



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:30 PM UTC

PDB ID : 3FIG / pdb\_00003fig  
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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

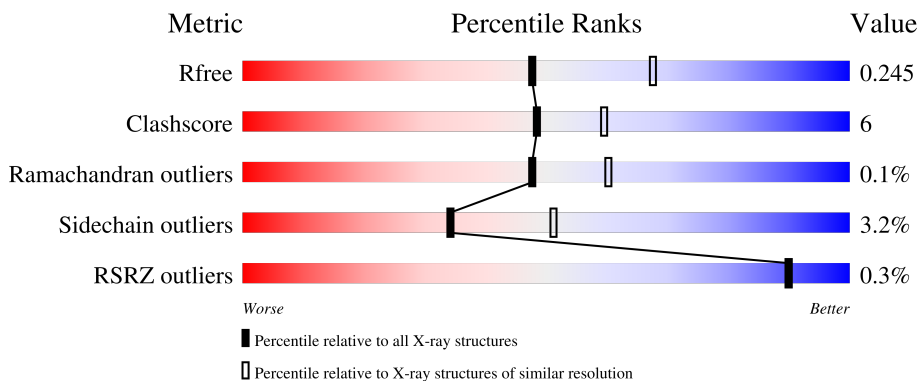
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.30 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))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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	 74%      13%      •      11%
1	B	646	 74%      14%      •      11%

## 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.

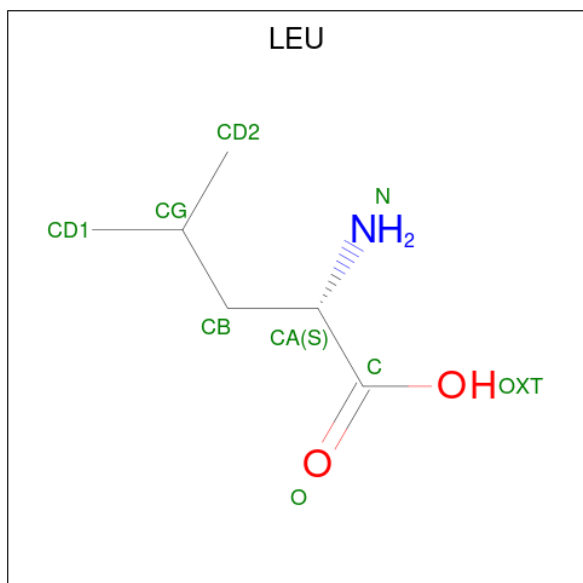
- Molecule 1 is a protein called 2-isopropylmalate synthase.

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

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 (CCD ID: 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 (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is water.

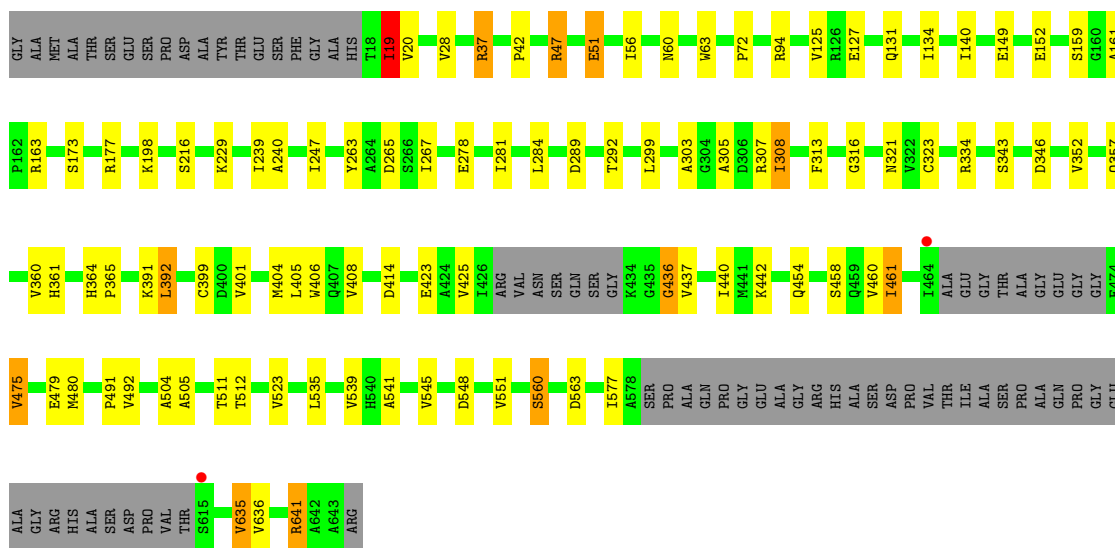
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	183	Total	O	0	0
			183	183		
5	B	183	Total	O	0	0
			183	183		

### 3 Residue-property plots

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.

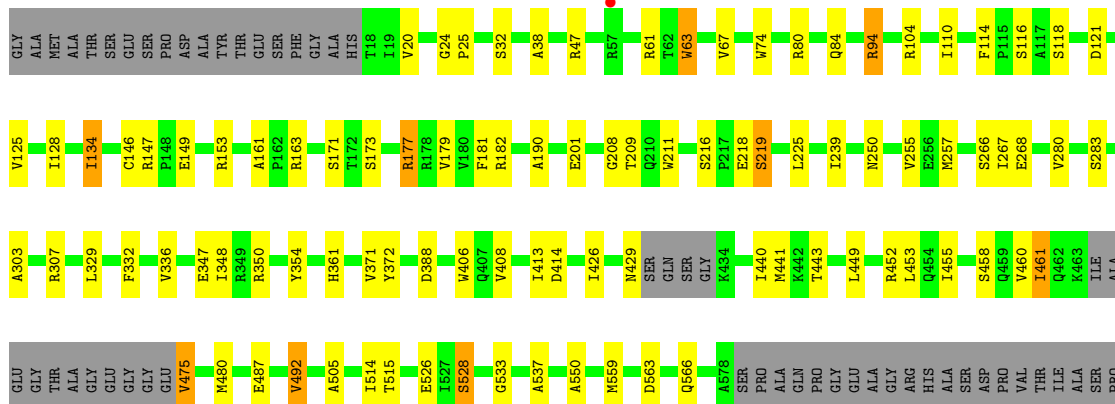
- Molecule 1: 2-isopropylmalate synthase

Chain A: 



- Molecule 1: 2-isopropylmalate synthase

Chain B: 



ALA	GLN	PRO	GLY	GLU	ALA	GLY	ARG	HIS	ALA	SER	ASP	PRO	VAL	I614	S615	I623	I627	S631	R644
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## 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 27.66 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (27.66-2.30) 99.7 (27.66-2.30)	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)	Xtrriage
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	Xtrriage
Anisotropy	0.240	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9159	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage'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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	1.44	24/4454 (0.5%)	1.35	27/6082 (0.4%)
1	B	1.45	16/4522 (0.4%)	1.32	19/6170 (0.3%)
All	All	1.45	40/8976 (0.4%)	1.33	46/12252 (0.4%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	25	PRO	CA-C	7.88	1.56	1.51
1	B	67	VAL	C-O	7.68	1.32	1.24
1	B	190	ALA	CA-CB	7.46	1.65	1.53
1	A	28	VAL	CA-CB	7.24	1.62	1.54
1	A	408	VAL	CA-CB	7.18	1.59	1.54
1	A	352	VAL	CA-CB	6.70	1.62	1.54
1	A	289	ASP	N-CA	6.64	1.54	1.46
1	B	280	VAL	CA-CB	6.60	1.62	1.54
1	B	110	ILE	CA-CB	6.59	1.62	1.54
1	A	523	VAL	CA-CB	6.55	1.61	1.53
1	B	413	ILE	C-O	6.40	1.30	1.23
1	A	541	ALA	CA-CB	6.25	1.63	1.53
1	A	19	ILE	CA-CB	6.12	1.61	1.54
1	A	577	ILE	CA-CB	6.05	1.60	1.53
1	A	475	VAL	CA-CB	5.95	1.61	1.54
1	A	539	VAL	CA-CB	5.89	1.62	1.54
1	A	134	ILE	CA-CB	5.83	1.59	1.53
1	A	125	VAL	CA-CB	5.73	1.61	1.54
1	A	20	VAL	CA-CB	5.57	1.60	1.54
1	A	635	VAL	N-CA	5.55	1.53	1.46
1	A	442	LYS	C-O	-5.54	1.17	1.24
1	B	134	ILE	CA-CB	5.45	1.60	1.54
1	B	537	ALA	CA-CB	5.44	1.61	1.53
1	B	267	ILE	C-O	-5.44	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	ILE	CA-C	5.42	1.58	1.52
1	B	336	VAL	CA-CB	5.42	1.60	1.54
1	A	636	VAL	CA-CB	5.41	1.61	1.54
1	A	551	VAL	CA-CB	5.39	1.60	1.54
1	B	455	ILE	CA-CB	5.37	1.60	1.54
1	B	74	TRP	N-CA	-5.37	1.39	1.46
1	A	308	ILE	CA-CB	5.27	1.61	1.54
1	A	360	VAL	CA-CB	5.24	1.60	1.54
1	A	140	ILE	CA-CB	5.23	1.61	1.54
1	A	161	ALA	N-CA	5.22	1.51	1.45
1	B	255	VAL	C-O	5.18	1.29	1.24
1	B	182	ARG	C-O	5.17	1.30	1.23
1	A	161	ALA	CA-CB	5.16	1.60	1.53
1	B	505	ALA	CA-CB	5.15	1.61	1.53
1	B	550	ALA	CA-CB	5.13	1.59	1.53
1	A	42	PRO	CA-C	5.10	1.57	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	TRP	CA-C-N	-7.96	111.59	119.87
1	B	63	TRP	C-N-CA	-7.96	111.59	119.87
1	B	533	GLY	CA-C-N	7.75	127.65	119.05
1	B	533	GLY	C-N-CA	7.75	127.65	119.05
1	A	545	VAL	CB-CA-C	7.59	120.91	111.65
1	A	299	LEU	CA-C-N	7.33	128.28	119.99
1	A	299	LEU	C-N-CA	7.33	128.28	119.99
1	A	545	VAL	N-CA-C	-7.09	105.91	112.43
1	B	372	TYR	N-CA-C	-6.70	103.70	112.41
1	A	635	VAL	N-CA-C	6.49	116.65	110.42
1	B	388	ASP	N-CA-C	6.38	118.77	111.11
1	A	47	ARG	CA-C-N	-6.32	113.44	119.89
1	A	47	ARG	C-N-CA	-6.32	113.44	119.89
1	A	399	CYS	N-CA-C	6.28	119.03	110.55
1	B	615	SER	N-CA-C	6.24	118.68	108.52
1	A	307	ARG	NE-CZ-NH1	-6.07	115.43	121.50
1	B	461	ILE	CB-CA-C	-6.04	102.79	112.16
1	A	425	VAL	N-CA-C	5.96	116.70	108.84
1	A	163	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	A	492	VAL	N-CA-C	-5.81	107.09	112.43
1	A	60	ASN	N-CA-C	5.68	119.07	111.24
1	A	240	ALA	CA-C-N	5.49	125.46	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ALA	C-N-CA	5.49	125.46	120.03
1	B	452	ARG	N-CA-C	-5.37	106.57	113.23
1	A	346	ASP	N-CA-C	5.36	117.54	111.11
1	B	219	SER	N-CA-C	-5.34	106.06	112.58
1	A	307	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	B	20	VAL	N-CA-C	5.28	115.56	108.17
1	A	163	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	B	161	ALA	CA-C-N	-5.18	114.32	119.56
1	B	161	ALA	C-N-CA	-5.18	114.32	119.56
1	A	491	PRO	N-CA-C	5.18	119.00	111.03
1	B	414	ASP	CA-C-N	-5.17	113.70	119.19
1	B	414	ASP	C-N-CA	-5.17	113.70	119.19
1	A	216	SER	CA-C-N	-5.17	113.38	119.84
1	A	216	SER	C-N-CA	-5.17	113.38	119.84
1	A	281	ILE	N-CA-C	-5.16	99.74	107.37
1	A	161	ALA	N-CA-C	5.12	115.87	109.57
1	B	208	GLY	N-CA-C	5.09	120.33	114.16
1	A	37	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	436	GLY	CA-C-N	5.04	127.01	120.56
1	A	436	GLY	C-N-CA	5.04	127.01	120.56
1	B	94	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	B	492	VAL	CB-CA-C	5.02	119.53	111.29
1	A	292	THR	N-CA-C	5.02	118.95	111.87
1	B	177	ARG	N-CA-C	-5.01	106.01	111.82

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	4350	0	4149	45	0
1	B	4412	0	4229	54	0
2	A	9	0	10	1	0
2	B	9	0	10	2	0
3	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	0	0
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	95	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 6.

All (95) 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:A:641:ARG:HH11	1:A:641:ARG:HG3	1.17	1.06
1:B:559:MET:HE1	1:B:623:ILE:HG23	1.49	0.93
1:B:559:MET:HE1	1:B:623:ILE:CG2	2.04	0.87
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:HE3	1:B:566:GLN:CB	2.15	0.77
1:A:641:ARG:HG3	1:A:641:ARG:NH1	1.94	0.72
1:A:440:ILE:HD12	1:A:480:MET:HE1	1.72	0.71
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:B:559:MET:HE3	1:B:566:GLN:HB2	1.73	0.70
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:B:80:ARG:HH11	1:B:84:GLN:CD	2.05	0.65
1:B:559:MET:HE3	1:B:566:GLN:HB3	1.79	0.63
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:LEU:CD1	1:A:635:VAL:CG2	2.85	0.55
1:B:559:MET:HE1	1:B:623:ILE:HG21	1.88	0.54
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
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: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: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: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:B:453:LEU:C	1:B:453:LEU:HD23	2.39	0.46
1:A:364:HIS:O	1:A:365:PRO:C	2.56	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:B:440:ILE:HG22	1:B:480:MET:HE1	1.98	0.45
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:B:559:MET:HE2	1:B:623:ILE:HG23	1.93	0.44
1:A:404:MET:HE3	1:A:404:MET:HB3	1.93	0.43
1:A:535:LEU:CD1	1:A:635:VAL:HG23	2.46	0.43
1:A:391:LYS:O	1:A:392:LEU:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:VAL:HG11	1:B:487:GLU:HG3	2.01	0.43
1:B:80:ARG:NH1	1:B:84:GLN:CD	2.74	0.42
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:O	1:B:461:ILE:HG22	2.18	0.42
1:A:239:ILE:HG13	1:A:247:ILE:HD12	2.02	0.42
1:B:24:GLY:HA3	1:B:38:ALA:HB3	2.02	0.41
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: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:80:ARG:HD2	1:B:80:ARG:C	2.45	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 [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	569/646 (88%)	551 (97%)	17 (3%)	1 (0%)	43 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	574/646 (89%)	558 (97%)	16 (3%)	0	100	100
All	All	1143/1292 (88%)	1109 (97%)	33 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	460	VAL

### 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	444/519 (86%)	428 (96%)	16 (4%)	31	47
1	B	457/519 (88%)	444 (97%)	13 (3%)	38	56
All	All	901/1038 (87%)	872 (97%)	29 (3%)	34	51

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	51	GLU
1	A	159	SER
1	A	229	LYS
1	A	278	GLU
1	A	343[A]	SER
1	A	343[B]	SER
1	A	392	LEU
1	A	401	VAL
1	A	437	VAL
1	A	454	GLN
1	A	458	SER
1	A	461	ILE
1	A	548	ASP
1	A	560	SER

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Mol	Chain	Res	Type
1	A	641	ARG
1	B	32[A]	SER
1	B	32[B]	SER
1	B	163	ARG
1	B	179	VAL
1	B	201	GLU
1	B	239	ILE
1	B	371	VAL
1	B	443	THR
1	B	475	VAL
1	B	492	VAL
1	B	526	GLU
1	B	528	SER
1	B	631	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	36	GLN
1	A	119	GLN
1	A	131	GLN
1	A	202	GLN
1	B	339	GLN
1	B	384	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 oligosaccharides in this entry.

## 5.6 Ligand geometry

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	0.42	0	5,5,5	0.35	0
2	LEU	A	645	-	6,8,8	1.30	1 (16%)	5,10,10	2.07	1 (20%)
2	LEU	B	646	-	6,8,8	0.75	0	5,10,10	1.39	1 (20%)
3	GOL	B	647	-	5,5,5	0.82	0	5,5,5	1.20	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
3	GOL	A	646	-	-	2/4/4/4	-
2	LEU	A	645	-	-	6/8/8/8	-
2	LEU	B	646	-	-	6/8/8/8	-
3	GOL	B	647	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	645	LEU	OXT-C	-2.82	1.21	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	645	LEU	OXT-C-O	-4.15	114.66	124.08
2	B	646	LEU	OXT-C-O	-2.35	118.76	124.08

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	645	LEU	N-CA-CB-CG
2	B	646	LEU	N-CA-CB-CG
2	B	646	LEU	C-CA-CB-CG
2	A	645	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
2	A	645	LEU	OXT-C-CA-N
2	B	646	LEU	OXT-C-CA-N
2	A	645	LEU	O-C-CA-N
2	B	646	LEU	O-C-CA-N

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	645	LEU	1	0
2	B	646	LEU	2	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, 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%)	-0.49	2 (0%) 90 90	12, 26, 42, 58	3 (0%)
1	B	577/646 (89%)	-0.56	1 (0%) 91 91	15, 26, 42, 56	5 (0%)
All	All	1151/1292 (89%)	-0.52	3 (0%) 90 90	12, 26, 42, 58	8 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	615	SER	3.0
1	A	464	ILE	2.8
1	B	57	ARG	2.3

### 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, 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(Å <sup>2</sup> )	Q<0.9
4	ZN	B	645	1/1	0.88	0.15	29,29,29,29	1
3	GOL	B	647	6/6	0.95	0.07	20,26,26,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	646	6/6	0.96	0.07	22,27,28,29	0
2	LEU	B	646	9/9	0.97	0.05	23,24,26,26	0
2	LEU	A	645	9/9	0.97	0.05	17,20,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.