



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 03:33 PM EDT

PDB ID : 3FIG  
Title : Crystal Structure of Leucine-bound LeuA from Mycobacterium tuberculosis  
Authors : Koon, N.; Squire, C.J.; Baker, E.N.  
Deposited on : 2008-12-11  
Resolution : 2.30 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](mailto: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.

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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	:	2.23.2
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)	:	2.23.2

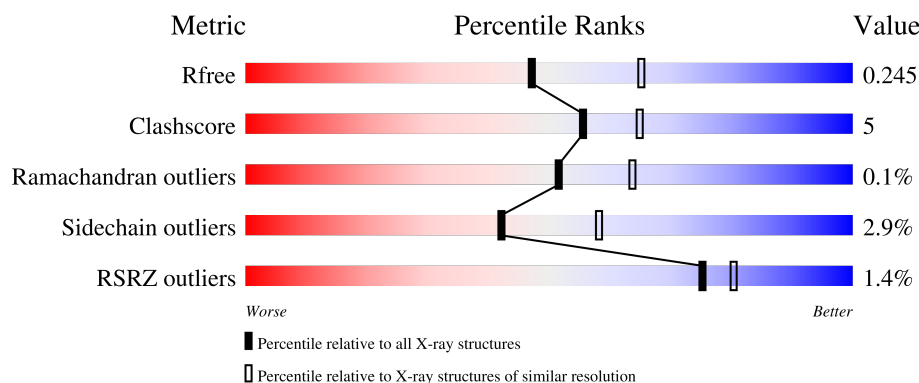
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	646	<div> <div></div> <div>77%</div> <div>10%</div> <div>•</div> <div>11%</div> </div>
1	B	646	<div> <div></div> <div>76%</div> <div>11%</div> <div>•</div> <div>11%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9159 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.

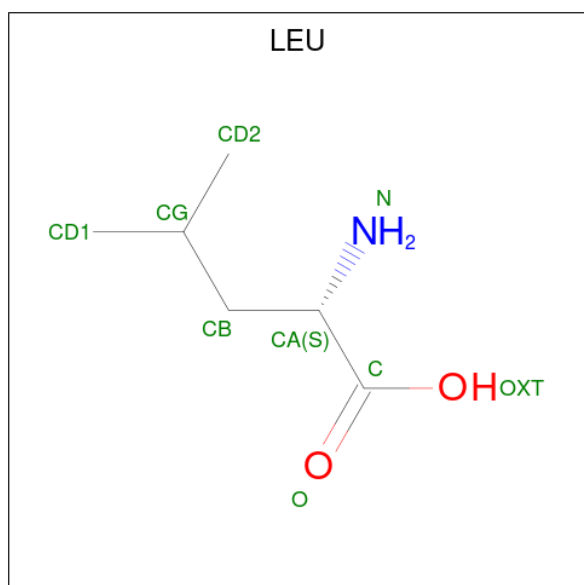
- Molecule 1 is a protein called 2-isopropylmalate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	574	Total	C	N	O	S	0	3	0
			4350	2741	752	837	20			
1	B	577	Total	C	N	O	S	0	5	0
			4412	2773	767	852	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P96420
A	0	ALA	-	expression tag	UNP P96420
A	2	ALA	THR	engineered mutation	UNP P96420
B	-1	GLY	-	expression tag	UNP P96420
B	0	ALA	-	expression tag	UNP P96420
B	2	ALA	THR	engineered mutation	UNP P96420

- Molecule 2 is LEUCINE (three-letter code: LEU) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	6	1	2		
2	B	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	183	Total	O	0	0
			183	183		
5	B	183	Total	O	0	0
			183	183		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.21Å 154.26Å 68.67Å 90.00° 97.99° 90.00°	Depositor
Resolution (Å)	27.66 – 2.30 27.07 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (27.66-2.30) 99.8 (27.07-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.166 , 0.244 0.166 , 0.245	Depositor DCC
$R_{free}$ test set	2509 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9159	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, 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	1.17	5/4454 (0.1%)	1.02	17/6082 (0.3%)
1	B	1.19	7/4522 (0.2%)	1.03	13/6170 (0.2%)
All	All	1.18	12/8976 (0.1%)	1.02	30/12252 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	155	PHE	CE1-CZ	6.66	1.50	1.37
1	B	190	ALA	CA-CB	6.24	1.65	1.52
1	B	423	GLU	CD-OE1	5.97	1.32	1.25
1	B	313	PHE	CE1-CZ	5.90	1.48	1.37
1	A	107	TYR	CD1-CE1	5.84	1.48	1.39
1	A	399	CYS	CB-SG	-5.35	1.73	1.81
1	B	486	GLU	CG-CD	5.28	1.59	1.51
1	B	77	VAL	CB-CG1	5.20	1.63	1.52
1	A	169	TYR	CG-CD1	5.18	1.45	1.39
1	A	554	TYR	CD2-CE2	5.13	1.47	1.39
1	A	541	ALA	CA-CB	5.12	1.63	1.52
1	B	99	PHE	CE1-CZ	5.09	1.47	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ARG	NE-CZ-NH1	-9.75	115.43	120.30
1	A	163	ARG	NE-CZ-NH2	8.32	124.46	120.30
1	A	163	ARG	NE-CZ-NH1	-8.13	116.23	120.30
1	A	307	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	A	37	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	A	392	LEU	CA-CB-CG	6.96	131.31	115.30
1	B	94	ARG	NE-CZ-NH2	6.86	123.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	B	644	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	544	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	544	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	B	644	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	177	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	B	499	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	177	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	B	47	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	414	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	A	633	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	94	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	A	233	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	177	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	272	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	A	414	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	506	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	136	ASP	CB-CG-OD1	5.26	123.04	118.30
1	B	350	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	641	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	59	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	B	414	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	545	VAL	CB-CA-C	5.00	120.91	111.40

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	4350	0	4149	43	0
1	B	4412	0	4229	49	0
2	A	9	0	10	1	0
2	B	9	0	10	2	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	183	0	0	3	0
5	B	183	0	0	4	0
All	All	9159	0	8414	88	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (88) 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:559:MET:HE1	1:B:623:ILE:HG23	1.31	1.08
1:A:641:ARG:HH11	1:A:641:ARG:HG3	1.17	1.06
1:B:559:MET:CE	1:B:623:ILE:HG23	2.05	0.86
1:B:426:ILE:HG21	1:B:461:ILE:HG21	1.63	0.80
1:A:641:ARG:HH11	1:A:641:ARG:CG	1.92	0.80
1:B:147:ARG:NH2	1:B:149:GLU:OE2	2.15	0.79
1:B:559:MET:HE1	1:B:623:ILE:CG2	2.14	0.77
1:A:641:ARG:HG3	1:A:641:ARG:NH1	1.94	0.72
1:A:535:LEU:HD11	1:A:635:VAL:CG2	2.20	0.71
1:B:118:SER:HB3	1:B:121:ASP:HB2	1.73	0.71
1:A:19:ILE:HG22	1:B:104:ARG:HG2	1.76	0.68
1:A:535:LEU:HD11	1:A:635:VAL:HG23	1.75	0.67
1:B:426:ILE:HG21	1:B:461:ILE:CG2	2.26	0.65
1:A:405:LEU:HD11	1:B:47:ARG:HG3	1.80	0.63
1:A:47:ARG:HD2	1:A:51:GLU:HG2	1.81	0.61
1:B:114:PHE:HE2	5:B:814:HOH:O	1.82	0.61
1:B:515[B]:THR:HG22	1:B:528:SER:OG	2.02	0.60
1:B:80:ARG:HH11	1:B:84:GLN:CD	2.05	0.60
1:A:361:HIS:HB3	5:A:819:HOH:O	2.00	0.59
1:A:63:TRP:HB3	1:A:303:ALA:HA	1.83	0.59
1:B:121:ASP:O	1:B:125:VAL:HG23	2.04	0.58
1:A:440:ILE:HD12	1:A:480:MET:CE	2.34	0.58
1:A:94:ARG:CZ	1:A:357:GLN:OE1	2.52	0.57
1:A:173:SER:O	1:A:177:ARG:HG3	2.04	0.56
1:B:361:HIS:HB3	5:B:811:HOH:O	2.07	0.55
1:A:535:LEU:CD1	1:A:635:VAL:CG2	2.85	0.55
1:A:284:LEU:HD21	1:A:305:ALA:HB2	1.89	0.54
1:B:218:GLU:O	1:B:219:SER:HB2	2.09	0.53
1:B:458:SER:HA	1:B:461:ILE:HD12	1.91	0.53
1:A:423:GLU:HA	1:A:423:GLU:OE2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ILE:HD12	1:A:480:MET:HE1	1.91	0.52
1:B:61:ARG:HD2	5:B:703:HOH:O	2.10	0.52
1:A:560:SER:HB2	5:A:669:HOH:O	2.09	0.51
1:B:116:SER:HA	1:B:153:ARG:HG2	1.92	0.51
1:B:209:THR:HB	1:B:211:TRP:CE2	2.46	0.50
1:B:559:MET:CE	1:B:623:ILE:CG2	2.84	0.50
1:B:63:TRP:HB3	1:B:303:ALA:HA	1.93	0.50
1:B:128:ILE:HG13	1:B:134:ILE:HD11	1.94	0.50
1:B:559:MET:HE2	1:B:566:GLN:CB	2.42	0.49
1:A:47:ARG:HB3	1:A:51:GLU:HG2	1.93	0.49
1:B:173:SER:O	1:B:177:ARG:HG3	2.13	0.48
1:A:475:VAL:HG13	1:A:479:GLU:HB3	1.94	0.48
1:B:559:MET:HE2	1:B:566:GLN:HB3	1.95	0.48
1:A:47:ARG:HD2	1:A:51:GLU:CG	2.44	0.48
1:B:559:MET:CE	1:B:566:GLN:HB3	2.44	0.48
1:B:225:LEU:HD21	1:B:266:SER:HB2	1.96	0.47
1:B:146:CYS:O	5:B:815:HOH:O	2.20	0.47
1:A:72:PRO:HG3	1:A:308:ILE:HD12	1.97	0.47
1:B:441:MET:HG3	1:B:449:LEU:HD11	1.96	0.47
1:A:436:GLY:O	1:A:440:ILE:HG13	2.14	0.46
1:A:56:ILE:HD13	1:A:265:ASP:OD2	2.15	0.46
1:A:316:GLY:HA3	1:A:321:ASN:ND2	2.30	0.46
1:A:505:ALA:HB2	1:A:511:THR:O	2.16	0.46
1:B:147:ARG:CZ	1:B:149:GLU:OE2	2.63	0.46
1:A:475:VAL:HG12	1:A:479:GLU:HB2	1.99	0.45
1:B:627:ILE:HD11	2:B:646:LEU:HG	1.99	0.45
1:B:329:LEU:HA	1:B:332:PHE:HB3	1.99	0.44
1:B:429:ASN:N	1:B:475:VAL:O	2.48	0.44
1:A:19:ILE:HD11	1:B:348:ILE:HG13	1.99	0.44
1:A:535:LEU:CD1	1:A:635:VAL:HG23	2.46	0.43
1:A:334:ARG:HD2	1:B:257:MET:O	2.18	0.43
1:A:535:LEU:CD1	1:A:635:VAL:HG21	2.48	0.43
1:A:461:ILE:CD1	1:A:480:MET:HG3	2.49	0.43
1:B:460:VAL:HG11	1:B:487:GLU:HG3	2.01	0.43
1:B:94:ARG:HG2	1:B:354:TYR:CZ	2.55	0.42
1:B:563:ASP:O	2:B:646:LEU:HB2	2.19	0.42
1:A:127:GLU:O	1:A:131:GLN:HB2	2.20	0.42
1:B:461:ILE:HG22	1:B:461:ILE:O	2.18	0.42
1:A:239:ILE:HG13	1:A:247:ILE:HD12	2.02	0.42
1:B:453:LEU:C	1:B:453:LEU:HD23	2.39	0.42
1:B:24:GLY:HA3	1:B:38:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:SER:HB2	1:B:307:ARG:HD3	2.02	0.41
1:A:263:TYR:O	1:A:267:ILE:HG12	2.20	0.41
1:A:563:ASP:O	2:A:645:LEU:HB2	2.20	0.41
1:A:406:TRP:CE3	1:A:414:ASP:HB2	2.56	0.41
1:A:149:GLU:HA	1:A:152:GLU:HG2	2.01	0.41
1:A:364:HIS:O	1:A:365:PRO:C	2.56	0.41
1:B:347:GLU:HA	1:B:350:ARG:NH1	2.35	0.41
1:B:487:GLU:OE2	1:B:644:ARG:HD3	2.21	0.41
1:A:37:ARG:HD3	5:A:747:HOH:O	2.21	0.41
1:B:171[A]:SER:HB3	1:B:181:PHE:HE1	1.86	0.41
1:A:313:PHE:HA	1:A:323:CYS:SG	2.60	0.41
1:B:216:SER:OG	1:B:250:ASN:HB3	2.21	0.41
1:B:268:GLU:HB2	1:B:303:ALA:HB1	2.03	0.41
1:A:198:LYS:HD2	1:A:198:LYS:HA	1.94	0.40
1:A:504:ALA:HA	1:A:512:THR:HG23	2.02	0.40
1:B:514:ILE:HD13	1:B:514:ILE:HG21	1.87	0.40
1:B:406:TRP:CH2	1:B:408:VAL:HG21	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	569/646 (88%)	551 (97%)	17 (3%)	1 (0%)	47	58
1	B	574/646 (89%)	558 (97%)	16 (3%)	0	100	100
All	All	1143/1292 (88%)	1109 (97%)	33 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	460	VAL

### 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	444/519 (86%)	429 (97%)	15 (3%)	37	51
1	B	457/519 (88%)	447 (98%)	10 (2%)	52	69
All	All	901/1038 (87%)	876 (97%)	25 (3%)	42	60

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	PHE
1	A	159	SER
1	A	163	ARG
1	A	278	GLU
1	A	343[A]	SER
1	A	343[B]	SER
1	A	392	LEU
1	A	401	VAL
1	A	454	GLN
1	A	458	SER
1	A	461	ILE
1	A	548	ASP
1	A	554	TYR
1	A	560	SER
1	A	641	ARG
1	B	66	ARG
1	B	114	PHE
1	B	163	ARG
1	B	427	ARG
1	B	443	THR
1	B	475	VAL
1	B	492	VAL
1	B	528	SER
1	B	554	TYR
1	B	631	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	321	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](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	$\# Z  > 2$
3	GOL	A	646	-	5,5,5	0.40	0	5,5,5	0.34	0
2	LEU	B	646	-	5,8,8	1.12	1 (20%)	6,10,10	1.44	1 (16%)
3	GOL	B	647	-	5,5,5	0.79	0	5,5,5	1.14	0
2	LEU	A	645	-	5,8,8	0.88	0	6,10,10	1.49	1 (16%)

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
3	GOL	A	646	-	-	2/4/4/4	-
2	LEU	B	646	-	-	4/4/8/8	-
3	GOL	B	647	-	-	0/4/4/4	-
2	LEU	A	645	-	-	4/4/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	646	LEU	CA-N	2.33	1.52	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	646	LEU	CG-CB-CA	2.44	130.85	116.29
2	A	645	LEU	CG-CB-CA	2.38	130.51	116.29

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	645	LEU	N-CA-CB-CG
2	A	645	LEU	C-CA-CB-CG
2	B	646	LEU	N-CA-CB-CG
2	B	646	LEU	C-CA-CB-CG
2	B	646	LEU	CA-CB-CG-CD1
2	A	645	LEU	CA-CB-CG-CD1
3	A	646	GOL	C1-C2-C3-O3
3	A	646	GOL	O2-C2-C3-O3
2	B	646	LEU	CA-CB-CG-CD2
2	A	645	LEU	CA-CB-CG-CD2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	646	LEU	2	0
2	A	645	LEU	1	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	574/646 (88%)	-0.36	8 (1%) 75 80	15, 26, 42, 58	0
1	B	577/646 (89%)	-0.38	8 (1%) 75 80	15, 26, 42, 56	0
All	All	1151/1292 (89%)	-0.37	16 (1%) 75 80	15, 26, 42, 58	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	ALA	3.9
1	A	28	VAL	3.4
1	B	57	ARG	3.1
1	B	397	ALA	3.0
1	B	396	ALA	2.9
1	A	399	CYS	2.9
1	B	398[A]	ASP	2.8
1	B	522	GLY	2.7
1	B	439	TYR	2.6
1	A	398	ASP	2.6
1	B	394	ALA	2.5
1	A	578	ALA	2.5
1	B	429	ASN	2.4
1	A	434	LYS	2.1
1	A	461	ILE	2.1
1	A	395	ASP	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, 95<sup>th</sup> 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
4	ZN	B	645	1/1	0.86	0.29	29,29,29,29	1
3	GOL	B	647	6/6	0.96	0.12	20,26,26,27	0
3	GOL	A	646	6/6	0.96	0.10	22,27,28,29	0
2	LEU	B	646	9/9	0.97	0.10	23,24,26,26	0
2	LEU	A	645	9/9	0.97	0.11	17,20,22,22	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.