:162:CYS:HA	1:C:165:ASP:OD1	2.09	0.53
1:B:154:LYS:HD3	1:B:275:MET:HE2	1.91	0.52
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: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: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:A:72:LYS:HZ2	2:A:1332:GOL:H32	1.79	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
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: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:D:147:TRP:CH2	1:D:275:MET:HE1	2.52	0.44
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: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: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:231:LYS:NZ	6:C:2204:HOH:O	2.51	0.40
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:D:288:LEU:HD12	1:D:288:LEU:C	2.41	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%)	25	14
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%)	47	41

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%)	273 (99%)	2 (1%)	84	83
1	B	282/286 (99%)	282 (100%)	0	100	100
1	C	288/286 (101%)	285 (99%)	3 (1%)	76	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	284/286 (99%)	280 (99%)	4 (1%)	67	62
All	All	1129/1144 (99%)	1120 (99%)	9 (1%)	86	80

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	THR
1	A	325	ILE
1	C	17	VAL
1	C	98	ARG
1	C	247	THR
1	D	175[A]	GLU
1	D	175[B]	GLU
1	D	316[A]	LYS
1	D	316[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	20	ASN
1	D	20	ASN

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 monosaccharides 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	$\#\|Z\| > 2$
5	OXM	D	1332	-	5,5,5	2.92	1 (20%)	4,6,6	1.80	1 (25%)
3	AJ1	C	1333	-	12,16,16	0.79	0	16,22,22	1.20	1 (6%)
4	MLI	B	1334	-	6,6,6	1.33	0	7,7,7	1.83	1 (14%)
4	MLI	D	1336	-	6,6,6	1.18	0	7,7,7	1.73	3 (42%)
3	AJ1	B	1333	-	12,16,16	0.72	0	16,22,22	1.10	1 (6%)
2	GOL	D	1333	-	5,5,5	0.37	0	5,5,5	0.69	0
4	MLI	A	1334	-	6,6,6	1.44	0	7,7,7	1.79	4 (57%)
2	GOL	B	1332	-	5,5,5	0.56	0	5,5,5	0.64	0
4	MLI	A	1335	-	6,6,6	1.16	0	7,7,7	1.68	2 (28%)
3	AJ1	D	1334	-	12,16,16	0.76	0	16,22,22	1.11	1 (6%)
4	MLI	D	1335	-	6,6,6	1.32	0	7,7,7	1.99	3 (42%)
2	GOL	C	1332	-	5,5,5	0.46	0	5,5,5	0.59	0
3	AJ1	A	1333	-	12,16,16	0.84	0	16,22,22	1.18	1 (6%)
4	MLI	C	1334	-	6,6,6	1.80	1 (16%)	7,7,7	1.44	1 (14%)
4	MLI	B	1335	-	6,6,6	1.04	0	7,7,7	2.26	4 (57%)
2	GOL	A	1332	-	5,5,5	0.51	0	5,5,5	0.87	0
4	MLI	C	1335	-	6,6,6	0.97	0	7,7,7	1.99	3 (42%)

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
5	OXM	D	1332	-	-	3/3/4/4	-
3	AJ1	C	1333	-	-	2/4/6/6	0/2/2/2
4	MLI	B	1334	-	-	2/4/4/4	-
4	MLI	D	1336	-	-	3/4/4/4	-
3	AJ1	B	1333	-	-	0/4/6/6	0/2/2/2
2	GOL	D	1333	-	-	2/4/4/4	-
4	MLI	A	1334	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	1332	-	-	4/4/4/4	-
4	MLI	A	1335	-	-	2/4/4/4	-
3	AJ1	D	1334	-	-	0/4/6/6	0/2/2/2
4	MLI	D	1335	-	-	2/4/4/4	-
2	GOL	C	1332	-	-	4/4/4/4	-
3	AJ1	A	1333	-	-	4/4/6/6	0/2/2/2
4	MLI	C	1334	-	-	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	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1332	OXM	C1-C2	-6.32	1.47	1.55
4	C	1334	MLI	C1-C3	2.33	1.54	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1335	MLI	O8-C3-C1	-3.30	112.43	122.08
4	B	1335	MLI	O8-C3-C1	-3.23	112.64	122.08
4	C	1335	MLI	O7-C2-O6	3.08	130.97	123.30
4	B	1334	MLI	O8-C3-C1	-2.92	113.53	122.08
3	A	1333	AJ1	C9-C8-N13	2.87	114.72	108.04
5	D	1332	OXM	O3-C2-C1	2.85	120.42	113.84
3	C	1333	AJ1	C9-C8-N13	2.84	114.66	108.04
4	D	1336	MLI	O7-C2-O6	2.77	130.21	123.30
4	B	1335	MLI	O6-C2-C1	-2.77	113.99	122.08
3	D	1334	AJ1	C9-C8-N13	2.75	114.45	108.04
3	B	1333	AJ1	C9-C8-N13	2.70	114.33	108.04
4	B	1335	MLI	O9-C3-O8	2.69	130.00	123.30
4	C	1335	MLI	O8-C3-C1	-2.67	114.26	122.08
4	A	1335	MLI	O7-C2-O6	2.58	129.74	123.30
4	D	1335	MLI	O9-C3-O8	2.56	129.67	123.30
4	A	1334	MLI	O9-C3-O8	2.54	129.63	123.30
4	A	1335	MLI	O6-C2-C1	-2.49	114.81	122.08
4	C	1334	MLI	C3-C1-C2	-2.44	104.30	112.87
4	D	1336	MLI	O8-C3-C1	-2.34	115.23	122.08
4	B	1335	MLI	C3-C1-C2	-2.28	104.88	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1334	MLI	O8-C3-C1	-2.27	115.44	122.08
4	D	1335	MLI	O7-C2-O6	2.20	128.79	123.30
4	A	1334	MLI	O7-C2-O6	2.19	128.76	123.30
4	D	1336	MLI	O9-C3-O8	2.12	128.58	123.30
4	A	1334	MLI	O6-C2-C1	-2.07	116.03	122.08
4	C	1335	MLI	O9-C3-O8	2.04	128.39	123.30

There are no chirality outliers.

All (42) 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
5	D	1332	OXM	N1-C1-C2-O2
5	D	1332	OXM	N1-C1-C2-O3
5	D	1332	OXM	O1-C1-C2-O2
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
3	A	1333	AJ1	C1-C2-N4-C5
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	C	1333	AJ1	C6-C5-N4-C2
4	B	1335	MLI	C3-C1-C2-O7
3	C	1333	AJ1	C10-C5-N4-C2
3	A	1333	AJ1	O3-C2-N4-C5
4	A	1335	MLI	C3-C1-C2-O7
4	C	1335	MLI	C3-C1-C2-O7
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	B	1335	MLI	C3-C1-C2-O6
4	C	1335	MLI	C3-C1-C2-O6
4	D	1336	MLI	C3-C1-C2-O7
4	C	1334	MLI	C3-C1-C2-O6

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Mol	Chain	Res	Type	Atoms
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	A	1334	MLI	C3-C1-C2-O7
4	B	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
5	D	1332	OXM	1	0
3	C	1333	AJ1	1	0
2	D	1333	GOL	1	0
3	A	1333	AJ1	1	0
2	A	1332	GOL	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.07	11 (3%)	45	46	16, 24, 47, 76	0
1	B	330/331 (99%)	-0.19	6 (1%)	68	70	16, 22, 39, 65	0
1	C	330/331 (99%)	-0.21	7 (2%)	63	65	18, 24, 39, 64	0
1	D	330/331 (99%)	0.10	9 (2%)	54	56	18, 27, 49, 63	0
All	All	1318/1324 (99%)	-0.09	33 (2%)	57	59	16, 24, 45, 76	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	PHE	5.3
1	B	281	GLY	4.7
1	D	331	PHE	4.5
1	B	14	GLU	4.4
1	A	1	ALA	4.2
1	D	118	PHE	4.0
1	C	238[A]	TYR	3.8
1	A	329	LEU	3.7
1	B	11	LEU	3.6
1	B	13	LYS	3.5
1	A	324	GLY	3.3
1	B	15	GLU	3.1
1	A	282	ILE	3.1
1	D	281	GLY	3.1
1	A	328	GLU	3.0
1	A	284	GLU	2.9
1	A	278	GLY	2.7
1	C	331	PHE	2.7
1	C	15	GLU	2.7
1	A	277	LYS	2.6
1	C	281	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	14	GLU	2.4
1	D	221	ALA	2.4
1	D	282	ILE	2.3
1	D	182	LEU	2.3
1	D	15	GLU	2.3
1	D	220	ASP	2.3
1	A	323	TRP	2.2
1	C	221	ALA	2.2
1	C	2	ALA	2.1
1	D	280	TYR	2.1
1	A	147	TRP	2.1
1	B	2	ALA	2.1

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 monosaccharides 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(Å^2)	Q<0.9
3	AJ1	C	1333	15/15	0.83	0.24	34,47,54,55	0
2	GOL	C	1332	6/6	0.84	0.15	43,44,46,48	0
3	AJ1	A	1333	15/15	0.84	0.24	29,40,43,43	0
2	GOL	A	1332	6/6	0.84	0.20	33,37,41,47	0
3	AJ1	D	1334	15/15	0.84	0.26	44,51,55,58	0
2	GOL	B	1332	6/6	0.88	0.15	39,42,42,44	0
5	OXM	D	1332	6/6	0.88	0.12	46,47,52,54	0
2	GOL	D	1333	6/6	0.89	0.20	32,36,37,39	0
4	MLI	A	1335	7/7	0.95	0.15	26,29,32,32	0
3	AJ1	B	1333	15/15	0.96	0.09	26,29,31,32	0
4	MLI	B	1335	7/7	0.97	0.07	23,24,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MLI	C	1334	7/7	0.97	0.07	23,25,27,29	0
4	MLI	D	1335	7/7	0.97	0.07	27,29,31,31	0
4	MLI	A	1334	7/7	0.97	0.08	24,27,31,32	0
4	MLI	B	1334	7/7	0.98	0.08	24,25,26,28	0
4	MLI	D	1336	7/7	0.98	0.13	25,25,27,28	0
4	MLI	C	1335	7/7	0.98	0.06	21,23,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.